

# RESUME

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### Qualifications

- 24 Years in industry and 5 years in government institute in structure/ligand-based drug design
- Disease areas include oncology, diabetes, inflammatory diseases, infectious diseases and neurodegeneration
- Optimized initial hits to IND track candidates (4 IND went to clinical trials)
- Expert in using MD simulations and free energy calculations for drug design
- Use of AI algorithms (e.g. DeepChem) for pharmacokinetic prediction and virtual screening
- Homology modeling, Quantum mechanics, Pharmacophore elucidation
- Management of chem/bio/PK databases
- Advanced use of Schrödinger Suite, Sybyl-X, DS-Modeling, Pipeline Pilot, KNIME
- Programming and scripting: C, C++, Fortran, Perl, Python and Bash. Wrote 6 major programs (4 published)
- Trilingual (English/Chinese/French)

### Professional Experience

- **Senior Director** (May 2023 – present), Architect Therapeutics (still in stealth), San Diego, CA
  1. Computational drug design in working with medicinal chemists and biologists for three confidential targets aiming at working all the way from hit ID to IND
  2. Acquired and managed Schrodinger Suite, LiveDesign, Dotmatics, cloud-based virtual cluster and workstation.
  3. Build virtual libraries with novel scaffolds synthesizable *via* CH-activation chemistries developed by Professor Jin-Quan Yu of Scripps Research Institute
- **Director** (July 2016 – May 2023), Arvinas, Inc.  
**Principal Research Investigator** (Aug 2013 – July 2016), Arvinas, Inc.
  1. One of the few in the startup team of Arvinas Inc., which went to public IPO in September 2018 and is now a clinical stage company with ARV-110, ARV-471 and ARV-766 in Phase I/II/III trials.
  2. Hiring manager, six direct reports ranking from Research Scientist to Principal Research Investigator.
  3. Acquired and managed hardware/software systems, including AWS virtual cluster to run Desmond with 200 GPUs, chembio databases and analysis tools (Seurat, ACAS and LiveDesign) and electronic notebook Arxspan. Facilitated remote working in groups.
  4. In working with few colleagues, quickly established PROTAC design systematic workflows based on modeling/simulation rationale and mechanistic understanding, recognized as the pioneer in the field.
  5. Proposed the main structures of ARV-110 (androgen receptor degrader) and ARV-471 (estrogen receptor degrader, being co-developed with Pfizer for clinical trials and marketing).
  6. Invented the Protein-Protein Interaction Inducing Technology (PPIIT, US patent application 20170281784).
  7. Published Dissociation Free Energy prediction method for protein-protein and protein-ligand binding potency (*Nature Sci. Rep.* 2022 <https://rdcu.be/cGvEu>).
  8. Collaborations with Merck, Genentech, Pfizer and Bayer.

