Molecular Profiling Research Center for Drug Discovery (MolProf), AIST

Semantic Analysis Service (SIO version)

User Manual

AIST
2015/07/24

Service		OWL classes corresponding to each input RDF
Blast	S	http://www.molprof.jp/ontologies/aistlssio.owl#BlastInput
CentroidFold	S	http://www.molprof.jp/ontologies/aistlssio.owl#CentroidFoldInput
ClustalW	S	http://www.molprof.jp/ontologies/aistlssio.owl#ClustalWInput
IPknot	S	http://www.molprof.jp/ontologies/aistlssio.owl#IPknotInput
Mafft	S	http://www.molprof.jp/ontologies/aistlssio.owl#MafftInput
Psipred	S	http://www.molprof.jp/ontologies/aistlssio.owl#PsiPredInput
Raccess	S	http://www.molprof.jp/ontologies/aistlssio.owl#RaccessInput
RactIP	S	http://www.molprof.jp/ontologies/aistlssio.owl#RactIPInput
Wolfpsort	S	http://www.molprof.jp/ontologies/aistlssio.owl#WolfPsortInput
Last	A	http://www.molprof.jp/ontologies/aistlssio.owl#LastInput
Modelling	A	http://www.molprof.jp/ontologies/aistlssio.owl#ModellingInput
PoodleL	A	http://www.molprof.jp/ontologies/aistlssio.owl#PoodleLInput
PoodleS	A	http://www.molprof.jp/ontologies/aistlssio.owl#PoodleSInput
Rassie	A	http://www.molprof.jp/ontologies/aistlssio.owl#RassieInput

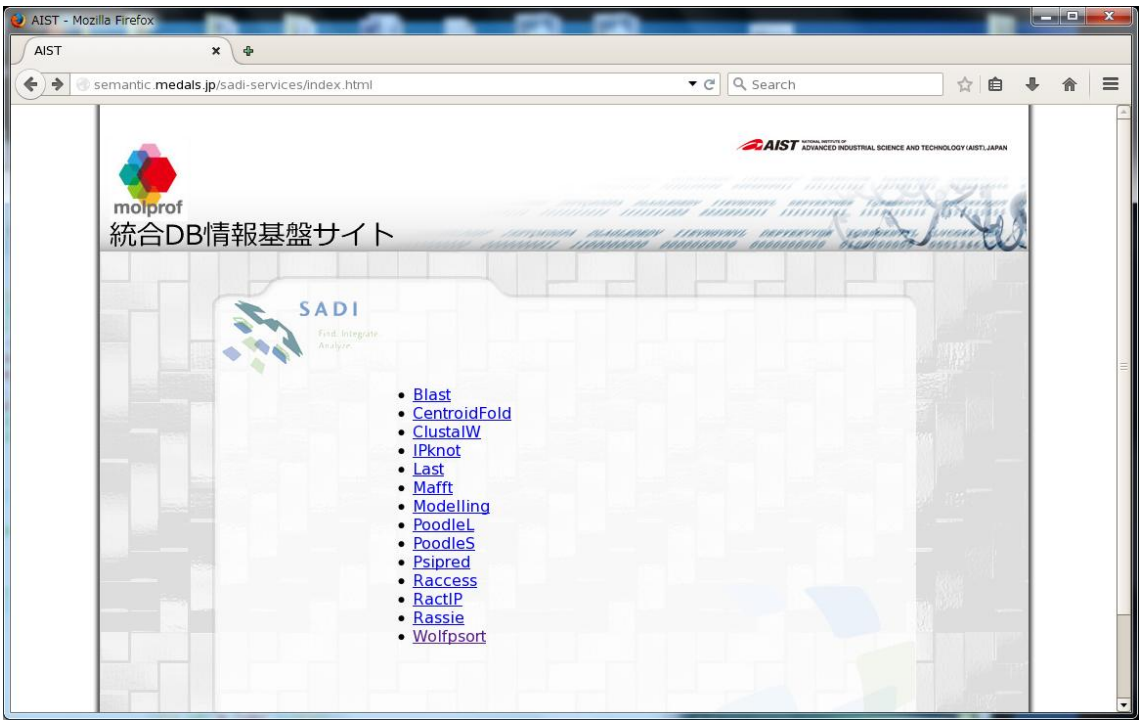
Figure 1-A Semantic web services and their input OWL class URLs

*** S: Synchronous, A: Asynchronous**

1. Synchronous type SADI services

1.0. Uses of synchronous type SADI services

The user can access “http://semantic.medals.jp:8090/sadi-services/index.html” and available SADI services are displayed on your web browser.



SADI service

Synchronous SADI services are Blast, CentroidFold, ClustalW, IPknot, Mafft, Psipred, Raccess, RactIP and Wolfpsort, and these services are executed by using the following cURL commands.

% curl --data-binary @"iput RDF file"
http://semantic.medals.jp:8090/sadi-services/"SADI service name" (Figure 1-A) -o "output RDF file name"

If the user would like to execute Wolfpsort SADI service with an input.rdf and to get an output.rdf stored Wolfpsort service results,

% curl --data-binary @input.rdf
http://semantic.medals.jp:8090/sadi-services/Wolfpsort -o output.rdf

This input RDF format is as follows:

```
<rdf:RDF
   xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
   xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#"
   xmlns:sio="http://semanticscience.org/resource/">
   <aistls:WolfPsortInput
rdf:about="http://www.molprof.jp/ontologies/wolfpsort.rdf#1">
       <sio:SIO_000230>
          <aistls:Kingdom rdf:about="#plant"/>
       </sio:SIO_000230>
       <aistls:SIO_000230>
          <sio:SIO_010015>
             <sio:SIO_000300>
   >sp|P35413|GPR3_MOUSE G-protein coupled receptor 3 OS=Mus musculus GN=Gpr3 PE=2 SV=1
   MMWGAGSSMAWFSAGSGSVNVSSVDPVEEPTGPATLLPSPRAWDVVLCISGTLVSCENAL
   VVAIIVGTPAFRAPMFLLVGSLAVADLLAGLGLVLHFAADFCIGSPEMSLMLVGVLAMAF
   TASIGSLLAITVDRYLSLYNALTYYSETTVTRTYVMLALVWVGALGLGLVPVLAWNCRDG
   LTTCGVVYPLSKNHLVVLAIAFFMVFGIMLQLYAQICRIVCRHAQQIALQRHLLPASHYV
   ATRKGIATLAVVLGAFAACWLPFTVYCLLGDADSPRLYTYLTLLPATYNSMINPVIYAFR
   NQDVQKVLWAICCCCSTSKIPFRSRSPSDV
             </sio:SIO_000300>
          </sio:SIO_010015>
       </aistls:SIO_000230>
   </aistls:WolfPsortInput>
</rdf:RDF>
```

Input RDF for Wolfpsort SADI service

- Black: start and end tag of RDF
- Green: name spaces and their corresponding URLs
- Red: subject (input OWL class to execute a SADI service (Figure 1-A), and an arbitrary string
  e.g. WolfPsort
  input OWL class : aistls:WolfPsortInput
  URL: http://www.molprof.jp/ontologies/wolfpsort.rdf#1

・ Blue: triples required to execute a SADI service

<e.g. Wolfpsort >

=Kingdon information=

Subject: WolfPsortInput

Predicate: SIO_000230 (has input)

Object: Kingdom (rdf:about="#plant" (animal, plant or fungi))

=Protein sequence=

Subject: WolfPsortInput

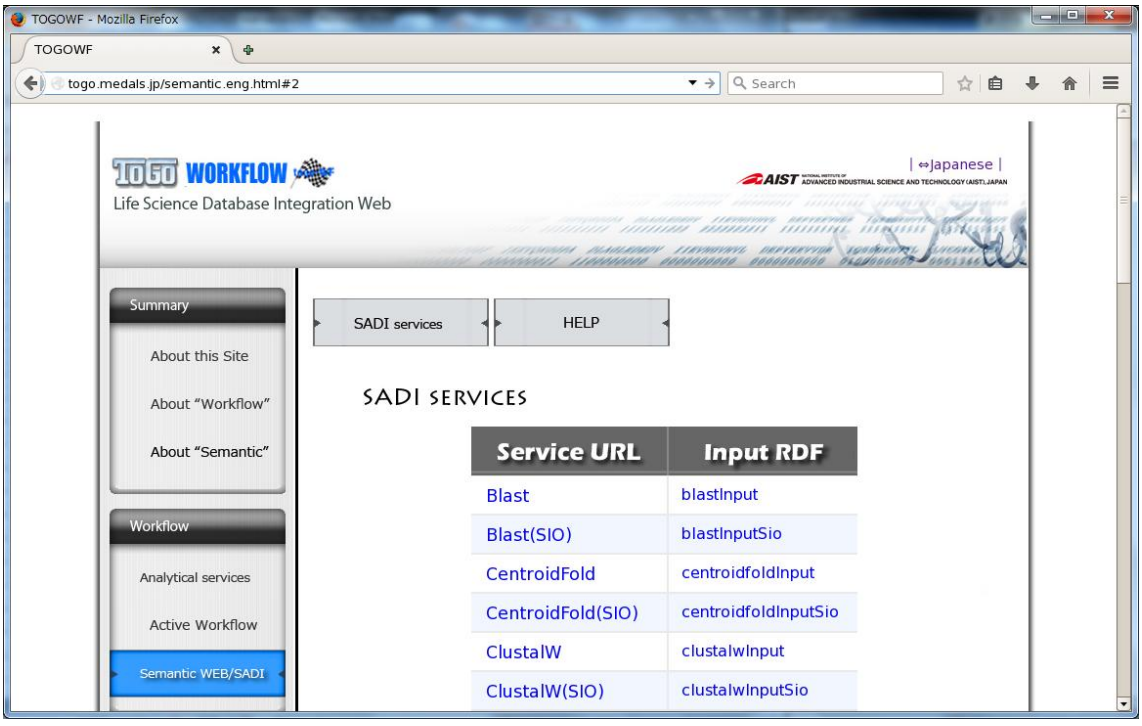
Predicate: SIO_000230 (has input)

Object (Subject): SIO_010015 (protein sequence)

Predicate: SIO_000300 (has value)

Object: string (protein sequence)

The user can download sample input RDFs on http://togo.medals.jp/semantic.eng.html#2 web page (click each links in “Input RDF” column (SIO))



SADI service page

A RDF stored execution results of WolfPsort is generated in the following format:

```
<rdf:RDF
    xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
    xmlns:sio="http://semanticscience.org/resource/"
    xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#">
    <aistls:WolfPsortOutput rdf:about="http://www.molprof.jp/ontologies/wolfpsort.rdf#2">
       <sio:SIO_000229>
          <sio:SIO_000785>
             <sio:SIO_000300># k used for kNN is: 14
    sp|P35413|GPR3_MOUSE cyto 7, extr 3, plas 2, E.R. 2, E.R._plas 2
             </sio:SIO_000300>
          </sio:SIO_000785>
       </sio:SIO_000229>
    </aistls:WolfPsortOutput>
</rdf:RDF>
```

Wolfpsort output RDF

- Red: output OWL class to execute a SADI service (Figure 1-A), and an arbitrary string
- Blue: triples required to display Wolfpsort execution result

  <e.g.Wolfpsort>

  Subject: WolfPsortOutput

  Predicate: SIO_000229 (has output)

  Object (Subject): SIO_000785 (answer)

  Predicate: SIO_000300 (has value)

  Object: string (WolfPsort result)

* If the user doesn't have cURL software, please visit a cURL web site.

http://curl.haxx.se/

1.1. Blast

1.1.1. Preparing input RDF

Blast input RDF format is as follows:

- RDF header:
  <rdf:RDF
    xmlns:rdf “http://www.w3.org/1999/02/22-rdf-syntax-ns#”
    xmlns:aistls “http://www.molprof.jp/ontologies/aistlssio.owl#”
    xmlns:sio “http://semanticscience.org/resource/”>
- Subject: BlastInput, rdf:about: an arbitrary string
  <aistls:BlastInput rdf:about=”http://www.molprof.jp/ontologies/blast.rdf#1”>
- Triple for a query sequence:
  Subject: BlastInput
  Predicate: SIO_000230 (has input)
  Object (Subject): SIO_000030 (biopolymer sequence)
    Predicate: SIO_000300 (has value)
    Object: string (query sequence)

```
<sio:SIO_000230>
    <sio:SIO_000030>
        <sio:SIO_000300>
            Query sequence
        <sio:SIO_000300>
    </sio:SIO_000030>
</sio:SIO_000230>
```

- Triple for Blast program
  Subject: BlastInput
  Predicate: SIO_000230 (has input)
  Object (Subject): BlastProgram (rdf:about="#blastp" (blastp, blastn, blastx, tblastn or tblastx))
  <sio:SIO_000230>

<aistls:BlastProgram rdf:about="#blastp"/>
</sio:SIO_000230>

- Triple for database:

Subject: BlastInput

Predicate: SIO_000300 (has input)

Object (Subject): BlastDatabase

Predicate: SIO_000300 (has value)

Object: 文字列 (SWISS, TREMBL, UNIPROT, PROTEIN, PDB etc.)

