

CURRICULUM VITAE

I. ACADEMIC BACKGROUND

A. PERSONAL DATA

Name: Khaled H. S. Barakat

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Nationality: Canadian

Language: Fluent in English and Arabic

B. EDUCATION AND TRAINING

04/2012-01/2014: Post-doctoral fellow in Virology; Department of Medical Microbiology and Immunology, Faculty of Medicine and Dentistry, University of Alberta, Edmonton (Alberta) Canada, under the supervision of the Nobel Laureate, Dr. Michael Houghton.

09/2007-03/2012: PhD in Biophysics; Department of Physics, Faculty of Science, University of Alberta, Edmonton (Alberta) Canada, under the supervision of Dr. Jack Tuszynski.

09/2003-09/2006: MSc in Engineering Physics; Faculty of Engineering, Cairo University, Cairo, Egypt, under the supervision of Dr. S. M. El-Sheikh and Dr. Noha. M. Salem.

09/2001-09/2003: Pre-Master's Preparation Courses, Faculty of Engineering, Cairo University, Cairo, Egypt.

05/1996- 05/2001 BSc, Electrical Engineering, Faculty of Engineering, Cairo University, Fayoum, Egypt.

C. ACADEMIC APPOINTMENTS

12/2015-present: Assistant Professor, Faculty of Pharmacy & Pharmaceutical Sciences, University of Alberta, Edmonton (Alberta) Canada.
01/2014-12/2015: Research Assistant Professor, Faculty of Pharmacy & Pharmaceutical Sciences, University of Alberta, Edmonton (Alberta) Canada.

D. AWARDS AND HONORS

2013 - 2014 Canadian Institute of Health Research (CIHR) postdoctoral fellowship, \$40,000 + Research Allowance (\$5000), for two years.
2012-2014 Alberta Innovates-Health Solutions (AIHS) postdoctoral fellowship, \$50,000 + Research Allowance (\$5000), for three years.
2011-2012 Dissertation award, \$22,000 + tuition fees (\$4,500), for one year.
2009-2010 Alberta Cancer Research Institute Studentship, \$20,000, for two years.
1999 Faculty of Engineering Distinction Award, E£200, for one year.
1998 Faculty of Engineering Distinction Award, E£200, for one year.
1997 Faculty of Engineering Distinction Award, E£200, for one year.

E. PROFESSIONAL ORGANIZATION MEMBERSHIP

1. Canadian Society for Pharmaceutical Sciences (CSPS)
2. American Chemical Society (ACS).
3. American Physical Society (APS).
4. Biophysical Society (BPS).
5. American Association for Cancer Research (AACR).
6. Association of Professional Engineers and Geoscientists of Alberta (APEGA)

II. SERVICE

A. STUDENTS' SUPERVISION

Graduate Students:

Completed:

Name	Degree	Period	Thesis Title	Current Position
Francesco Gentile	PhD	01/2014 – 12/2018	Computer-Aided Drug Design of DNA Repair Inhibitors Targeting the ERCC1-XPF Endonuclease.	Postdoctoral Fellow, UBC's Vancouver Prostate Centre, Canada.
*Horia Jalily Hasani	MSc	01/2015- 09/2017	A Comprehensive Dynamic Model for KCNQ1/KCNE1 Ion Channel: Structural & Functional Studies	Research Assistant, UofA, Canada.
*Tianhua Feng	MSc	09/2016- 09/2019	A Comprehensive Dynamic Model for Cav1.2 Ion Channel: Structural & Functional Studies	R&D technician at Neova Technology Inc., BC, Canada.
*Rui Chen	MSc	09/2017- 03/2020	Investigating the Mode(s) of Action of Human B7-1 Small-Molecule Inhibitors	Research Assistant, UofA, Canada.

* Principle supervisor

Current:

Name	Entry Date	Degree
Farag Mosa	06/2019	PhD
*Yasser Tabana	01/2018	PhD

* Principle supervisor

Awards received by the students during their tenure:

Name	Year	Award
<i>Yasser Tabana</i>	2020	Alberta Graduate Excellence Scholarship
<i>Yasser Tabana</i>	2020	Antoine Noujaim Graduate Scholarship in Pharmaceutical Sciences.
<i>Yasser Tabana</i>	2020	Shire Canada Inc Graduate Scholarship.
<i>Rui Chen</i>	2020	Shire Canada Inc Graduate Scholarship.
<i>Francesco Gentile</i>	2019	Ermenegildo Zegna Founder's Postdoctoral Fellowship.
<i>Francesco Gentile</i>	2019	SciNet International High-Performance Computing Summer School Scholarship.
<i>Francesco Gentile</i>	2019	Faculty of Science Dissertation Award, University of Alberta, Canada

<i>Francesco Gentile</i>	2019	International High-Performance Computing Summer School Scholarship, RIKEN Center for Computational Sciences, Kobe, Japan.
<i>Rui Chen</i>	2019	Graduate Student Travel Support to CSPA and AFPC.
<i>Yasser Tabana</i>	2020	Shire Canada Inc Graduate Scholarship.
<i>Rui Chen</i>	2018	Graduate Student Tuition Supplement, Winter Term.
<i>Yasser Tabana</i>	2018	Shire Canada Inc Graduate Scholarship.
<i>Tianhua Feng</i>	2018	Graduate Student Travel Support to CSPA and AFPC.
<i>Francesco Gentile</i>	2018	Novartis Pharmaceuticals Canada Inc. Graduate Scholarship.
<i>Francesco Gentile</i>	2018	Alberta Innovates Graduate Student Scholarship.
<i>Francesco Gentile</i>	2018	SciNet HPC Summer School Scholarship (Declined).
<i>Francesco Gentile</i>	2018	Canadian Cancer Society Travel Award.
<i>Francesco Gentile</i>	2017	Biophysical Society International Travel Award.
<i>Francesco Gentile</i>	2017	University of Alberta Graduate Students' Association Academic Travel Award.
<i>Francesco Gentile</i>	2016	University of Alberta Graduate Students' Association Academic Travel Award.
<i>Francesco Gentile</i>	2016	University of Alberta Graduate Students' Association Research Assistant Award.
<i>Francesco Gentile</i>	2014	Alumni Meritevoli Award.
<i>Horia Jalily Hasani</i>	2015	Mary Louise Imrie Graduate Student Award.
<i>Horia Jalily Hasani</i>	2017	Finalist in the 3MT competition at the University of Alberta.
<i>Horia Jalily Hasani</i>	2016	Novartis Pharmaceuticals Canada Inc Graduate Scholarship.
<i>Horia Jalily Hasani</i>	2016	Graduate Poster Award, Faculty of Pharmacy and Pharmaceutical Sciences Research Day
<i>Horia Jalily Hasani</i>	2016	People's Choice Poster Award, received at the Annual HPCS-CANHEIT 2016 Conference.
<i>Horia Jalily Hasani</i>	2015	Antoine Noujaim Graduate Scholarship in Pharmaceutical Sciences. This Scholarship is awarded on the basis of overall academic excellence and achievement.
<i>Horia Jalily Hasani</i>	2015	Graduate Student Tuition Award, Fall Term 2015 (September to December).
<i>Horia Jalily Hasani</i>	2015	Mary Louise Imrie Graduate Student Award. This award is to recognize outstanding graduate students of the faculty.
<i>Horia Jalily Hasani</i>	2016	Graduate Student Tuition Award, Winter Term 2016 (January to April).
<i>Tianhua Feng</i>	2017	Shoppers Drug Mart Graduate Scholarship in Pharmacy and Pharmaceutical Sciences.
<i>Tianhua Feng</i>	2016	Graduate Student Tuition Supplement, Winter Term.

Undergraduate & Intern Students:

Name	Period	Degree	Current Position
*Minwoo Ha [^]	05/2020-09/2020	Summer student	Science Undergraduate Student, University of Alberta, Canada.