- **Assistant Director** (Dec 2012 – Aug 2013)  
**Senior Research Investigator** (Jan 2010 – Dec 2012)  
**Research Investigator** (May 2005 – Dec 2009), Astellas-OSI Pharmaceuticals Inc, Long Island, New York (OSI was acquired by Astellas, the second largest pharma in Japan in June 2010).
  1. Head of the computational chemistry group. Maintained a most efficient and innovative computational chemistry platform for the company. Evaluated and acquired software like MEDIT for PDB data mining and fragment-based design, StarDrop for metabolic sites prediction, Muse for compound design and Desmond for MD simulation. Also developed own procedures. Coordinated with the computational chemistry and Fragment Evolution groups in Japan site, IT group and bioinformatics group. Worked from target identification through lead optimization.
  2. Computational chemist who supported mTOR kinase inhibitor project for colorectal cancers from project initiation (Aug. 2005) to IND track candidate OSI-027 (Aug. 2006) (went to Phase II clinical trial).
  3. Computational chemist who supported RON/MET kinase inhibitor project for gastric cancers from project initiation (June 2005) to IND track candidate OSI-296.
  4. Developed quantum “ReCore” technology which calculates conformational energy and ligand-protein interaction energy using advanced quantum chemistry methods. Achieved 100% success rate of prediction.
  5. Worked on epigenetic targets. Performed druggability calculations for over 40 acetyl/methyl lysine and arginine reader domains to help target identification. Performed structural comparison for 250 crystal/NMR structures to evaluate selectivity. Perform virtual screening against OSI database and Astellas corporate database for the bromodomains of a specific target.
- **Senior Scientist** (Nov. 2004 – May 2005), Accelrys, Inc., San Diego, CA.  
  1. Have repaired outstanding bugs in CHARMM, Decipher and Delphi modules of Insight II product and participated in Z-dock implementation. Working languages: C, C++ and Perl.
- **Principal Scientist** (Mar. 2002 – Oct. 2004)  
**Senior Scientist I** (Dec. 1997 – Feb. 2002), Cengent Therapeutics Inc - Structural Bioinformatics Inc, San Diego, CA.
  1. Have performed virtual screening of databases of commercially available compounds based on pharmacophores derived from protein structures, and obtained novel inhibitors/antagonists for PTP1B (Patent WO 03/032916), TNFR (Patent WO 00/032598), IKK $\beta$  (satisfying the milestone of Yamanouchi Co), hepatitis C virus protease (satisfying the milestone of BioChem Pharma Inc), HER2 kinase and Bcl2.
  2. Have designed a number of compounds that showed improved inhibitory activities for PTP1B with  $K_i$  up to 7 nM and efficacy in mice diabetes models with oral bioavailability.
  3. Awarded a NIH Small Business Innovation Research Grant (SBIR, 1R43CA101580-01) to convert EGF into small molecule antagonists.
  4. Lead Scientist in a major collaboration with DuPont Pharmaceuticals Company for TNF small molecule antagonist development.
  5. Recruited and trained three Ph.D.-level scientists with different seniorities.
- **Assistant Research Officer** (Feb. 1993 – Dec. 1997), Biotechnology Research Institute of the National Research Council of Canada, Montreal.
- **Postdoctoral fellow** (Sep. 1991 – Feb. 1993), M.R.C. Group in Membrane Biology, University of Toronto (Supervisor: Reinhart Reithmeier).

## Education

- **Ph. D.** in Molecular Biophysics (Computational Chemistry), University of Paris VII, September 1991. Supervisor: Alberte Pullman. Thesis in modeling of lipid layer structures and lipid-gramicidin A interactions.
- 1<sup>st</sup> place in the graduate program entrance exam in Beijing Medical University in 1985, thus selected to be one of the 108 students sent to Europe by the Education Ministry of China.
- **B. S.** in Medical Biophysics from Nankai University, China, in 1985.

## **Awards and honors**

- 2008 Certificate Of Appreciation of OSI for valuable contributions to discovery of OSI-296, a MET/RON kinase inhibitor IND track candidate.
- 2006 Certificate Of Appreciation of OSI for valuable contributions to discovery of OSI-027, an mTOR kinase inhibitor IND track candidate.

