Hao Zhu, Ph.D.

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Biomedical Informatics & Genomics Division
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Education

August 1998 - August 2002: Ph.D. degree in Computational Chemistry (Professor Gilles Klopman, advisor)
Department of Chemistry, Case Western Reserve University
Thesis Title: Quantitative structure-activity relationship studies of the cancer-related properties of organic molecules

August 1995 - June 1998: M.S. degree in Applied Chemistry (Professor Nai Shi, advisor)
Department of Technical Physics, Peking University, Beijing, China
Thesis Title: Activity and Conformation Changes of Dihydrofolate Reductase in Reverse Micelles

August 1991 - July 1995: B.S. degree in Inorganic Chemistry (Professor Yuwen Liu, research advisor)
Department of Chemistry, Jilin University, Changchun, Jilin, China
Research Project: Study of the Gas Sensitivity of Novel Porphyrin Films

Professional Experience

2023-present	Professor, Biomedical Informatics and Genomics Center, School of Medicine, Tulane University
2022-present	Professor, Department of Chemistry and Biochemistry, Rowan University
2021-present	Adjunct Professor, Division of Environmental & Population Health Biosciences, Environmental and Occupational Health Sciences Institute, Rutgers University, New Brunswick
2020-present	Member, NIEHS Center for Environmental Exposure and Disease, Environmental and Occupational Health Sciences Center, Rutgers University, New Brunswick
2016-present	Member, Joint Graduate Program in Toxicology, Rutgers University, New Brunswick
2021-2023	Member, National Academies Committee, National Academy of Sciences (NAS)
2020-2022	Professor, Department of Chemistry, Rutgers University, Camden
2011-2022	Member, The Rutgers Center for Computational & Integrative Biology

2017-2020	Graduate Program Director, Department of Chemistry, Rutgers University, Camden
2016-2020	Associate Professor, Department of Chemistry, Rutgers University, Camden
2015-2020	Associate Member, NIEHS Center for Environmental Exposure and Disease, Environmental and Occupational Health Sciences Center, Rutgers University, New Brunswick
2015-2019	Member, Scientific Advisory Committee on Alternative Toxicological Methods (SACATM) at National Institute of Environmental Health Sciences (NIEHS)
2011-2016	Assistant Professor, Department of Chemistry, Rutgers University, Camden
2014-2016	Visiting Professor, School of Chemistry and Chemical Engineering, Shandong University, China
2006-2011	Research Assistant Professor, School of Pharmacy, University of North Carolina, Chapel Hill
2002-2006	Postdoctoral Associate Department of Chemistry, Case Western Reserve University Research Advisor: Gilles Klopman, Ph.D.

Honors and/or Awards

2023	Society of Toxicology AACT SAFE Best Publication Award
2022	NIEHS Extramural Paper of the Month (August, 2022)
2021	Society of Toxicology Computational Toxicology Best Publication Award
2021	Chancellor’s Award for Outstanding Research and Creative Activity at Rutgers
2020	NIEHS Extramural Paper of the Month (July, 2020)
2019	NIEHS Extramural Paper of the Month (June, 2019)
2019	Colgate-Palmolive Research Grant Recipient
2017	Big Data Initiative Grant Recipient
2017	Colgate-Palmolive Research Grant Recipient
2016	Early Tenure Promotion in Department of Chemistry at Rutgers-Camden
2016	Rutgers University's Research Council Grant Recipient
2016-2018	Johns Hopkins Center for Alternatives to Animal Testing Grant Recipient
2015	Rutgers University's Environmental Health Pilot Grant Recipient
2013	Colgate-Palmolive Research Grant Recipient
2013	Rutgers University's Research Council Grant Recipient
2011	Colgate-Palmolive Research Grant Recipient
2008-2011	Johns Hopkins Center for Alternatives to Animal Testing Grant Recipient
1997	Guanghua Graduate Student Award, Peking University
1991-1995	Undergraduate Fellowship, Jilin University

Membership in Professional Societies:

2011 – present	American Society for Cellular and Computational Toxicology
2006 - present	Society of Toxicology
2006 - present	American Chemical Society
2006 - 2011	American Association of Colleges of Pharmacy

Bibliography

Citation statistics from Google Scholar:
https://scholar.google.com/citations?user=60zr_psAAAAJ&hl=en
Citation list can also be viewed via PubMed:
https://www.ncbi.nlm.nih.gov/myncbi/1LiV9MREf-iAb/bibliography/public/

Total peer reviewed journal publications: 90; Total citations: >6,500; h-index: 46; Number of articles with over 100 citations: 17

	2012	2013	2014	2015	2016	2017	2018	2019	2020	2021	2022	2023
Publications	5	5	5	3	12	9	2	5	14	6	7	6#
Citations	173	193	238	236	332	369	457	560	698	863	1045	702#

#till August, 2023

*** Indicates that I served as the corresponding author in the publication**

Government Act

1. National Academic of Sciences (NAS) committee members including **Zhu H** Transforming EPA Science to Meet Today's and Tomorrow's Challenges. ***NAS Consensus Study Report*** 2023, https://nap.nationalacademies.org/catalog/26602/transforming-epa-science-to-meet-todays-and-tomorrows-challenges

Book:

2. **Zhu H***, Xia M *High throughput screening in toxicology*. 2nd edition, Springer Science+Business Media LLC, 2022, New York, ISBN 978-1-0716-2213-1.

1. **Zhu H***, Xia M *High throughput screening in toxicology.* Springer Science+Business Media LLC, 2016, New York, ISBN 978-1-4939-6344-7.

Book chapters:

10. Yan X, Yue T, **Zhu H**, Yan B Bridging the Gap Between Nanotoxicological Data and the Critical Structure–Activity Relationships. In: *Advances in Toxicology and Risk Assessment of Nanomaterials and Emerging Contaminants* (Guo L. et al. Editor). Chapter 7, page 161-183, Springer Science+Business Media LLC, 2022, New York, ISBN 978-981-16-9115-7.

9. Ciallella H, Chung E, **Zhu H*** Automatic Quantitative Structure-Activity Relationship Modeling to Fill Data Gaps in High-Throughput Screening. In: *High throughput screening in toxicology 2nd edition* (Zhu, H. et al. Editor). Chapter 16, page 169-187, Springer Science+Business Media LLC, 2022, New York, ISBN 978-1-0716-2213-1.

8. Russo D, **Zhu H*** High-Throughput Screening Assay Profiling for Large Chemical Databases. In: *High throughput screening in toxicology 2nd edition* (Zhu, H. et al. Editor). Chapter 12, page 125-132, Springer Science+Business Media LLC, 2022, New York, ISBN 978-1-0716-2213-1.

7. Zhao L, **Zhu H*** Big data in computational toxicology: challenges and opportunities. In: *Computational toxicology – Risk assessment for chemicals* (by Ekins S Editor). Chapter 11, page 293-312, John Wiley & Sons, Inc., 2018, Hoboken, NJ 07030, USA, ISBN: 9781119282570.

6. Golbraikh A, Wang X S, **Zhu H,** Tropsha A Predictive QSAR modeling: Methods and applications in drug discovery and chemical risk assessment. In: *Handbook of computational chemistry* (by Leszczynski, J. et. al. Editor). Chapter 57, page 2303-2340, Springer-Verlag, 2017, GmbH Berlin Heidelberg, ISBN: 978-3-319-27281-8.

5. Kim M, Wang W, Sedykh A**, Zhu H*** Curating and Preparing High-Throughput Screening Data for Quantitative Structure-Activity Relationship Modeling. In: *High throughput screening in toxicology* (Zhu, H. et al. Editor). Springer Science+Business Media LLC, 2016, New York, ISBN 978-1-4939-6344-7.

4. Russo D P**, Zhu H*** Accessing the High-Throughput Screening Data Landscape. In: *High throughput screening in toxicology* (Zhu, H. et al. Editor). Springer Science+Business Media LLC, 2016, New York, ISBN 978-1-4939-6344-7.

3. **Zhu H***, Kim M, Zhang L, Sedykh A Computers instead of cells: Computational modeling of chemical toxicity. in: *Reducing, refining and replacing the use of animals in toxicity testing* (by Allen D, Waters M D Editor). Chapter 5, page 163-182, Royal Society of Chemistry, 2013, Burlington House, Piccadilly, London, ISBN: 978-1-84973-652-7.

2. **Zhu H*** From QSAR to QSIIR: Searching for enhanced computational toxicology models. In: *Computational toxicology volume II* (by Reisfeld B, Mayeno Ar N Editor). Chapter 3, page 53-65, Springer-Verlag, 2012, GmbH Berlin Heidelberg, ISBN 978-1-62703-058-8.

1. Golbraikh A, Wang X S, **Zhu H,** Tropsha A Predictive QSAR modeling: Methods and applications in drug discovery and chemical risk assessment. In: *Handbook of computational chemistry* (by Leszczynski, J. Editor). Chapter 37, page 1309-1342, Springer-Verlag, 2011, GmbH Berlin Heidelberg, ISBN: 978-94-007-0710-8.

Peer-reviewed articles:

90. Russo D P, Aleksunes L M, Goyak K, Qian H, **Zhu H*** Integrating concentration-dependent toxicity data and toxicokinetics to inform hepatotoxicity response pathways. ***Environ. Sci. Technol.,*** 2023, In press

89. Yan X, Yue T, Winkler D A, Yin Y, Jiang G, **Zhu H**, Yan B Converting Nanotoxicity Data to Information Using Artificial Intelligence and Simulation. ***Chem. Rev.***, 2023, In press

88. Jia X, Wang T, **Zhu H*** Advancing Computational Toxicology by Interpretable Machine Learning. ***Environ. Sci. Technol.,*** 2023, In press.

