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Toward potent immunotherapy drugs: Rational design of inhibitors of the immune checkpoints proteins

Immune checkpoints constitute a distinctive set of proteins that belong to the B7 family. The engagement of these transmembrane receptors with their ligands provides critical signals to inhibit T-cell activation and promote for immune tolerance. Tumor and infected cells can hide from the immune system by over expressing these proteins leading to T-cell exhaustion. Blocking these interactions emerged as a 'game changing' approach in anticancer and antiviral immunotherapy. Current immune checkpoints blockers are limited to antibodies and possess a unique mode of action; they reactivate exhausted T-cells, allowing them to proliferate and recognize and kill infected and tumor cells. Despite their outstanding success the ultimate therapeutic target or combination of targets from these proteins is still to be determined. They are highly limited by their substantial cost and severe side effects. Our team at the University of Alberta has been focused on developing less expensive and more controlled inhibitors for the immune checkpoints. Our approach combines state-of-the-art computational modeling techniques with cutting-edge experimental technologies to design and develop small molecule inhibitors for these proteins. During this talk, an overview about our program will be presented with updates on our recent progress toward this goal.

Biography

Khaled Barakat is an Assistant Professor at the School of Pharmacy at the University of Alberta, Canada. His research stands at the multidisciplinary interface of physics, biology and computer science. His major focus is on developing and applying state-of-the-art computational drug discovery tools to discover new antiviral and immunotherapeutic drugs. He has made great contributions in understanding the nature and biophysical processes underlying protein-drug, protein-protein and drug off-target interactions and predicting drug-mediated toxicity. He has also received numerous awards including the CIHR and AIHS Postdoctoral Fellowships, the prestigious University of Alberta Dissertation Award and many distinction awards throughout his undergraduate and graduate studies. He is also the Editor of the *Journal of Pharmaceutical Care & Health Systems* and serves as a Guest Reviewer for several journals.

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