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computer generated physical properties offers the environmental scientist a

basis to predict the properties of molecules and reengineer them to remove those properties that are harmful to the environment this technology is currently used in other fields and is now becoming popular in the environmental engineering field because of its pollution prevention and waste reduction capabilities this book interdisciplinary in scope treats the physical properties of matter as generated by computers it covers a wide variety of topics pointing towards synthesizing new molecules to substitute for reactants intermediaries and products in industrial processes with better physical and environmental properties than the original the author achieves this with a spreadsheet program called synprops that operates on a pc computer with optimization features a radar type graph one for each property visually sorts the various groups in order of their contribution to the property creating the necessity for a computer to obtain answers for the structure of the optimum molecules for substitution or synthesis the author discusses applications to biologically active molecules without side effects including antineoplastic drugs additionally he demonstrates model compounds and the applications of synprops optimization and substitution this book has everything you need to know about deriving properties and combinational chemistry from molecular structure

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the availability of machine learning algorithms and the immense computational power required to develop robust models with high accuracy has driven researchers to conduct extensive studies in forensic science particularly in the identification and examination of evidence found at crime scenes machine learning in forensic evidence examination discusses methodologies for the application of machine learning to the field of forensic science evidence analysis is the cornerstone of forensic investigations examined for either classification or individualization based on distinct characteristics artificial intelligence offers a powerful advantage by efficiently processing large datasets with multiple features enhancing accuracy and speed in forensic analysis to potentially mitigate human errors algorithms have the potential to identify patterns and

features in evidence such as firearms explosives trace evidence narcotics body fluids etc and catalogue them in various databases additionally they can be useful in the reconstruction and detection of complex events such as accidents and crimes both during and after the event this book provides readers with consolidated research data on the potential applications and use of machine learning for analyzing various types of evidence chapters focus on different methodologies of machine learning applied in different domains of forensic sciences such as biology serology physical sciences fingerprints trace evidence ballistics anthropology odontology digital forensics chemistry and toxicology as well as the potential use of big data analytics in forensics exploring recent advancements in machine learning coverage also addresses the challenges faced by experts during routine examinations and how machine learning can help overcome these challenges machine learning in forensic evidence examination is a valuable resource for academics forensic scientists legal professionals and those working on investigations and analysis within law enforcement agencies

the second edition of the handbook of medicinal chemistry is a carefully curated compilation of writing from global experts using their broad experience of medicinal chemistry project leadership and drug discovery from both industry academic and charity perspectives they provide unparalleled insight into the field in a single invaluable volume

titles of chemical papers in british and foreign journals included in quarterly journal v 1 12

the outcome of an american chemical society conference symposium held in los angeles sept 1988 chemical graph theory is a branch of mathematical chemistry that has concerned itself with the mathematical description and characterization of molecular species notational schemes and the enumeration

includes list of members 1882 1902 proceedings of the annual meetings and various supplements

the objective of the handbooks programme is the preparation of critical reviews and evaluations of evidence on the cancer preventive and other relevant properties of a wide range of potential cancer preventive agents and strategies by international working groups of experts in this volume on non steroidal anti inflammatory drugs the following drugs are reviewed aspirin sulindac piroxicam and indomethacin for each drug their chemical and physical characteristics occurrence production use analysis and human exposure metabolism kinetics and genetic variation are studied as well as their cancer preventive effects other beneficial effects carcinogenicity and other toxic effects a summary of data and recommendations for research are provided at the end

quantitative studies on structure activity and structure property relationships are powerful tools in directed drug research in recent years various strategies have been developed to characterize and classify structural patterns by means of molecular descriptors it has become possible not only to assess diversities or similarities of structure databases but molecular descriptors also facilitate the identification of potential bioactive molecules from the rapidly increasing number of compound libraries they even allow for a controlled de novo design of new lead structures this is the most comprehensive collection of molecular descriptors and presents a detailed review from the origins of this research field up to present day this practically oriented reference book gives a thorough overview of the different molecular descriptors representations and their corresponding molecular descriptors all descriptors are listed with their definition symbols and labels formulas some numerical examples data and molecular graphs while numerous figures and tables aid comprehension of the definitions cross references throughout a list of acronyms and notations allow easy access to the information needed to solve a specific research problem examples of descriptor calculations along with tables of descriptor values for a set of selected reference compounds and an up to date reference list add to the practical value of the book making it an invaluable guide for all those dealing with bioactive molecules as well as for researchers

evaluates the carcinogenic risks to humans posed by exposures in the dry cleaning industry by eight chlorinated solvents and related chemicals and by an additional group of seven industrial chemicals dry cleaning is evaluated in the first and most extensive monograph concerning exposures to specific chemicals tetrachloroethylene is identified as the most commonly used solvent during the last two to three decades the evaluation also considers exposure to the wide range of chemicals used in the treatment of spots a review of epidemiological studies on dry cleaning indicates that the risks for cancers at two sites urinary bladder and esophagus may be increased by employment in dry cleaning the monograph concludes that dry cleaning entails exposures that are possibly carcinogenic to humans a second group of monographs evaluates selected chlorinated solvents and related chemicals used in dry cleaning metal cleaning and degreasing as chemical intermediates and in the production of insecticides and herbicides trichloroethylene tetrachloroethylene and 1,2,3-trichloropropane were classified as probably carcinogenic to humans 1-chloro-2-methylpropene was classified as possibly carcinogenic to humans the remaining chemicals chloral and chloral hydrate dichloroacetic acid trichloroacetic acid and 3-chloro-2-methylpropene could not be classified for the remaining seven chemicals used in a diversity of industrial applications vinyl fluoride was classified as probably carcinogenic to humans furan benzofuran and vinyl acetate were classified as possibly carcinogenic to humans acrolein crotonaldehyde and furfural could not be classified

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