87. Chung E, Russo D P, Ciallella H L, Wang Y, Wu M, Aleksunes L M, **Zhu H*** Data-Driven Quantitative Structure-Activity Relationship (QSAR) Modeling for Human Carcinogenicity by Chronic Oral Exposure. ***Environ. Sci. Technol.,*** 2023, (57) 6573-6588. PMC10134506

86. Wang T, Russo D, Bitounis D, Demokritou P, Jia X, Huang H, **Zhu H*** Integrating structure annotation and machine learning approaches to develop graphene toxicity models. ***Carbon*** 2023, (204) 484-494

85. Liu M, Wang T, Wang Q, Zhou J, Wang B, Zhang B, Wang K, **Zhu H**, Zhang Y Structure-guided discovery of food-derived GABA-T inhibitors as hunters for anti-anxiety compounds. ***Food Funct.*** 2022, (13) 12674-12685

84. Jia X, Wen X, Russo D, Aleksunes L M, **Zhu H*** Mechanism-driven Modeling of Chemical Hepatotoxicity Using Structural Alerts and an In Vitro Screening Assay. ***J. Hazard. Mater.***, 2022, (436) 129193. (NIEHS Extramural Paper of the Month; Society of Toxicology AACT SAFE Best Publication Award)

83. Ciallella H, Russo D, Sharma S, Li Y, Sloter E, Sweet L, **Zhu H*** Predicting Prenatal Developmental Toxicity Based On the Combination of Chemical Structures and Biological Data. ***Environ. Sci. Technol.,*** 2022, (56) 5984–5998.

82. Marques E, Pfohl M, Wei W, Tarantola G, Ford L, Amaeze O, Alesio J, Ryu S, Jia X, **Zhu H**, Bothun G, Slitt A Replacement per- and polyfluoroalkyl substances (PFAS) are potent modulators of lipogenic and drug metabolizing gene expression signatures in primary human hepatocytes. ***Toxicol. Appl. Pharmacol.,*** 2022; (442) 1115991.

81. Yan J, Yan X, Hu S, **Zhu H**, Yan B Comprehensive Interrogation on Acetylcholinesterase Inhibition by Ionic Liquids Using Machine Learning and Molecular Modeling. ***Environ. Sci. Technol.,*** 2021, (55) 14720–14731.

80. **Zhu H***, Chen J, Huang R, Hong H Sustainable Management of Synthetic Chemicals. ***ACS Sustainable Chem. Eng.*** 2021, (9) 13703-13704 (Invited Editorial)

79. Ciallella H, Russo D, Aleksunes L M, Grimm F, **Zhu H*** Revealing Adverse Outcome Pathways from Public High-Throughput Screening Data to Evaluate New Toxicants by a Knowledge-Based Deep Neural Network Approach. ***Environ. Sci. Technol.,*** 2021, (55) 10875-10887. (Society of Toxicology Computational Toxicology Best Paper Award)

78. Mansouri K. and other 102 co-authors including **Zhu H** CATMoS: Collaborative Acute Toxicity Modeling Suite. ***Environ. Health Perspect.*** 2021, (129) 47013

77. Jia X; Ciallella H; Russo D; Zhao L; James M; **Zhu H*** Construction of a Virtual Opioid Bioprofile: a Data-driven QSAR Modeling Study to Identify New Analgesic Opioids. ***ACS Sustainable Chem. Eng.*** 2021, (9) 3909-3919. PMCID: PMC8259887

76. Ciallella H, Russo D, Aleksunes L M, Grimm F, **Zhu H*** Predictive Modeling of Estrogen Receptor Agonism, Antagonism, and Binding Activities Using Machine and Deep Learning Approaches. ***Lab Invest.***, 2021, (101) 490–502

75. Yan X, Zhang J, Russo D, **Zhu H*,** Yan B Prediction of Nano–Bio Interactions through Convolutional Neural Network Analysis of Nanostructure Images. ***ACS Sustainable Chem. Eng.*** 2020, (8) 19096–19104

74. Russo D, Yan X, Shende S, Huang H, Yan B, **Zhu H*** Virtual molecular projections and convolutional neural networks for end-to-end modeling of nanoparticle activities and properties. ***Anal. Chem.***, 2020; (92) 13971-13979.

73. Wang Y, Russo D, Liu C, Zhou Q, **Zhu H***, Zhang Y Predictive modeling of angiotensin I-converting enzyme (ACE) inhibitory peptides using various machine learning approaches. ***J. Agric. Food Chem.,*** 2020; (68):12132-12140.

72. Zhao L, Ciallella H, Aleksunes L M, **Zhu H*** Advancing computer-aided drug discovery (CADD) by big data and data-driven machine learning modeling. ***Drug Discov Today***, 2020 (25) 1624-1638. PMCID: PMC7572559 (Editor Invited Keynote Review)

71. Gao R, Guan N, Huang M, Foreman J, Kung M, Rong Z, Su Y, Sweet L, Zhu B, **Zhu H**, Zou H, Li B, Wang Y, Yin H, Yin Z, Zhang X Read-across: Principle, case study and its potential regulatory application in China. ***Regul. Toxicol. Pharmacol.,*** 2020; (116) 104728.

70. Yan X, Sedykh A, Wang W, Yan B, **Zhu H*** Construction of a web-based nanomaterial database by big data curation and modeling friendly nanostructure annotations. ***Nat. Commun,*** 2020; (11) 2519. (NIEHS Extramural Paper of the Month)

69. Zhou C, Shi W, **Zhu H**, Yu H, Liu J, Song M, Xia P, Chen Q, Wei S, Zhang X, Wang X Mechanistic in silico modeling of bisphenols to predict estrogen and glucocorticoid disrupting potentials. ***Sci. Total Environ.,*** 2020, (728) 138854.

68. Qi X, Li X, Yao H, Huang Y, Cai X, Chen J, **Zhu H** Predicting plant cuticle-water partition coefficients for organic pollutants using pp-LFER model. ***Sci. Total Environ.,*** 2020, (725) 138455.

67. Liu G, Yan X, Sedykh A, Pan X, Zhao X, Yan B, **Zhu H*** Analysis of model PM2.5-induced inflammation and cytotoxicity by the combination of a virtual carbon nanoparticle library and computational modeling. ***Ecotoxicol. Environ. Saf.,*** 2020; (191) 110216. PMCID: PMC7018436.

66. Liu Y, Wei Y, Zhang S, Yan X, **Zhu H**, Xu L, Zhao B, Xie H, Yan B Regulation of aryl hydrocarbon receptor signaling pathway and dioxin toxicity by novel agonists and antagonists. ***Chem. Res. Toxicol.,*** 2020; (33) 614-624.

65. Bai X, Wang S, Yan X, Zhou H, Zhan J, Liu S, Sharma V, Jiang G, **Zhu H**, Yan B Regulation of Cell Uptake and Cytotoxicity by Nanoparticle Core under the Controlled Shape, Size, and Surface Chemistries. ***ACS Nano,*** 2020; (14):289-302.

64. Zhao L, Russo D P, Wang W, Aleksunes L M, **Zhu H*** Mechanism-driven Read-Across of Chemical Hepatotoxicants Based on Chemical Structures and Biological Data. ***Toxicol. Sci.,*** 2020; (174) 178-188. PMCID: PMC7098374. (Featured by Society of Toxicology as monthly highlighted paper)

63. **Zhu H*** Big Data and Artificial Intelligence Modeling for Drug Discovery. ***Annual Rev. Pharm. Tox.,*** 2020; (20) 573-589. PMCID: PMC7010403. (Editor invited)

62. Wang Y, Li B, Xu X, Ren H, Yin J, **Zhu H**, Zhang Y FTIR spectroscopy coupled with machine learning approaches as a rapid tool for identification and quantification of artificial sweeteners. ***Food Chem.,*** 2020; (303) 125404.

61. Guo Y, Zhao L, Zhang X, **Zhu H*** Using a Hybrid Read-Across Method to Evaluate Chemical Toxicity Based on Chemical Structure and Biological Data. ***Ecotox. Environ. Saf.,*** 2019; (178) 178-187. PMCID: PMC6508079.

60. Yan X, Sedykh A, Wang W, Zhao X, Yan B, **Zhu H*** In silico profiling nanoparticles: predictive nanomodeling using universal nanodescriptors and various machine learning approaches. ***Nanoscale,*** 2019; (11) 8352–8362.

