

STN	Zdravotnícka informatika. Identifikácia liekov. Implementácia návodu pre dátové prvky a štruktúry pre jednoznačnú identifikáciu a výmenu regulovaných informácií o látkach (ISO 19844: 2015).	STN P CEN ISO/TS 19844 84 8125
------------	--	--

Health informatics - Identification of medicinal products - Implementation guidelines for data elements and structures for the unique identification and exchange of regulated information on substances (ISO/TS 19844:2015)

Táto norma obsahuje anglickú verziu európskej normy.
This standard includes the English version of the European Standard.

Táto norma bola oznámená vo Vestníku ÚNMS SR č. 03/16

Táto predbežná STN je určená na overenie. Pripomienky zasielajte ÚNMS SR najneskôr do apríla 2018.

Obsahuje: CEN ISO/TS 19844:2015, ISO/TS 19844:2015

122531

Úrad pre normalizáciu, metrológiu a skúšobníctvo SR, 2016
Podľa zákona č. 264/1999 Z. z. v znení neskorších predpisov sa môžu slovenské technické normy
rozmnžovať a rozširovať iba so súhlasom Úradu pre normalizáciu, metrológiu a skúšobníctvo SR.

TECHNICAL SPECIFICATION

CEN ISO/TS 19844

SPÉCIFICATION TECHNIQUE

TECHNISCHE SPEZIFIKATION

December 2015

ICS 35.240.80

English Version

**Health informatics - Identification of medicinal products -
Implementation guidelines for data elements and
structures for the unique identification and exchange of
regulated information on substances (ISO/TS 19844:2015)**

Informatique de santé - Identification des médicaments
- Lignes directrices pour la mise en oeuvre des
éléments de données et structures pour l'identification
unique et l'échange d'informations réglementées sur
les substances (ISO/TS 19844:2015)

Medizinische Informatik - Identifikation von
Arzneimitteln - Anwendungsleitfaden für die Struktur
und kontrollierten Vokabularien zur Identifikation und
Beschreibung von Substanzen und Inhaltsstoffen
(ISO/TS 19844:2015)

This Technical Specification (CEN/TS) was approved by CEN on 4 April 2016 for provisional application.

The period of validity of this CEN/TS is limited initially to three years. After two years the members of CEN will be requested to submit their comments, particularly on the question whether the CEN/TS can be converted into a European Standard.

CEN members are required to announce the existence of this CEN/TS in the same way as for an EN and to make the CEN/TS available promptly at national level in an appropriate form. It is permissible to keep conflicting national standards in force (in parallel to the CEN/TS) until the final decision about the possible conversion of the CEN/TS into an EN is reached.

CEN members are the national standards bodies of Austria, Belgium, Bulgaria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, Former Yugoslav Republic of Macedonia, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, Netherlands, Norway, Poland, Portugal, Romania, Slovakia, Slovenia, Spain, Sweden, Switzerland, Turkey and United Kingdom.



EUROPEAN COMMITTEE FOR STANDARDIZATION
COMITÉ EUROPÉEN DE NORMALISATION
EUROPÄISCHES KOMITEE FÜR NORMUNG

CEN-CENELEC Management Centre: Avenue Marnix 17, B-1000 Brussels

Contents	Page
European foreword.....	3

European foreword

This document (CEN ISO/TS 19844:2015) has been prepared by Technical Committee ISO/TC 215 "Health informatics" in collaboration with Technical Committee CEN/TC 251 "Health informatics" the secretariat of which is held by NEN.

Attention is drawn to the possibility that some of the elements of this document may be the subject of patent rights. CEN [and/or CENELEC] shall not be held responsible for identifying any or all such patent rights.

According to the CEN-CENELEC Internal Regulations, the national standards organizations of the following countries are bound to announce this Technical Specification: Austria, Belgium, Bulgaria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, Former Yugoslav Republic of Macedonia, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, Netherlands, Norway, Poland, Portugal, Romania, Slovakia, Slovenia, Spain, Sweden, Switzerland, Turkey and the United Kingdom.

Endorsement notice

The text of ISO/TS 19844:2015 has been approved by CEN as CEN ISO/TS 19844:2015 without any modification.

**Health informatics — Identification
of medicinal products —
Implementation guidelines for data
elements and structures for the
unique identification and exchange of
regulated information on substances**

Informatique de santé — Identification des médicaments — Lignes directrices pour la mise en oeuvre des éléments de données et structures pour l'identification unique et l'échange d'informations réglementées sur les substances





COPYRIGHT PROTECTED DOCUMENT

© ISO 2015, Published in Switzerland

All rights reserved. Unless otherwise specified, no part of this publication may be reproduced or utilized otherwise in any form or by any means, electronic or mechanical, including photocopying, or posting on the internet or an intranet, without prior written permission. Permission can be requested from either ISO at the address below or ISO's member body in the country of the requester.