## **Issued US Patents (first or coinventor):**

1. "Tetrahydronaphthalene and tetrahydroisoquinoline derivatives as estrogen receptor degraders" US 11,597,720 date 3/7/2023
2. "Indole derivatives as estrogen receptor degraders" US 11,584,743 date 2/21/2023
3. "Compounds and methods for the targeted degradation of bromodomain-containing proteins" US 11,554,171 date 1/17/2023
4. "Compounds and methods for the targeted degradation of bromodomain-containing proteins" US 11,512,083 date 11/29/2022
5. "Compounds and methods for the targeted degradation of androgen receptor" US 11,427,548 date 8/30/2022
6. "Modulators of estrogen receptor proteolysis and associated methods of use" US 11,384,063 date 7/12/2022
7. "Compounds and methods for the targeted degradation of androgen receptor" US 11,352,351 date 6/7/2022
8. "Compounds and methods for the targeted degradation of enhancer of zeste homolog 2 polypeptide", US 11,191,741 date 12/7/2021
9. "Compounds and methods for the targeted degradation of rapidly accelerated Fibrosarcoma polypeptide", US 11,173,211 date 11/16/2021
10. "Modulators of proteolysis and associated methods of use", US 11,161,841 date 11/2/2021
11. "Tetrahydronaphthalene and tetrahydroisoquinoline derivatives as estrogen receptor degraders", US 11,104,666 date 8/31/2021
12. "EGFR proteolysis targeting chimeric molecules and associated methods of use", US 10,994,015 date 5/4/2021
13. "Tank-binding kinase-1 PROTACs and associated methods of use", US 10,946,017 date 3/16/2021
14. "Tetrahydronaphthalene and tetrahydroisoquinoline derivatives as estrogen receptor degraders", US 10,899,742 date 1/26/2021
15. "Indole derivatives as estrogen receptor degraders", US 10,865,202 date 12/15/2020
16. "Compounds and methods for the targeted degradation of androgen receptor", US 10,844,021 date 11/24/2020
17. "Compounds and methods for the targeted degradation of bromodomain-containing proteins", US 10,772,962 date 9/15/2020
18. "Compounds and methods for the enhanced degradation of targeted proteins", US 10,730,870 date 8/4/2020
19. "Compounds and methods for the targeted degradation of rapidly accelerated fibrosarcoma polypeptides", US 10,723,717 date 7/28/2020
20. "Tetrahydronaphthalene and tetrahydroisoquinoline derivatives as estrogen receptor degraders", US 10,647,698 date 5/12/2020
21. "Modulators of estrogen receptor proteolysis and associated methods of use", US 10,604,506 date 3/31/2020
22. "Compounds and methods for the targeted degradation of androgen receptor", US 10,584,101 date 3/10/2020
23. "Estrogen-Related Receptor Alpha based PROTAC compounds and associated methods of use", US 10,071,164 date 9/11/2018
24. "Substituted pteridinones for the treatment of cancer", US 9,351,974 date 5/31/2016
25. "Fused bicyclic mTOR inhibitors", US patent 8,796,455 date 8/5/2014
26. "Substituted pyrrolo[2,3-b]pyridines and -pyrazines", US patent 8,592,448 date 11/26/2013
27. "Substituted imidazopyr- and imidazotri-azines", US patent 8,481,733 date 7/9/2013
28. "Fused bicyclic kinase inhibitors", US patent 8,445,510 date 5/21/2013
29. "7-aminofuropyridine derivatives", US patent 8,378,104 date 2/19/2013
30. "Fused bicyclic mTor inhibitors", US patent 8,314,111 date 11/20/2012
31. "2-aminopyridine kinase inhibitors", US Patent 8,178,668 date 5/15/2012
32. "Furo[3,2-C]pyridines", US patent 8,022,206 date 9/20/2011
33. "Fused bicyclic mTOR inhibitors" US patent 7,943,767 date 5/17/2011
34. "Fused bicyclic mTOR inhibitors" US patent 7,923,555 date 4/12/2011

35. "Fused bicyclic mTOR inhibitors" US patent 7,700,594 date 4/20/2010
36. "Thiazole and thiadiazole inhibitors of tyrosine phosphatases" US 7,381,736 date 6/3/2008

**International Patents (first or coinventor):**

37. "Substituted imidazopyr- and imidazotri- azines", Eur. Patent 09751280.0-2117
38. "Fused bicyclic kinase inhibitors", Eur. Patent 11721678.8-2101
39. "Substituted pyrrolo[2,3-b]pyridines and -pyrazines" PCT WO2010059771
40. "Fused heterobicyclic kinase inhibitors" Eur. Patent 07718344.0-2117, US2007001439
41. "Fused Bicyclic mTOR Inhibitors" Eur. Patent 11155268.3-2117
42. "Furo- and thieno[3,2-c]pyridines" Eur. Patent 09709265.4 – 2117, US2009033311
43. "Fused bicyclic mTOR inhibitors", Eur. Patent 11155270.9-2117
44. "Pyrrolopyridine kinase inhibiting compounds" (PDK1 inhibitors) PCT WO2007067537
45. "Fused heterobicyclic kinase inhibitors" WO2007084667 A2
46. "Derivatives of thiazole and thiadiazole inhibitors of tyrosine phosphatases" WO/2006/028970
47. "Oxygen/nitrogen heterocyclic inhibitors of tyrosine phosphatases" WO/2006/017124
48. "Trisubstituted nitrogen modulators of tyrosine phosphatases" WO/2006/009876
49. "Pyrrolopyridine kinase inhibiting compounds" (PDK1 inhibitors) PCT WO2007067537
50. "Fused heterobicyclic kinase inhibitors" WO2007084667 A2
51. "Derivatives of thiazole and thiadiazole inhibitors of tyrosine phosphatases" WO/2006/028970
52. "Oxygen/nitrogen heterocyclic inhibitors of tyrosine phosphatases" WO/2006/017124
53. "Trisubstituted nitrogen modulators of tyrosine phosphatases" WO/2006/009876
54. "Propeptide-based inhibitors of cysteine proteases." WO 03/097664 A2
55. "Organosulfur inhibitors of tyrosine phosphatases." WO 03/032916 A2
56. "Methods and Compositions for Treating Inflammatory Diseases Utilizing Inhibitors of Tumor Necrosis Factor Activity." WO 00/32598 A1

