Harry F. Ridgway, PhD | 575-654-2813 |ridgway@vtc.net | LinkedIn

Quick Profile Snapshot:

- PhD scientist, >10 years computational drug discovery/design (CADD) expertise
- Cross-disciplinary: CADD, materials science, environmental/industrial microbiology
- >100 publications/presentations: **15 new publications since 2022**
- Seasoned reliable professional, solid work ethos, passionate about my research
- Independent work style | communicative | collaborative and team-oriented
- Stakeholder engagement, CRO partnering/negotiations; team building, project management

Research Areas:

- **Drug Discovery and Design:** 10+ years CADD experience in industry/academia. Structure-based (SBDD) and ligand-based small-molecule design across a range of disease targets: adrenergic and opioid GPCRs, antiviral targets, biotoxins, RAS targets, transcription/regulatory factors
- **Materials Modeling:** Fully atomistic modeling of functional nanoporous polymers for drug delivery and water and gas separations | analytical thin-film (membrane) characterization
- **Reaction Modeling:** Coded specialized non-equilibrium QM/MM algorithms for modeling the reaction of small organics with halogen species in an aqueous background

Scientific/Technical Expertise *(100% hands on):*

- molecular dynamics (MD), VLS, QM/MM reaction modeling, some ML & QSAR modeling experience, QM calculations, bioinformatics, cheminformatics, focused and large library development, ligand ADMET profiling, polymer modeling, Tcl/tk and Python coding

Software I Use Routinely: Molsoft's ICMpro for cheminformatics of vast chemical space and VLS | Yasara Structure for GPU-accelerated VLS and fast MD algorithms | Numerous open-source codes

Recent Achievements:

- Discovery/modeling of next-generation angiotensin receptor blockers (ARBs)
- Coded novel MD algorithms for simulating small-molecule oxidation via free radicals
- Drug tunneling and docking to cryptic pockets in human furin via *neq*MD
- Designed a new first-in-class MAO-B antagonist for Parkinson's Disease (unpublished)
- Design/MD simulation of experimental charge-mosaic membranes

Professional Experience:

- **Current:** Founder & CSO, *THERAmolecular,* LLC, New Mexico, USA
- **Current:** Adjunct Professor, ISILC, Victoria University, Melbourne, AU
- **Current:** Ongoing collaborations with international academic/industry partners
- **Current:** Associate Real Estate Broker, CENTURY-21, Silver City, NM
- **Former:** Director Biotechnology Research, major CA water agency

Educational Background:

- 1971-**BSc,** Microbiology/Chemistry (minor), Academic Distinction, SDSU, San Diego, CA
- 1976-**PhD:** Microbiology/Biochemistry | Scripps Institute, UCSD, La Jolla, CA
- 1976-1981-**Postdoctoral Fellowships** (5 years): UCSD and UCI, CA

Distinguished Awards: Athalie Richardson Irvine Clarke Prize

Favorite Activities: mountain/gravel biking, cross-country running, photography

Recent Publications *(2017 to present):*

2026--GPCRs Share an Allosteric Regulatory Site Located Within the Extracellular Agonist-Binding Pocket: Cross-Binding of GPCR Ligands Can Knockout or Revitalize Receptors and Affect Tolerance and Addiction; Cells, pre-print (not peer-reviewed)

2025--Docking simulations of G-protein coupled receptors uncover crossover binding patterns of diverse ligands to angiotensin, alpha-adrenergic and opioid receptors: Implications for cardiovascular disease and addiction; Biomolecules

2025--Gating Mechanism for Biased Agonism at Angiotensin II Type 1 Receptors; https://doi.org/10.3390/molecules30112399

2024--Bisartans: Pursuing Next Generation Pan-Antiviral Therapeutics Targeting SARS-CoV-2, Influenza and RSV Viruses; Viruses 2024, 16(11), 1776; https://doi.org/10.3390/v16111776

2024--Novel benzimidazole angiotensin receptor blockers with anti-SARS-CoV-2 activity equipotent to that of nirmatrelvir: computational and enzymatic studies - *Expert Opinion on Therapeutic Targets*; https://doi.org/10.1080/14728222.2024.2362675

2024--Structural Features Influencing the Bioactive Conformation of Angiotensin II and Angiotensin A: Relationship between Receptor Desensitization, Addiction, and the Blood–Brain Barrier; International J. Molecular Sciences.

2023-- W254 in furin functions as a molecular gate promoting anti-viral drug binding: Elucidation of putative drug runneling and docking ny non-equilibrium molecular dynamics - Comput. Struc. Biotechnol. J.; https://doi.org/10.1016/j.csbj.2023.09.003

2023--Network-based prediction of side effects of repurposed anti-hypertensive Sartans against COVID-19 via proteome and drug-target interactomes; Proteomes 2023 Jun 8;11(2):21. doi:10.3390/proteomes11020021

2023- Computational and Enzymatic Studies of Sartans in SARS-CoV-2 Spike RBD-ACE2 Binding: The Role of Tetrazole and Perspectives as Antihypertensive and COVID-19 Therapeutics. Int. J. Mol. Sci. 24(9):8454. doi: 10.3390/ijms24098454

2023--Molecular Epidemiology of SARS-CoV-2: The Dominant Role of Arginine in Mutations and Infectivity – Viruses 15(2):309. doi: 10.3390/v15020309

2022--Actions of Novel Angiotensin Receptor Blocking Drugs, Bisartans, Relevant for COVID-19 Therapy: Biased Agonism at Angiotensin Receptors and the beneficial effects of Neprilysin in the Renin Angiotensin System – Molecules 27(15):4854. doi: 10.3390/molecules27154854

2022--Conference Talk: Synthesis and in-silico modeling of novel bisphenyltetrazole drugs for inactivation of rattlesnake venom components: *"Biology of the PitVipers4 Conference", 13-16 July 2022*

2022--Discovery of a new generation of angiotensin receptor blocking drugs: Receptor mechanisms and in silico binding to enzymes relevant to SARS-CoV-2 – Comput. Struct. Biotechnol. J. 20:2091-2111. doi: 10.1016/j.csbj.2022.04.010

2022--Understanding the Driving Forces That Trigger Mutations in SARS-CoV-2: Mutational Energetics and the Role of Arginine Blockers in COVID-19 Therapy – Viruses 14(5): 1029. doi:10.3390/v14051029

2022--The Human Myelin Proteome and Sub-Metalloproteome Interaction Map: Relevance to Myelin-Related Neurological Diseases – Brain Sci. 12(4):434. doi: 10.3390/brainsci12040434

2022--Diminazene Aceturate Reduces Angiotensin II Constriction and Interacts with the Spike Protein of Severe Acute Respiratory Syndrome Coronavirus 2 – Biomedicines 10(7):1731. doi:10.3390/biomedicines10071731

2019--Transformation of endocrine disrupting chemicals, pharmaceutical and personal care products during drinking water disinfection – Sci. Total Environ. 20;657:1480-1490. doi:10.1016/j.scitotenv

2018--Molecular dynamics simulation of gas-phase ozone reactions with sabinene and benzene – J. Molec. Graphics and Modelling 74,241-250. doi.org/10.1016/j.jmgm.2017.04.020

2018--Chlorination of oxybenzone and prediction of transformation products using non-equilibrium “forced” molecular dynamics – Desal. Water Treat. 114:31-50. doi: 10.5004/dwt.2018.22435

2017--Molecular simulations of polyamide membrane materials used in desalination and water reuse applications: Recent developments and future prospects – J. Membr. Sci. 524; 436-448. doi.org/10.1016/j.memsci.2016.11.061