*Please visit a below URL for further database information:

http://blast.ncbi.nlm.nih.gov/Blast.cgi

<sio:SIO_000230>
<aistls:BlastDatabase>
<sio:SIO_000300>
SWISS
</sio:SIO_000300>
</aistls:BlastDatabase>
</sio:SIO_000230>

- Tripe for E-value:

Subject: BlastInput

Predicate: SIO_000230 (has input)

Object (Subject): SIO_001021 (expected value)

Predicate: SIO_000300 (has value)

Object: double (E-value)

<sio:SIO_000230>
<sio:SIO_001021>
<sio:SIO_000300>
1.0e-30
</sio:SIO_000300>
</sio:SIO_001021>
</sio:SIO_000230>

Sample input RDF file is as follows:

```
<rdf:RDF
    xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
    xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#"
    xmlns:sio="http://semanticscience.org/resource/">

    <aistls:BlastInput rdf:about="http://www.molprof.jp/ontologies/blast.rdf#1">
       <sio:SIO_000230>
          <sio:SIO_000030>
             <sio:SIO_000300>
    >sp|P35413|GPR3_MOUSE G-protein coupled receptor 3 OS=Mus musculus GN=Gpr3 PE=2 SV=1
    MMWGAGSSMAWFSAGSGSVNVSSVDPVEEPTGPATLLPSPRAWDVVLCISGTLVSCENAL
    VVAIIVGTPAFRAPMFLLVGSLAVADLLAGLGLVLHFAADFCIGSPEMSLMLVGVLAMAF
    TASIGSLLAITVDRYLSLYNALTYYSETTVTRTYVMLALVWVGALGLGLVPVLAWNCRDG
    LTTCGVVYPLSKNHLVVLAIAFFMVFGIMLQLYAQICRIVCRHAQQIALQRHLLPASHYV
    ATRKGIATLAVVLGAFAACWLPFTVYCLLGDADSPRLYTYLTLLPATYNSMINPVIYAFR
    NQDVQKVLWAICCCCSTSKIPFRSRSPSDV
             </sio:SIO_000300>
          </sio:SIO_000030>
       </sio:SIO_000230>
       <sio:SIO_000230>
          <aistls:BlastDatabase>
             <sio:SIO_000300>nr</sio:SIO_000300>
          </aistls:BlastDatabase>
       </sio:SIO_000230>
       <sio:SIO_000230>
          <aistls:BlastProgram rdf:about="#blastp"/>
       </sio:SIO_000230>
       <sio:SIO_000230>
          <sio:SIO_001021>
             <sio:SIO_000300>1.0e-30</sio:SIO_000300>
          </sio:SIO_001021>
       </sio:SIO_000230>
    </aistls:BlastInput>
</rdf:RDF>
```

Blast input RDF

1.1.2. Execution command

% curl --data-binary @"input RDF file"
http://semantic.medals.jp:8090/sadi-services/Blast -o "output RDF file"

1.1.3. Execution result

Blast output RDF format is as follows:

- Triple for RDF:
  <rdf:RDF
    xmlns:rdf “http://www.w3.org/1999/02/22-rdf-syntax-ns#”
    xmlns:aistls “http://www.molprof.jp/ontologies/aistlssio.owl#”
    xmlns:sio “http://semanticscience.org/resource/”>
- Subject: BlastOutput, rdf:about: the string as same as specifying in the input RDF file
  <aistls:BlastOutput rdf:about=”http://www.molprof.jp/ontologies/blast.rdf#1”>
- Tripe for Blast result:
  Subject: BlastOutput
  Predicate: SIO_000229 (has output)
  Object (Subject): BlastResult
    Predicate: SIO_000008 (has attribute)
    Object (Subject): BlastParameter
      Predicate: SIO_000008 (has attribue)
      Object (Subject): BlastFilter
        Predicate: SIO_000300 (has value)
        Object: literal (“T” or “F”)
      Predicate: SIO_000008 (has attribute)
      Object (Subject): BlastMatrix
        Predicate: SIO_000300 (has value)
        Object: literal (bl62, bl50, pam250 and so on)
      Predicate: SIO_000216 (has measurement value)
      Object (Subject): scoreMismatch
        Predicate: SIO_000300 (has value)
        Object: integer
      Predicate: : SIO_000216 (has measurement value)
      Object (Subject): scoreMatch
        Predicate: SIO_000300 (has value)
        Object: integer

Predicate: SIO_000216 (has measurement value)
Object (Subject): gapOpenPenalty
Predicate: SIO_000300 (has value)
Object: integer
Predicate: SIO_000216 (has measurement value)
Object (Subject): gapExtendPenalty
Predicate: SIO_000300 (has value)
Object: integer
Predicate: SIO_000216 (has measurement value)
Object (Subject): SIO_001021 (expected value)
Predicate: SIO_000300 (has value)
Object: double (e.g. 10e-30)
Predicate: SIO_000008 (has attribute)
Object (Subject): BlastProgram
Predicate: SIO_000300 (has value)
Object: string (blastp, blastn, blastx, tblastn or tblastx)
Predicate: SIO_000008 (has attribute)
Object (Subject): SIO_000176 (reference)
Predicate: SIO_000300 (has value)
Object: string (reference)
Predicate: SIO_000008 (has attribute)
Object (Subject): SIO_000135 (definition)
Predicate: SIO_000300 (has value)
Object: literal
Predicate: SIO_000008 (has attribute)
Object (Subject): BlastDatabase
Predicate: SIO_000300 (has value)
Object: string (e.g. nr, swissprot and so on)
Predicate: SIO_000008 (has attribute)
Object (Subject): SIO_000654 (software version label)
Predicate: SIO_000300 (has value)
Object: literal (BLAST version)
Predicate: SIO_000008 (has attribute)
Object (Subject): BlastHit
Predicate: SIO_000008 (has attribute)
Object (Subject): SIO_000135 (definition)

Predicate: SIO_000300 (has value)
Object: literal
Predicate: SIO_000008 (has attribute)
Object (Subject): BlastAlignment
Predicate: SIO_000008 (has attribute)
Object (Subject): query
Predicate: SIO_000008 (has attribute)
Object (Subject): SIO_000030 (biopolymer sequence)
Predicate: SIO_000300 (has value)
Object: string (query sequence)
Predicate: SIO_000216 (has measurement value)
Object (Subject): frame
Predicate: SIO_000300 (has value)
Object: integer
Predicate: SIO_000216 (has measurement value)
Object (Subject): SIO_000791 (sequence start position)
Predicate: SIO_000300 (has value)
Object: integer
Predicate: SIO_000216 (has measurement value)
Object (Subject): SIO_000792 (sequence end position)
Predicate: SIO_000300 (has value)
Object: integer
Predicate: SIO_000008 (has attribute)
Object (Subject): subject
Predicate: SIO_000008 (has attribute)
Object (Subject): SIO_000030 (biopolymer sequence)
Predicate: SIO_000300 (has value)
Object: string (query sequence)
Predicate: SIO_000008 (has attribute)

Object (Subject): sequenceLength
Predicate: SIO_000300 (has value)
Object: integer
Predicate: SIO_000216 (has measurement value)
Object (Subject): frame
Predicate: SIO_000300 (has value)
Object: integer
Predicate: SIO_000216 (has measurement value)
Object (Subject): SIO_000791 (sequence start position)
Predicate: SIO_000300 (has value)
Object: integer
Predicate: SIO_000216 (has measurement value)
Object (Subject): SIO_000792 (sequence end position)
Predicate: SIO_000300 (has value)
Object: integer
Predicate: SIO_000008 (has attribute)
Object (Subject): SIO_010068 (pairwise sequence alignment)
Predicate: SIO_000300 (has value)
Object: string (alignment symbol)
Predicate: SIO_000216 (has measurement value)
Object (Subject): bitScore
Predicate: SIO_000300 (has value)
Object: double (e.g. 570.852)
Predicate: SIO_000216 (has measurement value)
Object (Subject): SIO_001021 (expected value)
Predicate: SIO_000300 (has vlaue)
Object: double (e.g. 10e-30)
Predicate: SIO_000216 (has measurement value)
Object (Subject): numberOfGap
Predicate: SIO_000300 (has vlaue)

Object: integer
Predicate: SIO_000216 (has measurement value)
Object (Subject:): numberOfIdentity
Predicate: SIO_000300 (has vlaue)
Object: integer
Predicate: SIO_000216 (has measurement value)
Object (Subject): alignmentLength
Predicate: SIO_000300 (has vlaue)
Object: integer
Predicate: SIO_000216 (has measurement value)
Object (Subject): score
Predicate: SIO_000300 (has vlaue)
Object: double (e.g. 1422.0)
Predicate: SIO_000216 (has measurement value)
Object (Subject): numberOfPositive
Predicate: SIO_000300 (has vlaue)
Object: integer
Predicate: SIO_000216 (has measurement value)
Object (Subject): sequenceLength
Predicate: SIO_000300 (has value)
Object: integer
Predicate: SIO_000216 (has attribute)
Object (Subject): SIO_000794 (count)
Predicate: SIO_000300 (has value)
Object: integer (number of hit count)
Predicate: SIO_000673 (has unique identifier)
Object (Subject): SIO_000729 (record identifier)
Predicate: SIO_000300 (has value)
Object: Literal (hit target ID)
Predicate: SIO_000216 (has measurement value)
Object (Subject): iteration
Predicate: SIO_000300 (has value)
Object: integer (number of iteration)
Predicate: SIO_000673 (has unique identifier)
Object (Subject): SIO_000675 (unique identifier)
Predicate: SIO_000300 (has value)

Object: integer (unique ID)

```
<sio:SIO_000229>
    <aistls:BlastResult>
        <sio:SIO_000008>
            <aistls:BlastHit>
                <sio:SIO_000008>
                    <aistls:BlastAlignment>
                        <sio:SIO_000216>
                            <aistls:numberOfPositive>
                                <sio:SIO_000300>503</sio:SIO_000300>
                            </aistls:numberOfPositive>
                        </sio:SIO_000216>
                        <sio:SIO_000008>
                            <aistls:query>
                                <sio:SIO_000008>
                                    <sio:SIO_000030>
                                        <sio:SIO_000300>
                                            Hit region (query sequence)
                                        </sio:SIO_000300>
                                    </sio:SIO_000030>
                                </sio:SIO_000008>
                                <sio:SIO_000216>
                                    <aistls:frame>
                                        <sio:SIO_000300>
                                            1
                                        </sio:SIO_000300>
                                    </aistls:frame>
                                </sio:SIO_000216>
                                <sio:SIO_000216>
                                    <sio:SIO_000792>
                                        <sio:SIO_000300>
                                            613
                                        </sio:SIO_000300>
                                    </sio:SIO_000792>
                                </sio:SIO_000216>
                                <sio:SIO_000216>
```

<sio:SIO_000791>
<sio:SIO_000300>
66
</sio:SIO_000300>
</sio:SIO_000791>
</sio:SIO_000216>
</aistls:query>
</sio:SIO_000008>
<sio:SIO_000216>
<aistls:alignmentLength>
<sio:SIO_000300>551</sio:SIO_000300>
</aistls:alignmentLength>
</sio:SIO_000216>
<sio:SIO_000216>
<aistls:score>
<sio:SIO_000300>828.0</sio:SIO_000300>
</aistls:score>
</sio:SIO_000216>
<sio:SIO_000008>
<sio:SIO_010068>
<sio:SIO_000300>
Alignment symbol
</sio:SIO_000300>
</sio:SIO_010068>
</sio:SIO_000008>
<sio:SIO_000216>
<aistls:numberOfGap>
<sio:SIO_000300>11</sio:SIO_000300>
</aistls:numberOfGap>
</sio:SIO_000216>
<sio:SIO_000216>
<aistls:bitScore>
<sio:SIO_000300>747.881</sio:SIO_000300>
</aistls:bitScore>
</sio:SIO_000216>
<sio:SIO_000216>

```
        <aistls:numberOfIdentity>
            <sio:SIO_000300>503</sio:SIO_000300>
        </aistls:numberOfIdentity>
    </sio:SIO_000216>
    <sio:SIO_000216>
        <sio:SIO_001021>
            <sio:SIO_000300>0.0</sio:SIO_000300>
        </sio:SIO_001021>
    </sio:SIO_000216>
    <sio:SIO_000008>
        <aistls:subject>
            <sio:SIO_000008>
                <sio:SIO_000030>
                    <sio:SIO_000300>
                        Hit region (target sequence)
                    </sio:SIO_000300>
                </sio:SIO_000030>
            </sio:SIO_000008>
            <sio:SIO_000216>
                <aistls:frame>
                    <sio:SIO_000300>
                        1
                    </sio:SIO_000300>
                </aistls:frame>
            </sio:SIO_000216>
            <sio:SIO_000216>
                <sio:SIO_000792>
                    <sio:SIO_000300>
                        543
                    </sio:SIO_000300>
                </sio:SIO_000792>
            </sio:SIO_000216>
            <sio:SIO_000216>
                <sio:SIO_000791>
                    <sio:SIO_000300>
                        1
```

