CURRICULUM VITAE

Rima Hajjo, B.Sc. Pharm., M.S., Ph.D.

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1. Personal Data

Nationality: Jordanian

2. Education

- 2018 – 2020 Graduate Certificate Degree – Bioinformatics (Genetics and Epigenetics), Harvard University, Cambridge, MA, USA.
- 2005 – 2010 Ph.D. in Pharmaceutical Sciences (Minor: Pharmacoinformatic and Pharmacogenetics), Eshelman School of Pharmacy University of North Carolina at Chapel Hill, NC, USA.
- 1999 – 2003 M.Sc., Pharmaceutical Sciences, University of Jordan, Amman, Jordan.
- 1994 – 1999 B.Sc. Pharm, University of Jordan, Amman, Jordan.

3. Ph.D. Dissertation

Dissertation title: *In silico* Strategies to Study Polypharmacology of G-protein Coupled Receptors). Thesis Supervisors: Prof. Alexander Tropsha for the Computational studies and Prof. Bryan Roth for the Pharmacological and Pharmacogenetics Studies. Scope of studies: Pharmacoinformatics, pharmacology and pharmacogenomics.

4. M.S. Thesis

Thesis title: Determination of Some Pesticide Residues in Selected Medicinal Plants Commonly Used in Jordan. Thesis Supervisors: Prof. Farma U. Afifi and Prof. Abdelkader Battah. Scope of studies: Phytochemistry, toxicology, experimental analysis, analytical analysis, mass spectrometry, gas chromatography.

5. Employment

Academic Positions

- Jan 2021, **Adjunct Professor**, Computational Chemical Biology, Eshelman School of Pharmacy, UNC-Chapel Hill, Chapel Hill, North Carolina, USA.
- Feb 2019 – Present, **Assistant Professor**, Pharmaceutical Sciences, Al-Zaytoonah University of Jordan, Amman, Jordan.
- Jan 2011 – Present, **Visiting Scholar**, Tropsha's Lab, UNC-Chapel Hill, Chapel Hill, North Caroline, USA.
- Aug 2006 – Jun 2007, **Teaching assistant**, Eshelman School of Pharmacy, UNC-Chapel Hill, North Caroline, USA.
- Aug 1999 – Aug 2005, **Teaching assistant**, School of Pharmacy, University of Jordan, Amman, Jordan.

Research And Development Positions

- Apr 2016 – Sep 2019, **Solution Scientist Consultant, Discovery and Translational Science** (Clarivate Analytics, formerly Thomson Reuters IP & Science, Boston, MA)
- Nov 2014 – Mar 2016, **Computational Chemist/Biologist** (FORMA Therapeutics, Watertown, MA)
- Jan 2013 – Oct 2014, **Senior Research Scientist** (TransTech Pharma, High Point, NC)
- Nov 2010 – Dec 2012, **Research Scientist** (TransTech Pharma, High Point, NC)
- Nov 2009 – Oct 2010, **Pre-doctoral Scientist** (TransTech Pharma, High Point, NC)

6. Research Interests

Research Specialties

Machine learning, artificial intelligence, computer-assisted drug design, cheminformatics, bioinformatics, computational genomics, microarrays, Next Genome Sequencing (NGS), proteomics, metabolomics, metagenomics, systems biology, pathway ontologies, network analysis, polypharmacology, pharmacogenomics, drug-repurposing, biomarker selection, drug target prioritization, quantitative structure-activity relationships (QSAR) modeling, model-based virtual screening, diversity metrics, molecular descriptors, multiple sequence alignment, homology modeling, docking and scoring, binding free energies, conformational search, pharmacophore modeling, small-molecule optimization, scaffold hopping.

Therapeutic Areas of Interest

Oncology, immuno-oncology, neuroscience, inflammatory regulators, diabetes, infectious disease, rare disease, and the human microbiome.

Technical Research Skills

- Operating Systems and Platforms: High-Performance Computing Cluster, Cloud-computing, UNIX, Linux, Windows & Mac.