59. Russo D P, Strickland, J, Karmaus A L, Wang W, Shende S, Hartung T, Aleksunes L M, **Zhu H*** Non-animal models for acute toxicity evaluations: applying data-driven profiling and read-across. ***Environ. Health Perspect.,*** 2019; (127) 47001. PMCID: PMC6785238. (NIEHS Extramural Paper of the Month. Featured by over 10 public medias. See details in "Media Reports")

58. Ciallella, H, **Zhu H*** Advancing Computational Toxicology in the Big Data Era by Artificial Intelligence: Data-Driven and Mechanism-Driven Modeling for Chemical Toxicity. ***Chem. Res. Tox.,*** 2019; (32) 536−547. PMCID: PMC6688471. (Editor invited perspective and featured as Chemical Research in Toxicology cover paper)

57. Wang W, Yan X, Zhao L, Russo D P, Wang S, Liu Y, Sedykh A, Zhao X, Yan B, **Zhu H*** Universal nanohydrophobicity predictions using virtual nanoparticle library. ***J. Cheminform.*****,** 2019, (11) 6. PMCID: PMC6689884

56. Russo D P, Zorn K M, Clark A M, **Zhu H**, Ekins S Comparing Multiple Machine Learning Algorithms and Metrics for Estrogen Receptor Binding Prediction. ***Mol. Pharm.***, 2018; (15) 4361-4370. PMCID: PMC6181119

55. Wang W, Sedykh A, Sun H, Zhao L, Russo D P, Zhou H, Yan B, **Zhu H*** Predicting Nano-bio Interactions by Integrating Nanoparticle Libraries and Quantitative Nanostructure Activity Relationship Modeling. ***ACS Nano***, 2017; (11) 12641-12649. PMCID: PMC5772766

54. Zhang L, Tan J, Han D, **Zhu H*** From machine learning to deep learning: progress in machine intelligence for rational drug discovery. ***Drug Discov. Today***, 2017; (22) 1680-1685. (Featured as Drug Discovery Today top citation paper of the year)

53. Liu Y, Su G, Wang F, Jia J, Li S, Zhao L, Shi Y, Cai Y, **Zhu H**, Zhao B, Jiang G, Zhou H, Yan B Elucidation of the Molecular Determinants for Optimal Perfluorooctanesulfonate Adsorption Using a Combinatorial Nanoparticle Library Approach. ***Environ. Sci. Technol.*****,** 2017; (51) 7120-7127. PMCID: PMC5784263

52. Zhao L, Wang W, Sedykh A, **Zhu H*** Experimental Errors in QSAR Modeling Sets: What We Can Do and What We Cannot Do. ***ACS Omega****,* 2017; (2) 2805-2812. PMCID: PMC5494643

51. Bai X, Liu F, Liu Y, Li C, Wang S, Zhou H, Wang W, **Zhu H**, Winkler D, Yan B Toward A Systematic Exploration of Nano-Bio Interactions. ***Toxicol. Appl. Pharmacol.*** 2017; (323) 66-73. PMCID: PMC5581002

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approaches for identifying acute systemic toxicity: Moving from research to regulatory testing. ***Toxicol. In Vitro*****,** 2017; (41) 245-259. PMCID: PMC5479748

49. Russo D P, Kim M, Wang W, Pinolini D, Shende S, Strickland J, Hartung T, **Zhu H*** CIIPro: A new read-across portal to fill data gaps using public large scale chemical and biological data. ***Bioinformatics*****,** 2017; (33) 464-466. PMCID: PMC6075082

48. Xiang J, Zhang Z, Mu Y, Xu X, Guo S, Liu Y, Russo D, **Zhu H**, Yan B, Bai X Discovery of Novel Tricyclic Thiazepine Derivatives as Anti-Drug-Resistant Cancer Agents by Combining Diversity-Oriented Synthesis and Converging Screening Approach. ***ACS Comb. Sci.***， 2016; (18) 230–235.

47. Ribay K, Kim M, Wang W, Pinolini D, **Zhu H*** Hybrid Modeling of Estrogen Receptor Binding Agents Using Advanced Cheminformatics Tools and Massive Public Data. ***Front. Environ. Sci.***， 2016; (4) 12. PMCID: PMC5023020

46. Kim M, Huang R, Sedykh A, Zhang J, Xia M, **Zhu H*** Mechanism profiling liver toxicants by using antioxidant response element assay data model and public big data. ***Environ. Health Perspect.***， 2016; (124) 634-641. PMCID: PMC4858396

45. Mu Y, Liu Y, Xiang J, Zhang Q, Zhai S, Russo D P, **Zhu H**, Bai X, Yan B From fighting depression to conquering tumors: a novel tricyclic thiazepine compound as a tubulin polymerization inhibitor ***Cell Death and Disease***， 2016; (7) e2143.

44. **Zhu H**, Bouhifd M, Kleinstreuer N, Kroese ED, Liu Z, Luechtefeld T, Pamies D, Shen J, Strauss V, Wu S, Hartung T Supporting read-across using biological data. ***ALTEX.***， 2016; (33) 167-182. PMCID: PMC4834201 (*ALTEX* cover paper. Featured together with following 5 *ALTEX* papers by *Science* Feb 12, 2016 “A crystal ball for chemical safety” and *Nature* Feb 11, 2016 “Legal tussle delays launch of huge toxicity database”)

43. Ball N, Cronin M T, Shen J, Adenuga M D, Blackburn K, Booth E D, Bouhifd M, Donley E, Egnash L, Freeman J J, Hastings C, Juberg D R, Kleensang A, Kleinstreuer N, Kroese E D, Luechtefeld T, Maertens A, Marty S, Naciff J M, Palmer J, Pamies D, Penman M, Richarz A N, Russo D P, Stuard S B, Patlewicz G, van Ravenzwaay B, Wu S, **Zhu H**, Hartung T Toward Good Read-Across Practice (GRAP) guidance. ***ALTEX.***， 2016; (33) 149-166. PMCID: PMC5581000

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41. Luechtefeld T, Maertens A, Russo D P, Rovida C, **Zhu H**, Hartung T Analysis of Draize eye irritation testing and its prediction by mining publicly available 2008-2014 REACH data. ***ALTEX.***， 2016; (33) 123-134.

40. Luechtefeld T, Maertens A, Russo D P, Rovida C, **Zhu H**, Hartung T Analysis of public oral toxicity data from REACH registrations 2008-2014. ***ALTEX.***， 2016; (33) 111-122.

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38. Zhang Y, Wang Y, Liu A, Xu S L, Zhao B, Zhang Y, Zou H, Wang W, **Zhu H**, Yan B Modulation of Carbon Nanotube's Perturbation to the Metabolic Activity of CYP3A4 in the Liver. ***Adv. Funct. Mater.***, 2016; (26) 841-850. (*Advanced Functional Materials* cover paper)

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36. Liu Y, Li F, Wu L, Wang W, **Zhu H**, Zhang Q, Zhou H, Yan B Improving both aqueous solubility and anti-cancer activity by assessing progressive lead optimization libraries. ***Bioorg. Med. Chem. Lett.,*** 2015; (25) 1971-1975.

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33. Zhang J, Hsieh J-H, **Zhu H*** Profiling animal toxicants by automatically mining public bioassay data: A big data approach for computational toxicology. ***PLoS One,*** 2014; (9) e99863. PMCID: PMC4064997

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20. Nakagawa-Goto K, Wu P, Lai C, Hamel E, **Zhu H**, Zhang L, Kozaka T, Bastow K F, Lee K H Antitumor agents 284. New desmosdumotin B analogues with bicyclic b-ring as potent cytotoxic and antitubulin agents. ***J. Med. Chem.,*** 2011; (54): 1244-1255.

19. Sedykh A, **Zhu H**, Tang H, Zhang L, Richard A, Rusyn I, Tropsha A Use of in vitro HTS-derived concentration-response data as biological descriptors improves the accuracy of QSAR models of in vivo toxicity. ***Environ. Health Perspect.,*** 2011; (119): 364-370.

18. Nakagawa-Goto K, Chang P, Lai C, Hung H, Chen T, Wu P, **Zhu H**, Sedykh A, Bastow K F, Lee K H Antitumor agents. 280. Multidrug resistance-selective desmosdumotin b analogues. ***J. Med. Chem.***, 2010; (53): 6699–6705.

17. Zhou T, Chen C H, Shi Q, **Zhu H,** Huang L, Ho P, Lee K H Anti-AIDS Agents 79. Design, synthesis, molecular modeling and structure-activity relationships of novel dicamphanoyl -2',2'-dimethyldihydropyranochromone (DCP) analogs as potent anti-HIV agents. ***Bioorg. Med. Chem.,*** 2010; (18): 6678-6689.

16. Rodgers A D, **Zhu H**, Fourches D, Rusyn I, Tropsha A Modeling adverse liver effects of drugs using kNN QSAR method. ***Chem. Res. Tox.,*** 2010; (23): 724-732.

15. **Zhu H**, Martin M T, Ye L, Sedykh A, Young M D, Tropsha A Combinatorial QSAR modeling of rat acute toxicity by oral exposure. ***Chem. Res. Tox.*** 2009; (22): 1913-1921. (Highlighted by *Chemical Research in Toxicology* Dec 21 2009 "In this issue")

14. **Zhu H**, Ye L, Richard A, Golbraikh A, Rusyn I, Tropsha A A novel two-step hierarchical quantitative structure activity relationship modeling workflow for predicting acute toxicity of chemicals in rodents. ***Environ. Health Perspect.*** 2009; (117): 1257-1264. (*Environmental Health Perspectives* cover paper)

13. Tetko I V, Sushko I, Pandey AK, **Zhu H**, Tropsha A, Papa E, Oberg T, Todeschini R, Fourches D, Varnek A Critical assessment of QSAR models of environmental toxicity against Tetrahymena pyriformis: focusing on applicability domain and overfitting by variable selection. ***J. Chem. Inf. Model.*** 2008; (48): 1733-1746.

12. Zhang L, **Zhu H**, Oprea T, Golbraikh A, Tropsha A QSAR modeling of the blood-brain barrier permeability for diverse organic compounds. ***Pharm. Res.***, 2008; (25): 1902-1914.

11. **Zhu H**, Rusyn I, Richard A, Tropsha A Use of cell viability assay data improves the prediction accuracy of conventional quantitative structure-activity relationship models of animal carcinogenicity. ***Environ. Health Perspect.,*** 2008; (116): 506-513. (Featured by *Chemical Research in Toxicology* March 17, 2008 "Spotlight")

10. **Zhu H**, Tropsha A, Fourches D, Varnek A, Papa E, Gramatica P, Oberg T, Dao P, Cherkasov A, Tetko I V. Combinatorial QSAR modeling of chemical toxicants tested against Tetrahymena pyriformis. ***J. Chem. Inf. Model.,*** 2008; (48): 766-784.

