UPOV
International Union for the Protection of New Varieties of Plants

E

Technical Working Party on Automation and Computer Programs **TWC/35/20**

Thirty-Fifth Session
Buenos Aires, Argentina, November 14 to 17, 2017

Original: English
Date: November 20, 2017

STANDARDS FOR DATABASES CONTAINING MOLECULAR INFORMATION

Document prepared by the Office of the Union

Disclaimer: this document does not represent UPOV policies or guidance

The Annex to this document contains a copy of a presentation on "Standards for databases containing molecular information" made by the Office of the Union at the thirty-fifth session of the Technical Working Party on Automation and Computer Programs (TWC).

[Annex follows]

Standards for databases containing molecular information

November 7, 2017

UPOV
International Union for the Protection of New Varieties of Plants

PREVIEW

- Databases
- WIPO ST.26
- WIPO ST.26 Software

2

Databases

- Organized array of information
- Place where you put things in, and you should be able to get them out again.
- Allows you to search.

UPOV

3

What you can store

- Fingerprints
  - 1-D electrophoresis gels scanned as bitmaps (RFLP, PFGE, Ribotyping, RAPD, DGGE & TGGE, etc.)
  - Sequencer chromatogram files (AFLP, VNTR, HDA, etc.)
  - Spectrophotometric files
  - MALDI & SELDI profiles
  - All other kinds of densitometric profiles
- Character data : Phenotypic test panels
  - Antibiotic resistance profiles
  - Fatty acid and quinolone profiles
  - Hybridization blots
  - Biochemical & morphological features
  - Microarray & Genechip data

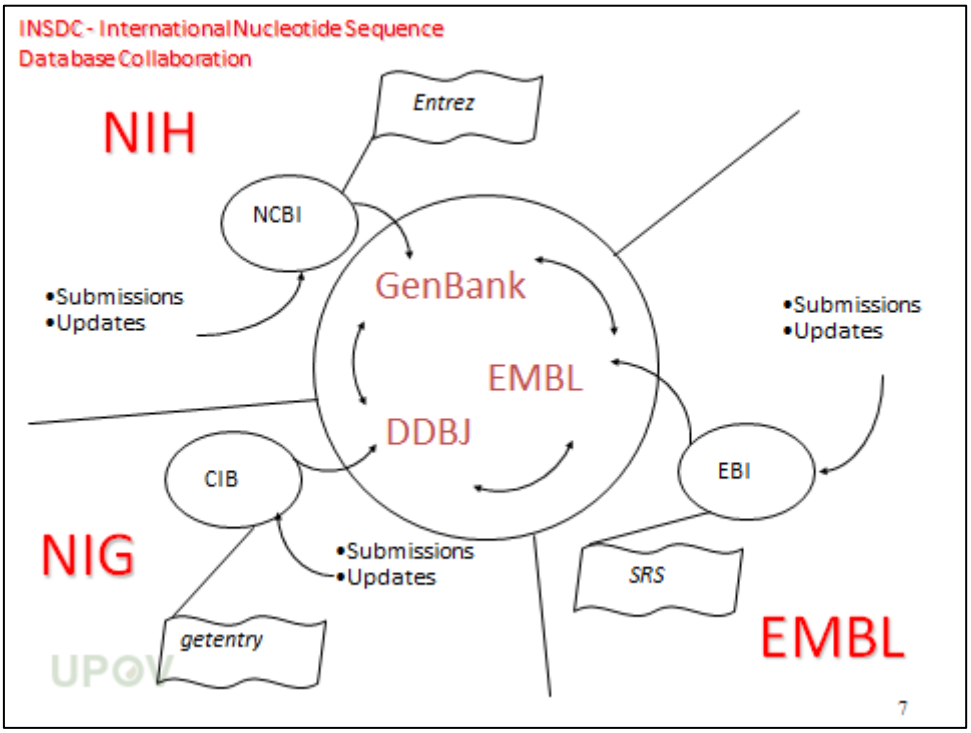
UPOV

What you can store (cont'd)

- Sequence data
  - Sequence trace (chromatogram) files
  - Formatted sequences from public databases (EMBL, GenBank)
  - Aligned sequences
  - Amino acid sequences