- Software Packages (Mastery): Bioconductor (The Bioconductor Project, Open Source); Galaxy Genomics Tools (Galaxy, Open Source); GenomeSpace and available tools: Cytoscape, Galaxy, GenePattern, Genomica, Integrative Genomics Viewer (IGV), and the UCSC Genome Table Browser (Genomespace.org); GenePattern (Broad Institute); GATK, Genome Analysis Toolkit (Broad Institute, Open-source); SAMtools (Open-source); JMP Genomics (SAS Institute); Partek Genomics and Pathway (Partek, Inc.); NCBI Bioinformatics Tools (National Center for Biotechnology Information - NCBI – NIH, Open Source), MetaCore and MetaBase Systems Biology Solutions (Clarivate Analytics); Key Pathway Advisror (Clarivate Analytics); IPA, Ingenuity Pathway Analysis (QIAGEN Bioinformatics); Integrity Drug Pipeline Database and APIs (Clarivate Analytics); GeneSeq Database for Biological Sequences (Clarivate Analytics); Drug Research Advisor- Target Draggability (Clarivate Analytics); SequenceBase Sequence Search Engine (SequenceBase); Maestro (Schrodinger); Glide, Phase, Prime, Jaguar, MacroModel, Core Hopping (Schrodinger); CANVAS (Schrodinger), Discovery Studio (Accelrys, Inc.); GOLD, LibDock and CDOCKER (Accelrys, Inc.); Pipeline Pilot (Accelrys); Molecular Operating Environment- MOE (Chemical Computing Group), MUSE (Tripos); OMEGA (OpenEye Scientific Software); LigandScout (InteLigand); JMP (SAS Institute); Partek (Partek); Dragon Molecular Descriptors (Talete); MolconnZ (eduSoft); ChemDraw Ultra (PerkinElmer), Marvin, Instant JChem (ChemAxon); kNN, SVM, CBA (MML-UNC-Chapel Hill); Sybyl (Tripos); Matlab (MathWorks); R (The R Project for Statistical Computing, Open-source), Spotfire (TIBCO); Jmol (Open-source), PyMol (Open-source), Vortex (Dotmatics); CRM for Customer Relationship Management (SalesForce).

- Software Packages (Familiarity): R-Shiny (R Project, Open-source); Coot X-rayCrytallography Model Building Toolkit (University of Oxford); Chimera (UCSF.edu); Rosetta (RosettaCommons); Torch (Cresset), Microbiome dataset analysis tools: QIIME1, mothur and DADA2 (NCBI, NIH).

- Programming Languages (Mastery and Familiarity): Python (expert), R (expert), Javascript, Java, HTML, JSON, Perl, Awk, SQL.

- Data types: Pre-clinical and clinical data, structure activity (SAR) data, chemical descriptors, high throughput screening (HTS) data, microarrays, next-generation sequencing (NGS), RNA-Seq, ChIP-seq, Cancer Cell Line Encyclopedia (CCLE), Genotype Tissue Expression (GTEx), gene expression, gene mutation/gene variant, metagenomics data,16S and ITS amplicon data, genomic and protein sequences, protein PDB data, protein x-ray structures, proteomics, metabolomics, patient genomic and drug response data.

7. Membership in Scientific Societies and Associations

- American Chemical Society (ACS) 2007 – Present

- American Association of Pharmaceutical Scientists (AAPS) 2007 - Present
- American Association for the Advancement of Science (AAAS) 2009 – Present
- Institute of Electrical and Electronics Engineers (IEEE) 2018 - Present
- Jordan Pharmaceutical Association (JPA) 1999 - Present

8. Honors and Awards

- **2017** Clarivate Analytics Century Club Award Recipient.
- **2016** Forma Therapeutics Distinguished Service Award.
- **2010** CINF- FIZ Scholarship for Scientific Excellence.
- **2010** ADDF Young Investigator Scholarship (Alzheimer's Drug Discovery Foundation).
- **2009** AAPS Young Innovator Award (American Association of Pharmaceutical Scientists).
- **2009** ADDF Young Investigator Scholarship (Alzheimer's Drug Discovery Foundation).
- **2005** Nominated for King Abdullah's Award for best thesis writing.
- **2004** The University of Jordan's scholarship to proceed with doctoral studies in the USA.
- **1994** The Jordanian Ministry of Higher Education's Scholarship to study Pharmaceutics.
- **1993** Jordanian Government's Academic Prize for the Scientific Creativity of Students.

9. Fellowships and Scholarships

- **2006-2010** University of North Carolina at Chapel Hill Graduate Studies Research Assistantship.
- **2004** The University of Jordan's scholarship to proceed with doctoral studies in the USA.
- **1994** The Jordanian Ministry of Higher Education's Scholarship to study Pharmaceutics.
- **1993** Jordanian Government's Academic Prize for the Scientific Creativity of Students.

