RICHARD **VAN**

Ph.D. Candidate in Computational Biochemistry | University of Oklahoma

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Education

Present	**Ph.D., Biochemistry**, University of Oklahoma, Norman, OK.
	Advisor : Dr. Yihan Shao
2019	**B.S., Chemistry**, University of Oklahoma, Norman, OK.

Research Experience (with Various Collaborators)

Dr. R. Rajan (OU)
Dr. J. Liu (UNT)

Machine learning assisted free energy simulations of CRISPR-Cas9 (2021 - Present)

- Improved the semi-empirical method (PM3) through reparameterization (PM3*) for Mg^{2+} systems.
- Implemented deep learning networks to investigate the free energy profile of Cas9 ntDNA cleavage, which can predict energy (forces) at *ab initio* QM level within 1 kcal/mol (1 kcal/mol/Å).
- Extending approach to investigate other RuvC domain containing enzymes (Cas12a, Ippo1).

Force Matching | DeePMD-kit | Adaptive String Method | Umbrella Sampling

Dr. L. McNally (OUHSC)

Rational design of low-pH insertion peptides (pHLIP) (2020 - Present)

- Delineated pH-dependent residue-membrane interactions through simulations of insertion dynamics.
- Acquired qualitative inference of thermodynamic properties in peptide insertion mechanism.
- Developed computational protocols to aid in the design of pH specific peptides.

Membrane Simulations | CpHMD | PROPKA | Thermodynamic Integration

Dr. S. Liang (Emory U.)

Positron emission tomography (PET) tracers (2019 - Present)

- Ranked and prioritized compounds for synthesis targetting the endocannabinoid system.
- Determined thermodynamic properties for lead compounds through biomolecular simulations.

Virtual Screening | Homology Modelling | MMPBSA/MMGBSA

Dr. C. Ran (HMS)

Chemiluminescent probes (2019 - 2020)

- Assisted in identifying π-conjugated compounds for proteins implicated in Alzheimer's disease.

Molecular Docking

Dr. I. Sharma (OU)
Dr. J. Lin (OUHSC)

Drug discovery for Bax/Bak inhibition (2018 - 2020)

- Identified lead candidates from large compound libraries and suggested a novel pocket to target.
- Assisted in the synthesis and structure-based modification to improve ligand-receptor interactions.
- Performed biochemical assays to quantify the inhibitory effects of the lead candidate.

Ensemble Docking | Structure Based Drug Discovery | Transition Metal Catalyzed Reactions | Liposome Dye Release Assay

Skills

Technical	Molecular dynamics study of small molecules, proteins, membranes, and DNA/RNA **(AMBER)**.
	Absolute binding free energy calculations for small molecules/proteins **(MMPBSA/MMGBSA)**.
	Free energy simulations of enzymatic reactions **(AMBER, Q-Chem, QMhub)**.
	Machine learning for biological systems **(PyTorch)**.
	Prediction of pKa **(CpHMD, PROPKA)**.
	Molecular Docking and virtual sceening **(AutoDock Vina)**.
	Sequence and structural analysis **(BLAST, Pfam, MUSCLE, HH suite, AlphaFold)**.
Programming/OS	Python, Bash; MacOS, Linux.
Misc.	LaTeX, Git, Blender, Adobe (Photoshop, Premiere).

