

# 8<sup>TH</sup> CARDIOVASCULAR NURSING & NURSE PRACTITIONERS MEETING

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## Paradigm shift cardiac technology advances

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There are several technological advances that may change the current standards of care for cardiology in the coming years. These new technologies are coming at the same time the U.S. healthcare system is undergoing major reforms and they may contribute to efforts to reduce costs, cut lengths of stay, enable easier delivery of care and reduce complication rates. This technology also might simplify management of patients with chronic cardiac conditions, like atrial fibrillation and heart failure. The newest technologies are also part of a larger trend in healthcare toward minimally invasive and noninvasive diagnostic and therapy options. These will eventually reduce the number of open-heart surgeries, diagnostic catheterizations and enable complex procedures such as heart valve replacement to be conducted as out-patient procedures. This technology update report will discuss advances across the cardiovascular subspecialties of interventional cardiology, electrophysiology, structural heart repair, heart valve repair and replacement, heart failure management and cardiac imaging. FDA cleared technologies entering practice include transcatheter aortic replacement (TAVR); left atrial appendage (LAA) occlusion; implantable cardiac monitors; leadless implantable cardioverter defibrillators (ICDs); and fractional flow reserve computed tomography (FFR-CT) for noninvasive assessment of coronary blockages. There are also several new technologies that may have major impacts on care in the future that are now entering FDA investigation device exemption trials or under current FDA review. These technologies include fully bioresorbable stents; transcatheter delivered leadless pacemakers; transcatheter mitral valves and annuloplasty systems; and implantable early warning monitors for new onset of myocardial infarction in previously treated heart attack patients.

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## Computational simulation of the effect of quantum chemical parameters on the molecular docking of HMG-CoA reductase drugs

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Density functional theory (B3LYP-6-31G(d)) was performed to study the effect of molecular and electronic structures, of 2-cyclopropyl-4-thiophenyl-quinoline mevalonolactones as potential hypocholesterolemic inhibitors, on their biological activities and discuss the correlation between the inhibition efficiency and quantum chemical parameters. Molecular docking was performed to investigate the mode of interactions between the investigated inhibitors and the active sites of the target Hydroxymethylglutaryl-Coenzyme A (HMG-CoA) reductase. The results could suggest further structural modifications to discover more potent and selective HMG-CoA reductase inhibitors. The catalytic active sites of HMGR have a positive electrostatic potential which is complemented with a negative electrostatic potential of the investigated drugs to form a stabilized complex. The presence of lipophobic groups, such as quinoline nucleus, cyclopropyl and substituted thiophenyl groups as well as a lactone moiety, is important for binding to the active sites. A good correlation between the experimental and theoretical data confirms that the quantum chemical methods and molecular docking studies are successful tools for enriching screening experiments aimed at the discovery of novel bioactive compounds.

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