10. Teaching Experience

Graduate Courses

- Molecular Molding and Drug Design for PhD students.
- Graduate Scientific Research Seminars for PhD students.

Undergraduate Courses

- Medicinal Chemistry (2&3)
- Phytotherapy & Alternative Medicine
- Medicinal Chemistry Lab

11. Grants

Hajjo, R., Sabbah, D., Aqel, D., The Development, Application and Experimental Validation of an Integrative Informatics Methodology to Identify Biomarkers, Pharmacological Targets and Pharmacotherapy for COVID-19
Grant 2020-2019/17/03, The Deanship of Scientific Research at Al-Zaytoonah University of Jordan (55,000 JD).

Al-Bawab, A., **Hajjo, R.**, Akour, A. Investigating the role of vitamin D in altering gut microbiome as a mechanism to alleviate prediabetes and type 2 diabetes mellitus. Grant XX, The Deanship of Scientific Research at Al-Zaytoonah University of Jordan (22, 850 JD).

12. Membership of Committees

- The Scientific Research Committee at the School of Pharmacy, Al-Zaytoonah University of Jordan (2019 – present)
- The Curriculum Committee at the School of Pharmacy, Al-Zaytoonah University of Jordan. (2020 – present).
- The Graduate Follow-up Committee at the School of Pharmacy, Al-Zaytoonah University of Jordan. (2020 – present).

13. Professional and Scientific Meetings

1. **Hajjo, R**. The ethical challenges of applying artificial intelligence and machine learning in cancer care. The First International Cancer Care Informatics Conference, Amman, Jordan, November 19-21, 2018.
2. **Hajjo, R.** Integrative informatics approaches for unraveling the mysteries of rare diseases: Shedding the light on Potocki-Shaffer syndrome. Oral Presentation, The 256th ACS National Meeting in Boston, MA, August 19-23, 2018.
3. **Hajjo, R.** A Biomarker-assisted systems biology approach to explore host-microbiome-drug interactions. The 17th Annual BioIT World Conference & Expo, Boston, MA, May 15-17, 2018.
4. **Hajjo, R.** Causal reasoning networks for the prioritization of clinically-relevant drug targets and disease-tracking biomarkers The 16th Annual BioIT World Conference & Expo, Boston, MA, May 15-17, 2018.
5. **Hajjo, R.** and Willis, C. Systems biology approaches to omics data analysis in complex diseases. Abstracts of papers, 253rd ACS National Meeting, San Francisco, CA, April 2-6, 2017. Abst BIOT 461.

6. **Hajjo, R.** and Tropsha, A. Chemogenomics-assisted anti-obesity drug discovery. Abstracts of papers, 250th ACS National Meeting, Boston, MA, August 16-20, 2015. Abst CINF 47.

7. **Hajjo, R.** Chemocentric informatics analysis of 'omics' data identifies novel links between HDACi and neuro-disease. Abstracts of papers, 250th ACS National Meeting, Boston, MA, August 16-20, 2015. Abst CINF 11.

8. **Hajjo, R.** and Tropsha, A. Chemocentric informatics analysis of 'omics' data identifies novel chemical-gene-disease associations in autism. Abstracts of papers, 247th ACS National Meeting, Dallas, TX, March 16-20, 2014. Abst COMP Sci-Mix 267.

9. **Hajjo, R.**; Setola, V.; Roth, B.L.; Tropsha, A. Integration of cheminformatics, chemical genomics, and network mining approaches to predict novel drug-gene-disease associations: applications to drug reprofiling for neuropsychiatric and neurodegenerative diseases. LINCS Symposium, Broad Institute, Cambridge, MA, November 18-19, 2013.

10. **Hajjo, R.**; Roth, B.L.; Tropsha, A. Computational Identification and Experimental Validation of Selective Estrogen Receptor Modulators as Ligands of 5-Hydroxytryptamine-6 Receptors and Potential Anti-Alzheimer's Agents. The Eighth Meeting of the Globalization of Pharmaceutics Education Network, November 10-12, 2010.

