EUROPEAN PATENT OFFICE
U.S. PATENT AND TRADEMARK OFFICE

CPC NOTICE OF CHANGES 742

DATE: JANUARY 1, 2020

PROJECT DP0209

The following classification changes will be effected by this Notice of Changes:

Action	**Subclass**	**Group(s)**
DEFINITIONS:		
Definitions Modified:	G16C	subclass
		10/00
		20/10
		20/20
		20/30
		20/40
		20/50
		20/60
		20/70
		20/80
		20/90
		60/00

No other subclasses/groups are impacted by this Notice of Changes.

This Notice of Changes includes the following *[Check the ones included]:*

1. CLASSIFICATION SCHEME CHANGES
   - ☐ A. New, Modified or Deleted Group(s)
   - ☐ B. New, Modified or Deleted Warning(s)
   - ☐ C. New, Modified or Deleted Note(s)
   - ☐ D. New, Modified or Deleted Guidance Heading(s)
2. DEFINITIONS
   - ☒ A. New or Modified Definitions (Full definition template)
   - ☐ B. Modified or Deleted Definitions (Definitions Quick Fix)
3. ☐ REVISION CONCORDANCE LIST (RCL)
4. ☐ CHANGES TO THE CPC-TO-IPC CONCORDANCE LIST (CICL)
5. ☐ CHANGES TO THE CROSS-REFERENCE LIST (CRL)

2. A. DEFINITIONS (modified)

G16C

Definition statement

This place covers:

Replace: Paragraphs 2 and 3 with the following new paragraphs:

Computational theoretical chemistry.

Computational materials science, i.e. 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.

Replace: In paragraph 4 the term “group” with “subclass”.

Relationships with other classification places

Replace: The existing paragraphs with the following new paragraphs:

This subclass covers 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.

Classification should be directed to subclass G16C for processing of data related to chemical entities in general, i.e. chemical particles, elements, compounds, mixtures and/or materials.

Classification should be directed to subclass G16B for processing of data related to molecules which are directly involved in molecular biology processes, i.e. molecules out of the groups of nucleic acids, proteins, peptides and amino acids.

G16C 10/00

Definition statement

This place covers:

Replace: The first paragraph with the following newly reformatted paragraph.

Computer-based calculations and theoretical analysis 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;
- related Monte Carlo (MC) methods, e.g. details on MC algorithms, conformation analysis or the like.

Replace: In paragraph 2 the term “place” with “group”.

G16C 20/10

Definition statement

This place covers:

Replace: The existing paragraph with the following newly reformatted paragraph.

Computer-assisted analysis and design of chemical reactions, processes and syntheses. The following are examples of the subjects covered:

- synthesis design;
- identifying a suitable pathway;
- reaction outcome prediction;
- crystallization/co-crystallization process prediction;
- mechanism elucidation.

G16C 20/20

Definition statement

This place covers:

Replace: The two existing paragraphs

> 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.

with the following three newly reformatted paragraphs:

> Computer-assisted, measurement-based identification of molecules, parts of molecules or their molecules structures, and of compositions of multi-component mixtures, e.g. computer-assisted structure elucidation (CASE).
>
> Computer-assisted, measurement-based, qualitative and quantitative analysis of samples.
>
> Measurement may be based on mass spectrometry (MS), nuclear magnetic resonance (NMR), spectroscopy, chromatography, electrophoresis or the like.

G16C 20/30

Definition statement

This place covers:.

Delete: The two existing paragraphs.

Insert: The following three new paragraphs.

Computer-assisted prediction of physical, physicochemical and biological properties of chemical compounds, compositions or mixtures. The following are examples of the subjects covered:

- computing and selecting molecular descriptors;
- computing structure-activity relationship (SAR) models;
- computing quantitative structure-activity relationship (QSAR) models;
- computing quantitative structure-property relationship (QSPR) models;
- computing absorption, distribution, metabolism, excretion and toxicity (ADME-Tox or ADMET) models; and
- computing pharmacokinetic/pharmacodynamic (PK/PD) models.

Computer-assisted prediction of a drug dosage or drug regimen.

Computer-assisted prediction of the concentration of a pharmaceutical active agent/drug based on molecular data, wherein the drug/active agent can be any molecule other than in the group of nucleic acids, proteins, peptides and their conjugates.

G16C 20/40

Definition statement

This place covers:

Replace: The existing paragraph with the following formatted text.

Database search of chemical structures or physicochemical data. The following are examples of the subjects covered:

- full structure search;
- substructure search;
- similarity search;
- combinations of similarity coefficients;
- pharmacophore search; and
- 3D structure search.

G16C 20/50

Definition statement

This place covers:

Replace: The existing paragraph with the following two paragraphs.

Computer-assisted design and modelling of molecules to be used for any purpose. The following are examples of the subjects covered:

- drug design with the emphasis on a therapeutic agent;
- ligand-biological target interactions;
- docking algorithms, and pharmacophore generation.

Computer-assisted drug formulation.

G16C 20/60

Definition statement

This place covers:

Delete: In the first paragraph, the following text and punctuations:

"(i.e. computer based)".

G16C 20/70

Definition statement

This place covers:

Replace: The two existing paragraphs with the following newly reformatted paragraphs.

Computer-assisted 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 any of:

- machine learning;
- statistical models;
- supervised and unsupervised learning techniques;

- pattern finding;
- knowledge discovery;
- rule extraction;
- correlation;
- clustering; and
- classification.

G16C 20/80

Definition statement

This place covers:

Replace: The second paragraph with the following newly reformatted paragraph.

The following are examples of the subjects covered:

- 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

Definition statement

This place covers:

Replace: The second paragraph with the following two newly reformatted paragraphs.

Database systems specially adapted for managing chemical data.

The following are examples of the subjects covered:

- ontologies;
- heterogeneous data integration;
- data warehousing;
- computing architectures.

Delete: The existing third paragraph “Encryption and compression algorithms specially adapted for chemical data, e.g. chemical fingerprints.”

Insert: The following new paragraph between the existing first and the new second paragraphs.

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

G16C 60/00

Definition statement

This place covers:

Replace: The first paragraph “Computer-implemented mathematical modelling of ... as the knowledge of the modelled materials” with the following two paragraphs.

Computer-assisted mathematical modelling of the structures (e.g. metals, polymers, ceramics, composites, biomaterials, nanomaterials) by applying the knowledge of physics, physical chemistry and chemistry.
In particular modelling of:

- structures of materials (e.g. structural defects and their resulting limitations);
- properties of materials (e.g. electronic, thermal, chemical, magnetic, optical); and/or
- behaviors of materials.

Computer-assisted investigation of existing materials and design of new ones.