<i>*Issar Arab</i>	08/2019- 11/2019	UARE ¹ Intern	MSc, Germany
<i>*Harsh Beesoon</i>	07/2019- 07/2019	HYRS ²	High School Student
<i>*Minwoo Ha</i>	06/2019- 08/2019	Summer student	Science Undergraduate Student, University of Alberta, Canada.
<i>*Anna Jutla[^]</i>	06/2019- 08/2019	Summer student	Pharmacy Undergraduate Student, University of Alberta, Canada.
<i>*Nawreen Hena[^]</i>	06/2019- 08/2019	Summer student	Science Undergraduate Student, University of Alberta, Canada.
<i>*Simaranjit Grewal</i>	06/2019- 08/2019	Summer student	Science Undergraduate Student, University of Alberta, Canada.
<i>*Jiay Tong</i>	03/2019- 05/2019	UARE Intern	MSc, Germany
<i>*Yanping Yang</i>	01/2019- 03/2019	UARE Intern	MSc, China
<i>*Ziwen Chen</i>	10/2018- 12/2018	CSC ³ Intern	MSc, China.
<i>*Guilherme Afonso</i>	02/2018- 05/2018	UARE Intern	MSc
<i>*Anna Jutla[^]</i>	04/2018- 09/2018	Summer Student	Pharmacy Undergraduate Student, University of Alberta, Canada.
<i>*Nawreen Hena[^]</i>	01/2017- 05/2017	Summer Student	Science Undergraduate Student, University of Alberta, Canada.
<i>*Theinmozhi Arulraj</i>	05/2017- 08/2017	UARE Intern	PhD Student, Germany.
<i>*Gyan Darshan</i>	05/2017- 08/2017	UARE Intern	MSc, India
<i>*Nathalia Dumas</i>	06/2017- 09/2017	UARE Intern	PhD student, Brazil
<i>*Min-haung chiang</i>	01/2017- 05/2017	UARE Intern	PhD student, New Zealand
<i>*Abhishek Pal</i>	05/2016- 08/2016	UARE Intern	MSc, India
<i>*Crystal Lui</i>	01/2016- 05/2016	Summer Student	Faculty of Medicine, University of Calgary, Canada.
<i>*Michael Heinzinger</i>	01/2016- 03/2016	UARE Intern	PhD student, Germany.
<i>*Amanda Ngo</i>	05/2015- 09/2015	Summer Student	Pharmacist, Edmonton, AB, Canada.
<i>*Jeffery Chow</i>	05/2015- 09/2015	Summer Student	Pharmacist, Edmonton, AB, Canada.

¹ UARE: University of Alberta Research Experience

²HYRS: Heritage Youth Researcher Summer (HYRS) Program

³ CSC: China Scholarship Council

* <i>Tianhua Feng</i>	04/2015- 07/2015	CSC intern	MSc, University of Alberta, Canada.
* <i>Summer Kassem</i>	09/2014- 01/2015	Intern Student	PhD, AUC ⁴ , Egypt.
* <i>Celment Vercil</i>	06/2014- 01/2015	Intern Student	PhD, France
* <i>Alessio Prunotto</i>	03/2012- 03/2012	Intern Student	PhD, Italy

^Joined my research group more than one time as a summer student

*Principle supervisor

Awards received by the undergraduate students during their tenure:

Name	Year	Award
Anna Jutla	2020	Alberta Innovates Summer Research Studentship
Minwoo Ha	2020	NSERC Undergraduate Student Research Assistantship Award
Anna Jutla	2019	Office of the Provost and VP (Academic) Summer Student Award
Anna Jutla	2019	Cathy Compton McNabb Summer Studentship.
Anna Jutla	2019	Alberta Cancer Foundation (ACF) Undergraduate Summer Research Studentship.
Anna Jutla	2018	Faculty of Pharmacy and Pharmaceutical Sciences Undergraduate Summer Research Studentship.
Anna Jutla	2018	Alberta Innovates Health Solutions (AIHS) Undergraduate Summer Research Studentship.

Examining Committees:

Candidate	Degree & Exam	Supervisor	Date
Fanchi Meng	PhD/Candidacy Exam	Lukasz Kurgan	13/06/2016
Meng Jie Yan	MSc/Final Exam	Paul Jurasz	28/09/2016
Cameron Smithers	phD/ Candidacy Exam	Michael Overduin	28/04/2018
Amir Tabatabaei	PhD/ Candidacy Exam	Carlos Velazquez	21/11/2018
Daniela Amaral Silva	PhD/ Candidacy Exam	Neal Davies & Raimar Loebenberg	05/03/2020

B. POSTDOCTORAL FELLOWS, RESEARCH ASSOCIATES & TECHNICIANS:

Postdoctoral Fellows:

Completed:

Name	Period	Current Position
*Subha Kalyanamoorthy	06/2016 – 09/2019	Assistant Professor, Department of Chemistry, University of Waterloo.

⁴ AUC: American University in Cairo

*Aravindhan Ganesan	05/2015 – 09/2019	Research Assistant Professor, School of Pharmacy, University of Waterloo.
*Marawan Ahmed	06/2014 – 10/2018	Senior data analyst, Alberta Health Services, Canada.
*Abdo Mohamed	02/2018 – 08/2018	Associate Professor, Faculty of Science, Cairo University, Egypt.

*Principle supervisor

Current:

Name	Period
*Surya Narayanan	10/2019 – Present

*Principle supervisor

Awards received by postdoctoral fellows during their tenure:

Name	Year	Award
Subha Kalyaanamoorthy	2019	Best basic science research award (Oral) at the 2019 Cardiac Society Research day, Edmonton, AB Canada.
Subha Kalyaanamoorthy	2018	NSERC post-doctoral fellowship, two years.
Subha Kalyaanamoorthy	2017	Wu Hong Memorial Poster Prize; Faculty of Pharmacy Research Day.
Marawan Ahmed	2016	Wu Hong Memorial Poster Prize; Faculty of Pharmacy Research Day.
Marawan Ahmed	2016	Wu Hong Memorial Poster Prize; Faculty of Pharmacy Research Day.

Research Associates:

Name	Period
*Tae Chul Moon	10/2015 – Present

*Principle supervisor

Technicians:

Name	Period
*Bethany Yoon	01/2016 – 03/2017

*Principle supervisor

C. COMMITTEES:

At the Faculty Level

2015- 2018 (Member)
2019-Current (Chair)

Research Day Committee

2015 -2017 (Member) 2019 – Current (Leader of the graduate students' awards sub-committee)	Student Awards Committee
2019- Current	Pharmaceutical Sciences working group for the PharmD Implementation Committee.
2018-2020 (Member)	Graduate Studies Committee
2018 -2019 (Member)	International Committee
2014 – 2015 (Chair)	Space-Safety & Information Technology Committee

At the University Level

2014 – 2015 (Member)	Environmental Health and Safety Senior Administrator's Committee at the University of Alberta.
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D. TEACHING

i. Undergraduate Courses:

Faculty of Pharmacy and Pharmaceutical Sciences, University of Alberta, Canada (2014-present):

Course	Role	#of students	Actual Contact Hrs/Yr	Preparation, Coordination & Office Hrs/Yr	Total Hrs/Yr
PHARM201 ^a	Contributor	~130	8L	40	48
PHARM327	Contributor	~130	1L	4	5
PHARM367	Contributor	~130	2L	8	8
PHARM487	Contributor	~130	1L	4	5
PHARM437	Contributor	~130	1L	4	5

^a course name changed from PHARM 301 to PHARM201 in 2019.

L – Lecture Hours

ii. Graduate Courses:

Faculty of Pharmacy and Pharmaceutical Sciences, University of Alberta, Canada (2014-present):

Course	Role	#of students	Actual Contact Hrs/Yr	Preparation, Coordination & Office Hrs/Yr	Total Hrs/Yr
PHARM580	Instructor/Contributor	5-10	37.5L/24LB	50	111.5
PHARM697	Coordinator/Contributor	10-15	3L/3S	7	13

L – Lecture Hours

LB – Lab Hours

S – Seminar Hours

iii. Other Teaching

Guest lecturer (2016-2017):

Course	Role	#of students	Actual Contact Hrs/Yr	Preparation, Coordination & Office Hrs/Yr	Total Hrs/Yr
CHEM 405/ 669	Contributor	30-40	1.5L	4	5.5

L – Lecture Hours

III. RESEARCH AND SCHOLARLY ACTIVITY

A. RESEARCH INTERESTS:

My research focuses on medicinal chemistry and computer modelling to fuel discoveries in two main research streams.

