

# ISO/TS 19844:2016-12 (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
1	Scope .....	1
2	Normative references .....	2
3	General background and history .....	2
4	Substance (Mandatory) .....	3
4.1	General .....	3
4.2	Defining substances .....	5
4.2.1	Substance type (Mandatory) .....	7
4.2.2	Substance ID (Mandatory) .....	10
4.3	Substance names (Mandatory) .....	11
4.3.1	Substance name .....	12
4.3.2	Substance name type .....	13
4.3.3	Language .....	14
4.3.4	Official name (Conditional) .....	14
4.4	Reference source (Conditional) .....	17
4.4.1	Public domain .....	17
4.4.2	Reference source type .....	18
4.4.3	Reference source class .....	18
4.4.4	Reference source ID .....	19
4.4.5	Reference source citation .....	19
4.5	Reference source document (Conditional) .....	19
4.5.1	Public domain .....	19
4.5.2	Reference source document .....	20
4.5.3	Reference source document type .....	20
4.5.4	Reference source document ID .....	21
4.5.5	Reference source document classification .....	21
4.5.6	Reference source document URL .....	21
4.6	Substance code (Conditional) .....	21
4.6.1	Code .....	22
4.6.2	Code system .....	22
4.6.3	Code system ID .....	23
4.6.4	Code system status .....	23
4.6.5	Code change date .....	24
4.6.6	Comment .....	24
4.6.7	Reference source .....	24
4.7	Reference information (Conditional) .....	24
4.7.1	Comment .....	25
4.7.2	Substance classification (Conditional) .....	25
4.7.3	Substance relationship (Conditional) .....	28
4.7.4	Target (Conditional) .....	30
4.7.5	Gene (Conditional) .....	33
4.7.6	Gene element (Conditional) .....	35
4.8	Structure .....	36
4.8.1	Structural Representation (Conditional) .....	36
4.8.2	Stereochemistry .....	42
4.8.3	Optical activity .....	43
4.8.4	Molecular Formula .....	44

4.8.5	Molecular Formula by Moiety .....	44
4.8.6	Molecular weight (Mandatory) .....	44
4.8.7	Isotope (Conditional) .....	44
4.9	Amount (Conditional) .....	46
4.9.1	Average .....	46
4.9.2	Low limit .....	47
4.9.3	High limit .....	47
4.9.4	Unit .....	47
4.9.5	Non-numeric Value .....	48
4.9.6	Reference Source (Conditional) .....	48
4.9.7	Reference source document (Conditional) .....	48
4.10	Source material (Conditional) .....	48
4.10.1	Source material class .....	49
4.10.2	Source material type .....	50
4.10.3	Source material state .....	50
4.10.4	Organism ID .....	50
4.10.5	Organism name .....	51
4.10.6	Parent substance ID .....	51
4.10.7	Parent substance name .....	51
4.10.8	Development stage .....	52
4.10.9	Part Description (CONDITIONAL) .....	52
4.10.10	Fraction (Conditional) .....	54
4.10.11	Organism (Conditional) .....	57
4.11	Modification (Conditional) .....	64
4.11.1	Modification type .....	66
4.11.2	Residue modified .....	66
4.11.3	Residue sites .....	66
4.11.4	Structural modification (Conditional) .....	67
4.11.5	Agent modification (Conditional) .....	69
4.11.6	Physical Modification (Conditional) .....	70
4.12	Property (Conditional) .....	72
4.12.1	Property type .....	72
4.12.2	Property name .....	73
4.12.3	Property parameters .....	73
4.12.4	Substance ID .....	73
4.12.5	Substance name .....	74
4.12.6	Amount type (Mandatory) .....	74
4.13	Version (Mandatory) .....	74
4.13.1	Version number .....	74
4.13.2	Effective date .....	75
4.13.3	Change made .....	75
5	Substance definitions .....	75
5.1	Chemical substance .....	75
5.1.1	Comment .....	76
5.1.2	Structure .....	77
5.1.3	Stoichiometric/Non-stoichiometric chemicals .....	77
5.1.4	Stoichiometric chemicals .....	78
5.1.5	Non-stoichiometric chemicals (Conditional) .....	81
5.1.6	Substance Name (Mandatory) .....	83
5.1.7	Substance Code (Conditional) .....	83
5.1.8	Version (Mandatory) .....	83
5.1.9	Reference information .....	83
5.1.10	Reference source (Conditional) .....	83
5.1.11	Reference source document (Conditional) .....	83
5.2	Proteins/peptides .....	83
5.2.1	Microheterogeneity .....	84
5.2.2	Sequence type .....	86
5.2.3	Number of subunits .....	86
5.2.4	Disulfide linkage .....	86
5.2.5	Comment .....	87
5.2.6	Protein subunit (Mandatory) .....	87

