Harry F. Ridgway, PhD

Founder & Chief Scientific Officer, THERAmolecular, LLC · Independent Computational Chemistry Consultant
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PROFESSIONAL SUMMARY

Senior computational chemist and drug-design scientist with 10+ years of hands-on CADD experience spanning industry, academia, and independent consulting. Specializes in structure- and ligand-based design for GPCRs (angiotensin, adrenergic, opioid), antiviral targets (furin, SARS-CoV-2), and RAAS pathway modulators. Known for mechanistic insight—molecular gates, cryptic pockets, non-equilibrium MD, biased agonism—and for delivering actionable designs, custom algorithms, and clear scientific communication. Founder of THERAmolecular, LLC; adjunct academic appointment; extensive publication record and cross-disciplinary background in materials modeling and biotech research management. Seeks high-value consulting, contract, and collaborative engagements that leverage deep expertise to accelerate client discovery programs.

CORE CONSULTING COMPETENCIES & SERVICE AREAS

Drug Discovery & Design
- Structure-based & ligand-based CADD
- GPCR modeling (AT1R, adrenergic, opioid)
- Antiviral targets (furin, spike, viral proteases)
- Virtual screening (focused & ultra-large libraries)
- ADMET profiling & cheminformatics pipelines
- Lead optimization & multi-target design

Advanced Simulation & Methods
- GPU-accelerated molecular dynamics (MD)
- Non-equilibrium / forced MD & drug tunneling
- Cryptic pocket detection & docking
- QM/MM reaction modeling & free-radical chemistry
- Custom algorithm & workflow development (Python/Tcl)
- Materials & membrane atomistic modeling

SELECTED ACHIEVEMENTS RELEVANT TO CLIENT WORK

- **Next-generation ARBs / Bisartans** — Discovery and computational modeling of novel angiotensin receptor blockers with dual antiviral potential; multiple peer-reviewed publications supporting mechanism and therapeutic rationale.
- **Furin molecular gate & drug tunneling** — Elucidated W254 as a molecular gate; demonstrated anti-viral drug binding pathways using non-equilibrium MD; published in Computational and Structural Biotechnology Journal.
- **GPCR allosteric / cross-binding insights** — Identified shared allosteric regulatory site within extracellular agonist-binding pockets; implications for receptor crosstalk, tolerance, and addiction (2025–2026 publications).
- **First-in-class MAO-B antagonist design** — Designed novel Parkinson's disease candidate (unpublished); demonstrates ability to generate proprietary IP-ready designs.
- **Custom MD algorithms** — Coded novel methods for simulating free-radical oxidation of small molecules; extends capability beyond off-the-shelf packages for specialized client problems.
- **Charge-mosaic membranes** — Design and MD simulation of experimental membranes for separations / delivery applications.

PROFESSIONAL EXPERIENCE

Founder & Chief Scientific Officer
THERAmolecular, LLC · New Mexico, USA · Current
Independent consulting and R&D; practice focused on computational drug design, molecular simulation, and cheminformatics. Delivers project-based CADD services, mechanistic studies, custom method development, and scientific advisory support to academic and industry partners. Manages client relationships, scoping, delivery, and IP considerations.

Adjunct Professor
ISILC, Victoria University · Melbourne, Australia · Current
Academic affiliation supporting collaborative research and knowledge exchange in computational and structural biology.

Ongoing International Academic & Industry Collaborations
Multiple partners · Current
Active multi-institutional collaborations producing peer-reviewed publications in GPCR pharmacology, antiviral design, and related areas. Demonstrates ability to integrate into distributed teams and deliver high-quality joint science.

Associate Real Estate Broker
CENTURY 21 · Silver City, NM · Current (part-time)
Client-facing professional practice requiring negotiation, relationship management, and clear communication—skills directly transferable to consulting engagements.