9. **Zhu H**, Sedykh A, Chakravarti S K, Klopman G A new group contribution approach to the calculation of logP. ***Curr. Comput.-Aided Mol. Design***, 2005; (1): 3-9.

8. Klopman G, **Zhu H** Recent methodologies for the estimation of n-octanol/water partition coefficients and their use in the prediction of membrane transport properties of drugs. ***Mini-Rev. Med. Chem.***, 2005; (5): 127-133.

7. Klopman G, **Zhu H**, Fuller M A, Saiakov R D Searching for an enhanced prediction tool for mutagenicity. ***SAR QSAR Environ. Res.,*** 2004; (15): 251-263.

6. Klopman G, Chakravarti S K, **Zhu H**, Ivanov J, Saiakov R D ESP: A method to predict toxicity and pharmacological properties of chemicals using multiple MCASE databases. ***J. Chem. Inform. Comput. Sci.*** 2004; (44): 704-715.

5. Klopman G, **Zhu H**, Ecker G, Chiba P MCASE study of the multidrug resistance reversal activity of propafenone analogs. ***J. Comput.-Aided Mol. Design,*** 2003; (17): 291-297.

4. Klopman G, **Zhu H** Estimation of the aqueous solubility of organic molecules by the group contribution approach. ***J. Chem. Inform. Comput. Sci.*** 2001; (41): 439-445.

3. **Zhu H**, Fan Y, Shi N, Zhou J Activity and conformation changes of dihydrofolate reductase in reverse micelles. ***Arch. Biochem. Biophy.***, 1999; (368): 61-66.

2. **Zhu H**, Fan Y, Shi N, Zhou J The enzymological researches in reverse micellar systems. ***Prog. Biochem. Biophy.*** 1998; (25): 204-210. (in Chinese)

1. Liu YW, Zhao YE, Wang LB, Wang RW, Liang HB, **Zhu H**, Cao XZ Synthesis of long aliphatic carbochain porphyrins and their LB films and study on their gas sensitivity. ***Chem. J. Chinese Univ.*** 1997; (18): 682-684. (in Chinese)

Refereed/Invited oral presentations:

52. Mechanistic computational modeling for chemical toxicity evaluations, 12th World Congress on Alternatives and Animal Use in the Life Sciences, Niagara Falls, Ontario, Canada, August, 2023

51. Professional Advantages of AOP Development for Graduate Students, 12th World Congress on Alternatives and Animal Use in the Life Sciences, Niagara Falls, Ontario, Canada, August, 2023

50. Advancing Computational Chemical Toxicology by Interpretable Machine Learning, Rutgers University-New Brunswick, Department of Chemistry invited seminar, Piscataway, NJ, April, 2023

49. Nanoinformatics: rational design of biocompatible nanomaterials by nanostructure annotations, Rensselaer Polytechnic Institute, Department of Chemistry and Chemical Biology invited seminar, Troy, NY, September, 2022

48. Adverse outcome pathways (AOP) to predict toxicity of new compounds, and illustrate relevant toxicity mechanisms, Drug Safety Gordon Research Conference invited seminar, Easton, MA, June 2022

47. Mechanistic machine learning modeling for chemical toxicity evaluations, The 26th Annual Green Chemistry & Engineering Conference invited seminar, Reston, VA, June, 2022

46. Nanoinformatics: rational design of biocompatible nanomaterials by nanostructure annotations, The Gold 2022 conference, the only global scientific event entirely dedicated to advances in gold-based high-tech materials, invited virtual seminar, February, 2022

45. Non-animal models for animal toxicity evaluations: applying data-driven and mechanistic modeling, Rutgers Cancer Institute of New Jersey invited virtual seminar, February, 2022

44. Non-animal models for animal toxicity evaluations: applying data-driven and mechanistic modeling, Rensselaer Polytechnic Institute, Department of Chemistry and Chemical Biology invited virtual seminar, February, 2022

43. Non-animal models for animal toxicity evaluations: applying data-driven and mechanistic modeling, ExxonMobil invited seminar, Lebanon, NJ, February, 2022

42. Non-animal models for animal toxicity evaluations: applying data-driven and mechanistic modeling, Oregon State University, Department of Environmental and Molecular Toxicology invited virtual seminar, October, 2021

41. Artificial Intelligence, Machine Learning, and Data Science in Toxicology Studies, John Hopkins University Bloomberg School of Health invited virtual seminar, April, 2021

40. Non-animal models for animal toxicity evaluations: applying data-driven profiling and read-across, Lush Prize Conference invited virtual seminar, November, 2020

39. Virtual Nanostructure Simulation (VINAS) Modeling for Rational Nanomaterial Design. Case Western Reserve University, Department of Chemistry invited virtual seminar, October, 2020

38. Rational design of biocompatible nanomaterials by nanostructure annotations and nanoinformatics modeling, The NTP Interagency Center for the Evaluation of Alternative Toxicological Methods (NICEATM) invited virtual seminar, June, 2020

37. Non-animal models for animal toxicity evaluations: applying data-driven profiling and read-across, Society of Toxicology invited virtual seminar, June, 2020

36. Big data, AI and intelligent modeling for modern computational toxicology, Case Western Reserve University, Department of Civil Engineering invited seminar, Cleveland, OH, November, 2019

35. Big data, AI and intelligent modeling for modern computational toxicology, Rutgers-ExxonMobil computational toxicology workshop invited seminar, Piscataway, NJ, September, 2019.

34. Digital nano: Rational Design of Biocompatible Nanomaterials by Virtual Nano Library Techniques and Artificial Intelligence, North Jersey American Chemical Society invited seminar, Somerset, NJ, May, 2019

33. Digital nano: rational design of biocompatible nanomaterials by digitalizing nanostructures. Rutgers University-New Brunswick, Department of Chemistry invited seminar, Piscataway, NJ, March, 2019.

32. Advanced Predictive Modeling of Hepatotoxicity by Big Data. John Hopkins Bloomberg School of Health invited seminar, Baltimore MD, November 2018. (**JHU Center of Alternatives to Animal Testing Keynote Seminar**)

31. Big data in computational toxicology: predictive animal toxicity modeling using data-driven profiling and mechanism-driven read-across. Midwest regional chapter of society of toxicology fall 2018 meeting invited seminar, Madison, WI, October 2018.

30. Big data in computational toxicology: predictive animal toxicity modeling using data-driven profiling and mechanism-driven read-across. Novartis invited seminar, East Hanover NJ, October 2018.

29. Big data in computational toxicology: predictive animal toxicity modeling using data-driven profiling and mechanism-driven read-across. Chinese Analytical Toxicology Society 10th annual meeting, Yichang, Hubei, China, July 2018. (**Chinese Analytical Toxicology Society 2018 Keynote Seminar**)

28. Virtual Nanostructure Simulation (VINAS): a toolbox to quantify nanomaterial structures for intelligent modeling and rational material design. American Chemical Society 255th national meeting, New Orleans, LA, March, 2018.

27. From QSAR to big data: Developing mechanism-driven predictive models for animal toxicity. Akron University, Department of Chemical and Biomolecular Engineering invited seminar, Akron, OH, November, 2017.

26. Quantitative Nano-structure Toxicity Relationship: Developing Predictive Cell Recognition Models for Gold Nanoparticles. The 33th International Conference of the Society for Environmental Geochemistry and Health (SEGH 2017), Guangzhou, Guangdong, China, July, 2017 (**SEGH 2017 Conference Keynote Seminar**)

25. From QSAR to big data: Developing mechanism-driven predictive models for drug induced liver injury. World Drug Safety Congress Americas invited seminar, Philadelphia, PA, May, 2017

24. From QSAR to big data: Developing mechanism-driven predictive models for animal toxicity. NTP Interagency Center for the Evaluation of Alternative Toxicological Methods (NICEATM) invited seminar, Research Triangle Park, NC, November, 2016

23. Cheminformatics education and research at home: the best way to teach graduate chemistry in the professional community. American Chemical Society 252th national meeting, Philadelphia, PA, August, 2016.

22. Quantitative Nano-structure Toxicity Relationship: Developing Predictive Cell Recognition Models for Gold Nanoparticles. Pan American Conference of Alternative Methods invited seminar, Baltimore, MD, April, 2016

21. Support read-across using biological data. US FDA, “Good Read-Across Practice (GRAP) Guidance” workshop invited seminar, College Park, MD, March, 2016

20. From QSAR to big data: Developing mechanism-driven predictive models for animal toxicity. University of Tennessee, Medical School invited seminar, Memphis, TN, February, 2016

19. From QSAR to big data: Developing mechanism-driven predictive models for animal toxicity. University of Connecticut, Department of Chemistry invited seminar, Storrs, CT, February, 2016

18. From QSAR to big data: Developing mechanism-driven predictive models for animal toxicity. The Rutgers CCIB-SEBS workshop invited seminar, Camden, NJ, October, 2015

17. From QSAR to big data: Developing mechanism-driven predictive models for animal toxicity. National Institute of Health workshop “Alternative Approaches for Identifying Acute Systemic Toxicity: Moving from Research to Regulatory Testing” invited seminar, Bethesda, MD, September, 2015.

16. From QSAR to big data: Developing mechanism-driven predictive models for animal toxicity. American Chemical Society 250th national meeting, Boston, MA, August, 2015.