- I. Develop small molecule inhibitors for the immune checkpoints. Immune checkpoints are T cell membrane receptors that can activate or inhibit T cell activity. Understanding how these receptors interact with their protein ligands can provide a unique tool to modulate the immune system. Since 2015, my lab has been leading a multidisciplinary research team to rationally design small molecule immune checkpoint inhibitors (see Appendix A for the full team picture). Our focus has been on two major targets, namely cytotoxic T-lymphocyte-associated antigen 4 (CTLA-4) and programmed cell death protein 1 (PD-1). Developing small molecule inhibitors for these targets can help overcome many of the clinical limitations associated with current anti-PD-1 and anti-CTLA-4 monoclonal antibodies (MABs) and reduce costs. Compared to available MAB therapies, small molecule immune checkpoint blockers can offer a more affordable, more easily administered, and more easily controlled treatments against a variety of cancers including hard to treat cancers such as advanced solid tumours and brain tumours.

- II. Understand cardiac ion channels off-target interactions. A major problem in drug discovery is the unexpected toxicity that can emerge from the interaction of drugs with unforeseen targets, such as ion channels and transporters. Cardiac ion channels form a significant class of these proteins, which can interact with many drugs. These unwanted interactions can lead to cardiotoxicity and, eventually, sudden heart arrest. This research is funded through a 5-year NSERC discovery grant (2015-2020) and was renewed for an additional 5 years until 2026). Our research harnesses the power of computer simulations to predict the interaction of drugs with cardiac ion channels (such as hERG, NAV and CAV channels). The ultimate goal is to understand how the

different drugs interact with these channels and suggest chemical modifications to these drugs to avoid these off-target interactions.

B. RESEARCH GRANTS

Received:

- 03/2020 –03/2026 **Funding source:** Natural Sciences and Engineering Research Council
Program: Discovery Grant
Title: Multiscale Computer Modeling to Evaluate Protein-Ligand Off-Target Interactions
Role: Principal Applicant. **Total funding:** 210,000 CAD.
Status: Active
- 03/2015 –03/2021 **Funding source:** Natural Sciences and Engineering Research Council
Program: Discovery Grant
Title: Atomistic Computational Models To Evaluate Protein-Ligand Off-Target Interactions
Role: Principal Applicant. **Total funding:** 150,000 CAD.
Status: Active
- 03/2015 – 03/2021 **Funding source:** Alberta Cancer Foundation & The Li Ka Shing Applied Virology Institute
Program: Transformative Ideas
Title: Developing Novel Cancer Immunotherapy Drugs: A Multidisciplinary Team
Role: Principal Applicant. **Total funding:** 5,386,000 CAD.
Status: Active.
- 07/2015 – 07/2018 **Funding source:** IC-IMPACTS Centres of Excellence
Title: Identification of high affinity ligands against Dengue virus NS1 for the development of an affordable point-of-care diagnostic kit
Program: Research Grant
Role: Co-Applicant. **Total funding:** 400,000 USD.
Status: Completed.
- 01/2015 – 01/2017 **Funding source:** Li Ka Shing Institute of Virology
Title: Developing a novel combination therapy for Dengue virus infection
Program: Translational Grant

Role: Co-Applicant. **Total funding:** 100,000 CAD.
Status: Completed.

01/2014 – 01/2016

Funding source: Li Ka Shing Institute of Virology
Program: Start-up Fund
Role: Principal Applicant. **Total funding:** 50,000 CAD.
Status: Completed.

10/2014 – 01/2015

Funding source: Alberta Cancer Foundation
Program: Transformative Ideas (seed fund)
Title: Developing Novel Cancer Immunotherapy Drugs: A Multidisciplinary Team
Role: Principal Applicant. **Total funding:** 20,000 CAD.
Status: Completed.

07/2014 – 08/2015

Funding source: Li Ka Shing Institute of Virology
Title: Computational Discovery of Novel Hepatitis C Virus NS5A inhibitors.
Program: Translational Grant
Role: Principal Applicant. **Total funding:** 50,000 CAD.
Status: Completed.

Pending:

Title of Grant	Source	Role	Total amount	Period of support
Toward Reducing Tyrosine Kinase Inhibitors-Induced Cardiotoxicity	Cancer Research Society	PI	120,000 CAD	2020-2022
A Multi-target Drug Identification Approach Against SARS-CoV-2 Replicase Machinery	University of Alberta	PI	40,000 CAD	2020-2021
A vaccine design to induce protective B and T cell immunity against hepatitis C virus.	NIH [^]	Co-PI	2,000,000 USD	2021-2026

[^] National Institutes of Health, USA.

C. RESEARCH COMMUNITY

Editorial board:

- Associate Editor, BMC Bioinformatics.
Country: United Kingdom
International Standard Serial Number (ISSN): 14712105

Reviewer for grant applications:

- Mitacs Elevate

- Saskatchewan Health Research Foundation (SHRF) Collaborative Innovation Development.
- The John R. Evans Leaders Fund (JELF), a program of the Canada Foundation for Innovation (CFI).
- Swiss National Supercomputing Center.
- French National Research Agency.
- University of Sharjah

Reviewer for Journals:

Journal	ISSN⁵
1 Scientific reports	20452322
2 eLife.	2050084X
3 PLOS ONE	19326203
4 Journal of Medicinal Chemistry	15204804
5 BMC Clinical Pathology	14726890
6 Journal of Molecular Modeling	09485023
7 Journal of Advanced Research	20901232
8 Viruses	19994915
9 Journal of pharmacy and pharmaceutical sciences	14821826
10 Drug Design, Development and Therapy	11778881
11 Toxins	20726651
12 Pharmaceutical Sciences	00223549
13 BMC Bioinformatics	14712105
14 Cancer Investigation	15324192
15 Chemical Biology & Drug Design	1747-0285
16 BMC Medical Genomics	17558794
17 Drug Design, Development and Therapy	11778881
18 OncoTargets and Therapy	11786930
19 Virology Journal	1743422X
20 Journal of Enzyme Inhibition And Medicinal Chemistry	14756366
21 Journal of Biological Physics	00920606
22 Journal of Gastroenterology	00029270
23 Enzyme Inhibition and Medicinal Chemistry	14756366
24 BMC Research Notes	17560500
25 Computational Biology and Chemistry	14769271
26 Asian Pacific Journal of Tropical Medicine	19957645
27 Cardiovascular Pharmacology and Therapeutics	10742484
28 Journal of Biological Physics	00920606
29 Journal of Molecular Graphics and Modelling	10933263
30 Marine Drugs	16603397
31 Current Drug Discovery Technologies	15701638
32 Medicines	22279059
33 Chemical Physics Letters	00092614
34 Cellular and Molecular Life Sciences	14209071
35 BMC Systems Biology	17520509
36 Journal of the American Chemical Society	00027863
37 Molecular and Cellular Proteomics	15359484
38 World Journal of Gastroenterology	10079327
39 British Journal of Pharmacology	00071188
40 Journal of Medical Virology	01466615

⁵ International Standard Serial Number

41	Medicinal Research Reviews	10981128
42	Bioelectrochemistry	15675394
43	Advances and Applications in Bioinformatics and Chemistry	11786949
44	Expert Opinion On Drug Discovery	17460441
45	The Journal of Physical Chemistry Letters	19487185
46	Computers in Biology and Medicine	00104825
47	Biophysical Chemistry	03014622
48	Bioorganic Chemistry	10902120
49	Future Medicinal Chemistry	17568927

D. PUBLICATIONS

Refereed Papers: (*corresponding author)

Published/In press:

1. Mosa, FES, , Suryanarayanan, C., Feng, T. and **Baraka, K.*** (2020). Effects of selective calcium channel blockers on ions' permeation through the human Cav1.2 ion channel: A computational study. *Journal of molecular graphics & modelling*, 102, 107776. (Impact Factor 2020=1.93, Citation=0)
2. Kalyaanamoorthy, S., Lamothe, S., Hou, X., Moon, T., Kurata, H., Houghton, M., **Barakat, K.*** (2020). A structure-based computational workflow to predict liability and binding modes of small molecules to hERG. *Scientific reports*, 1;10(1):16262. (Impact Factor 2020=4.12, Citation=1)
3. Chen, R., Ganesan, A., Okoye, I., Arutyunova, E., Elahi, S., Lemieux, M. J., & **Barakat, K.*** (2020). Targeting B7-1 in immunotherapy. *Medicinal research reviews*, 40(2), 654–682. (Impact Factor 2020=9.791, Citation=1)
4. Gentile, F., Elmenoufy, A. H., Ciniero, G., Jay, D., Karimi-Busheri, F., **Barakat, K.**, Weinfeld, M., West, F. G., & Tuszynski, J. A.* (2020). Computer-aided drug design of small molecule inhibitors of the ERCC1-XPF protein-protein interaction. *Chemical biology & drug design*, 95(4), 460–471. (Impact Factor 2020=2.256, Citation=3)
5. Jaballah, M. Y., Serya, R., Saad, N., Khojah, S. M., Ahmed, M., **Barakat, K.**, & Abouzid, K*. (2019). Towards discovery of novel scaffold with potent antiangiogenic activity; design, synthesis of pyridazine based compounds, impact of hinge interaction, and accessibility of their bioactive conformation on VEGFR-2 activities. *Journal of enzyme inhibition and medicinal chemistry*, 34(1), 1573–1589. (Impact Factor 2018=4.027, Citation=0)
6. Mitran, C. J., Mena, A., Gnidehou, S., Banman, S., Arango, E., Lima, B., Lugo, H., Ganesan, A., Salanti, A., Mbonye, A. K., Ntumngia, F., **Barakat, K.**, Adams, J. H., Kano, F. S., Carvalho, L. H., Maestre, A. E., Good, M. F., & Yanow, S. K.* (2019). Antibodies to cryptic epitopes in distant homologues underpin a mechanism of heterologous immunity between *Plasmodium vivax* PvDBP and *Plasmodium falciparum* VAR2CSA. *mBio*, 10(5), e02343-19. (Impact Factor 2020=6.50, Citation=3)
7. Ganesan, A., Ahmed, M., Okoye, I., Arutyunova, E., Babu, D., Turnbull, W. L., Kundu, J. K., Shields, J., Agopsowicz, K. C., Xu, L., Tabana, Y., Srivastava, N., Zhang, G., Moon, T. C., Belovodskiy, A., Hena, M., Kandadai, A. S., Hosseini, S. N., Hitt, M., Walker, J., ... **Barakat, K.*** (2019). Comprehensive in vitro characterization of PD-L1 small

- molecule inhibitors. *Scientific reports*, 9(1), 12392. (Impact Factor 2020=4.12, Citation=9)
8. Elmenoufy, A. H., Gentile, F., Jay, D., Karimi-Busheri, F., Yang, X., Soueidan, O. M., Weilbeer, C., Mani, R. S., **Barakat, K. H.**, Tuszynski, J. A., Weinfeld, M., & West, F. G.* (2019). Targeting DNA repair in umor ells via inhibition of ERCC1-XPF. *Journal of medicinal chemistry*, 62(17), 7684–7696. (Impact Factor 2020=6.26, Citation=4)
 9. Ahmed, M., Kumar, A., Hobman, T. C., & **Barakat, K.*** (2019). Structure-based screening and validation of potential dengue virus inhibitors through classical and QM/MM affinity estimation. *Journal of molecular graphics & modelling*, 90, 128–143. (Impact Factor 2020=1.93, Citation=0)
 10. Feng, T., Kalyaanamoorthy, S., Ganesan, A., & **Barakat, K.*** (2019). Atomistic modeling and molecular dynamics analysis of human CaV1.2 channel using external electric field and ion pulling simulations. *Biochimica et biophysica acta. General subjects*, 1863(6), 1116–1126. (Impact Factor 2020=3.74, Citation=3)
 11. Elsayed, N., Serya, R., Tolba, M. F., Ahmed, M., **Barakat, K.**, Abou El Ella, D. A., & Abouzid, K.* (2019). Design, synthesis, biological evaluation and dynamics simulation of indazole derivatives with antiangiogenic and antiproliferative anticancer activity. *Bioorganic chemistry*, 82, 340–359. (Impact Factor 2020=3.94, Citation=8)
 12. Groenendyk, J., Paskevicius, T., Urra, H., Viricel, C., Wang, K., **Barakat, K.**, Hetz, C., Kurgan, L., Agellon, L. B., & Michalak, M.* (2018). Cyclosporine A binding to COX-2 reveals a novel signaling pathway that activates the IRE1 α unfolded protein response sensor. *Scientific reports*, 8(1), 16678. (Impact Factor 2020=4.12, Citation=7)
 13. Ganesan, A., Moon, T. C., & **Barakat, K. H.*** (2018). Revealing the atomistic details behind the binding of B7-1 to CD28 and CTLA-4: A comprehensive protein-protein modelling study. *Biochimica et biophysica acta. General subjects*, 1862(12), 2764–2778. (Impact Factor 2020=3.74, Citation=0)
 14. Ganesan, A., Arulraj, T., Choulli, T., & **Barakat, K. H.*** (2018). A mathematical modelling tool for unravelling the antibody-mediated effects on CTLA-4 interactions. *BMC medical informatics and decision making*, 18(1), 37. (Impact Factor 2020=2.38, Citation=2)
 15. Gentile, F., **Barakat, K. H.**, & Tuszynski, J. A.* (2018). Computational characterization of small molecules binding to the human XPF active site and virtual screening to identify potential new DNA repair inhibitors targeting the ERCC1-XPF Endonuclease. *International journal of molecular sciences*, 19(5), 1328. (Impact Factor 2020=4.21, Citation=7)
 16. Gentile, F., Deriu, M. A., **Barakat, K.**, Danani, A., & Tuszynski, J.* (2018). A Novel Interaction Between the TLR7 and a Colchicine Derivative Revealed Through a Computational and Experimental Study. *Pharmaceuticals (Basel, Switzerland)*, 11(1), 22. (Impact Factor 2020=3.85, Citation=1)
 17. Kalyaanamoorthy, S., & **Barakat, K. H.*** (2018). Binding modes of hERG blockers: an unsolved mystery in the drug design arena. *Expert opinion on drug discovery*, 13(3), 207–210. (Impact Factor 2020=4.34, Citation=8)
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69. **Barakat, K.***, Ahmed, M., Tabana, Y., Ha, M., A “Deep Dive” into the SARS-Cov-2 Polymerase Assembly: Identifying Novel Allosteric Sites and Analyzing the Hydrogen Bond Networks and Correlated Dynamics. Submitted to JCIM.
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74. Mosa, F., **Barakat, K.***, Effects of temperature of the SARS-CoV-2 Envelope protein stability.
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78. Tabana, Y., Elahi, S., Siraki, A., **Barakat, K.***, Tackling therapeutic immune targets to modulate the tumor microenvironment of breast cancer.
79. Tabana, Y., Elahi, S., Siraki, A., **Barakat, K.***, Reversing T cell Exhaustion in immunotherapy: A survey on current approaches and limitations.
80. Chen, R., Kundu, J., Lemieux J., **Barakat, K.***, Understanding the Mode of Action of B7-1 Inhibitors: a Computational Study.

Book Chapters:

1. Feng, T., & **Barakat, K.*** (2018). Molecular Dynamics Simulation and Prediction of Druggable Binding Sites. Mohini Gore and Umesh B. Jagtap (eds.), In *Computational Drug Discovery and Design, Methods in Molecular Biology*, vol. 1762, © Springer Science+Business Media, LLC, part of Springer Nature.
2. Feng, T., Kalyanamoorthy, S., & **Barakat, K.*** (2018). L-Type Calcium Channels: Structure and Functions. In *Ion Channels in Health and Sickness*, 127. Kaneez Fatima Shad, K. F. eds. InTech open access publisher.
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Patents:

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Abstracts/Presentations: (*corresponding author)

1. Tabana, Y., Shahbaz, S., Babu D, Ahmed, M., Dunsmore, G., Okoye, I.S., Moon, T.C., Fahlman, R.P., West, F.G., Elahi, S., Siraki, A., & **Barakat, K.*** Identifying the mechanism of action for a potent small molecule immunomodulator. *Poster presentation*. 7th Pharmaceutical Sciences World Congress 2020 May 22-27.
2. Hena, N., Hasani, H.J., Kalyanamoorthy, S., Moon, T.C., & **Barakat K.*** A Multifaceted Approach to Study Binding Modes of Tyrosine Kinase Inhibitors to hERG Cardiac Ion Channel. *Poster presentation*. University of Alberta, Faculty of Pharmacy and Pharmaceutical Sciences Research Day 2019 Nov 28. Poster was also presented in the 6th Annual CRINA Research Day 2019 Nov 15.

