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Nota di contenuto	Preface (Arieh Warshel) -- Acknowledgments -- How should this text be read -- Chapter 1 Introduction (Silvano Coletti, Marcello Allegretti) -- Chapter 2 A European Drug Discovery Platform: From In Silico to Experimental Validation (Gianluca Palermo, Daniela Iaconis, Philip Gribbon) -- Chapter 3 The Drug Repurposing Strategy in the Exscalate4CoV Project: Raloxifene Clinical Trials (Andrea Beccari, Lamberto Dionigi, Emanuele Nicastri, Candida Manelfi, Elizabeth Gavioli) -- Chapter 4 The High-Performance Computing Resources for the Exscalate4CoV Project (Andrew Emerson, Federico Ficarelli, Gianluca Palermo, Freancesco Frigerio) -- Chapter 5 The Impact of the Scientific Metaverse on the Biotech Industry: How Virtual Reality Helped Researchers Fight Back Against COVID-19 (Carmine Talarico, Edgardo Leija) -- Chapter 6 From Genome to Variant Interpretation Through 3D Protein Structures (Janani Durairaj, Leila Tamara Alexander, Gabriel Studer, Gerardo Tauriello, Ingrid Guarnetti Prandi, Rosalba Lepore, Giovanni Chillemi, Torsten Schwede) -- Chapter 7 The Role of Structural Biology Task Force: Validation of the Binding Mode of Repurposed Drugs Against SARS-CoV-2 Protein Targets (Paola Storici, Elisa Costanzi, Stefano Morasso) -- Chapter 8 Drug Discovery and Big Data: From Research to the Community (Luca Barbanotti, Marta Cicchetti, Gaetano Varriale) -- Chapter 9 Exploiting Drug Discovery

Sommario/riassunto	This book highlights the different aspects of the research project "E4C Horizon 2020 European Project" aimed at fighting the coronavirus by combining the best supercomputing resources and artificial intelligence with state-of-the-art experimental facilities up through clinical validation. Coronavirus disease has become an important public issue across the globe since December 2019. There is an urgent need to develop potent anti-COVID-19 agents for the prevention of the outbreak and stop viral infections. To this aim, a public–private consortium composed by European and national infrastructures, center of excellence, universities, and a pharmaceutical company started the E4C Horizon 2020 European Project: Its core idea was to use the EXaSCale smArt pLatform Against paThogEns (EXSCALATE) supercomputing platform for a process known as "drug repurposing", namely to identify the most promising safe in man drugs for immediate treatment of the already infected population and then novel pan-coronavirus inhibitors to address future emergencies. This ambitious goal exploited a "chemical library" of 500 billion molecules, thanks to a processing capacity of more than 3 million molecules per second, made available by the computing power of the EXSCALATE platform.