</sio:SIO_000300>
</sio:SIO_000791>
</sio:SIO_000216>
</aistls:subject>
</sio:SIO_000008>
</aistls:BlastAlignment>
</sio:SIO_000008>
<sio:SIO_000216>
<aistls:sequenceLength>
<sio:SIO_000300>8162</sio:SIO_000300>
</aistls:sequenceLength>
</sio:SIO_000216>
<sio:SIO_000008>
<sio:SIO_000729>
<sio:SIO_000300>XM_004010367</sio:SIO_000300>
</sio:SIO_000729>
</sio:SIO_000008>
<sio:SIO_000008>
<sio:SIO_000135>
<sio:SIO_000300>PREDICTED: Ovis aries chromodomain helicase DNA binding protein 8 (CHD8), mRNA</sio:SIO_000300>
</sio:SIO_000135>
</sio:SIO_000008>
<sio:SIO_000216>
<sio:SIO_000794>
<sio:SIO_000300>58</sio:SIO_000300>
</sio:SIO_000794>
</sio:SIO_000216>
</aistls:BlastHit>
</sio:SIO_000008>
</aistls:BlastResult>
</sio:SIO_000300>

Sample output RDF file is as follows:

```
<rdf:RDF
   xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
   xmlns:sio="http://semanticscience.org/resource/"
   xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#">
  <aistls:BlastOutput rdf:about="http://www.molprof.jp/ontologies/blast.rdf#1">
    <sio:SIO_000229>
      <aistls:BlastResult>
        <sio:SIO_000008>
          <aistls:BlastHit>
            <sio:SIO_000008>
              <aistls:BlastAlignment>
                <sio:SIO_000008>
                  <aistls:subject>
                    <sio:SIO_000008>
                      <sio:SIO_000030>

<sio:SIO_000300>QLPSGPQGLLRSAVNPWDVLLCVSGTVIAGENAL-VVALIASTPALRTPMFVLVGSLATADLLAGCGLILH
FVFQYLVPSETVSLLMVGFLVASFA-ASVSSLLAITVDRYLSVYNALTYYSRRTLLGVHLLLAATWTVSLGLGLMPVLGWNCL-AEQ
ATCSVVRPLTRSHVALLSAAFFAVFGIMLHLYVRICQVVWRHAHQIALQQHCLAPPH-LAATRKGVGTLAVVLGTFGASWLPFAIYC
VVGSREDPAVYTYATLLPATYNSMINPIIYAFR-NQEIQRALWLLFCGCSQSKVPFRSRSPSEV</sio:SIO_000300>
                    </sio:SIO_000030>
                  </sio:SIO_000008>
                  <sio:SIO_000216>
                    <aistls:frame>
                      <sio:SIO_000300>0</sio:SIO_000300>
                    </aistls:frame>
                  </sio:SIO_000216>
                  <sio:SIO_000216>
                    <sio:SIO_000792>
                      <sio:SIO_000300>365</sio:SIO_000300>
                    </sio:SIO_000792>
                  </sio:SIO_000216>
                  <sio:SIO_000216>
……
……
            </sio:SIO_000216>
            <sio:SIO_000008>
              <sio:SIO_000729>
                <sio:SIO_000300>XP_005529726</sio:SIO_000300>
              </sio:SIO_000729>
            </sio:SIO_000008>
            <sio:SIO_000008>
              <sio:SIO_000135>
                <sio:SIO_000300>PREDICTED: G-protein coupled receptor 12-like [Pseudopodoces
humilis]</sio:SIO_000300>
              </sio:SIO_000135>
            </sio:SIO_000008>
            <sio:SIO_000216>
              <sio:SIO_000794>
                <sio:SIO_000300>60</sio:SIO_000300>
              </sio:SIO_000794>
            </sio:SIO_000216>
          </aistls:BlastHit>
        </sio:SIO_000008>
      </aistls:BlastResult>
    </sio:SIO_000229>
  </aistls:BlastOutput>
</rdf:RDF>
```

Blast output RDF

1.2. CentroidFold

1.2.1. Preparing input RDF

Centroid input RDF format is as follows:

- RDF header:
  <rdf:RDF
    xmlns:rdf “http://www.w3.org/1999/02/22-rdf-syntax-ns#”
    xmlns:aistls “http://www.molprof.jp/ontologies/aistlssio.owl#”
    xmlns:sio “http://semanticscience.org/resource/>
- Subject: CentroidFoldInput, rdf:about: an arbitrary string
  <aistls:CentroidFoldInput
rdf:about=”http://www.molprof.jp/ontologies/centroidfold.rdf#1”>
- Triple for an RNA sequence:
  Subject: CentroidFoldInput
  Predicate: SIO_000230 (has input)
  Object (Subject): SIO_010017 (ribonucleic acid sequence)
    Predicate: SIO_000300 (has value)
    Object: string (RNA sequence)
  <sio:SIO_000230>
    <sio:SIO_010017>
      <sio:SIO_000300>
        RNA sequence
      </sio:SIO_000300>
    </sio:SIO_010017>
  </sio:SIO_000230>
- Triple for a ClustalW multiple alignment (the user can specify this instead of an RNA sequence as input):
  Subject: CentroidFoldInput
  Predicate: SIO_000230 (has input)
  Object (Subject): ClustalWMultipleAlignment
    Predicate: SIO_000300 (has value)

Object: string (ClustalWExecution result)

<sio:SIO_000230 >

<aistls:ClustalWMultipleAlignment>

<sio:SIO_000300>

ClustalW multiple alignment

</sio:SIO_000300>

</aistls:ClustalWMultipleAlignment>

</sio:SIO_000230>

- Triple for command options:

Subject: CentroidFoldInput

Predicate: SIO_000230 (has input)

Object (Subject): SIO_000144 (parameter)

Predicate: SIO_000300 (has value)

Object: string (CentroidFold options)

<sio:SIO_000230>

<sio:SIO_000144>

<sio:SIO_000300>

-g 4

</sio:SIO_000300>

</sio:SIO_000144>

</sio:SIO_000230>

Sample input RDF file is as follows:

```
(use an RNA sequence)
<rdf:RDF
   xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
   xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#"
   xmlns:sio="http://semanticscience.org/resource/">
   <aistls:CentroidFoldInput
rdf:about="http://www.molprof.jp/ontologies/centroidfold.rdf#1">
       <sio:SIO_000230>
          <sio:SIO_010017>
             <sio:SIO_000300>
>FR123027|AF375583|transfer messenger RNA (tmRNA), 10Sa RNA|tmRNA|u1607 NONCODE
GATAGTTCGAGCTTGATTTGCGAGTCGGGGGGATCGTCCTCGTTATCAACGTCAAAGCCAATAATAACTG
GCAAAGAAAAACAAAACCTAGCTTTCGCTGCCTAATAAGCAGTAGCATAGCTGATCCTCCGTGCATCGCC
CATGTGCTACGGTAAGGGTCTCACTCTAAGTGGGCTACACTAGTTAATCTCCGTCTGAGGTTAAATAGAA
GAGCTTAATCAGACTAGCTGAATGGAAGCCTGTTACCGGGCTGATGTTTATGCGAAATGCTAATACGGTG
ACTACGCTCGTAGATATTCAAGTGCCGATATTTCTGGACGT
             </sio:SIO_000300>
          </sio:SIO_010017>
       </sio:SIO_000230>
       <sio:SIO_000230>
          <sio:SIO_000144>
             <sio:SIO_000300>-g 4</sio:SIO_000300>
          </sio:SIO_000144>
       </sio:SIO_000230>
   </aistls:CentroidFoldInput>
</rdf:RDF>


(use Multiple alignment)
<rdf:RDF
   xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
   xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#"
   xmlns:sio="http://semanticscience.org/resource/">
<aistls:CentroidFoldInput
rdf:about="http://www.molprof.jp/ontologies/centroidfold.rdf#2">
       <sio:SIO_000230>
          <aistls:ClustalWMultipleAlignment>
             <sio:SIO_000300>
CLUSTAL W (1.83) multiple sequence alignment
FR167351|CR382122_CR382124_CR3     GGTTCAATTCCCCGTCGCGGAG---
FR376599|AE016814_AE016815_AE0     GGTTCAATTCCCCGTCGCGGAG---
CR382135_CR382136_CR382137_CR3     GGTTCAATTCCCCGTCGCGGAG---
FR139547|J03573|transfer          GGTTCAATTCCCCGTCGGGGAG---
AJ347710_Y08491|transfer          GGTTCGATTCCCCGCAAGAGAG---
                                **  * *  *****      *
             </sio:SIO_000300>
          </aistls:ClustalWMultipleAlignment>
       </sio:SIO_000230>
       <sio:SIO_000230>
          <sio:SIO_000144>
             <sio:SIO_000300>-g 4</sio:SIO_000300>
          </sio:SIO_000144>
       </sio:SIO_000230>
   </aistls:CentroidFoldInput>
</rdf:RDF>
```

CentroidFold input RDF

1.2.2. Execution command

% curl --data-binary @"input RDF file"
http://semantic.medals.jp:8090/sadi-services/CentroidFold -o "output RDF file"

1.2.3. Execution result

Centroid output RDF format is as follows:

- RDF header:
  <rdf:RDF
  xmlns:rdf "http://www.w3.org/1999/02/22-rdf-syntax-ns#"
  xmlns:aistls "http://www.molprof.jp/ontologies/aistlssio.owl#"
  xmlns:sio "http://semanticscience.org/resource/">
- Subject: CentroidFoldOutput, rdf:about: the string as same as specifying in the input RDF file
  <aistls:CentroidFoldOutput
  rdf:about="http://www.molprof.jp/ontologies/centroidfold.rdf#1">
- Triple for CentroidFold results:
  Subject: CentroidFoldOutput
  Predicate: SIO_000229 (has output)
  Object (Subject): secondaryStructureModel
  Predicate: SIO_000300 (has value)
  Object: string (RNA secondary structure)

```
<sio:SIO_000229>
    <aistls:secondaryStructureModel>
        <sio:SIO_000300>
            RNA secondary structure
        </sio:SIO_000300>
    </aistls:secondaryStructureModel>
</sio:SIO_000229>
```

- Triple for PNG ->Base64 transformation:
  Subject: CentroidFoldOutput

Predicate: SIO_000229 (has output)

Object (Subject): Base64

Predicate: SIO_000300 (has value)

Object: string (Base64)

<sio:SIO_000229>

<aistls:Base64>

<sio:SIO_000300>

Base64

</sio:SIO_000300>

</aistls:Base64>

</sio:SIO_000229>

*if "-noimage" is specified at command options triple, CentroidFold doesn't generate PNG images (not contained in the output RDF file).

Sample output RDF file is as follows:

```
<rdf:RDF
   xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
   xmlns:sio="http://semanticscience.org/resource/"
   xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#">
  <aistls:CentroidFoldOutput
rdf:about="http://www.molprof.jp/ontologies/centroidfold.rdf#1">
   <sio:SIO_000229>
     <aistls:secondaryStructureModel>
       <sio:SIO_000300>&gt;FR014095|AJ316556|transfer
UCCGYGAUAGUUUAAUGGUYAGAAUKSGCGCYUGUCRCGUGCCAGAUCGGGGUUCAAUUCCCCGUCGCGGMG---
(((((((.................(((((.......)))))....(((((.......)))))))))))....
(g=4,th=0.2,e=-14.5964)
</sio:SIO_000300>
     </aistls:secondaryStructureModel>
   </sio:SIO_000229>
  </aistls:CentroidFoldOutput>
  <aistls:Base64/>
</rdf:RDF>
```

CentroidFold output RDF

1.3. ClustalW

1.3.1. Preparing input RDF

ClustalW input RDF format is as follows:

- RDF header:

<rdf:RDF
xmlns:rdf “http://www.w3.org/1999/02/22-rdf-syntax-ns#”
xmlns:aistls “http://www.molprof.jp/ontologies/aistlssio.owl#”
xmlns:sio “http://semanticscience.org/resource/”>

- Subject: ClustalWInput, rdf:about: an arbitrary string

<aistls:ClustalWInput
rdf:about=”http://www.molprof.jp/ontologies/clustalw.rdf#1”>

- Triple for multiple sequences

Subject: ClustalWInput
Predicate: SIO_000230 (has input)
Object (Subject): SIO_000030 (biopolymer sequence)
Predicate: SIO_000300 (has value)
Object: string (Multi-FASTA sequences)

<sio:SIO_000230>
<sio:SIO_000030>
<sio:SIO_000300>
Multi-FASTA sequences
</sio:SIO_000300>
</sio:SIO_000030>
</sio:SIO_000230>

- Triple for command options

Subject: ClustalWInput
Predicate: SIO_000230 (has input)
Object (Subject): SIO_000144 (parameter)
Predicate: SIO_000300 (has value)
Object: string (ClustalW options)

<sio:SIO_000230>
<sio:SIO_000144>
<sio:SIO_000300>
-GAPOPEN=10 -GAPEXT=0.5
</sio:SIO_000300>
</sio:SIO_000144>
</sio:SIO_000230>

