Title	DOI	Notes
Best-Practice DFT Protocols for Basic Molecular Computational Chemistry	https://doi.org/10.1002/anie.202205735	Perspective on best-practice protocols and guidance in the choice of robust quantum-chemical methods to model experiments as close a possible
A binding mode hypothesis for prothioconazole binding to CYP51 derived from first principles quantum chemistry	https://doi.org/10.1007/s10822-020-00331-z	Binding Mode Hypotheises for Prothioconazole
Flupyradifurone: a brief profile of a new butenolide insecticide	https://doi.org/10.1002/ps.3932	Discovery of Butenolides
Bayer's in silico ADMET platform: a journey of machine learning over the past two decades	https://doi.org/10.1016/j.drudis.2020.07.001	Overview of the Machine Learning Model Platform at Bayer Pharma with details on data curation, descriptors, and alorigthms.
MELLODDY: Cross-pharma Federated Learning at Unprecedented Scale Unlocks Benefits in QSAR without Compromising Proprietary Information	https://doi.org/10.1021/acs.jcim.3c00799	Main outcome of the IMI MELLODDY collaboration on Machine Learning across mutliple partners
MELLODDY GitHub Repository	https://github.com/melloddy	Open-source ML tool developed within the MELLODDY collaboration
Site of Metabolism Prediction Based on ab initio Derived Atom Representations	https://doi.org/10.1002/cmdc.201700097	Example of model improvements from QM-informed descriptors
!AIQU Announcement	https://www.linkedin.com/posts/tobias-morawietz_machinelearning-neuralnetworks-artificialintelligence-activity-6891744599526703104-t19W?utm_source=share&utm_medium=member_android	Public announcement of the !AIQU collaboration on combining QM and AI for accelerated molecular design
Machine learning-accelerated quantum mechanics-based atomistic simulations for industrial applications	https://doi.org/10.1007/s10822-020-00346-6	Overview of ML-accelerated QM simulations applied to industrial applications
An implementation of artificial neural-network potentials for atomistic materials simulations: Performance for TiO2	https://doi.org/10.1016/j.commatsci.2015.11.047	Open-source code for training Machine Learning models for atomistic simulations
ænet-PyTorch: A GPU-supported implementation for machine learning atomic potentials training	https://doi.org/10.1063/5.0146803	Extented code for efficient training on GPUs