Publications

15. **Van, Richard**, Pan, X., Liu, J., Rajan, R. & Shao, Y. Free energy profiles of cas9-catalyzed DNA cleavages within HNH and RuvC domains. *Manuscript in Preparation.*
14. Yao, S., **Van, Richard**, Pan, X., Park, J. H., Ma, Y., Mei, Y. & Shao, Y. Machine learning based implicit solvent model for aqueous-solution alanine dipeptide molecular dynamics simulations. *Manuscript in Preparation.*
13. Cheng, R., Fujinaga, M., Yang, J., Rong, J., Haider, A., Ogasawara, D., **Van, Richard S.**, Shao, T., Chen, Z., Zhang, X., Leon, E. R. C., Zhang, Y., Mori, W., Kumata, K., Yamasaki, T., Xie, L., Sun, S., Wang, L., Ran, C., Shao, Y., Cravatt, B., Josephson, L., Zhang, M.-R. & Liang, S. H. A novel monoacylglycerol lipase-targeted 18F-labeled probe for positron emission tomography imaging of brown adipose tissue in the energy network. *Acta Pharmacologica Sinica* **0,** 1-9 (2022).
12. Pan, X., **Van, Richard**, Epifanovsky, E., Liu, J., Pu, J., Nam, K. & Shao, Y. Accelerating ab initio QM/MM molecular dynamics simulations with multiple time step integration and a recalibrated semi-empirical QM/MM hamiltonian. *Journal of Physical Chemistry B* **126,** 4226-4235 (2022).
11. Zhu, B., Yang, J., **Van, Richard**, Yang, F., Yu, Y., Yu, A., Ran, K., Yin, K., Liang, Y., Shen, X., Yin, W., Choi, S. H., Lu, Y., Wang, C., Shao, Y., Shi, L., Tanzi, R. E., Zhang, C., Cheng, Y., Zhang, Z. & Ran, C. Epitope alteration by small molecules and applications in drug discovery. *Chemical Science* **13,** 8104-8116 (2022).
10. Chen, Z., Mori, W., Rong, J., Schafroth, M. A., Shao, T., **Van, Richard S.**, Ogasawara, D., Yamasaki, T., Hiraishi, A., Hatori, A., Chen, J., Zhang, Y., Hu, K., Fujinaga, M., Sun, J., Yu, Q., Collier, T. L., Shao, Y., Cravatt, B. F., Josephson, L., Zhang, M.-R. & Liang, S. H. Development of a highly-specific 18F-labeled irreversible positron emission tomography tracer for monoacylglycerol lipase mapping. *Acta Pharmaceutica Sinica B* **11,** 1686-1695 (2021).
9. Deng, X., Salgado-Polo, F., Shao, T., Xiao, Z., **Van, Richard**, Chen, J., Rong, J., Haider, A., Shao, Y., Josephson, L., Perrakis, A. & Liang, S. H. Imaging autotaxin in vivo with 18F-labeled positron emission tomography ligands. *Journal of Medicinal Chemistry* **64,** 15053-15068 (2021).
8. Haider, A., Xiao, Z., Xia, X., Chen, J., **Van, Richard S.**, Kuang, S., Zhao, C., Rong, J., Shao, T., Ramesh, P., Aravind, A., Shao, Y., Ran, C., Young, L. J. & Liang, S. H. Development of a triazolobenzodiazepine-based PET probe for subtype-selective vasopressin 1A receptor imaging. *Pharmacological Research* **173,** 105886 (2021).
7. Pan, X., Yang, J., **Van, Richard**, Epifanovsky, E., Ho, J., Huang, J., Pu, J., Mei, Y., Nam, K. & Shao, Y. Machine-learning-assisted free energy simulation of solution-phase and enzyme reactions. *Journal of Chemical Theory and Computation* **17,** 5745-5758 (2021).
6. Rong, J., Mori, W., Xia, X., Schafroth, M. A., Zhao, C., **Van, Richard S.**, Yamasaki, T., Chen, J., Xiao, Z., Haider, A., Ogasawara, D., Hiraishi, A., Shao, T., Zhang, Y., Chen, Z., Pang, F., Hu, K., Xie, L., Fujinaga, M., Kumata, K., Gou, Y., Fang, Y., Gu, S., Wei, H., Bao, L., Xu, H., Collier, T. L., Shao, Y., Carson, R. E., Cravatt, B. F., Wang, L., Zhang, M.-R. & Liang, S. H. Novel reversible-binding PET ligands for imaging monoacylglycerol lipase based on the piperazinyl azetidine scaffold. *Journal of Medicinal Chemistry* **64,** 14283-14298 (2021).
5. Yamasaki, T., Zhang, X., Kumata, K., Zhang, Y., Deng, X., Fujinaga, M., Chen, Z., Mori, W., Hu, K., Wakizaka, H., Hatori, A., Xie, L., Ogawa, M., Nengaki, N., **Van, Richard**, Shao, Y., Sheffler, D. J., Cosford, N. D. P., Liang, S. H. & Zhang, M.-R. Identification and

development of a new positron emission tomography ligand 4-(2-Fluoro-4-[11C] methoxyphenyl)-5-((1-methyl-1 H-pyrazol-3-yl) methoxy) picolinamide for imaging metabotropic glutamate receptor subtype 2 (mGlu2). *Journal of Medicinal Chemistry* **63,** 11469-11483 (2020).

