Mitochondria are essential cell organelles that are responsible for cellular respiration and apoptosis. Several degenerative diseases, including Parkinson’s disease, heart conditions, and cancer, have been attributed to dysfunctional mitochondria. Therefore, many efforts have been focused on the design of optimal mitochondrion-targeting drugs specifically delivered into the mitochondria. Triphenyl phosphonium (TPP) moieties are traditionally used to deliver a wide range of molecular cargo to mitochondria organelle. However, TPP uptake by mitochondria can result in charge accumulation, which will cause depolarization of the mitochondrial membrane. Additionally, this type of vector cannot deliver high molecular weight cargo. It is, therefore, necessary during the design of lipophilic cation as pro-drugs and drug transporters, to investigate the factors that can minimize the therapeutic concentration and improve its delivery ability.