

ISO/TS 19844:2015-12 (E)

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

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