ISO copyright office
Ch. de Blandonnet 8 • CP 401
CH-1214 Vernier, Geneva, Switzerland
Tel. +41 22 749 01 11
Fax +41 22 749 09 47
copyright@iso.org
www.iso.org

Contents

Page

Foreword.....	viii
Introduction.....	ix
1 Scope.....	1
2 Normative references.....	2
3 General background and history.....	2
4 Substance (Mandatory).....	3
4.1 Introduction.....	3
4.2 Defining Substances.....	5
4.3 Substance Types (Mandatory).....	7
4.4 Substance ID (Mandatory).....	10
4.5 Substance Names (Mandatory).....	11
4.5.1 Substance Name.....	12
4.5.2 Substance Name Type.....	12
4.5.3 Language.....	13
4.5.4 Official Name (repeat as necessary).....	13
4.6 Reference Sources (Mandatory).....	15
4.6.1 Public Domain.....	16
4.6.2 Reference Source Type.....	16
4.6.3 Reference Source Class.....	16
4.6.4 Reference Source ID.....	17
4.6.5 Reference Source Citation.....	17
4.6.6 Reference Source Document (new class to be included in the second edition of ISO 11238).....	17
4.6.7 Reference Source Document Type (new class to be included in the second edition of ISO 11238).....	18
4.6.8 Reference Source Document Classification (new class to be included in the second edition of ISO 11238).....	18
4.6.9 Reference Source URL (new class to be included in the second edition of ISO 11238).....	18
4.7 Substance Code (Conditional).....	18
4.7.1 Code.....	19
4.7.2 Code System.....	19
4.7.3 Code System ID.....	20
4.7.4 Code System Status.....	20
4.7.5 Code System Status Change Date.....	20
4.7.6 Comment.....	20
4.7.7 Reference Source.....	21
4.7.8 Substance Classification (repeat as necessary).....	21
4.7.9 Target.....	23
4.7.10 Gene.....	25
4.7.11 Gene Elements.....	26
4.7.12 Substance Relationship.....	27
4.8 Structure (repeat as necessary) (Conditional).....	29
4.8.1 Structural Representation Type.....	34
4.8.2 Structural Representation.....	35
4.8.3 Structural Representation Attachment.....	35
4.8.4 Stereochemistry.....	35
4.8.5 Optical Activity.....	36
4.8.6 Molecular Formula.....	36
4.8.7 Molecular Formula by Moieties (new class to be included in the second edition of ISO 11238).....	37
4.8.8 Isotope (repeat as necessary).....	37

4.9	Amount (Conditional)	38
4.9.1	Average	38
4.9.2	Low Limit	38
4.9.3	High Limit	39
4.9.4	Unit	39
4.9.5	Non-numeric Value	39
4.10	Source Material (Conditional)	39
4.10.1	Source Material Class	40
4.10.2	Source Material Type	41
4.10.3	Source Material state	41
4.10.4	Organism ID	41
4.10.5	Organism Name	41
4.10.6	Development Stage	42
4.10.7	Part Description (repeat as necessary)	42
4.10.8	Fraction (repeat as necessary)	42
4.10.9	Organism	43
4.11	Modification (repeat as necessary) (Conditional)	49
4.11.1	Modification Type	50
4.11.2	Residue Modified	51
4.11.3	Residue Site	51
4.11.4	Structural Modification	51
4.12	Property (Conditional)	55
4.12.1	Property Type	56
4.12.2	Property Name	56
4.12.3	Property Parameters (new class to be included in the second edition of ISO 11238)	56
4.12.4	Substance Name	57
4.12.5	Substance ID	57
4.12.6	Amount type	57
4.13	Version (repeat as necessary) (Mandatory)	57
4.13.1	Version Number	57
4.13.2	Effective date	58
4.13.3	Change Made	58
5	Substance definitions	58
5.1	Chemical Substance	58
5.1.1	Structure	59
5.1.2	Stoichiometric	59
5.1.3	Stoichiometric Chemicals	59
5.1.4	Comment	62
5.1.5	Non- Stoichiometric Chemicals	62
5.2	Proteins/ Peptides	64
5.2.1	Microheterogeneity	65
5.2.2	Sequence Type	66
5.2.3	Number of subunits	66
5.2.4	Disulfide Linkage	66
5.2.5	Comment	67
5.2.6	Protein Subunit (repeat as necessary)	67
5.2.7	Molecular Weight (repeat as necessary)	69
5.2.8	Glycosylation	69
5.2.9	Structure	71
5.2.10	Modification	71
5.2.11	Property	71
5.2.12	Molecular Weight	71
5.3	Nucleic Acids	72
5.3.1	Structure	73
5.3.2	Sequence Type	73
5.3.3	Number of Subunits	73
5.3.4	Area of hybridisation	74

