G16C

COMPUTATIONAL CHEMISTRY; CHEMOINFORMATICS; COMPUTATIONAL MATERIALS SCIENCE

Definition statement

This place covers:

Data processing methods or systems for the storage, retrieval, analysis, distribution or visualisation of physicochemical or structural data of chemical particles, elements, compounds, or mixtures.

Computational theoretical chemistry and computational materials science.

Data processing methods or systems for investigating physics or chemistry of new or existing materials or phenomena associated with their design, synthesis, processing, characterization, or utilisation.

This group also covers computational chemistry and computational materials science methods or systems where the digital data processing is inherent or implicit, although not explicitly mentioned.

Relationships with other classification places

This subclass covers computational chemistry, which comprises computational theoretical chemistry, chemoinformatics, and computational materials science, whereas subclass G16B covers bioinformatics.

In order to determine whether classification should be directed to this subclass or to subclass G16B, one has to take into account the type of molecule(s), whose characterising features are processed by a computational algorithm.

Following the definition statements of computational chemistry, computational materials science and bioinformatics, processing of data related to chemical entities (i.e. chemical particles, elements, compounds, mixtures) and/or materials should be classified under G16C.

Processing of data related to nucleic acids, proteins, peptides and/or amino acids should be classified under G16B.

References

Informative references

Attention is drawn to the following places, which may be of interest for search:

Investigating or analysing materials by determining their chemical or physical properties	G01N
Chromatographic signal analysis	G01N 30/86
Systems controlled by a computer	G05B 15/00
Computer input/output arrangements	G06F 3/00
Computer architectures or program control	G06F 9/00
Information retrieval; Database structures therefor; File system structures therefor	G06F 16/00
Complex mathematical operations	G06F 17/10
Computer-aided design	G06F 17/50
Pattern recognition	G06K 9/00
Computer systems using neural network models	G06N 3/02

Computer systems using knowledge representation, e.g. expert systems	G06N 5/02
Computer systems using probabilistic models	G06N 7/00
Machine learning	G06N 20/00
3D image rendering	G06T 15/00
3D modelling for computer graphics	G06T 17/00
Manipulating 3D models or images for computer graphics	G06T 19/00
Bioinformatics	G16B
Healthcare Informatics	G16H
Mass spectrometry apparatus	H01J 49/00

Glossary of terms

In this place, the following terms or expressions are used with the meaning indicated:

design	Software-based creation or planning
handling	Covers retrieval, analysis, visualisation or storage
quantum chemistry	Branch of chemistry, in which quantum mechanics is applied to theoretical studies of chemical systems
molecular mechanics	Branch of chemistry, in which classical mechanics is applied to model molecular systems
molecular dynamics	Computer-based simulation method for studying movements of atoms and molecules in time by applying Newton's equations of motion and molecular mechanics force fields
in silico	Performed on a computer or via computer simulations

Synonyms and Keywords

In patent documents, the following words/expressions are often used with the meaning indicated:

systems	includes apparatus

G16C 10/00

Computational theoretical chemistry, i.e. ICT specially adapted for theoretical aspects of quantum chemistry, molecular mechanics, molecular dynamics or the like

Definition statement

This place covers:

Computer based calculations and theoretical details of quantum mechanics (QM), e.g. density functional theory (DFT), molecular mechanics (MM), e.g. details related to force fields, molecular dynamics (MD), e.g. details on setting up simulations, Monte Carlo (MC) methods, e.g. details on MC algorithms, conformational analysis or the like.

Mere mention of modelling or simulation using QM, MM, MD, etc. is not sufficient to justify classification in this place.

G16C 20/00

Chemoinformatics, i.e. ICT specially adapted for the handling of physicochemical or structural data of chemical particles, elements, compounds or mixtures

Definition statement

This place covers:

Subject matter related to cheminformatics as specified in the subgroups.

G16C 20/10

Analysis or design of chemical reactions, syntheses or processes

Definition statement

This place covers:

Analysis and design of chemical reactions, processes and syntheses, e.g. synthesis design, identifying a suitable pathway, reaction outcome prediction, crystallization/co-crystallization process prediction, and mechanism elucidation.