Director, Biotechnology Research
Major California Water Agency · 1981–2002
Led biotech research programs; extensive experience in team building, project management, stakeholder engagement, CRO partnering, negotiations, and grantsmanship. Built foundation in applied microbiology, environmental systems, and technology translation.

EDUCATION & DISTINGUISHED AWARDS

PhD, Microbiology / Biochemistry — Scripps Institution of Oceanography / UC San Diego, La Jolla, CA (1976)
BSc, Microbiology / Chemistry (Academic Distinction) — San Diego State University, San Diego, CA (1971)
Two postdoctoral fellowships (5 years total) — UC San Diego and UC Irvine

Athalie Richardson Irvine Clarke Prize — Distinguished award recognizing scientific achievement

TECHNICAL TOOLKIT (HANDS-ON)

Simulation & Modeling: Molecular dynamics (GPU-accelerated), non-equilibrium MD, VLS, docking, QM/MM, QSAR, free-energy approaches, cryptic-pocket methods. **Platforms:** Yasara Structure, Molsoft ICMpro, GROMACS-compatible workflows, open-source servers (ProteinsPlus, PASSer, CryptoSite/CryptoBank, and others). **Cheminformatics & Data:** Large-library handling, ADMET profiling, focused library design, structure similarity & clustering. **Programming:** Python, Tcl/Tk — custom algorithms, pipeline automation, analysis scripts. **AI-augmented workflows:** Routine use of advanced AI models (including Grok) for calculation support, hypothesis generation, and literature synthesis.

SELECTED RECENT PUBLICATIONS (CLIENT-RELEVANT HIGHLIGHTS)

Full list available on request or via ORCID/Google Scholar. Emphasis below on GPCR, antiviral, ARB, and method papers most relevant to prospective consulting clients.

2026 — Sartans and Bisartans: Expanding Therapeutic Horizons Through Broad Receptor Interactions and Repurposing Potential. *Int. J. Mol. Sci.* 27, 8883.

2026 — The Crucial Role of Arginine Residues and the Arginine–Tetrazole Paradigm in Viral Infection: Therapeutic Opportunities for Tetrazole-Containing Angiotensin Receptor Blockers and Bisartans. *Pathogens* 15, 1134.

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).

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. *Molecules* 30(11), 2399.

2024 — Bisartans: Pursuing Next Generation Pan-Antiviral Therapeutics Targeting SARS-CoV-2, Influenza and RSV Viruses. *Viruses* 16(11), 1776.

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*.

2024 — Structural Features Influencing the Bioactive Conformation of Angiotensin II and Angiotensin A: Relationship between Receptor Desensitization, Addiction, and the Blood-Brain Barrier. *Int. J. Mol. Sci.*

2023 — W254 in furin functions as a molecular gate promoting anti-viral drug binding: Elucidation of putative drug tunneling and docking by non-equilibrium molecular dynamics. *Comput. Struct. Biotechnol. J.*

2023 — Network-based prediction of side effects of repurposed anti-hypertensive Sartans against COVID-19 via proteome and drug-target interactomes. *Proteomes* 11(2), 21.

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.

2023 — Molecular Epidemiology of SARS-CoV-2: The Dominant Role of Arginine in Mutations and Infectivity. *Viruses* 15(2), 309.

2022 — Actions of Novel Angiotensin Receptor Blocking Drugs, Bisartans, Relevant for COVID-19 Therapy: Biased Agonism at Angiotensin Receptors... *Molecules* 27(15), 4854.

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.

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.

2018–2017 — Selected materials / environmental papers: MD of membrane polymers for desalination & water reuse (*J. Membr. Sci.*); non-equilibrium MD for transformation-product prediction; gas-phase ozone reaction simulations.

Engagement models: Project-based CADD campaigns · Mechanistic / MD deep-dives · Retainer advisory support · Custom method & pipeline development · Expert reports for IP, due diligence, or grant applications · Training / knowledge transfer. Remote-first; flexible scoping. Contact to discuss how these capabilities can advance your discovery or development goals.