3. Tabana, Y., Okoye, I.S., Shahbaz, S., Ahmed, M., Babu, D., Moon, T.C., Fahlman, R., West, F., Elahi, S., Siraki, A., & **Barakat, K.*** Identifying the mechanism of action for a potent small molecule immunomodulator. *Poster presentation*. 6th Annual Cancer Research Institute of Northern Alberta (CRINA) Research Day, Canada. (Invited for oral presentation).
4. Jutla, A., Kumar, J., Ahmed, M., Overduin, M., & **Barakat, K.*** Cross-Validation of SHP2 Inhibitors Identified through Computational Methods. *Invited oral presentation*. Faculty of Pharmacy and Pharmaceutical Sciences Research Day, Canada.
5. Jutla, A., Kumar, J., Ahmed, M., Overduin, M., & **Barakat, K.*** Cross-Validation of SHP2 Inhibitors Identified through Computational Methods. *Poster presentation*. Faculty of Medicine and Dentistry Research Day 2019, Canada and at Cancer Research Institute of Northern Alberta (CRINA) Research Day 2019, Canada.
6. Jutla, A., Kumar, J., Ahmed, M., Overduin, M. & **Barakat, K.*** The Use of Computational, Biophysical and Molecular Biological Techniques to Screen and Identify Compounds for Juvenile Myelomonocytic Leukemia. *Poster presentation*. Festival of Undergraduate Research and Creative Activities 2019, Canada.
7. Kalyaanamoorthy, S., Lamothe, S.M., Hou, X. Moon, T.C., Kurata, H.T., Houghton, M. & **Barakat, K.*** Structure-based prediction of drug-induced hERG blockade. *Poster presentation*. Cardiac Society Research day 2019, Edmonton, AB Canada.
8. Kalyaanamoorthy, S., Co, J., & **Barakat, K.*** Computational study of the unbinding kinetics and mechanisms of hERG blockers. *Poster presentation*. Cardiac Society Research day 2019, Edmonton, AB Canada.
9. Feng, T., Kalyaanamoorthy, S., Ganesan, A., & **Barakat, K.*** Atomistic modeling of the human CaV1.2 channel: structural and mechanistic insights of cardiac ion permeation. *Poster presentation*. Cardiac Society Research day 2019, Edmonton, AB Canada.
10. Chen, R., Arutyunova, E., Ganesan, A., Lemieux, M.J., & **Barakat, K.*** Recombinant B7-1 (CD80) Preparation Towards Probing the Druggable Sites of B7-1. *Poster presentation*. CSPS/CC-CRS 2019 Symposium, Vancouver, British Columbia, Canada.
11. Feng, T., Kalyaanamoorthy, S., Ganesan, A., & **Barakat, K.*** Atomistic modeling of the human CaV1.2 channel: structural and mechanistic insights of cardiac ion permeation. *Poster presentation*. Cardiac Sciences Research Day 2019, Edmonton, AB, Canada.
12. Feng, T., Ganesan, A., Kalyaanamoorthy, S., & **Barakat, K.*** Modeling the near-open conformation of human CaV1.2 using external electric field and ion pulling simulations. *Poster presentation*. Faculty of Pharmacy Research Day 2018, Edmonton, AB, Canada.
13. Chen, R., Arutyunova, E., Moon, T.C., Ganesan, A., Lemieux, M.J., & **Barakat, K.*** Decoding the Druggable Sites of Human B7-1 for Targeting a Pyrazolocinnoline Series Small-molecule Inhibitor. CRINA Research Day 2018, Edmonton, Alberta, Canada.
14. Feng, T., Kalyaanamoorthy, S., & **Barakat, K.*** Modeling the dynamic gating mechanism and small-molecule binding in the CaV1.2 channel. *Poster presentation*. 2018 CSPS conference.
15. Gentile, F., & **Barakat, K.*** Computer-Aided Drug Design of ERCC1-XPF Inhibitors for Combination Cancer Therapy. *Oral presentation*. Western Canadian Medicinal Chemistry Workshop - 6th WCMCW, Saskatoon, SK, Canada, September 22, 2018.
16. Tabana, Y., Okoye, I.S., Shahbaz, S., Ahmed, M., Babu, D., Elahi, S., Siraki, A., & **Barakat, K.*** Studying the immunostimulatory activity of heterocyclic small molecules. *Poster*

- presentation*. 2018, 5th Annual Cancer Research Institute of Northern Alberta (CRINA) Research Day, Edmonton, Canada.
17. Chen, R., Arutyunova, E., Ganesan, A., Lemieux, M.J., & **Barakat, K.*** Does the IgC Domain of B7-1 (CD80) Impact Receptor Binding – A Key Process in T-cell Immunomodulation. *Poster presentation*. 2018 Faculty of Pharmacy and Pharmaceutical Sciences Research Day, Edmonton, AB, Canada.
 18. Mitran, C.J., Ganesan, A., Gnidehou, S., Ntumnia, F., Adams, J.H., **Barakat, K.**, Good, M. F., & **Yanow, S. K.*** A structurally defined epitope in *P. vivax* PvDBP that may mediate antibody cross-reactivity to similar epitopes in VAR2CSA. *Poster presentation.*, The Americal Society of Tropical Medicine & Hygine-2018, New Orleans, Louisiana, USA, October 28-November 1, 2018.
 19. Ganesan, A., & **Barakat, K.*** Structural bases of antibody-mediated effects on CTLA-4 revealed through molecular. *Poster presentation*. 101st Canadian Chemistry Conference and Exhibition, Edmonton, Alberta, Canada, 27-31 May 2018.
 20. Kilannamorthy, S., & **Barakat, K.*** Structural basis for the PIP2-mediated pharmacology in KCNQ3 channels. *Poster presentation*. 101st Canadian Chemistry Conference and Exhibition, Edmonton, Alberta, Canada, 27-31 May 2018.
 21. Ahmed, M., Kumar, A., THobman, T., & **Barakat, K.*** High Affinity Ligands against Dengue Virus NS1. *Poster presentation*. The 101st Canadian Chemistry Conference and Exhibition, Edmonton, AB (2018).
 22. Feng, T. Kalyaanamoorthy, S., & **Barakat, K.*** Modeling the dynamic gating mechanism and small-molecule binding in the CaV1.2 channel. *Poster presentation*. The Canadian Society for Pharmaceutical Sciences Conference Toronto 05/2018.
 23. Feng, T. Kalyaanamoorthy, S., & **Barakat, K.*** Modeling the dynamic gating mechanism and small-molecule binding in the CaV1.2 channel. *Poster presentaion*. 101st Canadian Chemistry Conference and Exhibition, Edmonton, Alberta, Canada, 27-31 May 2018.
 24. Mitran, C., Mena, A., Ganesan, A., Salanti, A., Maestre, A., Kano, F.S. , Carvalho, L., **Barakat, K.** Good, M. F. , & **Yanow, S. K.*** Defining a structural epitope within Plasmodium vivax PvDBP as a vaccine candidate against Plasmodium falciparum placental malaria. *Poster presentation*. 1st Malaria World Congress, Melbourne, Victoria, Australia, 1-5 July 2018.
 25. Tabana, Y., Dahham, S.S, **Barakat, K.**, Majid, A.M. Anti-angiogenic effects of β -caryophyllene against Human Colorectal Cancer Xenografts", 27-31 May (2018) Canada. *Poster presentation*. 101st Canadian Chemistry Conference and Exhibition (CSC2018).
 26. Gentile, F., **Barakat, K.**, Tuszynski, J.A.* Investigating the Structure of the XPF-ERCC1 Functional Endonuclease using a Computational Approach. *Poster presentation*. Biophysical Society 62nd Annual Meeting Moscone Center, San Francisco, CA, United States of America, February 18, 2018.
 27. Kalyaanamoorthy, S., & **Barakat, K.*** Binding site and interaction analysis of Kv7 modulators on KCNQ1 and KCNQ3 channels. *Poster presentation*. CRINA-Research Day 2017, Edmonton, Alberta, Canada, November 2017. (Awarded the WU Hong Memorial Poster Prize for Runner-up for the Poster Group D Postdoctoral Fellow Award award).
 28. Ganesan, A., Moon, T.C., **Barakat, K.*** How do the co-stimulatory CD28/B7-1 interactions differ from the co-inhibitory interactions of CTLA/B7-1 for orchestrating T-cell immune