G16C 20/20

Identification of molecular entities, parts thereof or of chemical compositions

Definition statement

This place covers:

Computer-assisted and measurement-based — e.g. by any of mass spectrometry (MS), nuclear magnetic resonance (NMR), spectroscopy, chromatography, electrophoresis — identification of molecules, parts thereof, their molecular structures, e.g. computer-assisted structure elucidation (CASE), compositions of multi-component samples or mixtures.

Computer-assisted and measurement-based (for example: see above paragraph) qualitative and quantitative analyses of samples.

G16C 20/30

Prediction of properties of chemical compounds, compositions or mixtures

Definition statement

This place covers:

Prediction of physical, physicochemical and/or biological properties of chemical compounds, compositions or mixtures, e.g. calculating and selecting molecular descriptors, details related to the development of structure-activity relationship (SAR)/quantitative structure-activity relationship (QSAR)/ quantitative structure-property relationship (QSPR) models, absorption, distribution, metabolism, excretion and toxicity (ADME-Tox or ADMET) models, and pharmacokinetic/pharmacodynamic (PK/ PD) models.

Prediction of a drug dosage or regimen, concentration of a pharmaceutical active agent based on molecular data, wherein the drug/active agent is any molecule excluding nucleic acids, proteins, peptides or their conjugates, e.g. oligonucleotide-peptides.

G16C 20/40

Searching chemical structures or physicochemical data

Definition statement

This place covers:

Database search of chemical structures or physicochemical data, e.g. full structure search, substructure search, similarity search, combinations of similarity coefficients, pharmacophore search, and 3D structure search.

G16C 20/50

Molecular design, e.g. of drugs

Definition statement

This place covers:

Design and modelling of molecules to be used for any purpose, e.g. drug design with the emphasis on a therapeutic agent, e.g. ligand-biological target interactions, docking algorithms, and pharmacophore generation.

G16C 20/60

In silico combinatorial chemistry

Definition statement

This place covers:

In silico (i.e. computer based) designing and screening of combinatorial chemical libraries of compounds other than nucleic acids, proteins, peptides, or amino acids.

Mere mention of combinatorial libraries of particular types of compounds is not sufficient to classify in this place.

G16C 20/70

Machine learning, data mining or chemometrics

Definition statement

This place covers:

Discovery and/or analysis of patterns within a vast amount of physicochemical data, wherein the emphasis is placed on the methods of analysis and is largely independent of the particular type of physicochemical data.

Analysis methods are based on machine learning, statistical models, supervised and unsupervised learning techniques including chemical pattern finding, knowledge discovery, rule extraction, correlation, clustering and classification.

G16C 20/80

Data visualisation

Definition statement

This place covers:

Visual representations specifically adapted to structural and/or physicochemical data, wherein the emphasis is placed on the method of visualisation and is largely independent of the particular type of structural and/or physicochemical data.

For example: graphics generation, map display (e.g. physical and/or chemical properties maps), chemical structure representations (e.g. chemical name-to-structure conversion algorithms).

G16C 20/90

Programming languages; Computing architectures; Database systems; Data warehousing

Definition statement

This place covers:

Software specially adapted to assist in programming procedures within computational chemistry.

Database systems specially adapted for managing chemical data. For example: ontologies, heterogeneous data integration, data warehousing, or computing architectures.

Encryption and compression algorithms specially adapted for chemical data, e.g. chemical fingerprints.

G16C 60/00

Computational materials science, i.e. ICT specially adapted for investigating the physical or chemical properties of materials or phenomena associated with their design, synthesis, processing, characterisation or utilisation

Definition statement

This place covers:

Computer-implemented mathematical modelling of the structures (including but not limited to structural defects and their resulting limitations), properties (including but not limited to electronic, thermal, chemical, magnetic, optical) and/or behaviours of materials (including but not limited to metals, polymers, ceramics, composites, biomaterials, nanomaterials) by applying the knowledge of physics, physical chemistry, and chemistry governing the said structures, properties and/or behaviours of the materials as well as the knowledge of the modelled materials.

Computational investigation of existing materials and design of new ones.