**Recent US Patent Applications (first or coinventor):**

57. "Compounds and methods for the targeted degradation of androgen receptor" US 20230331681 date 10/19/2023
58. "Compounds and methods for the targeted degradation of bromodomain-containing proteins" US 20230263893 date 8/24/2023
59. "Compounds and methods for the enhanced degradation of targeted proteins" US 20230203030 date 6/29/2023
60. "Cereblon ligands and bifunctional compounds comprising the same" US 20230183209 date 6/15/2023
61. "Methods of treating prostate cancer" US 20230128132 date 4/27/2023
62. "Indazole based compounds and associated methods of use" US 20230097358 date 3/30/2023
63. "Cereblon ligands and bifunctional compounds comprising the same" US 20230082997 date 3/16/2023
64. "Rapidly accelerating fibrosarcoma protein degrading compounds and associated methods of use" US 20230081501 date 3/16/2023
65. "Compounds and methods for the targeted degradation of androgen receptor and associated methods of use" US 20230084249 date 3/16/2023
66. "Compounds and methods for the targeted degradation of rapidly accelerated fibrosarcoma polypeptides" US 20230000994 date 1/5/2023
67. "Modulators of proteolysis and associated methods of use" US 20220402907 date 12/22/2022
68. "Modulators of BCL6 proteolysis and associated methods of use" US 20220395576 date 12/15/2022
69. "Tetrahydronaphthalene and tetrahydroisoquinoline derivatives as estrogen receptor degraders" US 20220388984 date 12/8/2022
70. "Compounds and methods for the targeted degradation of enhancer of zeste homolog 2 polypeptide" US 20220378726 date 12/1/2022
71. "Compounds and methods for targeted degradation of KRAS" US 20220370416 date 11/24/2022
72. "Modulators of BCL6 proteolysis and associated methods of use" US 20220323457 date 10/13/2022
73. "Tetrahydronaphthalene and tetrahydroisoquinoline derivatives as estrogen receptor degraders" US 20220274955 date 9/1/2022
74. "Modulators of estrogen receptor proteolysis and associated methods of use" US 20220267305 date 8/25/2022
75. "Compounds and methods for the targeted degradation of androgen receptor" US 20220259154 date 8/18/2022
76. "Methods of treating breast cancer with tetrahydronaphthalene derivatives as estrogen receptor degrader" US