11. **Hajjo, R.**; Wang, X.S.; Roth, B.L.; Tropsha, A. A Chemocentric Informatics Approach to Drug Discovery: An Application to the Identification and Experimental Validation of Selective Estrogen Receptor Modulators as Serotonin Receptor Subtype 6 Binders and Potential Anti-Alzheimer's Agents. Abstracts of papers, 240th ACS National Meeting, Boston, MA, United States, August 22-26, 2010.

12. **Hajjo, R.**; Wang, X.S; Roth, B.L.; Tropsha, A. QSAR Modeling of GPCR Receptor Families, Model Application for Virtual Screening, and Experimental Validation of Computational Hits. Abstracts of papers, 240th ACS National Meeting, Boston, MA, United States, August 22-26, 2010.

13. **Hajjo, R.**; Wang, X.S.; Roth, B.L.; Tropsha, A. A Novel Approach to Drug Discovery Integrating Chemogenomics and QSAR Modeling: Application to Anti-Alzheimer’s Agents. Submitted to 239th ACS National Meeting, San Francisco, CA, United States, March 21-25, 2010.

14. **Hajjo, R.**; Roth, B.L.; Tropsha, A. A Novel Chemogenomics Approach to Identify Receptor Mediated Clinical Effects of Chemicals. The 2009 AAPS Annual Meeting and Exposition, Los Angeles, CA, November, 2009.

15. **Hajjo, R.**; Fourches, D.; Roth, B.L.; Tropsha, A. *In silico* Strategies to Identify Novel 5-HT_6 Receptor Ligands as Potential Anti-Alzheimer's and Anti-Obesity Treatments. Abstracts of Papers, 238th ACS National Meeting, Washington, DC, United States, August 16-20, 2009.

16. Wang, X.S.; **Hajjo, R.**; Tropsha, A. A Computational Workflow to Identify and Validate the Druggable Allosteric Binding Sites. Abstracts of Papers, 238th ACS National Meeting, Washington, DC, United States, August 16-20, 2009.

17. **Hajjo, R.**; Grulke, C.; Golbraikh, A.; Roth, B.L.; Tropsha, A. QSAR Models of 5-HT_{2B} Receptor Ligands and their Application to Predicting Compounds that Could Cause Valvulopathy. Abstracts of Papers, 237th ACS National Meeting, Salt Lake City, UT, United States, March 22-26, 2009.

Selected Seminars

1. A Biomarker-assisted systems biology approach to explore host-microbiome-drug interactions. Yale Medical School, Yale University, New Haven, April 26, 2018.

2. Exploring the Drug Discovery Space for Microbiome-Based Therapies, November 15, 2017.

3. An Integrative Systems Biology Approach for Prioritizing Biomarkers and Drug Targets in Complex Diseases. Public Webinar. June 1, 2017.

4. Network Biology Approaches to 'Omics' Data Analysis in Complex Diseases. Yale University. Yale Medical School, Yale University, New Haven, April 17, 2017.

5. Network Biology Approaches to 'Omics' Data Analysis in Complex Diseases. Massachusetts Institute of Technology (MIT), Cambridge, MA, January 12, 2017.

6. Network Biology Approaches to 'Omics' Data Analysis in Complex Diseases. University of Illinois at Chicago (UIC), Chicago, IL, September 16, 2016.

7. ACS Chemical Information Division (CINF): The Growing Impact of Big Data in the World of Chemical Information. Title: Chemocentric informatics analysis of 'omics' data identifies novel links between HDACi and neuro-disease. The 250th ACS National Meeting, Boston, MA, August 16, 2015.

8. LINCS Symposium, 2013. Title: Integration of cheminformatics, chemical genomics, and network mining approaches to predict novel drug-gene-disease associations: applications to drug reprofiling for neuropsychiatric and

neurodegenerative diseases. LINCS Symposium, Broad Institute, Cambridge, MA, November 18-19, 2013.

9. AAPS 2009 Young Innovators Symposium. Title: A novel Chemogenomics Approach to Identify Receptor Mediated Clinical Effects of Chemicals. The 2009 AAPS Annual Meeting and Exposition, Los Angeles, CA, November, 2009.

10. Montreal International Biochemistry & Biophysics Forum. Title: Multi-Residue Pesticide Analysis of the Medicinal Plant Origanum syriacum. Montreal, Canada, November 3, 2011.