5.3.5	Comment	74
5.3.6	Nucleic Acid Subunit (repeat as necessary)	74
5.3.7	Modification	77
5.3.8	Property.....	77
5.3.9	Molecular Weight.....	77
5.4	Polymers –To be addressed in more detail in the next edition of this Technical Specification	78
5.4.1	Substance Name.....	79
5.4.2	Structure.....	79
5.4.3	Polymer Class	79
5.4.4	Polymer Geometry.....	80
5.4.5	Copolymer Sequence type.....	80
5.4.6	Comment	80
5.4.7	Monomer Description (repeat as necessary)	80
5.4.8	Structural Repeat (repeat as necessary).....	81
5.4.9	Molecular Weight (repeat as necessary).....	83
5.4.10	Property (repeat as necessary)	83
5.4.11	Reference Source (repeat as necessary)	83
5.5	Structurally-Diverse Substances	83
5.5.1	herbals and Substances Used in the Preparation of Plant-Based Allergenic Extracts	84
5.5.2	Vaccines — Annex addressing this will be included in the next edition of this Technical Specification.....	93
5.5.3	Purified Blood Products and Polyclonal Antibodies — Annex addressing this will be included in the next edition of this Technical Specification.....	93
5.5.4	Cells and Tissues — Annex addressing this will be included in the next edition of this Technical Specification	93
5.5.5	Minerals — Annex addressing this will be included in the next edition of this Technical Specification.....	93
5.6	Mixture Substance (repeat as necessary)	94
5.6.1	Mixture Type.....	94
5.6.2	Mixture Constituent (repeat as necessary)	94
6	specified substance (Optional)	95
6.1	specified substance Group 1 (repeat as necessary)	96
6.1.1	specified substance Group 1 ID.....	97
6.1.2	specified substance Group1 Name.....	97
6.1.3	Substance Name (repeat as necessary).....	97
6.1.4	Substance Code	97
6.1.5	Version (repeat as necessary).....	97
6.1.6	Reference Sources.....	97
6.1.7	Property (repeat as necessary)	97
6.1.8	Fraction (new class to be included in the second edition of ISO 11238).....	98
6.1.9	Modification	98
6.1.10	Reference Information (repeat as necessary).....	98
6.1.11	Constituent (repeat as necessary)	98
6.1.12	Physical Form (repeat as necessary).....	99
6.2	specified substance Group 1 intended for herbal Substance and herbal Preparation	100
6.2.1	specified substance Group 1 ID.....	101
6.2.2	specified substance Group1 Name.....	101
6.2.3	Reference Sources.....	101
6.2.4	Fraction (new class to be included in the second edition of ISO 11238).....	101
6.2.5	Modification (new classes to be included in the second edition of ISO 11238).....	102
6.2.6	Constituent (repeat as necessary)	102
6.2.7	Physical Form (repeat as necessary)	103
6.3	specified substance Group 2 (repeat as necessary)	104
6.3.1	specified substance Group2 ID.....	107
6.3.2	specified substance Group2 Name.....	107
6.3.3	Parent Substance ID.....	107
6.3.4	Manufacturing.....	107