Sample input RDF file is as follows:

```
<rdf:RDF
   xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
   xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#"
   xmlns:sio="http://semanticscience.org/resource/">

   <aistls:ClustalWInput rdf:about="http://www.molprof.jp/ontologies/clustalw.rdf#1">
      <sio:SIO_000230>
         <sio:SIO_000030>
            <sio:SIO_000300>
>1LYLA
FNDELRNRREKLAALRQQGVAFPNDFRRDHTSDQLHEEFDAKDNQELESLNIEVSVAGRM
MTRRIMGKASFVTLQDVGGRIQLYVARDSLPEGVYNDQFKKWDLGDIIGARGTLFKTQTG
ELSIHCTELRLLTKALRPLPDQEVRYRQRYLDLIANDKSRQTFVVRSKILAAIRQFMVAR
GFMEVETPMMQVIPGGASARPFITHHNALDLDMYLRIAPELYLKRLVVGGFERVFEINRN
FRNEGISVRHNPEFTMMELYMAYADYHDLIELTESLFRTLAQEVLGTTKVTYGEHVFDFG
KPFEKLTMREAIKKYRPETDMADLDNFDAAKALAESIGITVEKSWGLGRIVTEIFDEVAE
AHLIQPTFITEYPAEVSPLARRNDVNPEITDRFEFFIGGREIGNGFSELNDAEDQAERFQ
EQVNAKAAGDDEAMFYDEDYVTALEYGLPPTAGLGIGIDRMIMLFTNSHTIRDVILFPAM
RP
>1B8AA
MYRTHYSSEITEELNGQKVKVAGWVWEVKDLGGIKFLWIRDRDGIVQITAPKKKVDPELF
KLIPKLRSEDVVAVEGVVNFTPKAKLGFEILPEKIVVLNRAETPLPLDPTGKVKAELDTR
LNNRFMDLRRPEVMAIFKIRSSVFKAVRDFFHENGFIEIHTPKIIATATEGGTELFPMKY
FEEDAFLAESPQLYKEIMMASGLDRVYEIAPIFRAEEHNTTRHLNEAWSIDSEMAFIEDE
EEVMSFLERLVAHAINYVREHNAKELDILNFELEEPKLPFPRVSYDKALEILGDLGKEIP
WGEDIDTEGERLLGKYMMENENAPLYFLYQYPSEAKPFYIMKYDNKPEICRAFDLEYRGV
EISSGGQREHRHDILVEQIKEKGLNPESFEFYLKAFRYGMPPHGGFGLGAERLIKQMLDL
PNIREVILFPRDRRRLTP
>B64744 9209  proline--tRNA ligase (EC 6.1.1.15) - Escherichia coli
MRTSQYLLSTLKETPADAEVISHQLMLRAGMIRKLASGLYTWLPTGVRVLKKVENIVREE
MNNAGAIEVSMPVVQPADLWQESGRWEQYGPELLRFVDRGERPFVLGPTHEEVITDLIRN
ELSSYKQLPLNFYQIQTKFRDEVRPRFGVMRSREFLMKDAYSFHTSQESLQETYDAMYAA
YSKIFSRMGLDFRAVQADTGSIGGSASHEFQVLAQSGEDDVVFSDTSDYAANIELAEAIA
PKEPRAAATQEMTLVDTPNAKTIAELVEQFNLPIEKTVKTLLVKAVEGSSFPQVALLVRG
DHELNEVKAEKLPQVASPLTFATEEEIRAVVKAGPGSLGPVNMPIPVVIDRTVAAMSDFA
AGANIDGKHYFGINWDRDVATPEVADIRNVVAGDPSPDGQGRLLIKRGIEVGHIFQLGTK
YSEALKASVQGEDGRNQILTMGCYGIGVTRVVAAAIEQNYDERGIVWPDAIAPFQVAILP
MNMHKSFRVQELAEKLYSELRAQGIEVLLDDRKERPGVMFADMELIGIPHTIVLGDRNLD
NDDIEYKYRRNGEKQLIKTGDIVEYLVKQIKG
            </sio:SIO_000300>
         </sio:SIO_000030>
      </sio:SIO_000230>
      <sio:SIO_000230>
         <sio:SIO_000144>
            <sio:SIO_000300>-TYPE=PROTEIN -GAPOPEN=10 -GAPEXT=0.5</sio:SIO_000300>
         </sio:SIO_000144>
      </sio:SIO_000230>
   </aistls:ClustalWInput>
</rdf:RDF
```

ClustalW input RDF

1.3.2. Execution command

% curl --data-binary @"input RDF file"
http://semantic.medals.jp:8090/sadi-services/ClustalW -o "output RDF file"

1.3.3. Execution result

ClustalW output RDF format is as follows:

- RDF header:
  <rdf:RDF
    xmlns:rdf "http://www.w3.org/1999/02/22-rdf-syntax-ns#"
    xmlns:aistls "http://www.molprof.jp/ontologies/aistlssio.owl#"
    xmlns:sio "http://semanticscience.org/resource/">
- Subject: ClustalWOutput, rdf:about: the string as same as specifying in the input RDF file
  <aistls:ClustalWOutput
  rdf:about="http://www.molprof.jp/ontologies/clustalw.rdf#1">
- Triple for ClustalW results
  Subject: ClustalWOutput
  Predicate: SIO_000229 (has output)
  Object (Subject): ClustalWMultipleAlignment
    Predicate: SIO_000300 (has value)
    Object: string (ClustalW Execution result)

```
<sio:SIO_000229>
    <aistls:ClustalWMultipleAlignment>
        <sio:SIO_000300>
            ClustalW Execution result
        </sio:SIO_000300>
    </aistls:ClustalWMultipleAlignment>
</sio:SIO_000229>
```

Sample output RDF file is as follows:

```
<rdf:RDF
   xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
   xmlns:sio="http://semanticscience.org/resource/"
   xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#">
  <aistls:ClustalWOutput rdf:about="http://www.molprof.jp/ontologies/clustalw.rdf#1">
    <sio:SIO_000229>
      <aistls:ClustalWMultipleAlignment>
        <sio:SIO_000300>CLUSTAL 2.0.9 multiple sequence alignment


1ATIA           ------------------------------------AASSLDELVALCKRRGFIFQSSE
E64328          ------------------------------------MEKDIYEKIMDLAKRRGYLWSSFE
1B8AA           ------------------------------------------------MYRTHYSSEITEEL
1ASZB           ----------------------EDTAKDNYGKLPLIQSRDSDRTGQKRVKFVDLDEAKD
1SESA           ------------------------------------------------------MVDLKRL
A26400          ------------------------------------------------------MLDPNLL
JT0942          ----------------------MRTEYCGQLRLSHVGQQVTLCGWVNRRRDLGSLIFIDM
1LYLA           ---------------------------------FNDELRNRREKLAALRQQGVAFPNDFR
S56383          ------------------------------------------------------------
G64424          ------------------------------------------------------MIVMFQ
1ADJA           ------------------------------------------------------------TAR
B64744          --------------------------MRTSQYLLSTLKETPADAEVISHQLMLRAGMIRK
E64454          ----------------------------------------LEFSEWYSDILEKAEIYDVRY
1PYSA           ------------------------------------------------------------
y|Pyrococcus     ----------------------------------MRLGYNEKLVLLKLAELKNATVEEL
D64449          ------LRDNMKMLLIHSDYLEFEAKEKTKIAEETENLKGKLDECLACFIAVEREDENNP
G64930          MPVITLPDGSQRHYDHAVSPMDVALDIGPGLAKACIAGRVNGELVDACDLIENDAQLSII
……
……
…….
……
……

G64424          KKVIIVGEKELNEGKVTVKDMITGEQKLIGIDELTNF-----------------------
1ADJA           AFAGFLGEDELRAGEVTLKRLATGEQVRLSREEVPGYLLQALG-----------------
B64744          PHTIVLGDRNLDNDDIEYKYRRNGEKQLIKTGDIVEYLVKQIKG-----------------
E64454          VILVPFKEEIYNEELEEKVEATILGETEYKGNKYIAIAKTY-------------------
1PYSA           GLGVERLAMLRYGIPDIRYFFGGRLKFLEQFKGVL-------------------------
y|Pyrococcus     GIKVPVIAWGIGIDRLAMFKLGVDDIRYLFSYDLKWLRESKLIW-----------------
D64449          PYVVVIGDEEMESDKLTVTIREKSTLKKPYKEKMTLDELIERIKKETANYPYRPLPLPIR
G64930          PYMLVCGDKEVESGKVAVRTRRGKDLGSMDVNEVIEKLQQEIRSRSLKQLEE--------

1ATIA           --------
E64328          --------
1B8AA           --------
1ASZB           --------
1SESA           --------
A26400          --------
JT0942          VVKKAENN
1LYLA           --------
S56383          --------
G64424          --------
1ADJA           --------
B64744          --------
E64454          --------
1PYSA           --------
y|Pyrococcus     --------
D64449          CSLQPKFH
G64930          --------

</sio:SIO_000300>
     </aistls:ClustalWMultipleAlignment>
   </sio:SIO_000229>
  </aistls:ClustalWOutput>
</rdf:RDF>
```

ClustalW output RDF

1.4. IPknot

1.4.1. Preparing input RDF

IPknot input RDF format is as follows:

- RDF header:
  <rdf:RDF
    xmlns:rdf “http://www.w3.org/1999/02/22-rdf-syntax-ns#”
    xmlns:aistls “http://www.molprof.jp/ontologies/aistlssio.owl#”
    xmlns:sio “http://semanticscience.org/resource/”>
- Subject: IPknotInput, rdf:about: an arbitrary string
  <aistls:IPknotInput rdf:about=”http://www.molprof.jp/ontologies/ipknot.rdf#1”>
- Triple for an RNA sequence
  Subject: IPknotInput
  Predicate: SIO_000230 (has input)
  Object (Subject): SIO_010017 (ribonucleic acid sequence)
    Predicate: SIO_000300 (has value)
    Object: string (RNA sequence)

```
<sio:SIO_000230>
    <sio:SIO_010017>
        <sio:SIO_000300>
            RNA sequence
        </sio:SIO_000300>
    <sio:SIO_010017>
</sio:SIO_000230>
```

- Triple for ClustalW multiple alignment (the user can specify this instead of an RNA sequence as input):
  Subject: IPknotInput
  Predicate: SIO_000230 (has input)
  Object (Subject): ClustalWMultipleAlignment
    Predicate: SIO_000300 (has value)
    Object: string (ClustalW multiple alignment)

<sio:SIO_000230>
<aistls:ClustalWMultipleAlignment>
<sio:SIO_000300>
ClustalW multiple alignment
</sio:SIO_000300>
</aistls:ClustalWMultipleAlignment>
</sio:SIO_000230>

- Triple for command options

Subject: IPknotInput

Predicate: SIO_000230 (has input)

Object (Subject): SIO_000144 (parameter)

Predicate: SIO_000300 (has value)

Object: string (ClustalW options)

<sio:SIO_000230>
<sio:SIO_000144>
<sio:SIO_000300>
-i
</sio:SIO_000300>
</sio:SIO_000144>
</sio:SIO_000230>

Sample input RDF file is as follows:

```
<rdf:RDF
   xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
   xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#"
   xmlns:sio="http://semanticscience.org/resource/">

   <aistls:IPknotInput rdf:about="http://www.molprof.jp/ontologies/ipknot.rdf#1">
      <sio:SIO_000230>
         <sio:SIO_010017>
            <sio:SIO_000300>
>MIDV
UUCUUUUUUAGUGGCAGUAAGCCUGGGAAUGGGGGCGACCCAGGCGUAUGAACAUAGUGUAACGCUCCCC
            </sio:SIO_000300>
         </sio:SIO_010017>
      </sio:SIO_000230>
      <sio:SIO_000230>
         <sio:SIO_000144>
            <sio:SIO_000300></sio:SIO_000300>
         </sio:SIO_000144>
      </sio:SIO_000230>
   </aistls:IPknotInput>
</rdf:RDF>
```

IPknot input RDF

1.4.2. Execution command

% curl --data-binary @"input RDF file"
http://semantic.medals.jp:8090/sadi-services/IPknot -o "output RDF file"

1.4.3. Execution result

IPknot output RDF format is as follows:

- RDF header:
  <rdf:RDF
  xmlns:rdf "http://www.w3.org/1999/02/22-rdf-syntax-ns#"
  xmlns:aistls "http://www.molprof.jp/ontologies/aistlssio.owl#"
  xmlns:sio "http://semanticscience.org/resource/">
- Subject: IPknotOutput, rdf:about: the string as same as specifying in the input RDF file
  <aistls:IPknotOutput
  rdf:about="http://www.molprof.jp/ontologies/ipknot.rdf#1">
- Triple for IPknot results:
  Subject: IPknotOutput
  Predicate: SIO_000229 (has output)
  Object (Subject): SIO_000785 (answer)
  Predicate: SIO_000300 (has value)
  Object: string (IPknotExecution result)

```
<sio:SIO_000229>
    <sio:SIO_000785>
        <sio:SIO_000300>
            IPknotExecution result
        </sio:SIO_000300>
    </sio:SIO_000785>
</sio:SIO_000229>
```

Sample output RDF file is as follows:

```
<rdf:RDF
   xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
   xmlns:sio="http://semanticscience.org/resource/"
   xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#">
  <aistls:IPknotOutput rdf:about="http://www.molprof.jp/ontologies/ipknot.rdf#1">
    <sio:SIO_000229>
      <sio:SIO_000785>
        <sio:SIO_000300>&gt;MIDV
UUCUUUUUUAGUGGCAGUAAGCCUGGGAAUGGGGGCGACCCAGGCGUAUGAACAUAGUGUAACGCUCCCC
.....................(((((((...[[[[[[[.)))))))).................]]]]]]].
</sio:SIO_000300>
      </sio:SIO_000785>
    </sio:SIO_000229>
  </aistls:IPknotOutput>
</rdf:RDF>
```

