

Konferencja Użytkowników Komputerów Dużej Mocy - KUKDM 2024

Friday, 15 March 2024

S7 - Contributed session (12:50 - 14:50)

time	[id] title	presenter
12:50	[35] Ab Initio Molecular Dynamics Simulations of Aqueous LiTFSI Solutions – Structure, Hydrogen Bonding, and IR Spectra	EILMES, Andrzej
13:05	[36] Interaction Spheres for Molecular Interactions – Application in Drug Design	KURCZAB, Rafał
13:20	[37] Dynamic Disulfide Bonds in Molecular Dynamics Simulation	SMARDZ, Pamela
13:35	[38] Application of Fragment Molecular Orbital Method to Investigate G Protein Coupled Receptors	ŚLIWA, Paweł
13:50	[39] Theoretical Description of Peptide Bonds in Selected Systems Based on the ETS-NOCV Method	RÓZGA, Maria
14:05	[40] Analytical Inversion Regional Modeling System for Estimation of National-Scale CO ₂ Fluxes – Results of the CoCO ₂ Project	ZIMNOCH, Mirosław
14:20	[41] Big Data in Proton Beam Monitoring: LGAD Detectors Study	GRZANKA, Leszek
14:35	[42] Pedestrian Crossing Intention Detection within Challenging Road Conditions	MAZUREK, Szymon