5.2.7	Molecular weight (Conditional)	90
5.2.8	Glycosylation (Conditional)	91
5.2.9	Property (Conditional)	92
5.2.10	Structure (Mandatory)	93
5.2.11	Substance name (Mandatory)	93
5.2.12	Modification (Conditional)	93
5.2.13	Substance code (Conditional)	93
5.2.14	Source material (Conditional)	93
5.2.15	Version (Mandatory)	93
5.2.16	Reference information (Conditional)	93
5.2.17	Reference source (Conditional)	93
5.2.18	Reference source document (Conditional)	93
5.3	Nucleic acids	93
5.3.1	Structure (Conditional)	94
5.3.2	Sequence type	95
5.3.3	Number of subunits	95
5.3.4	Area of hybridisation	96
5.3.5	Comment	96
5.3.6	Nucleic acid subunit (Mandatory)	96
5.3.7	Modification (Conditional)	100
5.3.8	Property (Conditional)	100
5.3.9	Molecular weight (Conditional)	101
5.3.10	Substance Name (Mandatory)	101
5.3.11	Substance Code (Conditional)	101
5.3.12	Version (Mandatory)	101
5.3.13	Reference information (Conditional)	101
5.3.14	Reference source (Conditional)	101
5.3.15	Reference source document (Conditional)	101
5.4	Polymers	101
5.4.1	Polymer class	103
5.4.2	Polymer geometry	103
5.4.3	Copolymer sequence type	103
5.4.4	Comment	103
5.4.5	Substance name (Mandatory)	103
5.4.6	Structure (Mandatory)	104
5.4.7	Monomer description (Conditional)	104
5.4.8	Structural repeat (Conditional)	105
5.4.9	Molecular weight (Mandatory)	108
5.4.10	Property (Conditional)	108
5.4.11	Substance code (Conditional)	108
5.4.12	Version (Mandatory)	108
5.4.13	Reference information (Conditional)	108
5.4.14	Modification (Conditional)	108
5.4.15	Source material (Conditional)	109
5.4.16	Reference source (Conditional)	109
5.4.17	Reference source document (Conditional)	109
5.5	Structurally diverse substances	109
5.5.1	Comment	110
5.5.2	Substance name (Mandatory)	110
5.5.3	Structure (Mandatory)	110
5.5.4	Property (Conditional)	110
5.5.5	Molecular weight	111
5.5.6	Glycosylation (Conditional)	111
5.5.7	Modification (Conditional)	111
5.5.8	Source material (Conditional)	111
5.5.9	Substance code (Conditional)	111
5.5.10	Reference information (Conditional)	111
5.5.11	Version (Mandatory)	111
5.5.12	Reference source (Conditional)	111
5.5.13	Reference source document (Conditional)	111
5.5.14	Herbals and substances used in the preparation of plant-based allergenic extracts	111
5.5.15	Vaccines	114

5.5.16	Plasma-derived substance for human blood products and polyclonal antibodies .....	114
5.5.17	Allergens .....	114
5.5.18	Advance Therapies and Advanced Vaccines (Genes, Modified Viruses, Cells and Tissues as Substances) .....	115
5.5.19	Minerals .....	115
5.6	Mixture substance .....	116
5.6.1	Mixture type .....	116
5.6.2	Mixture constituent (Mandatory) .....	116
5.6.3	Modification (Conditional) .....	117
5.6.4	Source material (Conditional) .....	117
5.6.5	Substance name (Mandatory) .....	117
5.6.6	Substance code (Conditional) .....	117
5.6.7	Reference information (Conditional) .....	118
5.6.8	Version (Mandatory) .....	118
6	Specified substance (Optional) .....	118
6.1	Specified Substance Group 1 (repeat as necessary) .....	118
6.1.1	Specified substance Group 1 ID .....	119
6.1.2	Specified substance Group1 Name .....	120
6.1.3	Substance Name (Mandatory) .....	120
6.1.4	Substance Code (Conditional) .....	120
6.1.5	Version (Mandatory) .....	120
6.1.6	Reference source (Conditional) .....	120
6.1.7	Reference source document (Conditional) .....	120
6.1.8	Property (Conditional) .....	120
6.1.9	Fraction (Conditional) .....	121
6.1.10	Modification (Conditional) .....	125
6.1.11	Reference Information (Conditional) .....	125
6.1.12	Constituent (Mandatory) .....	125
6.1.13	Physical form (Conditional) .....	127
6.1.14	Specified substance particulars .....	128
6.2	Specified substance Group 2 .....	133
6.2.1	Specified Substance Group2 ID .....	135
6.2.2	Specified Substance Group2 Name .....	136
6.2.3	Parent Substance ID .....	136
6.2.4	Reference source (Conditional) .....	136
6.2.5	Reference source document (Conditional) .....	136
6.2.6	Manufacturing (Mandatory) .....	136
6.3	Specified Substance Group 2 for Herbal preparations .....	142
6.3.1	Specified Substance Group2 ID .....	142
6.3.2	Specified substance Group2 Name .....	142
6.3.3	Parent Substance ID .....	142
6.3.4	Manufacturing .....	143
6.3.5	Version .....	144
6.4	Specified Substance Group 3 .....	144
6.4.1	Specified Substance Group 3 ID .....	145
6.4.2	Specified Substance Group3 Name .....	145
6.4.3	Parent Substance ID .....	145
6.4.4	Grade (Mandatory) .....	145
6.4.5	Version (Mandatory) .....	146
6.4.6	Reference source (Conditional) .....	146
6.4.7	Reference source document (Conditional) .....	147
6.4.8	Substance name (Mandatory) .....	147
6.4.9	Substance code (Conditional) .....	147
6.4.10	Version (Mandatory) .....	147
7	Description of the information modelling principles and practices .....	147
Annex A (normative)	Choosing a Substance ID .....	148
Annex B (normative)	Chemical substance .....	150

<b>Annex C (normative) Protein substance .....</b>	<b>270</b>
<b>Annex D (normative) Nucleic acid substance .....</b>	<b>329</b>
<b>Annex E (normative) Structurally Diverse Substance - Herbal Substance/Herbal Specified Substance .....</b>	<b>348</b>
<b>Annex F (normative) Structurally Diverse Substance, Homeopathic substance .....</b>	<b>466</b>
<b>Annex G (normative) Structurally Diverse Substance - Plasma-derived substances .....</b>	<b>509</b>
<b>Annex H (normative) Polymer Substance .....</b>	<b>581</b>