- 20220193072 date 6/23/2022
- 77. "Compounds and methods for the targeted degradation of androgen receptor and associated methods of use" US 20220144809 date 5/12/2022
  - 78. "MDM2-based modulators of proteolysis and associated methods of use" US 20220127279 date 4/28/2022
  - 79. "Imide-based modulators of proteolysis and associated methods of use" US 20220089570 date 3/24/2022
  - 80. "Selective modulators of mutant LRRK2 proteolysis and associated methods of use" US 20220064168 date 3/3/2022
  - 81. "Protein-protein interaction inducing technology" US 20210315856 date 10/14/2021
  - 82. "Indazole based compounds and associated methods of use" US 20210315896 date 10/14/2021
  - 83. "EGFR proteolysis targeting chimeric molecules and associated methods of use" US 20210220475 date 7/22/2021
  - 84. "Compounds and methods for the targeted degradation of androgen receptor" US 20210196710 date 7/1/2021
  - 85. "Compounds and methods for the targeted degradation of bromodomain-containing proteins" US 20210187108 date 6/24/2021
  - 86. "Compounds and methods for the targeted degradation of androgen receptor", US 20210171470 date 6/10/2021
  - 87. "TANK-binding kinase-1 PROTACS and associated methods of use" US 20210145832 date 5/20/2021
  - 88. "Tetrahydronaphthalene and tetrahydroisoquinoline derivatives as estrogen receptor degraders" US 20210139458 date 5/13/2021
  - 89. "EGFR proteolysis targeting chimeric molecules and associated methods of use" US 10994015 date 5/4/2021
  - 90. "Methods of treating prostate cancer" US 20210113557 Date 4/22/2021
  - 91. "Methods of treating breast cancer with tetrahydronaphthalene derivatives as estrogen receptor degraders" US 20210060008 date 3/4/2021
  - 92. "Indole derivatives as estrogen receptor degraders" US 20210040081 date 2/11/2021
  - 93. "Compounds and methods for the targeted degradation of androgen receptor" US 20210040044 date 2/11/2021
  - 94. "Compounds and methods for the targeted degradation of androgen receptor" US 20210009528 date 1/14/2021
  - 95. "Compounds and methods for the enhanced degradation of targeted proteins" US 20200392131 date 12/17/2020
  - 96. "Modulators of estrogen receptor proteolysis and associated methods of use" US 20200199107 date 6/25/2020
  - 97. "Cereblon ligands and bifunctional compounds comprising the same" US 20200155689 date 5/21/2020
  - 98. "Cereblon ligands and bifunctional compounds comprising the same" US 20200155690 date 5/21/2020
  - 99. "Compounds and methods for the targeted degradation of rapidly accelerated fibrosarcoma polypeptides" US 20200129627 date 4/30/2020
  - 100. "Compounds and methods for the targeted degradation of androgen receptor" US 20200095205 date 3/26/2020
  - 101. "Compounds and methods for the targeted degradation of androgen receptor" US 20200055825 date 2/20/2020
  - 102. "BRM targeting compounds and associated methods of use" US 20200038378 date 2/6/2020
  - 103. "Modulators of proteolysis and associated methods of use" US 20190315732 date 10/17/2019
  - 104. "BRM targeting compounds and associated methods of use" US 20190300521 date 10/3/2019
  - 105. "Indole derivatives as estrogen receptor degraders" US 20190233408 date 8/1/2019
  - 106. "Tank-Binding Kinase-1 PROTACs and associated methods of use" US 20190192514 date 6/27/2019
  - 107. "Modulators of proteolysis and associated methods of use" US 20180353501 date 12/13/2018
  - 108. "Compounds and methods for the targeted degradation of androgen receptor" US 20180346461 date 12/6/2018
  - 109. "Modulators of estrogen receptor proteolysis and associated methods of use" US 20180237418 date 8/23/2018
  - 110. "Cereblon ligands and bifunctional compounds comprising the same" US 20180228907 date 8/16/2018
  - 111. "Cereblon ligands and bifunctional compounds comprising the same" US 20180215731 date 8/2/2018
  - 112. "EGFR proteolysis targeting chimeric molecules and associated methods of use" US 20180193470 date 7/12/2018
  - 113. "Compounds and methods for the targeted degradation of Rapidly Accelerated Fibrosarcoma Polypeptides" US 20180179183 date 6/28/2018
  - 114. "Compounds and methods for the targeted degradation of Enhancer of Zeste Homolog 2 Polypeptides" US 20180177750 date 6/28/2018
  - 115. "Tetrahydronaphthalene and tetrahydroisoquinoline derivatives as estrogen receptor degraders" US 20180155322 date 6/7/2018
  - 116. "Tank-Binding Kinase-1 PROTACs and associated methods of use" US 20180147202 date 5/31/2018
  - 117. "Compounds and methods for the targeted degradation of androgen receptor" US 20180099940 date 4/12/2018
  - 118. "Indole derivatives as estrogen receptor degraders" US 20180072711 date 3/15/2018
  - 119. "Compounds and methods for the targeted degradation of androgen receptor" US 20170327469 date 11/16/2017
  - 120. "Protein-Protein Interaction Inducing Technology" US 20170281784 date 10/5/2017

121. "Compounds and methods for the targeted degradation of bromodomain-containing proteins" US 20170065719 date 3/9/2017
122. "MDM2-based modulators of proteolysis and associated methods of use" US 20170008904 date 1/12/2017
123. "Compounds and methods for the enhanced degradation of targeted proteins" US 20160272639 date 9/22/2016
124. "Compounds and methods for the targeted degradation of androgen receptor" US 20160214972 date 7/28/2016
125. "Imide-based modulators of proteolysis and associated methods of use" US 20160058872 date 3/3/2016
126. "Estrogen-Related Receptor Alpha based PROTAC compounds and associated methods of use" US 20160045607 date 2/18/2016
127. "Imide-based modulators of proteolysis and associated methods of use" US 20150291562 date 10/15/2015