Podcasts

Hajjo, R. A Novel Chemogenomics Approach to Identify Receptor-Mediated Clinical Effects of Chemicals. A joint presentation of Pharmaceutical Technology and AAPS. Young Innovators of 2009: Interviews with AAPS Graduate Student Winners. Website link: http://www.pharmtech.com/pharmtech/AAPS-2009-Innovations--Chemogenomics/ArticleStandard/Article/detail/644071.

14. Participation in or organization of curricular and/or extra-curricular activities

Editor Responsibilities
Review Editor in Computational Toxicology and Informatics, (2020).

Reviewing Responsibilities
Reviewer for Annals of Palliative Medicine, (2020).

Research proposal peer reviewer
The Deanship of Scientific Research at University of Petra, Amman, Jordan, (2019).

Inspirational Speaker to High School Students
The International Academy Amman (IAA), Chemistry Class Students, (2018 – 2020).

Training workshops
Modern Teaching Strategies, Al-Zaytoonah University Accreditation and Quality Assurance Office, February 14-16th 2017.

15. Publications

Papers in peer-reviewed journals

1. **Hajjo, R.**; Sabbah, D.A.; Bardaweel, S.K. *A Chemocentric Informatics Analysis: Dexamethasone and Combination Therapy for COVID-19*. ACS Omega, ACS Omega, :acsomega.0c03597. https://doi.org/10.1021/acsomega.0c03597

2. **Hajjo, R.**; Tropsha, A. *A Systems Biology Workflow for Drug and Vaccine Repurposing: Identifying Small-Molecule BCG Mimics to Prevent COVID-19*

Mortality. Pharmaceutical Research, 37(11). https://doi.org/10.1007/s11095-020-02930-9.

3. **Hajjo, R.;** Sabbah, D.A. *Small Molecule Drugs are Still the Biggest Winners in the Post Genomic Era According to the 2019 FDA Drug Approvals: Do they Really Abide to Conventional Drug-Like Rules?* Submitted to Molecular Informatics. Manuscript ID: minf. 202060020.

4. **Hajjo, R.** *The Discovery of Highly Conserved Elements on SARS-CoV-2 Genomes*. Submitted to Medical Hypotheses, Manuscript ID: 595941.

5. **Hajjo, R**.; Tropsha, A. *Can the Flu Vaccine Lead to Severe Illness in Some COVID-19 Patients?* Submitted to mSpehere. Manuscript ID: mSphere01162-20.

6. Sabbah, D. A., Hasan, S. E., Abu Khalaf, R., Bardaweel, S.K., **Hajjo, R.**, Alqaisi, K. M., Sweidan, K. A., Al-Zuheiri, A. M. *Molecular Modeling, Synthesis and Biological Evaluation of N-Phenyl-4-Hydroxy-6-Methyl-2-Quinolone-3-CarboxAmides as Anticancer Agents*. *Molecules* 2020, 25, 5348.

7. Sabbah, D.A.; **Hajjo, R**.; Bardaweel, S.K.; Zhong, H.A. *An Updated Review on SARS-CoV-2 Main Proteinase (MPro): Protein Structure and Small-Molecule Inhibitors*. Current Topics in Medicinal Chemistry. Manuscript ID: BMS-CTMC-2020-184, Accepted on November 19, 2020.

8. Sabbah, D.A.; **Hajjo, R.**; Bardaweel, S.K.; Zhong, H.A. *An Updated Review on SARS-CoV-2 Inhibitors: A Focus on Host Entry Inhibitors*. Submitted on September 22nd, 2020 to Current Topics in Medicinal Chemistry, Manuscript ID: CTMC-2020-185.

9. Sabbah, D.A.; **Hajjo**, R.; Sweidan, K.; Zhong, H.A. *An Integrative Informatics Approach to Explain the Mechanism of Action of Novel N1-(Anthraquinon-2-yl) Amidrazones as BCR/ABL Inhibitors.* Curr Comput Aided Drug Des, 2020 Aug 19. doi: 10.2174/1573409916666200819113444. Online ahead of print

10. AL Bataineh, M.; Alzaatreh, A.; **Hajjo, R.**; Banimfreg, B. H.; Dash, N. *Human Gut Microbiome Composition and Functionality Correlation with Age*. Submitted on July 7th, 2020; Frontiers in Cellular and Infection Microbiology Microbiome in Health and Disease; Manuscript ID: 580947.