4. Yang, J., Yin, W., **Van, Richard**, Yin, K., Wang, P., Zheng, C., Zhu, B., Ran, K., Zhang, C., Kumar, M., Shao, Y. & Chongzhao, R. Turn-on chemiluminescence probes and dual-amplification of signal for detection of amyloid beta species in vivo. *Nature Communications* **11,** 1-14 (2020).
3. Zhang, X., Zhang, Y., Chen, Z., Shao, T., **Van, Richard**, Kumata, K., Deng, X., Fu, H., Yamasaki, T., Rong, J., Hu, K., Hatori, A., Xie, L., Yu, Q., Ye, W., Xu, H., Sheffler, D. J., Cosford, N. D. P., Shao, Y., Tang, P., Wang, L., Zhang, M.-R. & Liang, S. H. Synthesis and preliminary evaluation of 4-hydroxy-6-(3-[11C] methoxyphenethyl) pyridazin-3 (2H)-one, a 11C-labeled D-amino acid oxidase (DAAO) inhibitor for PET imaging. *Bioorganic & Medicinal Chemistry Letters* **30,** 127326 (2020).
2. Zhang, X., Zhang, Y., Chen, Z., Shao, T., **Van, Richard**, Kumata, K., Deng, X., Fu, H., Yamasaki, T., Rong, J., Hu, K., Hatori, A., Xie, L., Yu, Q., Ye, W., Xu, H., Sheffler, D. J., Cosford, N. D. P., Shao, Y., Tang, P., Wang, L., Zhang, M.-R. & Liang, S. H. Synthesis and preliminary studies of 11C-labeled tetrahydro-1, 7-naphthyridine-2-carboxamides for PET imaging of metabotropic glutamate receptor 2. *Theranostics* **10,** 11178 (2020).
1. Chen, Z., Mori, W., Fu, H., Schafroth, M. A., Hatori, A., Shao, T., Zhang, G., **Van, Richard S.**, Zhang, Y., Hu, K., Fujinaga, M., Wang, L., Belov, V., Ogasawara, D., Giffenig, P., Deng, X., Rong, J., Yu, Q., Zhang, X., Papisov, M. I., Shao, Y., Collier, T. L., Ma, J.-A., Cravatt, B. F., Josephson, L., Zhang, M.-R. & Liang, S. H. Design, synthesis, and evaluation of 18F-labeled monoacylglycerol lipase inhibitors as novel positron emission tomography probes. *Journal of Medicinal Chemistry* **62,** 8866-8872 (2019).

Oral Presentations

Poster **Richard Van**, Xiaoliang Pan, Caleb Chang, Yang Ga, and Yihan Shao.
"Catalytic Mechanism of HNH-like Domain of I-PpoI"
Oklahoma COBRE 10th Annual Symposium in Structural Biology (2022).

Poster **Richard Van**, Xiaoliang Pan, Alex Frickenstein, Lacey McNally, and Yihan Shao
"Towards a Rational Design of pHLIP via Constant pH Molecular Dynamics and Free Energy Simulation"
Pacifichem (2021).

Poster **Richard Van**, Xiaoliang Pan, Alex Frickenstein, Lacey McNally, and Yihan Shao
"Towards a Rational Design of pHLIP via Constant pH Molecular Dynamics and Free Energy Simulation"
EMBO Bioexcel Summer School on Biomolecular Simulations (2021).

Poster **Richard Van**, Nicholas Massaro, Xiaoliang Pan, Indrajeet Sharma, Jialing Li, and Yihan Shao.
"Drug Design : Small Molecule Inhibitor for Pro-Apoptotic BAX Proteins."
APS/ICTP-SAIFR Forum on Biological Physics : from Molecular to Macroscopic Scale (2020).

Poster **Richard Van**, Nicholas Massaro, Xiaoliang Pan, Indrajeet Sharma, Jialing Li, and Yihan Shao.
"Drug Design : Small Molecule Inhibitor for Pro-Apoptotic BAX Proteins."
7th Annual Symposium on Structural Biology (2019).

Poster **Richard Van**, Nicholas Massaro, Xiaoliang Pan, Indrajeet Sharma, Jialing Li, and Yihan Shao.
"Drug Design : Small Molecule Inhibitor for Pro-Apoptotic BAX Proteins"
4th Annual Pentasection Meeting of the Oklahoma Section of the American Chemical Society (2019).

Teaching

2021 Physical Chemistry I Lab
Instructor of record guiding 3-hour labs in the theory and application of fundamental physical chemistry.

2019 - 2020 **Provost's Certificate of Distinction in Teaching**
Awarded to the top 10% of graduate assistants across campus based on student evaluations.

2019 - 2020 General Chemistry II Lab and Recitation
Teaching assistant leading 1-hour discussions on foundations of chemical theory and 3-hour labs.

Membership and Outreach

2021 - Present	*Society of Chemical and Biochemical Researchers*, University of Oklahoma
	First Year Liason (2021-2022)
2021 - Present	*American Chemical Society*
2017 - Present	*Integrity Council*, University of Oklahoma
	Vice Chair of Membership (2019 - 2020), Vice Chair of Public Outreach (2018 - 2019), Secretary (2017 - 2018)