### **Peer-Reviewed Publications:**

1. S. Gough... **J. Wang**... I. Taylor "Oral estrogen receptor PROTAC® vepdegesterant (ARV-471) is highly efficacious as monotherapy and in combination with CDK4/6 or PI3K/mTOR pathway inhibitors in ER+ breast cancer models" *Clin. Cancer Res.* (submitted).
2. **J. Wang**, A. Ischchenko, W. Zhang, A. Razavi, D. Langley "Free Energy method to calculate protein–protein and protein–ligand binding potencies", *Nature Sci. Rep.* 2022, <https://doi.org/10.1038/s41598-022-05875-8>.
3. J. Cantley...**J. Wang**...R.L.Yauch *Nat Commun.* 2022 Nov 10;13(1):6814. doi: 10.1038/s41467-022-34562-5.
4. B.E. Smith...**J. Wang**...C.M. Crews. "Differential PROTAC substrate specificity dictated by orientation of recruited E3 ligase." *Nat. Commun.* 2019, Jan 10;10(1):131. doi: 10.1038/s41467-018-08027-7.
5. J. Salaami... **J. Wang**...C.M. Crews. "Androgen receptor degradation by the proteolysis-targeting chimera ARCC-4 outperforms enzalutamide in cellular models of prostate cancer drug resistance." *Commun Biol.* 2018 Aug 2;1:100. doi: 10.1038/s42003-018-0105-8.
6. D.P. Bondeson... **J. Wang**...C.M. Crews. "Lessons in PROTAC design from selective degradation with a promiscuous warhead." *Cell Chem Biol.* 2018 Jan 18;25(1):78-87.e5. doi: 10.1016/j.chembiol.2017.09.010.
7. G.M. Burslem... **J. Wang**...C.M. Crews. "The advantages of targeted protein degradation over inhibition: an RTK case study." *Cell Chem Biol.* 2018 Jan 18;25(1):67-77.e3. doi: 10.1016/j.chembiol.2017.09.009.
8. A.P. Crew... **J. Wang**...C.M. Crews. "Identification and characterization of Von Hippel-Lindau-Recruiting Proteolysis Targeting Chimeras (PROTACs) of TANK-Binding Kinase 1." *J Med Chem.* 2018 Jan 25;61(2):583-598. doi: 10.1021/acs.jmedchem.7b00635.
9. K. Raina...**J. Wang** et al. "PROTAC-induced BET protein degradation as a therapy for castration-resistant prostate cancer." *Proc Natl Acad Sci U S A.* 2016 Jun 28;113(26):7124-9. doi: 10.1073/pnas.1521738113.
10. J. Lu... **J. Wang**...C.M. Crews. "Hijacking the E3 ubiquitin ligase cereblon to efficiently target BRD4." *Chem Biol.* 2015 Jun 18;22(6):755-63. doi: 10.1016/j.chembiol.2015.05.009.
11. K.R. Hornberger...**J. Wang** et al. "Discovery of 7-aminofuro[2,3-c]pyridine inhibitors of TAK1: optimization of kinase selectivity and pharmacokinetics." *Bioorg Med Chem Lett.* 2013 Aug 15;23(16):4511-6. doi: 10.1016/j.bmcl.2013.06.054.
12. K.R. Hornberger...**J. Wang** et al. "Discovery and optimization of 7-aminofuro[2,3-c]pyridine inhibitors of TAK1." *Bioorg Med Chem Lett.* 2013 Aug 15;23(16):4517-22. doi: 10.1016/j.bmcl.2013.06.053.
13. A.G. Steinig, A.H. Li, **J. Wang** et al. "Novel 6-aminofuro[3,2-c]pyridines as potent, orally efficacious inhibitors of cMET and RON kinases." *Bioorg. Med. Chem. Lett.* 2013, **23**, 4381-4387.
14. M. Jin, **J. Wang** et al. "Discovery of potent, selective and orally bioavailable imidazo[1,5-a]pyrazine derived ACK1 inhibitors." *Bioorg. Med. Chem. Lett.* 2013, **23**, 979-984.
15. M. Jin, **J. Wang**, E. Buck, M.J. Mulvihill. "Small-molecule ATP-competitive dual IGF-1R and insulin receptor inhibitors: structural insights, chemical diversity and molecular evolution." *Future Med. Chem.* 2012, **4**, 315-328.
16. A.P. Crew, S.V. Bhagwat...**J. Wang** et al. "Imidazo[1,5-a]pyrazines: orally efficacious inhibitors of mTORC1 and mTORC2." *Bioorg. Med. Chem. Lett.* 2011, **21**, 2092-2097.
17. **J. Wang**, S. Steinbacher, M. Augustin, P. Schreiner, D. Epstein, M.J. Mulvihill, A.P. Crew "The crystal structure of a constitutively active mutant RON kinase suggests an intramolecular autophosphorylation hypothesis." *Biochemistry* 2010, **49**, 7972-7974.
18. **J. Wang**, S. Chan, K. Ramnarayan. "Structure-based prediction of free energy changes of binding of PTP1B inhibitors." *Journal of Computer-Aided Molecular Design* 2003, **17**, 495-513.
19. S. Chowdhury, J. Sivaraman, **J. Wang**, G. Devanathan, P. Lachance, H. Qi, R. Menard, J. Lefebvre, Y. Konishi, M. Cygler, T. Sulea, E. Purisima. "Design of non-covalent inhibitors of human cathepsin L. From the 96-residue proregion to optimized tripeptides." *Journal of Medicinal Chemistry* 2002, **45**, 5321-5329.