IPknot output RDF

1.5. Mafft

1.5.1. Preparing input RDF

Mafft input RDF format is as follows:

- RDF header:
  <rdf:RDF
    xmlns:rdf “http://www.w3.org/1999/02/22-rdf-syntax-ns#”
    xmlns:aistls “http://www.molprof.jp/ontologies/aistlssio.owl#”
    xmlns:sio “http://semanticscience.org/resource/”>
- Subject: MafftInput, rdf:about: an arbitrary string
  <aistls:MafftInput rdf:about=”http://www.molprof.jp/ontologies/mafft.rdf#1”>
- Triple for multiple sequences:
  Subject: MafftInput
  Predicate: SIO_000230 (has input)
  Object (Subject): SIO_000030 (biopolymer sequence)
    Predicate: SIO_000300 (has value)
    Object: string (Multi-FASTA sequences)
  <sio:SIO_000230>
    <sio:SIO_000030>
      <sio:SIO_000300>
        Multi-FASTA sequences (at least more than two sequences)
      </sio:SIO_000300>
    </sio:SIO_000030>
  </sio:SIO_000230>
- Triple for command options:
  Subject: MafftInput
  Predicate: SIO_000230 (has input)
  Object (Subject): SIO_000144 (parameter)
    Predicate: SIO_000300 (has value)
    Object: string (Mafft options)
  <sio:SIO_000230 >

```
        <sio:SIO_000144>
            <sio:SIO_000300>
                --retree 2 --maxiterate 0 --bl 62 --op 1.53 --ep 0.0 --clustalout
            </sio:SIO_000300>
        </sio:SIO_000144>
    </sio:SIO_000230>
```

Sample input RDF file is as follows:

```
<rdf:RDF
   xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
   xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#"
   xmlns:sio="http://semanticscience.org/resource/">

   <aistls:MafftInput rdf:about="http://www.molprof.jp/ontologies/mafft.rdf#1">
      <sio:SIO_000230>
         <sio:SIO_000030>
            <sio:SIO_000300>
>X02729 Methanococcus vannielli. #
tatctattaccctaccctggggaatggcttggcttgaaacgccgatgaaggacgtggtaa
gctgcgataagcctaggcgaggcgcaacagcctttgaacctaggatttccgaatgggact
tcctacttttgtaatccgtaaggattggtaacgcgggggattgaagcatcttagtacccg
caggaaaagaaatcaactgagattccgttagtagaggcgattgaacacggatcagggcaa
actgaatcccttcggggagatgtggtgttatagggccttctttttcgcctgttgagaaaag
ctgaagttgactggaacgtcacactatagagggtgaaagtcccgtaagcgcaatcgattc
aggtttgaagtgtccctgagtaccgtgcgttggatatcgcgcgggaatttgggaggcatc
aacttccaactctaaatacgtttcaagaccgatagcgtactagtaccgcgagggaaagct
gaaaagcacccttaacagggtggtgaaaagagcctgaaacccaggtaggtatggaatggc
gtggccccaaaggcaactgttctgaaggaaaccgtcgcaaggcggctgtacgaagaacag
agccagggttgcgtcctccgtttcgaaaaacgggccggggagtgtattgttgtggcgagc
ttaagatcttcacgatcgaaggcgtagggaaaccaacaagtccgcagaatctttagggac
ggggtcttaagggcccggagtcacagcaatacgacccgaaaccgggcgatctaggccggg
gcaaggtgaagtccctcaattgagggatggaggcctgcagagttgttgccgttcgaagca
ctcttctgacctcggtctaggggtgaaaggccaatcgagcccggagatagctggttcccc
……
……
……
aaagcggggcctcacgatccttctgacctttgggttttaagcaggaggtgtcagaaaag
ttaccacagggataactggcttgtggcggccaagcgttcatagcgacgtcgcttttttgat
ccttcgatgtcggctcttcctatcattgtgaagcagaattcgccaagcgttggattgttc
acccactaatagggaacgtgagctgggtttagaccgtcgtgagacaggttagttttaccc
tactgatgatgtgttgttgccatggtaatcctgctcagtacgagaggaaccgcaggttca
gacatttggtgtatgtgcttggctgaggagccaatggggcgaagctaccatctgtgggat
tatgactgaacgcctctaagtcagaatcccgcccaggcgaacgatacggcagcgccgcgg
agcctcggttggcctcggatagccggtcccccgcctgtccccgccggcgggccgccccc
cctccacgcgcccgccgcgcgggagggcgcgtgcccgccgcgcgccgggaccggggtccg
gtgcggagtgcccttcgtcctgggaaacggggcgcggccggaaaggcggccgccccctcg
cccgtcacgcaccgcacgttcgtggggaacctggcgctaaaccattcgtagacgacctgc
ttctgggtcggggtttcgtacgtagcagagcagctccctcgctgcgatctattgaaagtc
agccctcgacacaagggtttgtc
            </sio:SIO_000300>
         </sio:SIO_000030>
      </sio:SIO_000230>
      <sio:SIO_000230>
         <sio:SIO_000144>
            <sio:SIO_000300>
               --retree 2 --maxiterate 0 --bl 62 --op 1.53 --ep 0.0 --clustalout
            </sio:SIO_000300>
         </sio:SIO_000144>
      </sio:SIO_000230>
   </aistls:MafftInput>
```

Mafft input RDF

1.5.2. Execution command

% curl --data-binary @"input RDF file"
http://semantic.medals.jp:8090/sadi-services/Mafft -o "output RDF file"

1.5.3. Execution result

Mafft output RDF format is as follows:

- RDF header:
  <rdf:RDF
    xmlns:rdf "http://www.w3.org/1999/02/22-rdf-syntax-ns#"
    xmlns:aistls "http://www.molprof.jp/ontologies/aistlssio.owl#"
    xmlns:sio "http://semanticscience.org/resource/">
- Subject: MafftOutput, rdf:about: the string as same as specifying in the input RDF file
  <aistls:MafftOutput rdf:about="http://www.molprof.jp/ontologies/mafft.rdf#1">
- Triple for Mafft results:
  Subject: MafftOutput
  Predicate: SIO_000229 (has output)
  Object (Subject): ClustalWMultipleAlignment
    Predicate: SIO_000300 (has value)
    Object: string (Mafft multiple alignment)

```
<sio:SIO_000229>
    <aistls:ClustalWMultipleAlignment>
        <sio:SIO_000300>
            Mafft multiple alignment
        </sio:SIO_000300>
    </aistls:ClustalWMultipleAlignment>
</sio:SIO_000229>
```

Sample output RDF file is as follows:

```
<rdf:RDF
   xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
   xmlns:sio="http://semanticscience.org/resource/"
   xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#">
  <aistls:MafftOutput rdf:about="http://www.molprof.jp/ontologies/mafft.rdf#1">
    <sio:SIO_000229>
      <aistls:ClustalWMultipleAlignment>
        <sio:SIO_000300>CLUSTAL format alignment by MAFFT FFT-NS-2 (v6.717b)


X02729          ----------tatctattaccctaccctggggaatggcttggcttgaaacgccgatgaag
X15364          ----------ctttttttatgcc--gtctgggggatggcttggcttgagtcgctgatgaag
M61738          ------------ttcttacgcc--tgtcagtggatggctcggttcggg-tgccgacgaag
M64487          ---cggcgaa------tatccc--ggccggtggatggctcggctc-gggcgccgacgaag
M32298          -------gtgctctgctaatct--gcctagaggatggcttggttc-gggcgccgaagaag
M64487          ---ggggcagagaacctaagcc--gtctggtggatggctcggctcggggcgccgacgaag
X03407          -------g-tggctactgtgcc--acctggtggatagctcggctcgga-tgccgacgaag
M67497          tatatcaactggctactgtgcc--agctggtggatagctcggctcgag-agccgatgacg
X13738          -------gttggctactatgcc--agctggtggattgctcggctcagg-cgctgatgaag
X05481          ----------ggctactatgcc--aactggtgaatagctcggctcgag-tgccgatgaag
X05481          ---gcacgg------tcaagcc--gcccggtggatggctcggctc-gggcgccgaggaag
X14835          ---cggc-g------ctaagcc--acccggtggatggctcggctc-gggcgccgaggaag
M67495          ---tacccag-gggccgaagcc--tcccggtggatggctcggctc-gggcaccgaagaag
X05480          ---cgac-g--------acgcc--gcccggtggatggctcggctc-gggcgccgaggaag
M67498          -----ggtcaaggt-actaagggcacgcggtggatgccttggcggcgggaggcgatgaag
X12612,         -----ggtcaagat-ggtaagggcccacggtggatgcctcggc-acccgagccgatgaag
X07408          tttgtggtcaagct-attaagggcgtatgggggatgtcttggtatcagaaggcgatgaag
M62806          -------------n-acgaagggcgcatgggggatgcctaggctctcagaggcgaagaag
X06485          -----aatcaagcgcgagaagggcgtttggtggatgccttggcagcaagaggcgatgaag
……
……
……
K00637          -----t---------
X01387          -----a---------
X53361          ctgacagagtgggtg
Y00055          t--ctgggact----
X14553          tcacaagatct----
V01159          ttttgtcggc-----
X54512          tccttagatttat--
X54004          tccttagatttat--
X16108          ttttctgatttgttc
J01355          ttgtctgatttgt--
M11585          cgcacggattcgt--
X52320          cgctaagattcga--
X58118          cgcttcgattcgt--
X03680          tgattgagttttttg
X53538          atctacgatttgt--
M21017          cttgatgattcg---
X00136          ccaagc---------
X00525          cacaagggtttgt--
X01069          cacaagggtttgt--
M11167          cacaagggtttgt-c

</sio:SIO_000300>
     </aistls:ClustalWMultipleAlignment>
   </sio:SIO_000229>
  </aistls:MafftOutput>
</rdf:RDF>
```

Mafft output RDF

1.6. Psipred

1.6.1. Preparing input RDF

Psipred input RDF format is as follows:

- RDF header:
  <rdf:RDF
  xmlns:rdf “http://www.w3.org/1999/02/22-rdf-syntax-ns#”
  xmlns:aistls “http://www.molprof.jp/ontologies/aistlssio.owl#”
  xmlns:sio “http://semanticscience.org/resource/”>
- Subject: PsiPredInput, rdf:about: an arbitrary string
  <aistls:PsiPredInput
  rdf:about=”http://www.molprof.jp/ontologies/psipred.rdf#1”>
- Triple for a protein sequence:
  Subject: PsiPredInput
  Predicate: SIO_000230
  Object (Subject): SIO_010015 (protein sequence)
  Predicate: SIO_000300 (has value)
  Object: string (protein sequence)

```
<sio:SIO_000230>
    <sio:SIO_010015>
        <sio:SIO_000300>
            Protein sequence
        </sio:SIO_000300>
    </sio:SIO_010015>
</sio:SIO_000230>
```

Sample input RDF file is as follows:

```
<rdf:RDF
    xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
    xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#"
    xmlns:sio="http://semanticscience.org/resource/">

    <aistls:PsiPredInput rdf:about="http://www.molprof.jp/ontologies/psipred.rdf#1">
       <sio:SIO_000230>
          <sio:SIO_010015>
             <sio:SIO_000300>
>sp|P04156|PRIO_HUMAN Major prion protein OS=Homo sapiens GN=PRNP PE=1 SV=1
MANLGCWMLVLFVATWSDLGLCKKRPKPGGWNTGGSRYPGQGSPGGNRYPPQGGGGWGQP
HGGGWGQPHGGGWGQPHGGGWGQPHGGGWGQGGGTHSQWNKPSKPKTNMKHMAGAAAAGA
VVGGLGGYMLGSAMSRPIIHFGSDYEDRYYRENMHRYPNQVYYRPMDEYSNQNNFVHDCV
NITIKQHTVTTTTKGENFTETDVKMMERVVEQMCITQYERESQAYYQRGSSMVLFSSPPV
ILLISFLIFLIVG
             </sio:SIO_000300>
          </sio:SIO_010015>
       </sio:SIO_000230>
    </aistls:PsiPredInput>
</rdf:RDF>
```

Psipred input RDF

1.6.2. Execution command

% curl --data-binary @"input RDF file"
http://semantic.medals.jp:8090/sadi-services/Psipred -o "output RDF file"

1.6.3. Execution result

Psipred output RDF format is as follows:

- RDF header:
  <rdf:RDF
  xmlns:rdf “http://www.w3.org/1999/02/22-rdf-syntax-ns#”
  xmlns:aistls “http://www.molprof.jp/ontologies/aistlssio.owl#”
  xmlns:sio “http://semanticscience.org/resource/”>
- Subject: PsiPredOutput, rdf:about: the string as same as specifying in the input RDF
  <aistls:PsiPredOutput
  rdf:about=”http://www.molprof.jp/ontologies/psipred.rdf#1”>
- Triple for Psipred results:
  Subject: PsiPredOutput
  Predicate: SIO_000229 (has output)
  Object (Subject): SIO_000785 (answer)
  Predicate: SIO_000300 (has value)
  Object: string (Psipred execution result)

```
<sio:SIO_000229>
    <sio:SIO_000785>
        <sio:SIO_000300>
            Psipred execution result
        </sio:SIO_000300>
    </sio:SIO_000785>
</sio:SIO_000229>
```