Database Examples in Bioinformatics

	Primary database	Secondary database
Synonyms	Archival database	Curated database; knowledgebase
Source of data	Direct submission of experimentally-derived data from researchers	Results of analysis, literature research and interpretation, often of data in primary databases
Examples	✓ GenBank/EMBL/DDBJ (nucleotide sequence) ✓ Protein Data Bank (PDB, coordinates of three-dimensional macromolecular structures) ✓ Medline (literature) ✓ IMEx databases (protein interactions) ✓ ArrayExpress Archive and GEO (functional genomics data)	✓ InterPro(protein families, motifs and domains) ✓ UniProt Knowledgebase - SwissProt (sequence and functional information on proteins) ✓ Ensembl (variation, function, regulation and more layered onto whole genome sequences)



PREVIEW

- Databases
- WIPO ST.26
- WIPO ST.26 Software

8

What is WIPO ST.26?

- ST.26 is the recommended standard for the presentation of nucleotide and amino acid sequence listings using XML
- It defines the sequence disclosures in a patent application required to be included in a sequence listing

9

WIPO ST.26

- Based on INSDC specifications
- Faciliates searching of the sequence data
- Allows sequence data to be exchanged in electronic form and introduced into computerized databases.

UPOV

Sequence Listing in XML
General information part

- ApplicationIdentification : Mandatory
  - IPOfficeCode
  - ApplicationNumberText
  - FilingDate
- ApplicantFileReference: Optional
- EarliestPriorityApplicationIdentification : Mandatory if Priority is claimed
- ApplicantName : Mandatory
- ApplicantNameLatin : Optional
- InventorName: Optional
- InventorNameLatin: Optional
- InventionTitle: Mandatory in the language of filing
- SequenceTotalQuantity: Mandatory

UPOV

Sequence Listing in XML
Sequence Data part

- One or more SequenceData elements
- Each SequenceData has a mandatory attribute sequenceIDNumber

Element	Description	Mandatory/Not Included	
		Sequences	Intentionally Skipped Sequences
INSDSeq_length	Length of the sequence	Mandatory	Mandatory with no value
INSDSeq_moltype	Molecule type	Mandatory	Mandatory with no value
INSDSeq_division	Indication that a sequence is related to a patent application	Mandatory with the value "PAT"	Mandatory with no value
INSDSeq_feature-table	List of annotations of the sequence	Mandatory	Must NOT be included
INSDSeq_sequence	Sequence	Mandatory	Mandatory with the value "000"

UPOV

Feature Keys and Qualifiers

- Nucleic Acid Sequences
  - Agreed upon by the International Nucleotide Sequence Database Collaboration (INSDC)
  - 49 feature keys and 80 qualifiers for nucleic acid sequences: INSDC feature keys/qualifiers not relevant for patent data not included

UPOV

13

Sequence Listing in XML

Sequence Data part

Feature Table

- Information on location and roles of various regions within a particular sequence
- One or more INSDFeature elements

Element	Description	Mandatory\Optional
INSDFeature_key	A word or abbreviation indicating a feature	Mandatory
INSDFeature_location	Region of the presented sequence which corresponds to the feature	Mandatory
INSDFeature_quals	Qualifier containing auxiliary information about a feature	Mandatory where the feature key requires one or more qualifiers, e.g. source; otherwise, Optional

UPOV

Variety

qualifier	variety
definition	variety (= varietas, a formal Linnaean rank) of organism from which sequence was derived.
value format	free text (NOTE: this value may require translation for national/regional procedures)
example	<INSDqualifier_value>insularis</INSDqualifier_value>
comment	use the cultivar qualifier for cultivated plant varieties, i.e., products of artificial selection; varieties other than plant and fungal varietas should be annotated via a note qualifier, e.g. with the value <INSDqualifier_value>breed:cukorova</INSDqualifier_value>

UPOV

Example: PP28388

- Variety: CIMAP-KHUSINOLIKA
- Species/Crop: VETIVER (CHRYSOPOGON ZIZANIODES)
- Phenotype: PRODUCES KHUSINOL RICH ESSENTIAL OIL UNDER SHORT DURATION CULTIVATION
- What is stored: ISSR-PCR primers

