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[논문]

1. Unveiling Local and Global Conformational Changes and Allosteric Communications in SOD1 Systems using Molecular Dynamics Simulation and Network Analysis. Basitha S, Manavalanb B, Lee G. Comput Biol Med. 2024 Jan;168:107688
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Integration of multiomics for understanding nanotoxicity

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Exposure to nanoparticles leads to their accumulation in the brain, but drug development to counteract this nanotoxicity remains challenging. Here we assessed the effect of silica-coated-magnetic nanoparticles containing the rhodamine B isothiocyanate dye [MNPs@SiO2(RITC)] on microglia through integration of transcriptomics, proteomics, and metabolomics. Intracellular reactive oxygen species production, an inflammatory response, and morphological activation of cells were greater, but glucose uptake was lower in MNPs@SiO2(RITC)-treated BV2 microglia and primary rat microglia. Expression of 121 genes, and levels of 45 proteins and 17 metabolites related to the above phenomena changed in MNPs@SiO2(RITC)-treated microglia. We integrated the three omics datasets and generated a single network using a machine learning algorithm. We screened 19 compounds and predicted their effects on nanotoxicity within the triple-omics network. A combination of glutathione and citrate attenuated nanotoxicity induced by MNPs@SiO2(RITC) and ten other nanoparticles in vitro and in the murine brain, protecting mostly the hippocampus and thalamus.