6.4	specified substance Group 2 for herbal preparations.....	111
6.4.1	specified substance Group2 ID	111
6.4.2	specified substance Group2 Name.....	111
6.4.3	Parent Substance ID.....	111
6.4.4	Manufacturing.....	112
6.4.5	Version (repeat as necessary).....	113
6.5	specified substance Group 3 (repeat as necessary).....	113
6.5.1	specified substance Group3 ID	114
6.5.2	specified substance Group3 Name.....	114
6.5.3	Parent Substance ID.....	114
6.5.4	Grade	115
6.5.5	Reference Source (repeat as necessary)	115
6.5.6	Version (repeat as necessary).....	115
6.5.7	Reference Source (repeat as necessary)	116
6.5.8	Version (repeat as necessary).....	116
Annex A	(normative) Choosing a Substance ID	117
A.1	Requesting a Substance ID and providing information.....	117
Annex B	(normative) Chemical Substance	119
B.0	Introduction.....	119
B.0.1	Proposal for the update of the ISO 11238 Substance standard	120
B.0.2	Outline of Annex B	122
B.1	Scope.....	123
B.2	Terms and definitions	123
B.3	Chemical Substance subtypes and Mixture Substance.....	132
B.3.1	Substance type, Chemical substance.....	132
B.3.2	Solid state forms of the Substance	132
B.3.3	Need to substantiate the chemical structure, molecular formula and molecular weight.....	135
B.3.4	Polymorphism.....	136
B.3.5	Non-Stoichiometric chemical substances	137
B.3.6	Mixture substance	138
B.3.7	Multi substance material	139
B.4	Discussion of the key elements of a chemical substance	142
B.4.1	Identity of material	142
B.4.2	Nomenclature	142
B.4.3	Molecular formula	142
B.4.4	Molecular weight.....	143
B.4.5	Substance Structure	143
B.4.6	Geometric Isomerism	146
B.4.7	Stereo-descriptors in systematic nomenclature: Substance with one centre of Asymmetry.....	147
B.4.8	Substance with two centres of Asymmetry, Epimers, Diastereomers.....	148
B.4.9	Anomers	148
B.4.10	Substance with more than two centres of Asymmetry (Mixture of stereoisomers)	151
B.4.11	Conclusion for the Key elements.....	152
B.4.12	Decision tree for a new Substance ID	152
B.5	Discussing other elements of importance regarding the characteristics of a substance.....	153
B.5.1	Introduction.....	153
B.5.2	Naming Vegetable Oils	153
B.5.3	Castor Oil and related products.....	169
B.5.4	Properties to be captured, related to liquids (Gas), Nitrous oxide	172
B.6	Examples	177
B.6.1	Example 1: Amlodipine besilate.....	178
B.6.2	Example 2: Ponatinib hydrochloride.....	185
B.6.3	Example 3: Benzathine Benzylpenicillin tetrahydrate, sterilised	201
B.6.4	specified substance Group 2 information level	206
B.6.5	specified substance Group 3 information level	207
B.7	Radiopharmaceutical substance	207
B.7.1	Introduction.....	207

B.7.2	Example: Florbetapir ¹⁸F	208
B.7.3	Identity of material, combining the elements for Florbetapir ¹⁸F, Substance and specified substance information level.	209
B.7.4	specified substance Group 2 information level	214
Annex C (normative) Protein Substance		215
C.1	Scope	215
C.2	Introduction	215
C.3	Peptide Substances	216
C.3.1	Example IIIa: Protein Substance: Vasopressin	216
C.3.2	Example IIIb: Desmopressin	219
C.3.3	Example IIIc: Desmopressin Acetate	223
C.3.4	Example IIId: Calcitonin Salmon	227
C.3.5	Example IIIe: Human Insulin	233
C.4	Element Group Protein, specified substance Group 1	235
C.4.1	Example IVa: Insulin Human Zinc Suspension (Amorphous), taken from EP/USP Monographs for Zinc Suspensions	235
C.4.2	Example IVb: Insulin Human Zinc Suspension (Crystalline), taken from EP/USP Monographs for Zinc Suspensions	236
C.4.3	Example IVc: Insulin Human Zinc Suspension taken from EP/USP Monographs for Zinc Suspensions, including discussion for specified substance Group 3 information	237
C.5	Element Group Protein, specified substance Group 2	240
C.5.1	Example Va: Synthetic Calcitonin Salmon-Manufacturer Company Acme	240
C.5.2	specified substance Group 2 information level	240
C.5.3	Example Vb: Recombinant Calcitonin Salmon-- Company Acme	241
C.6	Element Group Protein, specified substance Group 3	241
C.6.1	Example: Calcitonin Salmon (Synthetic) specified substance Group 3	242
C.6.2	Example: Calcitonin Salmon (Recombinant) specified substance Group 3	242
C.7	Example Protein Substance Example of a Monoclonal Antibody conjugated Toxin	243
C.8	Addendum: Microheterogeneity	248
Annex D (normative) Nucleic Acid Substance		249
D.1	Scope	249
D.2	Introduction	249
D.3	Examples	250
D.3.1	Example: 5-Methylcytosine	250
D.3.2	Example: A 5'-phosphate ribonucleotide	251
D.4	Substances	252
D.4.1	Example: Mipomersen Sodium information	252
D.4.2	Example: Oligonucleotide Elements	252
D.4.3	Example: Anti-sense RNA	257

Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

Attention is drawn to the possibility that some of the elements of this document may be the subject of patent rights. ISO shall not be held responsible for identifying any or all such patent rights. Details of any patent rights identified during the development of the document will be in the Introduction and/or on the ISO list of patent declarations received (see www.iso.org/patents).