Sample output RDF file is as follows:

```
<rdf:RDF
    xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
    xmlns:sio="http://semanticscience.org/resource/"
    xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#">
  <aistls:PsiPredOutput rdf:about="http://www.molprof.jp/ontologies/psipred.rdf#1">
    <sio:SIO_000229>
      <sio:SIO_000785>
        <sio:SIO_000300># PSIPRED HFORMAT (PSIPRED V2.5 by David Jones)

Conf: 965203422130431010011012789987678875689888999888869888899988
Pred: CCCCHHHHHHHHHHHHHHCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
  AA: MANLGCWMLVLFVATWSDLGLCKKRPKPGGWNTGGSRYPGQGSPGGNRYPPQGGGGWGQP
            10       20       30       40       50       60


Conf: 888898988888989888889898888767788724334688777333143200001124
Pred: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCHHHHHCCHHHHH
  AA: HGGGWGQPHGGGWGQPHGGGWGQPHGGGWGQGGGTHSQWNKPSKPKTNMKHMAGAAAAGA
            70       80       90      100      110      120


Conf: 541000354322320732104774303456665664762125411243285453031100
Pred: HHHHHHHHHHHHHHCCCEECCCCCCCCHHHHHHHHHHCCCCCEECCCHHHCCCCCCEEEEE
  AA: VVGGLGGYMLGSAMSRPIIHFGSDYEDRYYRENMHRYPNQVYYRPMDEYSNQNNFVHDCV
           130      140      150      160      170      180


Conf: 1156400333103787543334899999998764235432234654328605885697 30
Pred: EEEEEEEEEEECCCCCCCCHHHHHHHHHHHHHHHHHHHHHHHHHHHHHCCCEEEEECCCCC
  AA: NITIKQHTVTTTTKGENFTETDVKMMERVVEQMCITQYERESQAYYQRGSSMVLFSSPPV
           190      200      210      220      230      240


Conf: 3333668832009
Pred: HHHHHHHHHHCCC
  AA: ILLISFLIFLIVG
           250

</sio:SIO_000300>
     </sio:SIO_000785>
   </sio:SIO_000229>
  </aistls:PsiPredOutput>
</rdf:RDF>
```

Psipred output RDF

1.7. Raccess

1.7.1. Preparing input RDF

Raccess input RDF format is as follows:

- RDF header:
  <rdf:RDF
    xmlns:rdf “http://www.w3.org/1999/02/22-rdf-syntax-ns#”
    xmlns:aistls “http://www.molprof.jp/ontologies/aistlssio.owl#”
    xmlns:sio “http://semanticscience.org/resource/”>
- Subject: RaccessInput, rdf:about: an arbitrary string
  <aistls:RaccessInput
  rdf:about=”http://www.molprof.jp/ontologies/raccess.rdf#1”>
- Triple for an RNA sequence:
  Subject: RaccessInput
  Predicate: SIO_000230 (has input)
  Object (Subject): SIO_010017 (ribonucleic acid sequence)
    Predicate: SIO_000300 (has value)
    Object: string (RNA sequence)

```
<sio:SIO_000230>
    <sio:SIO_010017>
        <sio:SIO_000300>
            RNA sequence
        </sio:SIO_000300>
    </sio:SIO_010017>
</sio:SIO_000230>
```

- Triple for command options:
  Subject: RaccessInput
  Predicate: SIO_000230 (has input)
  Object (Subject): SIO_000144 (parameter)
    Predicate: SIO_000300 (has value)
    Object: string (Raccess execution result)

<sio:SIO_000230>
    <sio:SIO_000144>
        <sio:SIO_000300>
            -access_len=50
        </sio:SIO_000300>
    </sio:SIO_000144>
</sio:SIO_000230>

Sample input RDF file is as follows:

```
<rdf:RDF
    xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
    xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#"
    xmlns:sio="http://semanticscience.org/resource/">

    <aistls:RaccessInput rdf:about="http://www.molprof.jp/ontologies/raccess.rdf#1">
        <sio:SIO_000230>
            <sio:SIO_010017>
                <sio:SIO_000300>
>gi|187607315|ref|NM_014909.4| Homo sapiens vasohibin 1 (VASH1), mRNA
GCCCCTGCGCGCCGCCCGAGCCGGTCCCGCTGAGCCGCGGGCCCCGTGCCCTGCGATGGCTCGGCTGGTG
CAGCGCGGCGCCAGGTGCCAGCCGTCCTCCCGCTGAGACGCGCCCGAGTGGGGACCCGCTGGGCCTCGGG
GCTCGCAGCCTTCGCCTCCCCGCCGCGCCCGCTCCCTTTCTGGGGACTCCGCCGCTGTTTCTGGGGACGA
GGGGACAGGGGACCCAGACAAAGCCCACTTTGTGCAGGGAGTTGGCCGCAGGCGGGGAATGTGCGCGTCG
GCGCGCGCCCCCTCCCCGCTCCCGGCCAGCTGCGAGTCTTGGCTCCCGGACTTGTCTCGTCGCGTCGGAG
AAATCGCCCCCCCAGCGCCGCTCTCCCGCCCGGGGGTCTTGGTTCCGAGCTCGCGCGGCCGGGGAGTCGCCT
CGGTCTTCCTTGGGGCGCGCGCAGATGTGAGCGTGCGAGAGTTGTGTAGGGGATTTTGTTCCCTCCGAAA
CTGAGACCCAGGGCGCCCAGTGGGCACCCGTGCCTTGACTCTGTCCTTTCTGCAGCCGCTGGTCCGAGCT
GTCTGGCCTCAGTTTCCCTCCGACTTTTCTCCGCTCTGCCAGCCCTCACTGCTGCCCGTCATTGTTCTCG
CAGTTAGATGGGGGTGCTTTGTGACGGCTGCCAAGTTGGGGTGTGTTCTCTTTATTCCGTTTTTCAAACA
GAACAAGGCCTCCAAGGCTGACCCCAGACAACCCACCCCCTCGGACCCTAATTCACCTTATTGCACTGAT
TTTTTTTATCAAGTCGTATTTTATTGTACAGGAGCCACGCCCTGATTTCTTAAAGGCGCCTTGCACTCTG
GCCATGTGTTATCTCTGCAGCCGGTGTGTGGGAGGCCTCTTGTGAGCCAGTTGTTTTCCCGCCTCCACCA
CCCCCCTCGAAGATTTAGGGATGCCAGGGGGGAAGAAGGTGGCTGGGGGTGGCAGCAGCGGTGCCACTCC
AACGTCCGCTGCGGCCACCGCCCCCTCTGGGGTCAGGCGTTTGGAGACCAGCGAAGGAACCTCAGCCCAG
AGAGATGAGGAGCCAGAAGAGGAAGGGGAAGAGGACCTGCGAGACGGAGGCGTCCCCTTCTTTGTCAACC
GGGGTGGGCTACCTGTGGATGAGGCCACCTGGGAAAGGATGTGGAAACACGTGGCCAAGATCCACCCCGA
TGGAGAGAAGGTGGCGCAACGGATCCGTGGGGCCACAGACCTGCCCAAGATCCCCATACCGAGTGTGCCT
ACGTTCCAGCCGTCTACACCTGTCCCTGAGCGCCTGGAAGCTGTGCAGCGCTACATCAGAGAGCTGCAGT
ACAATCACACAGGGACACAGTTCTTTGAAATTAAGAAGAGCAGACCTCTGACAGGGCTGATGGACCTGGC
CAAGGAAATGACCAAAGAGGCCCTGCCAATCAAATGCCTGGAAGCCGTGATCCTGGGAATTTACCTCACC
AACAGCATGCCCACCCTGGAGCGCTTCCCCATCAGCTTCAAGACCTACTTCTCAGGGAACTACTTCCGCC
……
……
……
GCTCCATCTTGGTCCTCCGGAGTCCCAAGTTTCCTTTTCATCAAATCTGACAAGAGAGAAGAAACATGGG
TGTGCTTGGCCCACAGGGCCTGGTGGTGATGGACCTCCCCGCTCCCTCAAGCTCTGGATGGCTGCAGTGT
TGTACTAGACTTTGTTCAGGCTGTTCTCATCTCAGTATTGCCCCTTCCTTTCACTTTCACACTTCATCTC
ATTCCTGTTGTCACTTTCCCCGAAACGAATAAAGTCTCCCCAGCTCCTGCTGTGTAGGCTGGGCAGAAAC
CACAACACGT
                </sio:SIO_000300>
            </sio:SIO_010017>
        </sio:SIO_000230>
        <sio:SIO_000230>
            <sio:SIO_000144>
                <sio:SIO_000300></sio:SIO_000300>
            </sio:SIO_000144>
        </sio:SIO_000230>
    </aistls:RaccessInput>
</rdf:RDF>
```

Raccess input RDF

1.7.2. Execution command

% curl --data-binary @"input RDF file"
http://semantic.medals.jp:8090/sadi-services/Raccess -o "output RDF file"

1.7.3. Execution result

Raccess output RDF format is as follows:

- RDF header:
  <rdf:RDF
    xmlns:rdf “http://www.w3.org/1999/02/22-rdf-syntax-ns#”
    xmlns:aistls “http://www.molprof.jp/ontologies/aistlssio.owl#”
    xmlns:sio “http://semanticscience.org/resource/”>
- Subject: RaccessOutput, rdf:about: the string as same as specifying in the input RDF
  <aistls:RaccessOutput
  rdf:about=”http://www.molprof.jp/ontologies/raccess.rdf#1”>
- Triple for Raccess results:
  Subject: RaccessOutput
  Predicate: SIO_000229 (has output)
  Object (Subject): SIO_000785 (answer)
    Predicate: SIO_000300 (has value)
    Object: string (Raccess execution result)

```
<sio:SIO_000229>
    <sio:SIO_000785>
        <sio:SIO_000300>
            Raccess execution result
        </sio:SIO_000300>
    </sio:SIO_000785>
</sio:SIO_000229>
```

Sample output RDF file is as follows:

```
<rdf:RDF
    xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
    xmlns:sio="http://semanticscience.org/resource/"
    xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#">
  <aistls:RaccessOutput rdf:about="http://www.molprof.jp/ontologies/raccess.rdf#1">
    <sio:SIO_000229>
      <sio:SIO_000785>
        <sio:SIO_000300>&gt;gi|187607315|ref|NM_014909.4| Homo sapiens vasohibin 1 (VASH1),
mRNA
6020    6029    0.62373
6019    6028    0.623859
6018    6027    0.623156
6017    6026    0.622921
6016    6025    0.648241
6015    6024    1.34601
6014    6023    2.08364
6013    6022    2.71933
6012    6021    4.96686
6011    6020    5.51342
6010    6019    5.52994
6009    6018    6.77058
6008    6017    8.45003
6007    6016    9.02248
6006    6015    9.61892
6005    6014    8.96482
6004    6013    8.98464
6003    6012    9.37755
6002    6011    9.11376
6001    6010    9.45949
6000    6009    8.523
5999    6008    9.24843
……
……
……
23      32      5.6887
22      31      7.51701
21      30      10.8552
20      29      12.0541
19      28      11.9882
18      27      10.2528
17      26      10.2699
16      25      10.0945
15      24      9.04197
14      23      10.665
13      22      11.1913
12      21      11.1897
11      20      11.5702
10      19      11.5887
9       18      11.4777
8       17      11.4848
7       16      13.0533
6       15      12.7788
5       14      10.5224
4       13      11.3123
3       12      10.8754
2       11      10.6341
1       10      9.07663
0       9       6.90453

</sio:SIO_000300>
      </sio:SIO_000785>
    </sio:SIO_000229>
  </aistls:RaccessOutput>
</rdf:RDF>
```

Raccess output RDF

1.8. RactIP

1.8.1. Preparing input RDF

RactIP input RDF format is as follows:

- RDF header:
  <rdf:RDF
    xmlns:rdf “http://www.w3.org/1999/02/22-rdf-syntax-ns#”
    xmlns:aistls “http://www.molprof.jp/ontologies/aistlssio.owl#”
    xmlns:sio “http://semanticscience.org/resource/”>
- Subject: RactIPInput, rdf:about: an arbitrary string
  <aistls:RactIPInput rdf:about=”http://www.molprof.jp/ontologies/ractip.rdf#1”>
- Triple for a query RNA sequence:
  Subject: RactIPInput
  Predicate: SIO_000230 (has input)
  Object (Subject): SIO_010017 (ribonucleic acid sequence)
    Predicate: SIO_000300 (has value)
    Object: string (RNA sequence)
  <sio:SIO_000230 >
    <sio:SIO_010017>
      <sio:SIO_000300>
        RNA sequence
      </sio:SIO_000300>
    </sio:SIO_010017>
  </sio:SIO_000230>
- Triple for a target RNA sequence:
  Subject: RactIPInput
  Predicate: SIO_000230 (has input)
  Object (Subject): SIO_010017 (ribonucleic acid sequence)
    Predicate: SIO_000300 (has value)
    Object: string (RNA sequence)
  <sio:SIO_000230 >

<sio:SIO_010017>
<sio:SIO_000300>
RNA sequence
</sio:SIO_000300>
</sio:SIO_010017>
</sio:SIO_000230>

- Triple for command options:

Subject: RactIPInput

Predicate: SIO_000230 (has input)