- responses? *Poster presentation*. Cancer Research Institute of Northern Alberta 2017, Edmonton, Alberta, Canada. (Awarded top poster award).
29. Kalyaanamoorthy, S., & **Barakat, K.*** Molecular determinants for blocking the hERG channel. *Poster presentation*. Faculty of Pharmacy and Pharmaceutical Sciences Research Day, University of Alberta (2017).
 30. Hasani, H.J., Ganesan, A., Ahmed, M., **Barakat, K.*** The effects of protein-protein interactions and ligand-binding on the ion permeation through KCNQ1 channel revealed by computational simulations. *Poster presentation*. Faculty of Pharmacy Research Day, University of Alberta, Edmonton, Alberta, Canada.
 31. Ganesan, A., Arulraj, T., Choulli, T., **Barakat, K.*** Mathematical modelling and analyses of antibody-induced changes in the co-stimulatory interactions. Faculty of Pharmacy Research Day. *Poster presentation*. University of Alberta, Edmonton, Alberta, Canada.
 32. Ahmed, M., Kumar, A., Hobman, T., & **Barakat, K.*** Identification of High Affinity Ligands against Dengue Virus NS1 for the Development of an Affordable Point-of-care Diagnostic Kit. *Poster presentation*. Faculty of Pharmacy and Pharmaceutical Sciences Research Day, University of Alberta (2017).
 33. Gentile, F., & **Barakat, K.**, Tuszynski, J.A.* Rational design of inhibitors of the XPF-ERCC1 heterodimerization for combination cancer therapy. *Oral and poster presentations*. Cancer Research Institute of Northern Alberta Research Day 2017, University of Alberta, Edmonton, AB, Canada, November 25, 2017.
 34. Feng, T., Kalyaanamoorthy, S., & **Barakat, K.*** Modeling dynamic structure and investigating properties of the CaV1.2. *Poster presentation*. The Faculty of Pharmacy and Pharmaceutical Sciences Research Day 10/2017.
 35. Ahmed, M., & **Barakat, K.*** The Too Many Faces of PD-L1: A Comprehensive Conformational Analysis Study. *Poster presentation*. Canadian Cancer Research Conference (CCRC) November 5-7, 2017, Vancouver BC, Canada.
 36. Gentile, F. **Barakat, K.**, Tuszynski, J.A.* Virtual screening of DNA repair inhibitors targeting the XPF active site for combination cancer therapy. *Poster presentation*. 4th Canadian Cancer Research Conference 2017, Vancouver Convention Center, Vancouver, BC, Canada, November 5, 2017.
 37. Ahmed, M., Ganesan, A., Kumar, A., Hobman, T., & **Barakat, K.*** Identification of high affinity ligands against dengue virus NS1 for the development of an affordable point-of-care diagnostic kit. *Poster presentation*. IC-Impacts India Workshop Series, December 4-5 2017, Pune, Maharashtra, India.
 38. Ganesan, A., & **Barakat, K.*** Modelling the interactions of CD28:B7-1 complexes: Towards understanding the control of immune responses against cancers. *Poster presentation*. CRINA-Research Day 2016, Edmonton, Alberta, Canada, 12 November 2016. (Awarded top poster award).
 39. Ganesan, A., Ahmed, M., Hasani, H.J. & **Barakat, K.*** Exploration of sodium permeation in the human Nav1.5 channel. *Poster presentation*. Toxicology Symposium 2016, University of Alberta, Canada, 18 May 2016.
 40. Ahmed, M. Elahi, S., Nieman, J., Xu, L., Okoye, I., Zhang, G., Kandadai, A.S., Hena, M., Belovodskiy, A., Hosseini, S.N, Arutyunova, E., Moon, T.C., Yoon, B., Shields, J., Agopsowicz, K.C., Srivastava, N., West, F., Hitt, M., Walker, J., Smylie, M., Lemieux, J.,

- Siraki, A., Tyrrell, D.L., Houghton, M., & **Barakat, K.*** Rational Design and Validation of Of Small Molecular Inhibitors For The PD-1/PD-L1 Immune Checkpoint Pathway. *Poster presentation*. CRINA research day (2016).
41. Ahmed, M., Elahi, S., Nieman, J., Xu, L., Okoye, I., Zhang, G., Kandadai, A.S., Hena, H., Belovodskiy, A., Hosseini, S.N., Arutyunova, E., Chul, T.C., Yoon, B., Shields, J., Agopsowicz, K.C., Srivastava, N., West, F., Hitt, M., Walker, J., Smylie, M., Lemieux, J., Siraki, A., Tyrrell, D.L., Houghton, M., & **Barakat, K.*** Rational Design and Validation of Of Small Molecular Inhibitors For The PD-1/PD-L1 Immune Checkpoint Pathway. *Poster presentation*. Faculty of Pharmacy and Pharmaceutical Sciences Research Day, University of Alberta (2016).
 42. Ahmed, M., Ganesan, A., Hasani, H.J., & **Barakat, K.*** Investigating The Ion Permeation Pathway Of Nav1.5 Ion Channel. *Poster presentation*. University of Alberta, Faculty of Pharmacy Toxicology symposium (2016).
 43. Ahmed, M., Ganesan, A., Hasani, H.J., & **Barakat, K.*** Investigating The Ion Permeation Pathway And Drug Blockade Of Nav1.5 Ion Channel. *Poster presentation*. CANHEIT, HPCS (2016).
 44. Gentile, F. & **Barakat, K.*** Computational Drug Design of Nucleotide Excision DNA Repair Inhibitors for Improved Cancer therapy. *Poster presentation*. American Society for Cell Biology 2016 Annual Meeting, Moscone Center, San Francisco, CA, United States, December 5, 2016.
 45. Gentile, F., & **Barakat, K.*** Modeling the Human XPF Nuclease Domain for Structure-Based Drug Design of Nucleotide Excision Repair and Interstrand Crosslink Repair Inhibitors. *Poster presentation*. Pharmacy Research Day 2016, University of Alberta Hospital, Edmonton, AB, Canada, November 25, 2016.
 46. Ahmed, M., Pal, A., Houghton, M., & **Barakat, K.*** A Comprehensive Computational Analysis For The Binding Modes Of HCV NS5A Inhibitors: The Question Of Symmetry. *Poster presentation*. University Of Alberta - UARE Symposium, University of Alberta, Edmonton, AB, Canada, November 12, 2016.
 47. Gentile, F., & **Barakat, K.*** A Novel Model Of The Human XPF Nuclease Domain For The Rational Design Of DNA Repair Inhibitors. *Poster presentation*. Cancer Research Institute of Northern Alberta Research Day 2016, University of Alberta, Edmonton, AB, Canada, November 12, 2016.
 48. Ganesan, A., Ahmed, M., Hasani, H.J., & **Barakat, K.*** Revealing ion exchange mechanisms in Nav1.5 channel using steered molecular dynamics simulations. *Oral presentation*. CANHEIT-HPCS 2016, University of Alberta, Edmonton, Canada, 2016.
 49. Heinzinger, M., Ganesan, A., Feng, T., & **Barakat, K.*** Taking protein-protein interactions to the maximum speed: Applying coarse-graining simulations. *Poster presentation*. CANHEIT-HPCS 2016, University of Alberta, Edmonton, Canada, 2016.
 50. Ganesan, A., Ahmed, M., Hasani, H.J., & **Barakat, K.*** Exploration of sodium permeation in the human Nav1.5 channel using steered molecular dynamics simulations. *Poster presentation*. Toxicology Symposium 2016, University of Alberta, Edmonton, Canada, 2016.
 51. Ahmed, M., Pal, A., Houghton, M., & **Barakat, K.*** A Comprehensive Computational Analysis For The Binding Modes Of HCV NS5A Inhibitors: The Question Of Symmetry. *Poster presentation*. University of UARE Symposium.