UPOV

```
<ST26SequenceListing dtdVersion="V1_0 " fileName="PP28388.xml" productionDate="2013-12-17">
  <ApplicationIdentification>
    <IPOfficeCode>US</IPOfficeCode>
    <ApplicationNumberText>14/545,762</ApplicationNumberText>
    <FilingDate>06-15-2015</FilingDate>
  </ApplicationIdentification>
  <ApplicantFileReference/>
  <InventionTitle languageCode="en">CIMAP-KHUSINOLIKA</InventionTitle>
  <SequenceTotalQuantity>10</SequenceTotalQuantity>
  <SequenceData sequenceIDNumber="1">
    <INSDSeq>
      <INSDSeq_length>17</INSDSeq_length>
      <INSDSeq_moltype>DNA</INSDSeq_moltype>
      <INSDSeq_division>PAT</INSDSeq_division>
      <INSDSeq_feature-table>
        <INSDFeature>
          <INSDFeature_key>source</INSDFeature_key>
          <INSDFeature_location>1..17</INSDFeature_location>
          <INSDFeature_quals>
            <INSDQualifier>
              <INSDQualifier_name>organism</INSDQualifier_name>
              <INSDQualifier_value>Artificial</INSDQualifier_value>
            </INSDQualifier>
            <INSDQualifier>
              <INSDQualifier_name>Cultivar</INSDQualifier_name>
              <INSDQualifier_value>VETIVER ( CHRYSOPOGON ZIZANIODES )</INSDQualifier_value>
            </INSDQualifier>
            <INSDQualifier>
              <INSDQualifier_name>Phenotype</INSDQualifier_name>
              <INSDQualifier_value>PRODUCES KHUSINOL RICH
ESSENTIAL OIL UNDER SHORT DURATION CULTIVATION</INSDQualifier_value>
            </INSDQualifier>
              <INSDQualifier>
              <INSDQualifier_name>Variety</INSDQualifier_name>
              <INSDQualifier_value>CIMAP-KHUSINOLIKA</INSDQualifier_value>
```


UPOV

ISSR Primer


```
            <INSDQualifier>
              <INSDQualifier_name>note</INSDQualifier_name>
              <INSDQualifier_value>A synthetic ISSR Primer</INSDQualifier_value>
            </INSDQualifier>
          </INSDFeature_quals>
        </INSDFeature>
      </INSDSeq_feature-table>
      <INSDSeq_sequence>agagagagag agagagt </INSDSeq_sequence>
    </INSDSeq>
  </SequenceData>
```


UPOV

Example: PP16174

- Variety: B12
- Sepecies/Crop: ST. AUGUSTINE GRASS
- Prior application number: AU PBR 2002/342
- What is stored: Primer
  - ccgcatctac

UPOV


```xml
<?xml version="1.0" encoding="UTF-8"?>
<!DOCTYPE ST26SequenceListing SYSTEM "D:\Users\madhour\Desktop\IFREZ\03-26-ii_v1-1.dtd">
<ST26SequenceListing dtdVersion="V1_0 " fileName="PP16174.xml" productionDate="2013-12-17">
  <ApplicationIdentification>
    <IPOfficeCode>US</IPOfficeCode>
    <ApplicationNumberText>10/663,928</ApplicationNumberText>
    <FilingDate>09-16-2003</FilingDate>
  </ApplicationIdentification>
  <ApplicantFileReference/>
  <EarliestPriorityApplicationIdentification>
    <IPOfficeCode>AU</IPOfficeCode>
    <ApplicationNumberText>AU PBR 2002/342</ApplicationNumberText>
  </EarliestPriorityApplicationIdentification>
  <InventionTitle languageCode="en">ST. AUGUSTINE GRASS NAMED 'B12'</InventionTitle>
  <SequenceTotalQuantity>1</SequenceTotalQuantity>
  <SequenceData sequenceIDNumber="1">
    <INSDSeq>
      <INSDSeq_length>10</INSDSeq_length>
      <INSDSeq_moltype>DNA</INSDSeq_moltype>
      <INSDSeq_division>PAT</INSDSeq_division>
      <INSDSeq_feature-table>
        <INSDFeature>
          <INSDFeature_key>source</INSDFeature_key>
          <INSDFeature_location>1..9</INSDFeature_location>
          <INSDFeature_quals>
            <INSDQualifier>
              <INSDQualifier_name>organism</INSDQualifier_name>
              <INSDQualifier_value>Artificial</INSDQualifier_value>
            </INSDQualifier>
            <INSDQualifier>
              <INSDQualifier_name>Cultivar</INSDQualifier_name>
              <INSDQualifier_value>ST. AUGUSTINE GRASS</INSDQualifier_value>
            </INSDQualifier>
              <INSDQualifier>
            <INSDQualifier_name>Variety</INSDQualifier_name>
            <INSDQualifier_value>B12</INSDQualifier_value>
            </INSDQualifier>
```


