



Mendeleev 2019

XI International Conference on Chemistry
for Young Scientists

CONFERENCE PROGRAM

4 session "Computer modeling and cheminformatics"
(lecture hall 116)

ORAL REPORTS

10:00-10:15	<u>Pats K.M., Molnár F.</u> STUDY OF ALLOSTERIC COMMUNICATIONS IN VITAMIN D RECEPTOR BY MOLECULAR DYNAMICS
10:15-10:30	<u>Pavlov S.V., Kislenko S.A.</u> MODELING OF THE EFFECT OF GRAPHENE EDGES ON THE ELECTRON TRANSFER KINETICS
10:30-10:45	<u>Polynski M.V., Ananikov V.P.</u> MODELING (DE)ACTIVATION AND EVOLUTION OF PALLADIUM CATALYTIC SYSTEMS IN COUPLING REACTIONS
10:45-11:00	<u>Ragovja E. G., Matulis V.E.</u> DFT STUDY OF ABSORPTION AND EMISSION SPECTRA OF BODIPY DYES
11:00-11:15	<u>Rakhimbekova A., Nugmanov R.I., Gimadiev T.R., Madzhidov, Varnek A.</u> BENCHMARKING ANALYSIS OF APPLICABILITY DOMAIN DEFINITION: CHEMICAL REACTIONS CASE
11:15-11:30	<u>Shilyaeva E.A., Novakovskaya Yu.V</u> THE STRUCTURE OF GRAPHITE OXIDE AND ROLE OF WATER
15:00-15:15	<u>Smirnov A.N., Odintsova O.V., Solovyeva E.V.</u> THE SMALL CLUSTER MODEL SYSTEMS FOR QUANTUM CHEMICAL SIMULATIONS OF SERS: THE STUDY OF STILBENES ADSORBED ON AG NANOPARTICLES