52. Hasani, H.J., Ahmed, M., & **Barakat, K.*** Modelling the Human KCNQ1 Potassium ion Channel: Application of Computational Approaches To Cardiotoxicity. *Poster presentation*. CANHEIT, HPCS (2016).
53. Ahmed, M., Ganesan, A., Hasani, H.J., & **Barakat, K.*** Investigating The Ion Permeation Pathway And Drug Blockade Of Nav1.5 Ion Channel. *Poster presentation*. CANHEIT, HPCS (2016).
54. Ahmed, M., Ganesan, A., Hasani, H.J., & **Barakat, K.*** Investigating The Ion Permeation Pathway Of Nav1.5 Ion Channel. *Poster presentation*. University of Alberta, Faculty of Pharmacy Toxicology symposium (2016).
55. Gentile, F., Tuszynski, J. A.*, & **Barakat, K.*** Hybrid Ligand/Target-Based Virtual Screening Protocol to Identify Inhibitors for the XPA-ERCC1 Protein-Protein Interaction. *Poster presentation*. Pharmacy Research Day, November 27, 2015. University of Alberta Hospital, Edmonton, Canada.
56. Gentile, F., Tuszynski, J. A.*, & **Barakat, K.*** Identifying novel inhibitors for the XPA-ERCC1 protein-protein interaction. *Poster presentation*. Cancer Research Institute of Northern Alberta (CRINA) Research Day, November 14, 2015. University of Alberta, Edmonton, Canada.
57. Ahmed, M., Hasani, H.J., & **Barakat, K.*** SHP2 Directly Interact With PD-1 In A Favoured Conformation: A Comprehensive Modelling Study. *Poster presentation*. The Cancer Research Institute of Northern Alberta's (CRINA) Research Day (November, 2015).
58. Hasani, H.J., Ahmed, M., & **Barakat, K.*** Modelling The PD-L1:B7-1 Protein-Protein Interaction In The Tumor Microenvironment. *Poster presentation*. The Cancer Research Institute of Northern Alberta's (CRINA) Research Day (November, 2015).
59. Ahmed, M., Hasani, H.J., & **Barakat, K.*** A Comprehensive Atomistic Model For The Human Nav1.5 Sodium Ion Channel: Toward Understanding The Molecular Origin Behind Cardiotoxicity. *Poster presentation*. University of Alberta Faculty of Pharmacy and Pharmaceutical Sciences Research Day (November, 2015).
60. Ahmed, M. Hasani, H.J., & **Barakat, K.*** A Comprehensive Atomistic Model For The Human Nav1.5 Sodium Ion Channel: Toward Understanding the Molecular Origin Behind Cardiotoxicity. *Poster presentation*. Ion Channel Retreat, Vancouver BC, Canada. July 2015.
61. Hasani, H.J., Ahmed, M. & **Barakat, K.*** Knowledge-Based Flexible Docking Reveals A Comprehensive Model For Human PDL-1 Bound To Human B7-1. *Poster presentation*. HPCS 2015, Montreal, Québec, Canada. June 2015.
62. Ahmed, M. & **Barakat, K.*** Toward A Full Model For The PD-1 Pathway: Modeling The Interaction Between PD-1 And SHP2. *Poster presentation*. HPCS 2015, Montreal, Québec, Canada. June 2015
63. Ahmed, M. & **Barakat, K.*** Human PD-1 binds differently to its human ligands. *Poster presentation*. HPCS 2015, Montreal, Québec, Canada. June 2015.
64. **Barakat, K.*** Rational Design of Immune Checkpoints' Small Molecule Inhibitors." CIHR Institute Of Infection And Immunity New Investigator Forum. *Poster presentation*. LE MANOIR DU LAC DELAGE, QC, Canada. May 2015.
65. Viricel, C. Ahmed, M., & **Barakat, K.*** Rational Design of Small Molecule Immune Checkpoints' Inhibitors. *Poster presentation*. February 2015, Tumor Immunology: Multidisciplinary Science Driving Combination Therapy (J7)."

66. **Barakat, K.*** Toward Potent Immunotherapy Drugs: Rational Design of Inhibitors of the PD-1 Pathway”. *Poster presentation*. November 2014 CIHR, IG, ICR, ICRH New Principal Investigators 13th meeting.
67. **Barakat, K.,** Tyrrell, D.L., Evans, D., & Houghton, M.* Mode Of Binding of Daclatasvir”. *Poster presentation*. HCV meeting, September 2014, Banff, Canada, Canada.
68. **Barakat, K.,** Law, J., Prunotto, A., Tyrrell, D.L., Evans, D., Tuszynski, J., & Houghton, M.* Computational Modeling of the HCV Polymerase active site and drug screening in silico. *Poster presentation*. 2nd Li Ka Shing Institute of Virology Symposium, May 2013, Edmonton, AB, Canada.
69. Anwar-Mohamed, A., Barakat, K. Hockman, D. Thomas, B, Tyrrell, D.L., & Houghton, M.* Mechanisms Of Fatal Human Cardiotoxicity By The HCV Drug BMS-986094. *Poster presentation*. 2nd Li Ka Shing Institute of Virology Symposium, May 2013, Edmonton, AB, Canada.
70. **Barakat, K.,** Jordheim, L.P., Houghton, M. Dumontet, C. and Tuszynski, J.*, Virtual screening suggests novel inhibitors for the XPf-ERCC1 interaction. *Poster presentation*. 6th Drug Discovery and Medicinal Chemistry Conference, June 2012, San Diego, CA, USA.
71. Friesen, D., **Barakat, K.,** Fenske, B., Mane, J., Tseng, C.Y., & Tuszynski, J.*. Identification of γ -tubulin Paclitaxel and Colchicine Binding Locations for Novel Dual Inhibitors of γ and β III-tubulin. *Poster presentation*. 17th Canadian Symposium on Theoretical Chemistry, University of Alberta, July 2010.
72. **Barakat, K.,** Issack, B., Stepanova, M., & Tuszynski, J.* Effects of Temperature on the Binding Interactions and Collective Dynamics of p53-DNA: Comparing the Wild type to the R248Q Mutant. *Poster presentation*. 17th Canadian Symposium on Theoretical Chemistry, University of Alberta, July 2010.
73. Friesen, D., **Barakat, K.,** & Tuszynski, J.* Blind docking predicts potential binding sites for Human Polynucleotide kinase inhibitors. *Poster presentation*. Alberta Cancer Research Institute Meeting, November 2009, Banff, Edmonton, AB, Canada. The same poster was presented at the IGTC Summit, October 2010, Naramata Centre, Naramata, BC.
74. **Barakat, K.,** & Tuszynski, J.* Relaxed complex scheme predicts novel inhibitors for the lyase activity of DNA polymerase beta. *Poster presentation*. Alberta Cancer Research Institute Meeting, November 2009, Banff, Edmonton, AB, Canada.
75. Craddock, Travis J. A., **Barakat, K. H.,** and Tuszynski, Jack A., “Computational Determination of Putative Binding Sites of Anesthetics to the Cytoskeleton”, *Poster Presentation* at The Seventh Canadian Computational Chemistry Conference. July 2009, Halifax, Nova Scotia, Canada.
76. **Barakat, K.,** Tuszynski, J.* Ensemble Virtual Screening Reveals Potential Inhibitors for the MDM2-p53 Interaction. *Poster Presentation*. Seventh Canadian Computational Chemistry Conference in Halifax, Nova Scotia, Canada. July 2009, the abstract being included in the conference proceedings.
77. **Barakat, K.,** & Tuszynski, J.* Ensemble Virtual Screening Reveals Potential Inhibitors for the MDM2-p53 Interaction., *Poster Presentation*. Chemical Biophysics Symposium, Toronto, Canada, April 2009, the abstract being included in the conference proceedings.
78. **Barakat, K.,** Huzil, J. T., & Tuszynski, J. * Virtual Screening and MD simulations suggest potential inhibitors of the Nucleotide Excision Repair pathway. *Poster Presentation*. Western

Canadian Medicinal Chemistry Workshop, at the University of Saskatchewan, Saskatoon, in September of 2008, the abstract being included in the conference proceedings.