20. P. Carter, ... **J. Wang**, ... C. Decicco. "Photochemically enhanced binding of small molecules to the tumor necrosis factor receptor-1 inhibits the binding of TNF- $\alpha$ ." *Proceedings of the National Academy of Sciences of USA* 2001, **98**, 11879-11884.
21. **J. Wang** and K. Ramnarayan. "Toward designing drug-like libraries: a novel computational approach for prediction of drug feasibility of compounds." *Journal of Combinatorial Chemistry* 1999, **1**, 524-533.
22. K. Ramnarayan, D. Rideout, **J. Wang**, H. Zhu, E. Maggio. "Unification of bioinformatics, combinatorial chemistry and chemoinformatics with a structure based approach." CICSJ Bulletin (Chemical Information and Computer Sciences of Japan) 1998, **16(4)**, 12-17.
23. Y. Cheng, J. Slon-Usakiewicz, **J. Wang**, E. Purisima, Y. Konishi. "Thermodynamic investigation of enzyme and inhibitor interactions with high affinity." In "Techniques in Protein Chemistry VIII" 1997, 513-521.
24. C. Illy, O. Quraishi, **J. Wang**, E. Purisima, T. Vernet, J. Mort. "Role of the Occluding loop in cathepsin B activity." *Journal of Biological Chemistry* 1997, **272**, 1197-1202.
25. Y. Cheng, J. Slon-Usakiewicz, **J. Wang**, E. Purisima, Y. Konishi. "Nonpolar interactions of thrombin and its inhibitors at the fibrinogen recognition exosite: thermodynamic analysis." *Biochemistry* 1996, **35**, 13021-13029.
26. **J. Wang** and E. Purisima. "Analysis of thermodynamic determinants in helix propensities of nonpolar amino acids through a novel free energy calculation." *Journal of the American Chemical Society* 1996, **118**, 995-1001.
27. Y. Tsuda, Z. Szewczuk, **J. Wang**, S. Yue, E. Purisima, Y. Konishi. "Interactions of hirudin-based inhibitor with thrombin: critical role of the Ile<sup>H59</sup> side chain of the inhibitor." *Biochemistry* 1995, **34**, 8708-8714.
28. K.A. Williams, M. Glibowicka, Z. Li, H. Li, A.R. Khan, Y. Chen, **J. Wang**, D.A. Marvin, C.M. Deber. "Packing of coat protein amphipathic and transmembrane helices in filamentous bacteriophage M13: role of small residues in protein oligomerization." *Journal of Molecular Biology* 1995, **252**, 6-14.
29. **J. Wang**, Z. Szewczuk, S. Yue, Y. Tsuda, Y. Konishi, E. Purisima. "Calculation of relative binding free energies and configurational entropies: a structural and thermodynamic analysis of the nature of non-polar binding of thrombin inhibitors based on hirudin<sup>55-65</sup>." *Journal of Molecular Biology* 1995, **253**, 473-492.
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