15. Advancing predictive toxicity modeling by big data, Shandong University, College of Chemistry and Chemical Engineering invited seminar, Jinan, Shandong, China, June, 2015

14. Advancing predictive toxicity modeling by big data, Rensselaer Polytechnic Institute, Department of Chemistry and Chemical Biology invited seminar, Troy, NY, May, 2015

13. Advancing predictive toxicity modeling by big data, Cleveland State University, Department of Chemistry invited seminar, Cleveland, OH, April, 2015

12. Advancing predictive toxicity modeling by big data, Rutgers Environmental and Occupational Health Sciences Institute invited seminar, Piscataway, NJ, April, 2015

11. Advancing predictive modeling by big data, Research Institute for Fragrance Materials invited seminar, Woodcliff Lake, NJ, February, 2015

10. The big data of chemical toxicology: swimming of a bioassay in the big data pool, Shandong University, College of Chemistry and Chemical Engineering invited seminar, Jinan, Shandong, China, May, 2014

9. Predictive computational toxicity modeling using advanced cheminformatics techniques, Miami University, College of Engineering and Computing invited seminar, Oxford, OH, February, 2014

8. Virtual profiling animal toxicants by automatic mining public bioassay data, American Chemical Society 246th national meeting, Indianapolis, IN, September, 2013

7. Profiling animal toxicants by automatically data mining, The 10th International Symposium on Persistent Toxic Substances, Edmonton, Alberta, Canada August, 2013

6. Predictive computational toxicity modeling using advanced cheminformatics techniques, University of Massachusetts Chemistry Department invited seminar, Boston, MA, April, 2013

5. Predictive computational toxicity modeling using advanced cheminformatics techniques, The Rutgers CCIB invited seminar, Camden, NJ, September, 2012

4. Application of combinatorial QSAR approaches to facilitate drug discovery and environmental toxicity assessment, Beijing Institute of Technology invited seminar, Beijing, China, January, 2012

3. Improved quantitative models of chemical toxicity based on combined application of chemical and biological molecular descriptors, The 2009 monthly meetings of EPA's Chemical Prioritization Community of Practice (CPCP), RTP, NC, September, 2009

2. Using Quantitative High Throughput Screening (q-HTS) results as biological descriptors to assist modeling of acute rat toxicity, American Chemical Society 238th national meeting, Washington, DC, August, 2009

1. The use of hybrid chemical/biological descriptors in QSAR modeling improves the accuracy of in vivo chemical toxicity prediction, The 32nd Annual Midwest Biopharmaceutical Statistics Workshop, Muncie, IN, May, 2009

Refereed poster presentations:

49. Russo D P, **Zhu H*** Hierarchical concentration-response modeling for adverse outcome pathway-based evaluations using public big data resources. Society of Toxicology 62nd Annual Meeting, Nashville, Tennessee, March 2023.

48. Wang T, Russo, D, Bitounis D, Demokritou P, Jia X, Huang H, **Zhu H*** Integrating Structure Annotation and Machine Learning Approaches to Develop Graphene Toxicity Models. Society of

Toxicology 62nd Annual Meeting, Nashville, Tennessee, March 2023. (**2023 CTSS Graduate Student Award**)

47. Jia X, Russo D, Wang T, **Zhu H*** Integrating Adverse Outcome Pathway and Biological Pathway Knowledge in Interpretable Deep Learning Modeling of Hepatotoxicity. Society of Toxicology 62nd Annual Meeting, Nashville, Tennessee, March 2023. (**2023 Colgate-Palmolive Award for Student Research Training in Alternative Research**)

46. Chung E, Jia X, Ciallella H, Russo D, Aleksunes L, **Zhu H*** Integrating High throughput Toxicokinetics Data and Knowledge based Deep Neural Network (k DNN) Methodology to Advance a Computational Adverse Outcome Pathway Framework for Assessing Hepatotoxicity. Society of Toxicology 62nd Annual Meeting, Nashville, Tennessee, March 2023. (**2023 CTSS Graduate Student Award**)

45. Jia X, Wen X, Russo D, Aleksunes L, **Zhu H*** Mechanism-Driven Modeling of Drug-Induced Liver Injury Using Structural Alerts and an Oxidative Stress Screening Assay. Society of Toxicology 61st Annual Meeting, San Diego, California, March 2022.

44. Chung E, Russo D, Ciallella H, Aleksunes L, **Zhu H*** A Data-Driven Computational Modeling Study to identify and prioritize potential human carcinogens using public data. Society of Toxicology 61st Annual Meeting, San Diego, California, March 2022.

43. Russo D, Zhang Y, **Zhu H*** Extensive data-driven modeling of food-derived bioactive peptides that inhibit the angiotensin I-converting enzyme. American Chemical Society 257th national meeting, Orlando, FL, August, 2019.

42. Ciallella H, Russo D, **Zhu H*** Predictive Multitask Deep Learning Modeling of Estrogen Receptor Activity. Society of Toxicology 58th Annual Meeting, Baltimore, Maryland, March 2019.

41. Russo D, **Zhu H*** Developing Mechanism-Based Animal Toxicity Models: A Chemocentric Approach Using Big Data. American Society for Cellular and Computational Toxicology 6th Annual Meeting, Bethesda, MD, September 2018. (**2018 Toxicology in 21th Century student award presentation**)

40. Russo D, Zorn K, Clark AM, Korotocov A, Tkachenko V, **Zhu H**, Ekins S Comparison of multiple machine learning algorithms, descriptors, and metrics for estrogen receptor binding. Society of Toxicology 57th Annual Meeting, San Antonio, TX, March 2018.

39. Zhao L, Wang W, Russo D, Aleksunes LM, **Zhu H*** Mechanism-Driven Computational Modeling of Hepatotoxicity Based on Chemical Information, Biological Data, and Toxicity Pathways. Society of Toxicology 57th Annual Meeting, San Antonio, TX, March 2018.

38. Wang W, Russo D, Huang R, Xia M, **Zhu H*** Mechanistic evaluation of chemicals that induce oral acute toxicity by mitochondrial membrane disruption: big data profiling and analysis. American Society for Cellular and Computational Toxicology 6th Annual Meeting, Gaithersburg, MD, September 2017. (**2017 Toxicology in 21th Century student award presentation**)

37. Russo D, Wang W, Strickland J, Shende S, **Zhu H*** CIIProCluster: Developing read--across predictive toxicity models using big data. Society of Toxicology 56th Annual Meeting, Baltimore, MD, March 2017.

36. Wang W, Sedykh A, Sun H, Zhao L, Russo D, Yan B, **Zhu H*** Virtual gold nanoparticle library: simulation, modeling, and experimental validation. Society of Toxicology 56th Annual Meeting, Baltimore, Maryland, March 2017. (**Emil A. Pfitzer Drug Discovery Student Award presentation**)

35. Wang Y, Wang W, **Zhu H*** Profiling Pesticide Landscape from Different Regulatory Agencies: Prioritize Potential Environmental Hazard Compounds by Comparing the Chemical and Biological Diversities. Society of Toxicology 56th Annual Meeting, Baltimore, Maryland, March 2017.

34. Zhao L, Wang W, Sedykh A, **Zhu H*** Experimental errors in QSAR modeling sets: what we can do and what we cannot do. American Chemical Society 252nd national meeting, Philadelphia, PA, August, 2016.

33. Wang W, Sedykh A, Zhao L, Yan B, **Zhu H*** Virtual Gold Nanoparticles. American Chemical Society 252nd national meeting, Philadelphia, PA, August, 2016.

32. Wang W, Russo D, Kim M, Zhao L, Huang R, Xia M, Hartung, T, **Zhu H*** Profiling and Evaluating Environmental Chemicals that Induce Oral Acute Toxicity Using Mitochondrial Membrane Potential Disruption Assay, Big Data and New Read-across Strategy. Society of Toxicology 55th Annual Meeting, New Orleans, LA, March 2016.

31. Kim M T, **Zhu H*** From QSAR to big data: Developing mechanism-driven predictive models for animal toxicity. American Chemical Society 250th national meeting, Boston, MA, August, 2015.

30. Russo D P, Wang W, Kim M T, Pinolini D, **Zhu H*** CIIPro: An online cheminformatics portal for large scale chemical data analysis. American Chemical Society 250th national meeting, Boston, MA, August, 2015.

29. Kim T M, Wang W, Sedykh A, Huang R, Xia M, **Zhu H*** From individual datasets to big data: developing mechanism-driven predictive liver toxicity models. Society of Toxicology 54th Annual Meeting, San Diego, CA, March 2015. (**2015 Jean Lu Student Scholarship Award presentation**)

28. Wang W, Sedykh A, Yan B, **Zhu H*** Quantitative nanostructure toxicity relationship: Developing predictive cell recognition models for gold nanoparticles. Society of Toxicology 54th Annual Meeting, San Diego, CA, March 2015.

27. Kim T M, Sedykh A, Zhang J, Huang R, Xia M, **Zhu H*** Profiling environmental chemicals that induce the antioxidant response pathway using cell-based assays and cheminformatics tools. Society of Toxicology 53rd Annual Meeting, Phoenix, AZ, March 2014.

26. Kim T M, Lallier B, Zhang J, Russo D, Mayer-Bacon C, Boison A, Kotchoni S O, Martin J V, **Zhu H*** Computational profiling of the binding mechanisms of $GAPA_A$ receptor ligands. American Chemical Society 245th national meeting, Indianapolis, IN, September, 2013.

25. Zhang J, **Zhu H*** Applying novel data mining techniques to create a new chemical database of environmental interest. American Chemical Society 244th national meeting, Philadelphia, PA, August, 2012.