11. Bardaweel, S.K.; **Hajjo, R**.; Sabbah, D.A. *Sitagliptin: A Potential Drug for the Treatment of COVID-19?* Acta Pharm. 71 (2021) xxx–xxx. https://doi.org/10.2478/acph-2021-0013

12. Al-Zyoud, W.; **Hajjo, R.**; Abu-Siniyeh, A; Hajjaj, S. *Salivary Microbiome and Cigarette Smoking: A First of Its Kind Investigation in Jordan*. International Journal of Environmental Research and Public Health 17 (1), 256.

13. Sabbah, D.A.; **Hajjo**, R.; Sweidan, K. *Review on Epidermal Growth Factor Receptor (EGFR) Structure, Signaling Pathways, Interactions, and Recent Updates of EGFR Inhibitors*. Current Topics in Medicinal Chemistry, 2020.

14. Bardaweel, S.K.; **Hajjo, R**.; Sabbah, D.A. *COVID-19 Pandemic Impact on Female Researchers in Jordan: A call for equality!* Submitted on September 27th, 2020 to Global Health Action.

15. Almomani, E.; Qablan, A.M.; Atrooz, F.Y.; Almomany, A.M.; **Hajjo, R**.; Almomani, H.Y. The influence of Coronavirus Diseases 2019 (COVID-19) pandemic and the quarantine practices on university students' beliefs about the online learning experience in Jordan. Submitted on September 8th, 2020 to Frontiers Public Health. Manuscript ID: 595874

16. **Hajjo, R.**; Setola, V.; Roth, B.L.; Tropsha, A. *Chemocentric Informatics Approach to Drug Discovery: Identification and Experimental Validation of Selective Estrogen Receptor Modulators as Ligands of 5-Hydroxytryptamine-6 Receptors and as Potential Cognition Enhancers*. *J. Med. Chem. 2012, 55, 5704−5719*.

17. **Hajjo, R.;** Grulke, C.; Golbraikh; A., Setola, V.; Huang, XP; Roth, B.L.; Tropsha, A. *Development, Validation, and Use of Quantitative Structure-Activity Relationship Models of 5-Hydroxytryptamine (2B) Receptor Ligands to Identify Novel Receptor Binders and Putative Valvulopathic Compounds among Common Drugs*. J. Med. Chem. 2010, 53(21): 7573-7586.

18. **Hajjo, R.;** Roth, B.L.; Tropsha, A. *In Silico* Receptoromics: QSAR Modeling of Catecholamine and Sigma Receptor Families, Model Application for Virtual Screening, and Experimental Validation of Computational Hits. (Submitted: *J. Med. Chem.*).

19. **Hajjo, R.**; Afifi, F.U.; Battah, A.H. *Analysis of Multi-Component Pesticide Residues in Origanum syriacum.* Food Additives and Contaminants 2007, 24(3), 274-279.

20. **Hajou, R.**; Afifi, F.U.; Battah, A.H. *Determination of Multi-Pesticide Residues in Mentha piperita.* Pharmaceutical Biology 2005, 43(6), 554-562.

21. **Hajou, R.**; Afifi, F.U.; Battah, A.H. *Comparative Determination of Multi-Pesticide Residues in Pimpinella anisum Using Two Different AOAC methods.* Food Chemistry 2004, 88 (3), 469-478.

Books and Book Chapters

Afifi, F.U.; **Hajjo, R.M.**; Battah, A.H. *Medicinal Plants, Pesticide Residues, and Analysis. In Handbook of Pesticides,* Part III: Pesticides and the Environment. Ed. Leo M.L. Nollet and Hamir S. Rathore. CRC Press, Taylor and Francis Group. Boca Raton, FL. (2009).

Conference Presentations

18. **Hajjo, R**. *The ethical challenges of applying artificial intelligence and machine learning in cancer care.* The First International Cancer Care Informatics Conference, Amman, Jordan, November 19-21, 2018.

19. **Hajjo, R.** *Integrative informatics approaches for unraveling the mysteries of rare diseases: Shedding the light on Potocki-Shaffer syndrome.* Oral Presentation, The 256th ACS National Meeting in Boston, MA, August 19-23, 2018.

20. **Hajjo, R.** *A Biomarker-assisted systems biology approach to explore host-microbiome-drug interactions.* The 17th Annual BioIT World Conference & Expo, Boston, MA, May 15-17, 2018.