Any trade name used in this document is information given for the convenience of users and does not constitute an endorsement.

For an explanation on the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the WTO principles in the Technical Barriers to Trade (TBT) see the following URL: [Foreword - Supplementary information](#)

The committee responsible for this document is ISO/TC 215, *Health informatics*.

Introduction

This Technical Specification is a guide for implementing ISO 11238, *Health informatics — Identification of medicinal products — Data elements and structures for the unique identification and exchange of regulated information on substances*. This Technical Specification was developed in response to a worldwide demand for guidance on the implementation of internationally harmonised specifications for medicinal products. It is one of a group of four implementation guides for a total of five ISO standards which together provide the basis for the unique identification of medicinal products. The other standards in this group are:

- ISO 11615, *Health informatics — Identification of medicinal products — Data elements and structures for the unique identification and exchange of regulated medicinal product information*
- ISO 11616, *Health informatics — Identification of medicinal products — Data elements and structures for the unique identification and exchange of regulated pharmaceutical product information*
- ISO 11239, *Health informatics — Identification of medicinal products — Data elements and structures for the unique identification and exchange of regulated information on pharmaceutical dose forms, units of presentation, routes of administration and packaging*
- ISO 11240, *Health informatics — Identification of medicinal products — Data elements and structures for the unique identification and exchange of units of measurement*

The standards for the Identification of Medicinal Products (IDMP) support the activities of medicines regulatory agencies worldwide by jurisdiction. These include a variety of regulatory activities related to development, registration and life cycle management of medicinal products as well as pharmacovigilance and risk management.

The business objective of this implementation guide is to provide a means for exchanging regulatory substance information. To meet the primary objectives of the regulation of medicines and pharmacovigilance, it is necessary to exchange medicinal product information in a robust and reliable manner.

For the purposes of this Technical Specification, all conditions (e.g. mandatory, conditional, optional) correspond to the necessary requirements to uniquely and unambiguously identify a substance. Implementation of the ISO IDMP standards may dictate that mandatory elements for identification be tagged as conditional or optional, based on regional requirements. If a section is identified as 'optional' but is implemented in a specific region, conformance described within that section is applicable. The scope of this Technical Specification is to identify the scientifically necessary elements for the unique identification of substances/specified substances.

Health informatics — Identification of medicinal products — Implementation guidelines for data elements and structures for the unique identification and exchange of regulated information on substances

1 Scope

This Technical Specification is used in the implementation of ISO 11238. This Technical Specification defines substances based on their scientific identity (i.e. what they are) rather than on their use or method of production.

ISO 11238 provides the conceptual framework for defining substances and specified substances and for assigning unique identifiers in the context of the ISO IDMP standards. ISO 11238 describes general concepts for defining and distinguishing substances and a high level model for the structuring of information for substances. This Technical Specification provides detailed explanations of each type or grouping of substance information, an element-by-element description for implementation of ISO 11238, and examples for a variety of substances and specified substances.

This first edition of the Technical Specification will only address substances, and Groups 1 to 3 of the specified substances as defined in ISO 11238 and Annexes A, B, C, and D. It is anticipated that specified substances Group 4, as defined in ISO 11238, will be addressed in a subsequent edition of this Technical Specification. Some information that would typically fall under specified substances Group 4 may be covered in the Annexes of this Technical Specification. This information, although not defining of either a substance or a specified substance Group 1, may be essential to distinguishing substances.

This Technical Specification addresses the following:

- Data elements necessary for defining substances and specified substances Groups 1 to 3;
- The logical use of data elements as defined in ISO 11238;
- Substances and specified substances Groups 1 to 3 business rules for
 - determining necessary data elements,
 - distinguishing and defining materials according to ISO 11238,
 - triggering the assignment of identifiers.

This Technical Specification does not address the following:

- Business processes for data management;
- Implementation of a specific data information system (e.g. a relational database schema);
- Normative messaging standards for substances;
- The maintenance of controlled vocabularies;
- The specific global identifier system that should be used;
- Nomenclature standards for substances.

2 Normative references

The following referenced documents are indispensable for the application of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO 8601, *Data elements and interchange formats — Information interchange — Representation of dates and times*

ISO 11238, *Health informatics — Identification of medicinal products — Data elements and structures for the unique identification and exchange of regulated information on substances*

koniec náhľadu – text ďalej pokračuje v platenej verzii STN