24. Kim T M, **Zhu H*** Combinatorial Quantitative Structure-Activity Relationship (QSAR) modeling of oral bioavailability. American Chemical Society 244th national meeting, Philadelphia, PA, August, 2012.

23. **Zhu H*** Solimeo R L Quantitative Structure-Activity Relationship modeling of animal ocular toxicity. Society of Toxicology 51st Annual Meeting, San Francisco, CA, March 2012.

22. **Zhu H,** Zhang L, Staab J, Sedykh A, Tang H, Gomez S, Rusyn I, Tropsha A. Incorporation of ToxCast in vitro assay data and relevant toxicity pathway information improves the external prediction accuracy of Quantitative Structure-Activity Relationship (QSAR) models of chemical hepatotoxicity. Society of Toxicology 50th Annual Meeting, Washington DC, March 2011.

21. Low Y, Uehara T, Minowa Y, Yamada H, Ohno Y, Urushidani T, Sedykh A, Fourches D, **Zhu H,** Rusyn I, Tropsha A Predictive value of chemical and toxicogenomic descriptors for drug-induced hepatotoxicity. Society of Toxicology 50th Annual Meeting, Washington DC, March 2011.

20. Zhang L, **Zhu H,** Afantitis A, Melagraki G, Sarimveis H, Rusyn I, Tropsha A Quantitative Structure-Activity Relationship (QSAR) modeling of Estrogen Receptor (ER) binding affinity and virtual screening for potential Endocrine Disrupting Compounds (EDCs). Society of Toxicology 50th Annual Meeting, Washington DC, March 2011.

19. Afantitis A, Melagraki G, Sarimveis H, Zhang L, **Zhu H,** Tropsha A. Combinatorial QSAR modeling of toxicity data using 2D & 3D chemical descriptors. Book of abstract, 18th European Symposium on Quantitative Structure Activity Relationships, Rhodes, Greece September 2010.

18. Tang H, **Zhu H,** Sedykh A, Zhang L, Richard A M, Rusyn I, Tropsha A Toxicity reference database (ToxRefDB) to develop predictive toxicity models and prioritize compounds for future toxicity testing. American Chemical Society 240th national meeting, Boston, MA, August, 2010.

17. Zhang L, **Zhu H,** Sedykh A, Tang H, Richard A M, Rusyn I, Tropsha A Using ToxCast in vitro assays in the hierarchical Quantitative Structure-Activity Relationship (QSAR) modeling for predicting in vivo toxicity of chemicals. Abstract 192; The 49th National Meeting of the Society of Toxicology, Salt Lake City, UT, March 2010.

16. Sedykh A, **Zhu H**, Tang H, Zhang L, Richard A, Rusyn I, Tropsha A Using *in vitro* dose-response profiles to enhance QSAR modeling of *in vivo* toxicity. Abstract 185; The 49th National Meeting of the Society of Toxicology, Salt Lake City, UT, March 2010.

15. Zhang L, **Zhu H**, Rusyn I, Judson R, Dix D, Houck K, Martin M, Richard A, Kavlock R, Tropsha A Cheminformatics analysis of EPA ToxCast chemical libraries to develop predictive toxicity models and prioritize compounds for in vivo toxicity testing. EPA ToxCast Data Analysis Summit, RTP, NC, May 2009.

14. **Zhu H**, Sedykh, A, Zhang, L, Rusyn I, Tropsha A Using ToxCast cell-viability and gene-expression assays as biological descriptors in QSAR modeling of animal toxicity endpoints. EPA ToxCast Data Analysis Summit, RTP, NC, May 2009.

13. **Zhu, H**; Martin, T M, Ye L, Young D M, Tropsha A Combinatorial QSAR modeling of rat acute toxicity by oral exposure. Abstract 1125; The 48th National Meeting of the Society of Toxicology, Baltimore, MD, March 2009.

12. Eastling M, Tropsha A, Ye L, **Zhu H,** Martin T, Moudgal C Quantitative Structure Toxicity Relationships (QSTR) models for predicting acute/sub-acute and sub-chronic/chronic adverse effect levels. Abstract 1124; The 48th National Meeting of the Society of Toxicology, Baltimore, MD, March 2009.

11. Zhang L, **Zhu H,** Rusyn I, Judson R, Dix D, Houck K, Martin M, Richard A, Kavlock R, Tropsha A Cheminformatics analysis of EPA ToxCast chemical libraries to identify domains of applicability for predictive toxicity models and prioritize compounds for toxicity testing. Abstract 1088; The 48th National Meeting of the Society of Toxicology, Baltimore, MD, March 2009.

10. Ye L, **Zhu H,** Golbraikh A, Tropsha A Establishing a balance between prediction accuracy and applicability domain of QSAR models. American Chemical Society 235th national meeting, New Orleans, LO, March 2008.

9. Tropsha A, Golbraikh A, **Zhu H** Applicability domains, space coverage, and predictive power of QSAR models. American Chemical Society 235th national meeting, New Orleans, LO, March 2008.

8. Golbraikh A, **Zhu H,** Ye L, Wang-Bell M, Tang H, Tropsha A Automatic detection of outliers prior to QSAR studies. American Chemical Society 235th national meeting, New Orleans, LO, March 2008.

7. **Zhu H**, Ye L, Rusyn I, Richard A, Golbraikh A, Tropsha A Two-step quantitative structure activity relationship modeling of in vivo toxicity using in vitro cytotoxicity data. Abstract 245; The 47th National Meeting of the Society of Toxicology, Seattle, WA, March 2008.

6. Rodgers A D, **Zhu H,** Rusyn I, Tropsha A QSAR modeling of human liver adverse effects database using kNN method. Abstract 244; The 47th National Meeting of the Society of Toxicology, Seattle, WA, March 2008

5. Zhang L, **Zhu H**, Oprea T, Tropsha A QSAR modeling of blood–brain barrier permeability of diverse organic compounds. Book of abstracts, American Chemical Society 234th national meeting, Boston, MA, August 2007.

4. **Zhu H**, Rusyn I, Richard A, Tropsha A The utilization of NTP-HTS data in predictive ADME/tox modeling. U.S. EPA International Science Forum on Computational Toxicology, Research Triangle Park, NC, May, 2007.

3. **Zhu H**, Fourches D, Varnek A, Papa E, Gramatica P, Tetko I V, Öberg T, Cherkasov A, Tropsha A Combinational QSAR modeling of chemical toxicants tested against Tetrahymena pyriformis, U.S. EPA International Science Forum on Computational Toxicology, Research Triangle Park, NC, May, 2007.

2. **Zhu H**, Wang K, Rusyn I, Richard A, Tropsha A The utilization of NTP-HTS data in predictive ADME/tox modeling. The 46th National Meeting of Society of Toxicity, Charlotte, NC, March, 2007.

1. **Zhu H**, Shi N, Fan Y, Zhou J Activity and conformation changes of dihydrofolate reductase induced by denaturants, The 7th National Conference on Enzymology, Haikou, China, 1997. (In Chinese)

Research Grants

Active:

NIEHS (R01ES031080) Zhu (PI) 05/19/20 - 02/28/25
Mechanism-Driven Virtual Adverse Outcome Pathway Modeling for Hepatotoxicity. Total cost: $2,271,161

NSF (2245158) Zhu (leading PI of the multi-PI project) 09/01/22 - 08/31/26
Collaborative Research: III: Medium: New Machine Learning Empowered Nanoinformatics System for Advancing Nanomaterial Design. Total cost: $800,000 ($350,000 to Zhu lab).

NIGMS (R01GM148743) Zhu (PI) 05/01/23 – 01/31/27
Virtual nanostructure simulation (VINAS) portal. Total cost: $1,048,277

NIEHS (R35ES031709) Zhu (co-I) 07/16/21- 6/30/29
Discovering Chemical Activity Networks-Predicting Bioactivity Based on Structure. Subaward to Zhu lab: $576,818, PI: Robyn Tanguay at Oregon State University

ExxonMobil Zhu (PI) 01/01/20 - 12/31/23
Predictive and validated estrogen receptor models. Total cost: $350,000

Pending:

NIH (UHD113039A) Zhu (PI of the multi-PI project, 20% effort) Requested duration: 5 years
Integrated Transporter Elucidation Center. Total cost: $5,830,000
Received **15 impact score** from a NIH study section. Award is pending.