Object (Subject): SIO_000144 (parameter)

Predicate: SIO_000300 (has value)

Object: string (RactIP options)

<sio:SIO_000230>
<sio:SIO_000144>
<sio:SIO_000300>
-i
</sio:SIO_000300>
</sio:SIO_000144>
</sio:SIO_000230>

Sample input RDF file is as follows:

```
<rdf:RDF
   xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
   xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#"
   xmlns:sio="http://semanticscience.org/resource/">

   <aistls:RactIPInput rdf:about="http://www.molprof.jp/ontologies/ractip.rdf#1">
      <sio:SIO_000230>
         <sio:SIO_010017>
            <sio:SIO_000300>
>R1inv
GGCAACGGAUGGUUCGUUGCC
            </sio:SIO_000300>
         </sio:SIO_010017>
      </sio:SIO_000230>
      <sio:SIO_000230>
         <sio:SIO_010017>
            <sio:SIO_000300>
>R2inv
GCACCGAACCAUCCGGUGC
            </sio:SIO_000300>
         </sio:SIO_010017>
      </sio:SIO_000230>
      <sio:SIO_000230>
         <sio:SIO_000144>
            <sio:SIO_000300></sio:SIO_000300>
         </sio:SIO_000144>
      </sio:SIO_000230>
   </aistls:RactIPInput>
</rdf:RDF>
```

RactIP input RDF

1.8.2. Execution command

% curl --data-binary @"input RDF file"
http://semantic.medals.jp:8090/sadi-services/RactIP -o "output RDF file"

1.8.3. Execution result

RactIP output RDF format is as follows:

- RDF header:
  <rdf:RDF
  xmlns:rdf "http://www.w3.org/1999/02/22-rdf-syntax-ns#"
  xmlns:aistls "http://www.molprof.jp/ontologies/aistlssio.owl#"
  xmlns:sio "http://semanticscience.org/resource/">
- Subject: RactIPOutput, rdf:about: the string as same as specifying in the input RDF
  <aistls:RactIPOutput
  rdf:about="http://www.molprof.jp/ontologies/ractip.rdf#1">
- Triple for RactIP results:
  Subject: RactIPOutput
  Predicate: SIO_000229 (has output)
  Object (Subject): SIO_000785 (answer)
  Predicate: SIO_000300 (has value)
  Object: string (RactIP execution result)

```
<sio:SIO_000229>
    <sio:SIO_000785>
        <sio:SIO_000300>
            RactIP execution result
        </sio:SIO_000300>
    </sio:SIO_000785>
</sio:SIO_000229>
```

Sample output RDF file is as follows:

```
<rdf:RDF
   xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
   xmlns:sio="http://semanticscience.org/resource/"
   xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#">
  <aistls:RactIPOutput rdf:about="http://www.molprof.jp/ontologies/ractip.rdf#1">
   <sio:SIO_000229>
     <sio:SIO_000785>
       <sio:SIO_000300>GLPK Simplex Optimizer, v4.51
160 rows, 30 columns, 234 non-zeros
*    0: obj =   0.000000000e+00  infeas =  0.000e+00 (0)
*   37: obj =   1.604045469e+01  infeas =  0.000e+00 (0)
OPTIMAL SOLUTION FOUND
GLPK Integer Optimizer, v4.51
160 rows, 30 columns, 234 non-zeros
30 integer variables, all of which are binary
Integer optimization begins...
+   37: mip =    not found yet &lt;=            +inf       (1; 0)
+   37: &gt;&gt;&gt;&gt;&gt;  1.604045469e+01 &lt;=   1.604045469e+01   0.0% (1; 0)
+   37: mip =   1.604045469e+01 &lt;=    tree is empty   0.0% (0; 1)
INTEGER OPTIMAL SOLUTION FOUND
&gt;R2inv
GCACCGAACCAUCCGGUGC
(((((((((((.)))))))
&gt;R1inv
GGCAACGGAUGGUUCGUUGCC
(((((((.]]]]]]]]]]]))))
</sio:SIO_000300>
     </sio:SIO_000785>
   </sio:SIO_000229>
  </aistls:RactIPOutput>
</rdf:RDF>
```

RactIP output RDF

1.9. Wolfpsort

1.9.1. Preparing input RDF

Wolfpsort input RDF format is as follows:

- RDF header:
  <rdf:RDF
  xmlns:rdf “http://www.w3.org/1999/02/22-rdf-syntax-ns#”
  xmlns:aistls “http://www.molprof.jp/ontologies/aistlssio.owl#”
  xmlns:sio “http://semanticscience.org/resource/”>
- Subject: WolfPsortInput, rdf:about: an arbitrary string
  <aistls:WolfPsortInput
  rdf:about=”http://www.molprof.jp/ontologies/wolfpsort.rdf#1”>
- Triple for kingdom information:
  Subject: WolfPsortInput
  Predicate: SIO_000230 (has input)
  Object: Kingdom (rdf:about="#plant" (animal, plant or fungi))
  <sio:SIO_000230>
  <aistls:Kingdom rdf:about=”#animal”>
  </sio:SIO_000230>
- Triple for a protein sequence:
  Subject: WolfPsortInput
  Predicate: SIO_000230 (has input)
  Object (Subject): SIO_010015 (protein sequence)
  Predicate: SIO_000300 (has value)
  Object: string (protein sequence)
  <sio:SIO_000230>
  <sio:SIO_010015>
  <sio:SIO_000300>
  Protein sequence
  </sio:SIO_000300>
  </sio:SIO_010015>

</sio:SIO_000230>

Sample input RDF file is as follows:

```
<rdf:RDF
    xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
    xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#"
    xmlns:sio="http://semanticscience.org/resource/">
    <aistls:WolfPsortInput rdf:about="http://www.molprof.jp/ontologies/wolfpsort.rdf#1">
        <sio:SIO_000230>
            <aistls:Kingdom rdf:about="#animal"/>
        </sio:SIO_000230>
        <aistls:SIO_000230>
            <sio:SIO_010015>
                <sio:SIO_000300>
>sp|P35413|GPR3_MOUSE G-protein coupled receptor 3 OS=Mus musculus GN=Gpr3 PE=2 SV=1
MMWGAGSSMAWFSAGSGSVNVSSVDPVEEPTGPATLLPSPRAWDVVLCISGTLVSCENAL
VVAIIVGTPAFRAPMFLLVGSLAVADLLAGLGLVLHFAADFCIGSPEMSLMLVGVLAMAF
TASIGSLLAITVDRYLSLYNALTYYSETTVTRTYVMLALVWVGALGLGLVPVLAWNCRDG
LTTCGVVYPLSKNHLVVLAIAFFMVFGIMLQLYAQICRIVCRHAQQIALQRHLLPASHYV
ATRKGIATLAVVLGAFAACWLPFTVYCLLGDADSPRLYTYLTLLPATYNSMINPVIYAFR
NQDVQKVLWAICCCCSTSKIPFRSRSPSDV
                </sio:SIO_000300>
            </sio:SIO_010015>
        </aistls:SIO_000230>
    </aistls:WolfPsortInput>
</rdf:RDF>
```

Wolfpsort input RDF

1.9.2. Execution command

% curl --data-binary @"input RDF file"
http://semantic.medals.jp:8090/sadi-services/Wolfpsort -o "output RDF file"

1.9.3. Execution result

WolfPsort output RDF format is as follows:

- RDF header:
  <rdf:RDF
  xmlns:rdf “http://www.w3.org/1999/02/22-rdf-syntax-ns#”
  xmlns:aistls “http://www.molprof.jp/ontologies/aistlssio.owl#”
  xmlns:sio “http://semanticscience.org/resource/”>
- Subject: WolfPsortOutput, rdf:about: the string as same as specifying in the input RDF
  <aistls:WolfPsortOutput
  rdf:about=”http://www.molprof.jp/ontologies/wolfpsort.rdf#1”>
- Triple for Wolfpsort results:
  Subject: WolfPsortOutput
  Predicate: SIO_000229 (has output)
  Object (Subject): SIO_000785 (answer)
  Predicate: SIO_000300 (has value)
  Object: string (Wolfpsort execution result)

```
<sio:SIO_000229>
    <sio:SIO_000785>
        <sio:SIO_000300>
            Wolfpsort execution result
        </sio:SIO_000300>
    </sio:SIO_000785>
</sio:SIO_000229>
```

Sample output RDF file is as follows:

```
<rdf:RDF
   xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
   xmlns:sio="http://semanticscience.org/resource/"
   xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#">
  <aistls:WolfPsortOutput rdf:about="http://www.molprof.jp/ontologies/wolfpsort.rdf#2">
    <sio:SIO_000229>
      <sio:SIO_000785>
        <sio:SIO_000300># k used for kNN is: 14
sp|P35413|GPR3_MOUSE cyto 7, extr 3, plas 2, E.R. 2, E.R._plas 2
</sio:SIO_000300>
      </sio:SIO_000785>
    </sio:SIO_000229>
  </aistls:WolfPsortOutput>
</rdf:RDF>
```

Wolfpsort output RDF

2. Asynchronous type SADI services

2.0. Uses asynchronous type SADI services

Asynchronous type SADI services are Last, Modelling, PoodleL, PoodleS and Rassie.

Each SADI service is executed by the following three procedures:

1） Getting polling URL

% curl --data-binary @"input RDF file"
http://semantic.medals.jp:8090/sadi-services/"SADI service name" (Figure 1-A)

If the user would like to execute PoodleL SADI service, the user specify below command:

% curl --data-binary @input.rdf
http://semantic.medals.jp:8090/sadi-services/PoodleL

An RDF-format stored a polling URL is displayed in command lines as below.

```
<rdf:RDF
    xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
    xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#">
    <aistls:PoodleLOutput rdf:about="http://www.molprof.jp/ontologies/poodle1.rdf#1">
        <rdfs:isDefinedBy
        rdf:resource="http://semantic.medals.jp:8090/sadi-services/PoodleL?poll=1"/>
    </aistls:PoodleLOutput>
</rdf:RDF>
```

RDF stored a polling URL (e.g. PoodleL)

2） Polling to SADI server

% curl http://semantic.medals.jp:8090/sadi-services/”SADI service name”?poll=”random polling number”

If the user asks to the SADI server whether PoodleL execution is completed or not:

%curl http://semantic.medals.jp:8090/sadi-services/PoodleL?poll=1

If the service is completed, a URL to the RDF file stored the results is displayed in command lines as below:

% curl http://semantic.medals.jp:8090/sadi-services/PoodleL?poll=1
COMPLETE: http://semantic.medals.jp/tmp/xxx/yyyy/poodleLResult.rdf
*This result is displayed in command lines only one time.

3） Getting execution results

% curl http://semantic.medals.jp/tmp/xxx/yyyy/ poodleLResult.rdf -o “output RDF file”

Please visit a chapter 1.0 for further input and output RDF format information.

2.1. Last

2.1.1. Preparing input RDF

Last input RDF format is as follows:

- RDF header:
  <rdf:RDF
    xmlns:rdf “http://www.w3.org/1999/02/22-rdf-syntax-ns#”
    xmlns:aistls “http://www.molprof.jp/ontologies/aistlssio.owl#”
    xmlns:sio “http://semanticscience.org/resource/”>
- Subject: LastInput, rdf:about: an arbitrary string
  <aistls:LastInput rdf:about=”http://www.molprof.jp/ontologies/last.rdf#1”>
- Triple for a query sequence:
  Subject: LastInput
  Predicate: SIO_000230 (has input)
  Object (Subject): SIO_000030 (biopolymer sequence)
    Predicate: SIO_000300 (has value)
    Object: string (query sequence)
  <sio:SIO_000230>
    <sio:SIO_000030>
      <sio:SIO_000300>
        Query sequence
      </sio:SIO_000300>
    </sio:SIO_000030>
  </sio:SIO_000230>
- Triple for a target sequence:
  Subject: LastInput
  Predicate: SIO_000230 (has input)
  Object (Subject): SIO_000030 (biopolymer sequence)
    Predicate: SIO_000300 (has value)
    Object: string (target sequence)
  <sio:SIO_000230>

<sio:SIO_000030>
<sio:SIO_000300>
Target sequence
</sio:SIO_000300>
</sio:SIO_000030>
</sio:SIO_000230>

- Triple for command options for Lastdb:
  Subject: LastInput
  Predicate: SIO_000230 (has input)
  Object (Subject): lastdbParameter
  Predicate: SIO_000300 (has value)
  Object: string (Lastdb options)

<sio:SIO_000230>
<aistls:lastdbParameter>
<sio:SIO_000300>
-m110 -w1
</sio:SIO_000300>
</aistls:lastdbParameter>
</sio:SIO_000230>

- Triple for command options for Lastal:
  Subject: LastInput
  Predicate: SIO_000230 (has input)
  Object (Subject): lastalParameter
  Predicate: SIO_000300 (has value)
  Object: string (Lastal options)

<sio:SIO_000230>
<aistls:lastdbParameter>
<sio:SIO_000300>
-j4 -u0 -m10 -l1 -k1 -w0 -g1.0 -s2 -e30
</sio:SIO_000300>
</aistls:lastdbParameter>
</sio:SIO_000230>

