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Nota di contenuto	Frontmatter -- Preface of the Book of Proceedings of the Virtual Conference on Computational Science (VCCS-2019) -- Contents -- Corresponding authors -- 1 Structural and spectroscopic properties of 3-halogenobenzaldehydes: DFT and TDDFT simulations -- 2 Atomistic insight into the significantly enhanced photovoltaic cells of monolayer GaTe2 via two-dimensional van der Waals heterostructures engineering -- 3 Fluorescent styryl chromophores with rigid (pyrazole) donor and rigid (benzothiophenedioxide) acceptor – complete density functional theory (DFT), TDDFT and nonlinear optical study -- 4 Comparative studies of excited state intramolecular proton transfer (ESIPT) and azohydrazone tautomerism in naphthalene-based fluorescent acid azo dyes by computational study -- 5 Theoretical examination of efficiency of anthocyanidins as sensitizers in dye-sensitized solar cells -- 6 Selection of oxypeucedanin as a potential antagonist from molecular docking analysis of HSP90 -- 7 Mechanistic insight into the interactions between thiazolidinedione derivatives and PTP-1B combining 3D QSAR andmolecular docking in the treatment of type 2 diabetes -- 8 Review of research of nanocomposites based on graphene quantum dots -- 9 A computational study of the SNAr reaction of 2-ethoxy-3,5-dinitropyridine and 2-methoxy-3, 5-dinitropyridine with piperidine --

	10 Synthesis, characterization and computational studies of 1,3-bis[(E) -furan-2-yl)methylene]urea and 1,3-bis[(E)-furan-2-yl)methylene] thiourea -- 11 Computational studies of biologically active alkaloids of plant origin: an overview -- 12 Investigating the biological actions of some Schiff bases using density functional theory study -- 13 Molecular mechanics approaches for rational drug design: forcefields and solvation models -- Index
Sommario/riassunto	Computational Chemistry serves as a complement to experimental chemistry where the tools are limited. Using computational programs to solve advanced problems is widely used in the design and analysis of for example new molecules, surfaces, drugs and materials. This book will present novel innovations in the field, with real-life examples of where computational technologies serves as an indispensible tool.