NIH (R01HD114277) Zhu (PI, 20% effort) Requested duration: 4 years
Predictive modeling of chemical developmental toxicity by data-driven explainable machine learning approaches Total cost: $2,821,384

NSF Zhu (PI) Requested duration: 3 years
NSF Nanoinformatics Center Total cost: $1,500,000

Completed:

ExxonMobil Zhu (PI) 01/01/20 - 12/31/22
Predictive and validated estrogen receptor models. Total cost: $240,005

NIEHS (R15ES023148) Zhu (PI). 08/09/13 - 07/31/22
Mechanistic evaluation of chemicals that induce oral acute toxicity by novel read-across approaches using public big data. Total cost: $940,888

Lubrizol Zhu (PI) 05/01/20 - 12/31/20
Develop a hybrid DART model based on both chemical descriptors and biological data obtained from public domain. Total cost: $25,000

Colgate-Palmolive Zhu (PI) 5/1/17–6/30/20

Support read-across study of animal acute toxicity using public biological data. Total cost: $80,000

Rutgers Provost multidisciplinary research grant Zhu (PI) 1/1/18–12/31/19
Digital Nano: Developing Virtual Nanomaterial Simulation (VINAS) Toolbox for Intelligent Nanomodeling Total cost: $14,000

The Johns Hopkins Center for Alternatives to Animal Testing Zhu (PI) 3/1/16–2/28/19
Advance Predictive Modeling of Acute Toxicity by Big Data. Total cost: $70,000

Rutgers ORED-RUN-RBHS Grant in Big Data Analytics Zhu (PI) 7/1/17–6/30/18
Big Data, Modeling and Validation to Advance Hepatotoxicity Prediction. Total cost: $40,000

Rutgers Provost research grant Zhu (PI) 1/1/17–12/31/17
CIIPro: a new read-across ADME-Tox predictor based on big data tool. Total cost: $3,390

Rutgers University's Research Council Zhu (PI) 7/1/16–6/30/17
Advance QSAR to Big Data Profiling. Total cost: $3,920

Rutgers University's Environmental Health Pilot Grant Zhu (PI) 1/1/17–3/31/17
From QSAR to big data profiling: the new generation of animal toxicity modeling. Total cost: $4,800

Rutgers University's Environmental Health Pilot Grant Zhu (PI) 7/1/15–2/29/16
From QSAR to big data profiling: the new generation of animal toxicity modeling. Total cost: $15,000

Colgate-Palmolive Zhu (PI) 4/1/13–6/30/15
Profiling chemicals based on public bioassay data for the development of predictive computational acute toxicity model. Total cost: $40,000

Rutgers University's Research Council Zhu (PI) 4/30/13–5/1/14
Quantitative structure in vitro-in vivo relationship. Total cost: $3,000

Colgate-Palmolive Zhu (PI) 7/1/11–6/30/13
Predictive Quantitative Structure Activity Relationship (QSAR) modeling of reproductive and developmental toxicity using integrated chemical and biological (HTS profiles) descriptors of molecules. Total cost: $35,414

The Johns Hopkins Center for Alternatives to Animal Testing Zhu (PI) 2/1/08–1/31/11
Use of high throughput screening methods improves computational models for in vivo acute toxicity tests. Total cost: $45,000

EPA (RD832720) Zhu (co-PI of project 2) 9/1/05 – 8/31/10

Carolina environmental bioinformatics research center. Total cost: $4,500,000 (co-PI of $725,000 sub-award, PI: Tropsha)

Teaching Activities

Summary of Courses Taught:

Term	Course ID	Course Title	Credit Hours	Responsibility	Number of students
Fall 2023	43487	Biochemistry	4	80%	35
Spring 2022	56:121:555	CHEMINFORMATICS	3	100%	8
Fall 2021	50:115:403 56:115:511	GEN BIOCHEMISTRY I, BIOCHEMISTRY I	3	100%	26
Fall 2020	56:160:515	PHARM CHEM	3	100%	26
Spring 2020	56:160:602	SEMINAR IN CHEMISTRY	1	100%	10
Fall 2019	50:115:403 56:115:511	GEN BIOCHEMISTRY I, BIOCHEMISTRY I	3	100%	54
	56:160:515	PHARM CHEM	3	100%	14
	56:160:601	SEMINAR IN CHEMISTRY	1	100%	2
Spring 2019	56:121:555	CHEMINFORMATICS	3	100%	10
	56:160:602	SEMINAR IN CHEMISTRY	1	100%	2
Fall 2018	50:115:403 56:115:511	GEN BIOCHEMISTRY I, BIOCHEMISTRY I	3	100%	47
	56:160:515	PHARM CHEM	3	100%	9
	56:160:601	SEMINAR IN CHEMISTRY	1	100%	2
Spring 2018	56:121:555	CHEMINFORMATICS	3	100%	10
	56:160:602	SEMINAR IN CHEMISTRY	1	100%	3

Fall 2017	50:115:403 56:115:511	GEN BIOCHEMISTRY I, BIOCHEMISTRY I	3	100%	27
	56:160:515	PHARM CHEM	3	100%	11
	56:160:601	SEMINAR IN CHEMISTRY	1	100%	3
Spring 2017	56:121:555	CHEMINFORMATICS	3	100%	4
Fall 2016	50:115:403 56:115:511, 56:121:510	GEN BIOCHEMISTRY I, BIOCHEMISTRY I, ESSENT BIOL CHEM I	3	100%	35
	56:160:515	PHARM CHEM	3	100%	12
Spring 2016	56:121:555	CHEMINFORMATICS	3	100%	6
Fall 2015	50:115:403 56:115:511, 56:121:510	GEN BIOCHEMISTRY I, BIOCHEMISTRY I, ESSENT BIOL CHEM I	3	100%	60
	56:160:515	PHARM CHEM	3	100%	10
Fall 2014	50:115:403	GEN BIOCHEMISTRY I	3	100%	24
	56:115:511, 56:121:510	BIOCHEMISTRY I, ESSENT BIOL CHEM I	3	100%	2
	56:160:515	PHARM CHEM	3	100%	13
Spring 2014	56:121:555	CHEMINFORMATICS	3	100%	9
	50:115:494	ELEMENTARY CHEMINFORMATICS	3	100%	5
Fall 2013	50:115:403	GEN BIOCHEMISTRY I	3	100%	31
	56:115:511, 56:121:510	BIOCHEMISTRY I, ESSENT BIOL CHEM I	3	100%	5
	56:160:515	PHARM CHEM	3	100%	14
Spring 2013	56:121:555	CHEMINFORMATICS	3	100%	12
Fall 2012	50:115:403	GEN BIOCHEMISTRY I	3	100%	42
	56:115:511, 56:121:510	BIOCHEMISTRY I, ESSENT BIOL CHEM I	3	100%	10
Spring 2012	56:121:555	CHEMINFORMATICS	3	100%	9

Fall 2011	50:115:403, 56:115:511	GEN BIOCHEMISTRY I	3	100%	39

Advising:

Doctorals:

Dr. Marlene T Kim (CCIB, Ph.D. in 2016 and graduated with honor) 2012-2016 (advisor)
Developing advanced rules and tools to improve in vivo *QSAR models*

Dr. Wenyi Wang (CCIB, Ph.D. in 2018 and graduated with honor) 2013-2018 (advisor)
From QSAR to QNAR, searching for enhanced models for drug discovery

Dr. Sruthi Murlidaran (CCIB, Ph.D. in 2018) 2015-2018 (committee member)
Mechanisms underlying effects of genetic variance and general anesthetics on pentameric ligand gated ion channels

Dr. Daniel Russo (CCIB, Ph.D. in 2019 and graduated with honor) 2014-2019 (advisor)
Chemical-in vitro-in vivo profiling portal

Dr. Xiliang Yan (CCIB, Exchange Ph.D. student, Ph.D. in 2020) 2017-2019 (advisor)
Virtual nanostructure simulations

Dr. Linlin Zhao (CCIB, Ph.D. in 2020) 2017-2020 (advisor)
Computational modeling for chemical toxicity assessment in the big data era: combining data driven profiling and mechanism-driven read-across

Dr. Sung Won Oh (CCIB, Ph.D. in 2020) 2017-2020 (committee member)
Biochemical Sensing Circuits Based on Catalytic Swinging Arms

Dr. Heather Ciallella (CCIB, Ph.D. in 2022 and graduated with honor) 2017-2022 (advisor)
Predicting developmental and reproductive toxicity with AI and high-throughput screening data

Xuelian Jia (Rowan University, Ph.D. candidate) since 2019 (advisor)
Predictive hepatotoxicity modeling

Elena Chung (Rowan University, Ph.D. candidate) since 2020 (advisor)
Mechanistic modeling of chemical toxicity in liver

Tong Wang (Rowan University, Ph.D. candidate) since 2021 (advisor)
Nanoinformatics

Nada Daood (Rowan University, Ph.D. candidate) since 2021 (advisor)
Computational Immunotoxicology

Yitao Shen (Rowan University, Ph.D. candidate) since 2023 (advisor)
Public chemical toxicity portal

Masters:

Renee Solimeo (Chemistry, M.S. in 2012) 2011-2012 (advisor)
Predicting chemical ocular toxicity using a combinatorial QSAR approach

Chris Mayer-Bacon (CCIB, M.S. in 2014 and graduated with honor) 2012-2014 (advisor)
Predictive modeling of CYP3A4 inhibition by comparing different binding mechanisms

Daniel Russo (Biology, M.S. in 2014 and graduated with honor) 2012-2014 (advisor)
Quantitative structure activity relationship modeling of 5-hydroxytryptamine type 6 receptor antagonists

Abena Boison (Chemistry, M.S. in 2014) 2012-2014 (advisor)
Complying and curating public bioassay data for chemical toxicity and drug discovery studies

Brian Lallier (Biology, M.S. in 2014) 2012-2014 (committee member)
Characterization of bioactive anxiolytic compounds from Annona muricata leaf extract: a computational and experimental approach

Daniel Pinolini (CCIB, M.S. in 2015) 2013-2015 (advisor)
Profile chemicals with drug-drug interaction potentials by big data

Kyle Jenkins (CCIB, M.S. in 2015) 2015 (committee member)
The Effect of Annona Muricata extracts on the $GABA_A$ Receptor

Kathryn Ribay (Chemistry, M.S. in 2016 and graduated with honor) 2014-2016 (advisor)
Predictive modeling of Estrogen Receptor binding agents using advanced cheminformatics tools and massive public data

Nauf Aljuhani (Chemistry, M.S. in 2017) 2016-2017 (committee member)
A calcium oxalate phase stability and dissolution study

John Collins (Chemistry, M.S. in 2017 and graduated with honor) 2016-2017 (committee member)
Exploring Global and Micro-Environment Conditions for Affecting Enzyme Activities and Functional Transitions

Jinnie C Anstice (Chemistry, M.S. in 2018) 2012-2018 (committee member)
A microfluidic investigation of calcium oxalate crystallization