21. **Hajjo, R.** *Causal reasoning networks for the prioritization of clinically-relevant drug targets and disease-tracking biomarkers*. The 16th Annual BioIT World Conference & Expo, Boston, MA, May 15-17, 2018.

22. **Hajjo, R.** and Willis, C. *Systems biology approaches to omics data analysis in complex diseases.* Abstracts of papers, 253rd ACS National Meeting, San Francisco, CA, April 2-6, 2017. Abst BIOT 461.

23. **Hajjo, R.** and Tropsha, A. *Chemogenomics-assisted anti-obesity drug discovery*. Abstracts of papers, 250th ACS National Meeting, Boston, MA, August 16-20, 2015. Abst CINF 47.

24. **Hajjo, R.** *Chemocentric informatics analysis of 'omics' data identifies novel links between HDACi and neuro-disease*. Abstracts of papers, 250th ACS National Meeting, Boston, MA, August 16-20, 2015. Abst CINF 11.

25. **Hajjo, R.** and Tropsha, A. *Chemocentric informatics analysis of 'omics' data identifies novel chemical-gene-disease associations in autism.* Abstracts of papers, 247th ACS National Meeting, Dallas, TX, March 16-20, 2014. Abst COMP Sci-Mix 267.

26. **Hajjo, R.**; Setola, V.; Roth, B.L.; Tropsha, A. *Integration of cheminformatics, chemical genomics, and network mining approaches to predict novel drug-gene-disease associations: applications to drug reprofiling for neuropsychiatric and*

neurodegenerative diseases. LINCS Symposium, Broad Institute, Cambridge, MA, November 18-19, 2013.

27. **Hajjo, R.**; Roth, B.L.; Tropsha, A. *Computational Identification and Experimental Validation of Selective Estrogen Receptor Modulators as Ligands of 5-Hydroxytryptamine-6 Receptors and Potential Anti-Alzheimer's Agents.* The Eighth Meeting of the Globalization of Pharmaceutics Education Network, November 10-12, 2010.

28. **Hajjo, R.**; Wang, X.S.; Roth, B.L.; Tropsha, A. *A Chemocentric Informatics Approach to Drug Discovery: An Application to the Identification and Experimental Validation of Selective Estrogen Receptor Modulators as Serotonin Receptor Subtype 6 Binders and Potential Anti-Alzheimer's Agents.* Abstracts of papers, 240th ACS National Meeting, Boston, MA, United States, August 22-26, 2010.

29. **Hajjo, R.**; Wang, X.S; Roth, B.L.; Tropsha, A. *QSAR Modeling of GPCR Receptor Families, Model Application for Virtual Screening, and Experimental Validation of Computational Hits.* Abstracts of papers, 240th ACS National Meeting, Boston, MA, United States, August 22-26, 2010.

30. **Hajjo, R.**; Wang, X.S.; Roth, B.L.; Tropsha, A. *A Novel Approach to Drug Discovery Integrating Chemogenomics and QSAR Modeling: Application to Anti-Alzheimer's Agents.* Submitted to 239th ACS National Meeting, San Francisco, CA, United States, March 21-25, 2010.

31. **Hajjo, R.**; Roth, B.L.; Tropsha, A. *A Novel Chemogenomics Approach to Identify Receptor Mediated Clinical Effects of Chemicals.* The 2009 AAPS Annual Meeting and Exposition, Los Angeles, CA, November, 2009.

32. **Hajjo, R.**; Fourches, D.; Roth, B.L.; Tropsha, A. *In silico Strategies to Identify Novel 5-HT$_6$ Receptor Ligands as Potential Anti-Alzheimer's and Anti-Obesity Treatments.* Abstracts of Papers, 238th ACS National Meeting, Washington, DC, United States, August 16-20, 2009.

33. Wang, X.S.; **Hajjo, R.**; Tropsha, A. *A Computational Workflow to Identify and Validate the Druggable Allosteric Binding Sites.* Abstracts of Papers, 238th ACS National Meeting, Washington, DC, United States, August 16-20, 2009.

34. **Hajjo, R.**; Grulke, C.; Golbraikh, A.; Roth, B.L.; Tropsha, A. *QSAR Models of 5-HT$_{2B}$ Receptor Ligands and their Application to Predicting Compounds that Could Cause Valvulopathy.* Abstracts of Papers, 237th ACS National Meeting, Salt Lake City, UT, United States, March 22-26, 2009.