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| Autore                  | Lee Wen Ho                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
| Titolo                  | Computer simulation of shaped charge problems [[electronic resource] /] / Wen Ho Lee                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
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| Descrizione fisica      | 1 online resource (220 p.)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
| Disciplina              | 623.4/545                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| Soggetti                | Shaped charges - Computer simulation<br>Shaped charges - Mathematical models<br>Flow visualization - Computer simulation<br>Penetration mechanics - Computer simulation<br>Lagrange equations                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
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| Note generali           | Description based upon print version of record.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
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| Nota di contenuto       | Contents; A Personal Introduction; Chapter 1 Small Molecules for Chemogenomics-based Drug Discovery Edgar Jacoby, Ansgar Schuffenhauer, Kamal Azzaoui, Maxim Popov, Sigmar Dressler, Meir Glick, Jeremy Jenkins, John Davies and Silvio Roggo; 1. Introduction; 2. Compound Categories; 2.1. Natural products and derivatives; 2.2. Primary metabolites, co-substrates, co-factors, and marketed drugs; 2.3. Peptides and peptido-mimetics; 2.4. Diversity oriented synthesis molecules; 3. Designing Comprehensive Chemogenomics Screening Compound Collections<br>4. Essential Properties and Selection Processes along the Discovery Pipeline5. Molecular Information Systems and Annotated Compound Libraries; 6. Conclusion; Acknowledgements; References; Chapter 2 Mapping the Chemogenomic Space Jordi Mestres; 1. The Chemogenomic Space; 2. Annotation and Classification Schemes for Proteins; 2.1. Enzymes; 2.2. Receptors; 2.2.1. Channel receptors; 2.2.2. G Protein-coupled receptors; 2.2.3. Nuclear receptors; 3. Structural Representativity of Protein Families; 4. Annotation and Classification |

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 2.4. Library design based on privileged structures  
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 dehydrogenase5.5. Position of the PSSC concept in drug development  
 and chemogenomics; 6. Conclusions; Acknowledgments; References;  
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 Drug Molecules and Focused Libraries Roger Crossley and Martin Slater;  
 1. Introduction; 2. Molecular Recognition and Vicinity Analysis<sup>TM</sup>; 3.  
 Thematic Analysis<sup>TM</sup>; Examples of Themes; 4. Family B and C GPCRs; 5.  
 Classification of GPCRs; 6. Pharmacophore Maps  
 7. Library Design Using Thematic Analysis<sup>TM</sup>

#### Sommario/riassunto

Devoted to the subject of shape charge design using numerical  
 methods, this book offers the defense and commercial industries  
 unique material not contained in any other single volume. The coverage  
 of the Lagrangian and Eulerian methods as well as the equation of state  
 provides first hand help to engineers working on shape charge  
 problems. The book includes detailed descriptions of oil-well  
 perforation not available from any other sources and, coupled with the  
 material flow physics discussed in Chapters 2 and 3 and Appendix B,  
 readers can design the fuel rod configurations for a nuclear reactor