Ariel Lane (Chemistry, M. S. Candidate) 2014 (committee member)
Logic gated control of biochemical reactions

Dalia Al-Shahrani (Chemistry, M. S. in 2018) 2016-2018 (committee member)
Understanding the self-assembly of Lignin-based biomaterials

Nouf Alzahrani (Chemistry, M. S. in 2018) 2016-2018 (committee member)
Study co-aggregations of nucleic acid nanostructures with tetracycline molecules and their potential applications in smart drug delivery

Swati Sharma (CCIB, M. S. in 2020) 2018-2020 (advisor)
Hybrid modeling of reproductive and developmental toxicity

Brienne M Sprague (Chemistry, M.S. candidate) 2012-2013 (advisor)
Design, synthesis and experimental validate novel chemopreventive agents by employing cheminformatics modeling techniques

Kaitlyn Nguyen (Chemistry, M. S. in 2022) 2011-2022 (committee member)
Investigation of Negatively Charged Biopolymers for Stabilizing Enzymes and Preventing Aggregation

Yitao Shen (Chemistry, M.S. candidate) 2021-2022 (advisor)
Informatics science in Chemistry

Undergraduate:

Lisa H Darji (Chemistry) Fall 2012 (independent study advisor)

Joanna Kopko (Chemical Biology, Stevens Institute of Technology) Summer 2020 (independent study advisor)

Kayla Golliday (Chemistry) Fall 2020 (independent study advisor)

Post Doctoral:

Dr. Jun Zhang (CCIB, Post-doc) 2012-2014 (advisor)
Dr. Daniel Russo (Chemistry, Post-doc) 2020-2022 (advisor)

Visiting Scholar:

Dr. Daniel Russo (Rowan University) 2022-present (advisor)

Visiting Scholar:

Dr. Alexander Sedykh (CCIB) 2013-2015 (advisor)
Dr. Jun Zhang (CCIB) 2014-2015 (advisor)
Dr. Yutang Wang (CCIB) 2016-2017 (advisor)
Dr. Min Wu (CCIB) 2017-2018 (advisor)
Dr. Jin Liu (CCIB) 2018-2019 (advisor)

Professional Services

Within the Professions:

2022	Ad Hoc Reviewer, Florida Department of Health Biomedical Research Program Grant
2021	Ad Hoc Reviewer, Dutch Research Council Talent Programme Grant
2021-present	Associate Editor, Ecotoxicology and Environmental Safety
2021	Ad Hoc Reviewer, European Research Council Consolidator Grant
2021	Guest editor, Journal of Hazardous Materials
2020	Guest editor, ACS Sustainable Chemistry & Engineering

2019-present	Associate editor, Frontiers in Toxicology, Computational Toxicology and Informatics
2019	Ad Hoc Reviewer, NCATS ASPIRE Design Challenge Grant
2017-present	Editorial board member, Ecotoxicology and Environmental Safety
2017-present	ASCCT Annual Meeting Organizing Committee
2016	Ad Hoc Reviewer, US Army Grant
2016-present	Peer reviewer of US EPA's draft Provisional Peer-Reviewed Toxicity Values
2015	Ad Hoc Reviewer, U.S. EPA STAR Fellowship
2014-2019	Member, Acute Toxicity Study Group

Industrial Collaborations/Consultants:

2020-present	Lubrizol, Cleveland, OH
2019-present	ExxonMobil, Clinton, NJ
2011-present	MultiCase Inc., Cleveland, OH
2017	Sanofi, Bridgewater, NJ
2014	Sigmapharm Laboratories, Bensalem, PA
2013	Biofunc Research, Cleveland, OH

Reviewing manuscripts for professional journals:

Nature Machine Intelligence
Nature Climate Change
Nature Communications
Environmental and Health Perspective
Environmental Science and Technology
Chemical Review
Science Advances
Nucleic Acids Research
Environmental Pollution
Nano Today
NanoImpact
Journal of Chemical Information and Modeling
ACS Sustainable Chemistry and Engineering
ACS Infectious Diseases
Journal of Computational Chemistry
Risk Analysis
Toxicological Sciences
Toxicological Research
Chemical Research in Toxicology
Journal of Medicinal Chemistry
Frontier Toxicology
Medicinal Chemistry
SAR and QSAR in Environmental Research
Plos One

Scientific Reports
Toxicology and Applied Pharmacology
Bioorganic and Medicinal Chemistry Letters
Frontiers in Pharmacology
Applied In Vitro Toxicology
Molecular Pharmaceutics
Toxicology Research
Nano-Micro Letters
Ecotoxicology and Environmental Safety
BMC Bioinformatics
Bioorganic and Medicinal Chemistry
Achieve of Toxicology
Chemosphere
npj Computational Materials

Services within the Schools

Rowan University

2022-present	Tenure, Recontracting and Promotion (TRAP) Committee

Department of Chemistry, Rutgers

2019	Appointments and Promotions Committee
2019	Faculty Search Committee
2018	Appointments and Promotions Committee
2017-2020	Graduate Program Director
2017	Faculty Search Committee
2013	Faculty Search Committee
2012	Faculty Search Committee

Center for Computational and Integrative Biology, Rutgers

2015-present	Undergraduate Curriculum Committee
2013	Faculty Search Committee
2011-2014	Executive Committee
2011-2014	Admission Committee

Rutgers University:

2016-present	Appointments and Promotions Committee (Natural Science)
2012-2014	Rutgers China Office Advisory Council

Media Reports and Interviews

"NIH Awards Prestigious Grant to Support Research on Preventing Medical Toxicity in New Medications"
https://news.camden.rutgers.edu/2020/07/nih-awards-prestigious-grant-to-support-research-on-preventing-medical-toxicity-in-new-medications/

"Et si les algorithmes remplaçaient les tests sur les animaux?"

http://www.slate.fr/story/175986/sciences-tests-laboratoires-produits-chimiques-algorithme-animaux

“An end to animal testing?”
https://sciencenode.org/feature/An%20end%20to%20animal%20testing.php

“What Are the Alternatives to Animal Testing?”
https://www.livescience.com/65401-animal-testing-alternatives.html

“A new algorithm outperforms animal testing for spotting toxic chemicals”
https://www.theweek.in/news/health/2019/04/18/A-new-algorithm-outperforms-animal-testing-for-spotting-toxic-chemicals.html

“Animal-free chemical toxicity testing may become outdated with a new algorithm”
https://www.innovationtoronto.com/2019/04/animal-free-chemical-toxicity-testing-may-become-outdated-with-a-new-algorithm/

“New algorithm could save thousands of animals from toxic testing”
https://www.siliconrepublic.com/machines/algorithm-animal-testing-breakthrough

“Rutgers team predicts toxicity by mining PubChem data”
https://chemicalwatch.com/76839/rutgers-team-predicts-toxicity-by-mining-pubchem-data

“Low-cost, high-speed algorithm may allow animal-free chemical toxicity testing”
https://www.news-medical.net/news/20190417/Low-cost-high-speed-algorithm-may-allow-animal-free-chemical-toxicity-testing.aspx

“New Algorithm Allows for Faster, Animal-Free Chemical Toxicity Testing”
https://www.labmanager.com/news/2019/04/new-algorithm-allows-for-faster-animal-free-chemical-toxicity-testing

“New algorithm allows for faster, animal-free chemical toxicity testing”
https://www.sciencedaily.com/releases/2019/04/190416170918.htm

“Can an algorithm replace animal testing for chemicals”
https://www.futurity.org/animal-testing-chemicals-algorithm-2038082/

“New algorithm allows for faster, animal-free chemical toxicity testing”
https://phys.org/news/2019-04-algorithm-faster-animal-free-chemical-toxicity.html

“New Algorithm Allows Faster, Animal-Free Chemical Toxicity Testing”
https://www.rutgers.edu/news/new-algorithm-allows-faster-animal-free-chemical-toxicity-testing

“Computational and Integrative Biology Doctoral Student Daniel Russo Receives Tox21 Student Award”
https://fas.camden.rutgers.edu/2019/01/10/computational-and-integrative-biology-doctoral-student-daniel-russo-receives-tox21-student-award/

“Norcross Announces Over $1.4 Million for Medical Research & Training at South Jersey Universities”

https://norcross.house.gov/media-center/press-releases/norcross-announces-over-14-million-medical-research-training-south

"We R Arts and Sciences: Wenyi Wang and Dr. Hao Zhu"
https://fas.camden.rutgers.edu/2017/11/28/we-r-arts-and-sciences-wenyi-wang-and-dr-hao-zhu/

"Student Research Creates Pathway to Success for Chemistry Graduates"
http://news.camden.rutgers.edu/2016/10/student-research-creates-pathway-to-success-for-chemistry-graduates/

"Big Data in Modern Computational Toxicology"
http://ceed.rutgers.edu/big-data-in-modern-computational-toxicology/

"A crystal ball for chemical safety"
http://science.sciencemag.org/content/351/6274/651

"Legal tussle delays launch of huge toxicity database"
http://www.nature.com/news/legal-tussle-delays-launch-of-huge-toxicity-database-1.19365

"Trial data mining project flags up Qsar issues"
https://chemicalwatch.com/21201/trial-data-mining-project-flags-up-qsar-issues

"Chemistry Scholar Producing Toxicity Database for Researchers"
http://news.camden.rutgers.edu/2013/11/chemistry-scholar-producing-toxicity-database-for-researchers/

"We R Arts And Sciences: Dr. Hao Zhu"
http://fas.camden.rutgers.edu/2014/02/04/we-r-arts-and-sciences-dr-hao-zhu/