UPOV

Primer


```
<INSDQualifier>
  <INSDQualifier_name>note</INSDQualifier_name>
  <INSDQualifier_value>Primer</INSDQualifier_value>
</INSDQualifier>
</INSDFeature_quals>
</INSDFeature>
</INSDSeq_feature-table>
<INSDSeq_sequence>ccgcatctac</INSDSeq_sequence>
</INSDSeq>
</SequenceData>
</ST26SequenceListing>
```


UPOV

Example: PP15792

- Variety: BEINEKE 8
- Species/Crop: Black walnut
- What is stored: 18 primers
  - gacgacgaag gtgtacggat
  - ccatgaaact tcatgcgttg
  - ……
  - ttgaacaaaa ggccgttttc

UPOV

Example: PCT/US2015/055339

- TOMATO PLANTS WITH IMPROVED DISEASE RESISTANCE
- UPOV TG/44/11 Char 57: resistance to Tomato yellow leaf curl virus
- What is stored: probes and primers

UPOV


```
<SequenceData sequenceIDNumber="9">
<INSDSeq>
  <INSDSeq_length>10</INSDSeq_length>
  <INSDSeq_moltype>DNA</INSDSeq_moltype>
  <INSDSeq_division>PAT</INSDSeq_division>
  <INSDSeq_feature-table>
    <INSDFeature>
      <INSDFeature_key>source</INSDFeature_key>
      <INSDFeature_location>10..21</INSDFeature_location>
      <INSDFeature_quals>
                <INSDQualifier>
          <INSDQualifier_name>note</INSDQualifier_name>
          <INSDQualifier_value>Probe</INSDQualifier_value>
        </INSDQualifier>
      </INSDFeature_quals>
    </INSDFeature>
  </INSDSeq_feature-table>
  <INSDSeq_sequence>ctaatggtgt aactccccaa g</INSDSeq_sequence>
</INSDSeq>
</SequenceData>
<SequenceData sequenceIDNumber="10">
<INSDSeq>
  <INSDSeq_length>10</INSDSeq_length>
  <INSDSeq_moltype>DNA</INSDSeq_moltype>
  <INSDSeq_division>PAT</INSDSeq_division>
  <INSDSeq_feature-table>
    <INSDFeature>
      <INSDFeature_key>source</INSDFeature_key>
      <INSDFeature_location>10..21</INSDFeature_location>
      <INSDFeature_quals>
                <INSDQualifier>
          <INSDQualifier_name>note</INSDQualifier_name>
          <INSDQualifier_value>Primer</INSDQualifier_value>
        </INSDQualifier>
      </INSDFeature_quals>
    </INSDFeature>
  </INSDSeq_feature-table>
  <INSDSeq_sequence>cctggccctt ccgaaagaa</INSDSeq_sequence>
</INSDSeq>
</SequenceData>
```


UPOV

PREVIEW

- Databases
- WIPO ST.26
- WIPO ST.26 Software

UPOV

25

WIPO ST.26 Software

- Editing or importing sequences in ST.26 format
- Validation of sequences
- Transformation of ST.25 sequences to ST.26
- Importing existing sequence data in industry format, e.g. GenBank, EMBL and FASTA
- Presentation of XML in human readable format
- Multi language support: interface, message
- "Free text" translation support (the "free text" must be in Basic Latin in the sequence listing)

UPOV

Timelines

- End of 2017: Proof of concept
- 2018: Testing and upgrades

UPOV

[End of Annex and of document]