Invited Speaker:

1. April 2020, "Rational design of Small Molecule Inhibitors For COVID-19", COVID-19 Conference organized by DiscoveryLab, University of Alberta, Edmonton, AB, Canada.
2. April 2019, "Computational Drug Discovery of Membrane Proteins", Northern lights seminar series, University of Alberta, Edmonton, AB, Canada.
3. November 2018, "Developing Small Molecule Immune Checkpoints Inhibitors", LKS Translational Research Symposium, Edmonton (Alberta), Canada.
4. October 2018, "Atomistic Computational Models to Predict Drug-mediated Cardiotoxicity", CVRC Seminar Series, Edmonton (Alberta), Canada.
5. September 2018, "New trends in Computational Drug Discovery", Invited Talk, Faculty of Pharmacy, Ain Shams University, Cairo, Egypt
6. April 2018, "Atomistic Computational Models To Predict Drug-mediated Cardiotoxicity", **Keynote Speaker**, International Conference on Pharmacy and Pharmaceutical Sciences, Dubai, United Arab Emirates.
7. April 2018, "Atomistic Computational Models To Predict Drug-mediated Cardiotoxicity", Visit to Al-Ain University, United Arab Emirates.
8. March 2018, "Rational Design And Development Of Small Molecule Inhibitors Of The Immune Checkpoints: A Slide Set Focused On A PD-1 & CTLA-4 Antagonists", TecEdmonton Industrial day, Calgary, AB, Canada.
9. December 2017, "Identification Of High Affinity Ligands Against Dengue Virus NS1 For The Development Of An Affordable Point-of-care Diagnostic Kit", 2017 Pune IC-IMPACTS workshop, Pune, India.
10. October 2017, "Rational Design Of Small Molecule Immune Checkpoints' Inhibitors: The PD-1 Challenge", **Keynote Speaker**, Applied microbiology Conference, Toronto, Ontario, Canada.
11. May 2017, "Rational Design Of Small Molecule Immune Checkpoints' Inhibitors: The PD-1 Challenge", Vaccine Innovation Conference, Montreal, QC, Canada.
12. April 2017, "HEKA THERAPEUTICS: Spin Off For The Immune Checkpoints Program At The University Of Alberta, Canada", visit to Merck Research Labs (MRL), NJ, USA.
13. December 2016 "Computational Drug Discovery Applied To Cancer Immunotherapy And Hepatitis C Virus", **Keynote Speaker**, ICDDDT-2016, Cairo, Egypt.
14. December 2016 "Computational Drug Discovery: A Candle In The Dark", Invited Talk, Ain Shams University, Cairo, Egypt.
15. December 2016 "Computational Drug Discovery: A Candle In The Dark", Invited Talk, American University in Cairo (AUC), Cairo, Egypt.
16. March 2016 "Toward Potent Immunotherapy Drugs: Rational Design of Inhibitors of the Immune Checkpoints Proteins" **Keynote Speaker**, 6th Euro Virology Congress and Expo, Madrid, Spain.

17. February 2016 “Computational Drug Discovery: A Candle In The Dark”, Invited Talk, University of Sharjah, Sharjah, UAE.
18. February 2016 “Computational Drug Discovery: A Candle In The Dark”, Invited Talk, Al-Ain Univeristy, Al-Ain, UAE.
19. February 2016 “Computational Drug Discovery Applied To Cancer Immunotherapy And Hepatitis C Virus”, 7th International Conference on Drug Discovery and Therapy, University of Sharjah, Sharjah, UAE.
20. February 2016 “Computational Drug Discovery Applied To Cancer Immunotherapy And Hepatitis C Virus”, 7th International Conference on Drug Discovery and Therapy, University of Sharjah, Sharjah, UAE.
21. December 2015 “Rational Design Of Small Molecule Immune Checkpoints’ Inhibitors”, Virology 2015, Atlanta, GA, USA
22. April 2015 “Structure-Based Algorithms to Predict Drug-Mediated Toxicity” Bio-IT World, Boston, USA.
23. February 2015 “Rational Design of Small Molecule Immune Checkpoints’ Inhibitors” Short talk at the Tumor Immunology: Multidisciplinary Science Driving Combination Therapy (J7).
24. November 2014 “Toward Potent Immunotherapy Drugs: Rational Design of Inhibitors of the PD-1 Pathway” Short talk at the CIHR, IG, ICR, ICRH New Principal Investigators 13th meeting.
25. September 2014 “Computational Drug Discovery Applied to HCV” **Plenary Speaker** at the HCV meeting 2014.
26. June 2014, “Rational Drug Design” Department of Medical Genetics, University of Alberta, Edmonton, Canada.
27. September 2011, Virtual screening reveals dual inhibitors for the ERCC1-XPF interaction, 2nd Symposium on Graduate Physics Research, University of Alberta, Edmonton, AB, Canada.
28. May 2010, Sharcnnet research day, York university, Toronto, Canada,” Ensemble-based virtual screening reveals dual-inhibitors of the p53-MDM2/MDMX interactions”.
29. November 2009, Northern Lights seminar series – University of Alberta, Edmonton, AB, Canada: “Molecular Drug Design: Receptor-Based Virtual Screening (RBVS)”.
30. October 2009, Graduate Biophysics Class – University of Alberta, Edmonton, AB, Canada: “A An introductory lecture on Bioinformatics and Bioinformatics tools”.
31. December 2006, Dept. of Engineering Physics, Cairo *University*, Egypt: "Phase transitions of tetrahedral molecules using molecular dynamics simulations".
32. October 2006, Physics Department, *American University in Cairo*, Egypt: "Phase transitions in solid Methane".

IV. VOLUNTEER AND PUBLIC SERVICE

2016 Volunteer at the Alberta Cancer Foundation (ACF) longest baseball game fundraising event.

- 2015 Volunteer at the Cash & Cars fundraising for the Alberta Cancer Foundation (ACF).
- 2015 Volunteer for minor soccer association (MSA), serving as a soccer coach for minor kids
- 2011 President of the Graduate Physics Student Association (GPSA)
- 2011 Vice President of the Egyptian Student Association (ESA).

V. MEDIA INTERVIEWS

1. **TheScientist:** <https://offers.the-scientist.com/rising-stars-in-cancer-research-multisponsored-ebook>
2. **Folio:** <https://www.folio.ca/u-of-a-researchers-move-closer-to-magic-cancer-treatment/>
3. **CBC news:** <https://www.cbc.ca/news/canada/edmonton/cancer-u-of-a-research-khaled-barakat-immunotherapies-immune-system-arno-siraki-1.5301121>
4. **Mashable:** <https://in.mashable.com/tech/7201/researchers-are-working-on-a-magic-cancer-treatment>
5. **Vantage point:** <https://seekingalpha.com/article/4027531-vantage-point-going-small-hit-big>
6. **Edmonton Sun:** <https://edmontonsun.com/2015/06/24/magic-cancer-drug-being-developed-by-university-of-alberta/wcm/cf843ea0-672a-45b1-8163-612961e79454>
7. **CTV National:** <http://www.ctvnews.ca/health/alberta-team-assembled-to-develop-cancer-curing-magic-drug-1.2439593>
8. **CTV Edmonton:** <http://edmonton.ctvnews.ca/the-fight-against-cancer-gets-multimillion-dollar-boost-1.2438643>
9. **Global Edmonton:** <http://globalnews.ca/news/2073234/edmonton-partnership-hopes-to-develop-magic-drug-for-cancer-patients/>
10. **Eureka alert:** <http://www.techienews.co.uk/9734974/researchers-take-the-fight-against-cancer-at-molecular-level/>
11. **Science News:** <https://www.sciencenews.org/article/new-cancer-drugs-wake-sleeping-killer-t-cells>
12. **Dinner Television:** <http://www.dinnertelevision.ca/videos/4335349992001/>
13. **Leap Magazine:** <http://myleapmagazine.ca/2015/09/research-rock-star-the-beat-goes-on/>
14. **University of Alberta Website:** <http://pharm.ualberta.ca/news/2015/june/small-but-mighty-molecules>

VI. SPINOFF COMPANIES

1. **Heka Therapeutics INC:** Small molecule inhibitors for the immune checkpoints' proteins.
2. **Achlys:** Predicting off-target toxicity for small molecule drugs.