Sample input RDF file is as follows:

```
<rdf:RDF
   xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
   xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#"
   xmlns:sio="http://semanticscience.org/resource/">

   <aistls:LastInput rdf:about="http://www.molprof.jp/ontologies/last.rdf#1">
      <sio:SIO_000230>
         <sio:SIO_000030>
            <sio:SIO_000300>
>chickenMito
AATTTTATTTTTTAACCTAACTCCCCTACTAAGTGTACCCCCCCCTTTCCC
CAGGGGGGGTATACTATGCATAATCGTGCATACATTTATATACCACATAT
ATTATGGTACCGGTAATATATACTATATATGTACTAAACCCATTATATGT
ATACGGGCATTAACCTATATTCCACATTTCTCCCAATGTCCATTCTATGC
ATGATCTAGGACATACTCATTTACCCTCCCCATAGACAGTTCCAAACCAC
TATCAAGCCACCTAACTATGAATGGTTACAGGACATAAATCTCACTCTCA
TGTTCTCCCCCCAACAAGTCACCTAACTATGAATGGTTACAGGACATACA
TTTAACTACCATGTTCTAACCCATTTGGTTATGCTCGCCGTATCAGATGG
ATTTATTGATCGTCCACCTCACGAGAGATCAGCAACCCCTGCCTGTAATG
……
……
……
GAAACAAAAGAAACACCCAAACTCACTAACCACCCACATCCTATCACAGA
CGCTACCACCAACCCCACCACCCCATAATACGGCGAAGGATTAGACGCCA
CAGCTAAAACCCCCAGCATAAAACAAATCCCAAGAAAAATCACAAAATAA
GTCATATTATTCCCGCTTGGTTAGACCCCAAGGACTACGGCTTGAAAAGC
CATTGTTGTTCTCAACTACGGGAAC
            </sio:SIO_000300>
         </sio:SIO_000030>
      </sio:SIO_000230>
      <sio:SIO_000230>
         <sio:SIO_000030>
            <sio:SIO_000300>
>fuguMito
GCTAGCGTAGCTTAACCAAAGCAGAGTACTGAAGATGCTAAGATGGGCCC
TGAAAAGTCCCGCAGGCACAAAAGCTTGGTCCTGACTTTACTAACAACTC
TGATCAAACTTACACATGCAAGTATCCGCATCCCAGTGAAaatgcccccc
gccccccgtcCGGAAATAGGGAGTTGGTATCAGGCACACAAATTTGTAGC
CCATGACACCTAGCTTTGCCACGCCCCCAAGGGAATTCAGCAGTGATAAA
CATTAAGCCATAAGTGAAAACTTGACTTAGTTATGATCTAAAGAGTCGGT
……
……
……
TAGGAGAGACCTTTAAGTTTGAACCAAGCTCTCCActtaattaaatattc
atcatattattatcatatattataatattataataatataattatat
            </sio:SIO_000300>
         </sio:SIO_000030>
      </sio:SIO_000230>
      <sio:SIO_000230>
         <aistls:lastdbParameter>
            <sio:SIO_000300>-m110 -w1</sio:SIO_000300>
         </aistls:lastdbParameter>
      </sio:SIO_000230>
      <sio:SIO_000230>
         <aistls:lastalParameter>
            <sio:SIO_000300>-j4 -u0 -m10 -l1 -k1 -w0 -g1.0 -s2 -e30</sio:SIO_000300>
         </aistls:lastalParameter>
      </sio:SIO_000230>
   </aistls:LastInput>
</rdf:RDF>
```

Last input RDF

2.1.2. Execution command

% curl --data-binary @"input RDF file"
http://semantic.medals.jp:8090/sadi-services/Last

Last is an asynchronous SADI service, and first an RDF stored a URL polling for the SADI server is displayed in command lines as below. Next, the user asks to the SADI server using the URL defined in "isDefinedBy" tag whether Last execution is completed or not.

```
<rdf:RDF
    xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
    xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#">
    <aistls:LastOutput rdf:about="http://www.molprof.jp/ontologies/last.rdf#1">
        <rdfs:isDefinedBy
rdf:resource="http://semantic.medals.jp:8090/sadi-services/Last?poll=8"/>
        </aistls:LastOutput>
</rdf:RDF>
```

RDF stored the URL to poll for the SADI server

% curl http://semantic.medals.jp:8090/sadi-services/Last?poll=8 (in this case)
%

If Last execution is completed, the URL of an output RDF file stored Last results is displayed in command lines.
% curl http://semantic.medals.jp:8090/sadi-services/Last?poll=8
COMPLETE: http://semantic.medals.jp/tmp/xxx/yyyy/seq1_seq2Result.rdf
%

The user can get the RDF file as follows:
% curl http://semantic.medals.jp/tmp/xxx/yyyy/seq1_seq2Result.rdf -o "output RDF file"

2.1.3. Execution result

Last output RDF format is as follows:

- RDF header:
  <rdf:RDF
  xmlns:rdf “http://www.w3.org/1999/02/22-rdf-syntax-ns#”
  xmlns:aistls “http://www.molprof.jp/ontologies/aistlssio.owl#”
  xmlns:sio “http://semanticscience.org/resource/”>
- Subject: LastOutput, rdf:about: the string as same as specifying in the input RDF file
  <aistls:LastOutput rdf:about=”http://www.molprof.jp/ontologies/last.rdf#1”>
- Triple for Last results:
  Subject: LastOutput
  Predicate: SIO_000229 (has output)
  Object (Subject): SIO_000785 (answer)
  Predicate: SIO_000300 (has value)
  Object: string (Last execution result)

```
<sio:SIO_000229>
    <sio:SIO_000785>
        <sio:SIO_000300>
            Last execution result
        </sio:SIO_000300>
    </sio:SIO_000785>
</sio:SIO_000229>
```

- Triple for PNG ->Base64 transformation:
  Subject: LastOutput
  Predicate: SIO_000229 (has output)
  Object (Subject): Base64
  Predicate: SIO_000300 (has value)
  Object: string (Last PNG ->Base64 transformation)

```
<sio:SIO_000229>
    <aistls:Base64>
        <sio:SIO_000300>
```

Base64

<sio:SIO_000300>

</aistls:Base64>

</sio:SIO_000229>

</aistls:requiresResultInBase64BinaryFormat>

*if "-noimage" is specified at command options triple, Last doesn't generate PNG images (not contained in the output RDF file).

Sample output RDF file is as follows:


```
<rdf:RDF
   xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
   xmlns:sio="http://semanticscience.org/resource/"
   xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#">
  <aistls:LastOutput rdf:about="http://www.molprof.jp/ontologies/last.rdf#1">
   <sio:SIO_000229>
     <aistls:Base64>

<sio:SIO_000300>iVBORw0KGgoAAAANSUhEUgAAA9MAAAPmCAAAAADC0ZOHAAAOaElEQVR42u3dQVLbMABAUd3
/sj5C
mHHiISxgoAtX+nqvlDCli6DkI8lJnHEAJcMQgKZZ4ZYd48fvXp/QNIsk/X3KP/8fNM2cs/Tp7Pa8
eH59fTz/+bowXppmjXn6a8efH8fXT6LWNAs3PTStaUpNn3/ev61pTbPMfvq6ePv6VfX7Vtp+WtMs
OmujaTpztlHYs+kHsDxNg6YBTQOaBjQNmtY0aBrQNKBpQNOgaU2DpgFNA5oGNA2a1jRoGtA0oGlA
………
………
………
aRpaTQ9Ng6g1DaLWNOwYtaahFbWmoRW1pqEVtaahFbWmoRW1pqEVtaahFbWmoRW1pqEVtaahFbWm
oRW1pqEVtaahFbWmoRW1pqEV9Qf2BZeqhG6eZQAAAABJRU5ErkJggg==</sio:SIO_000300>
     </aistls:Base64>
   </sio:SIO_000229>
   <sio:SIO_000229>
     <sio:SIO_000785>
       <sio:SIO_000300># LAST version 58
#
# a=7 b=1 c=100000 e=30 d=18 x=27 y=10
# u=0 s=2 m=10 l=1 k=1 i=134217728 w=0 t=0.910239 g=1 j=4
# seq1
#
#    A  C  G  T
………
………
………
a score=40
s fuguMito    13752 126 + 16447
AACTGCTCGAAGAGCCCCCCGACCCAGCCCCCGCACCAGCTCTAATACTACAAGCAACGTCAATAACAAGACCCAGGCCCCCAATAG
TAATACTCCCCCACCGCTAGAATATATAAGTGAAACCCC
s chickenMito 16186 126 + 16775
AACCGCCCGAATTGCCCCCCGAGACAACCCCACGCACAAGCTCTAGTACAACAAACAAAGCTAACAACAAACCTCACCCAGCCACCAA
AAACAACCCAACCCCACATGAATAAAACACCGCAACTCC
p 0.681 0.832 0.883 0.9 0.95 0.967 0.973 0.989 0.995 0.997 0.997 0.998 0.998 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 0.999 0.999 0.998 0.996 0.988 0.985 0.984 0.98 0.979 0.976 0.967 0.963 0.962 0.959 0.958
0.958 0.957 0.955 0.948 0.945 0.945 0.942 0.941 0.941 0.94 0.938 0.937 0.935 0.934 0.933
0.933 0.93 0.93 0.929 0.929 0.928 0.928 0.925 0.924 0.922 0.921 0.921 0.92 0.918 0.911 0.89
0.828 0.807 0.745 0.724 0.717 0.696 0.69 0.687 0.68 0.678 0.671 0.65 0.588 0.567 0.505
# CPU time: 0.22 seconds
</sio:SIO_000300>
     </sio:SIO_000785>
   </sio:SIO_000229>
  </aistls:LastOutput>
</rdf:RDF>
```


Last output RDF

2.2. Modelling

2.2.1. Preparing input RDF

Modelling input RDF format is as follows:

- RDF header:
  <rdf:RDF
  xmlns:rdf “http://www.w3.org/1999/02/22-rdf-syntax-ns#”
  xmlns:aistls “http://www.molprof.jp/ontologies/aistlssio.owl#”
  xmlns:sio “http://semanticscience.org/resource/”>
- Subject: ModellingInput, rdf:about: an arbitrary string
  <aistls:ModellingInput
  rdf:about=”http://www.molprof.jp/ontologies/modelling.rdf#1”>
- Triple for a protein sequence:
  Subject: ModellingInput
  Predicate: SIO_000230 (has input)
  Object (Subject): SIO_010015 (protein sequence)
  Predicate: SIO_000300 (has value)
  Object: string (protein sequence)

```
<sio:SIO_000230>
    <sio:SIO_010015>
        <sio:SIO_000300>
            Protein sequence
        </sio:SIO_000300>
    </sio:SIO_010015>
</sio:SIO_000230>
```

- Triple for BLAST program name:
  Subject: ModellingInput
  Predicate: SIO_000230 (has input)
  Object (Subject): BlastSearch
  Predicate: SIO_000008 (has attribute)
  Object: BlastProgram (rdf:about=”#BLAST” (BLAST or PSI-BLAST))

<sio:SIO_000230>
<aistls:BlastSearch>
<sio:SIO_000008>
<aistls:BlastProgram rdf:about="#PSI-BLAST"/>
</sio:SIO_000008>
</aistls:BlastSearch>
</sio:SIO_000230>

- Triple for iteration number (for PSI-BLAST):

Subject: ModellingInput
Predicate: SIO_000230 (has input)
Object (Subject): BlastSearch
Predicate: SIO_000216 (has measurement value)
Object (Subject): iteration
Predicate: SIO_000300 (has value)
Object: integer (iteration number >1)

<sio:SIO_000230>
<aistls:BlastSearch>
<sio:SIO_000216>
<aistls:iteration>
<sio:SIO_000300>2</sio:SIO_000300>
</aistls:iteration>
</sio:SIO_000216>
</aistls:BlastSearch>
</sio:SIO_000230>

- Triple for E-value:

Subject: ModellingInput
Predicate: SIO_000230 (has input)
Object (Subject): BlastSearch
Predicate: SIO_000216 (has measurement value)
Object (Subject): SIO_001021 (expected value)
Predicate: SIO_000300 (has value)
Object: double (e.g. 10e-30)

<sio:SIO_000230>
<aistls:BlastSearch>
<sio:SIO_000216>
<sio:SIO_001021>

<sio:SIO_000300>0.00005</sio:SIO_000300>
</sio:SIO_001021>
</sio:SIO_000216>
</aistls:BlastSearch>
</sio:SIO_000230>

- Triple for a coverage threshold for BLAST hit regions:
  Subject: ModellingInput
  Predicate: SIO_000230 (has input)
  Object (Subject): BlastSearch
  Predicate: SIO_000216 (has measurement value)
  Object (Subject): coverage
  Predicate: SIO_000300 (has value)
  Object: double (coverage threshold for BLAST hit regions)

<sio:SIO_000230>
<aistls:BlastSearch>
<sio:SIO_000216>
<aistls:coverage>
<sio:SIO_000300>55.0</sio:SIO_000300>
</aistls:coverage>
</sio:SIO_000216>
</aistls:BlastSearch>
</sio:SIO_000230>

- Triple for an identity threshold for BLAST hit regions:
  Subject: ModellingInput
  Predicate: SIO_000230 (has input)
  Object (Subject): BlastSearch
  Predicate: SIO_000216 (has measurement value)
  Object (Subject): identity
  Predicate: SIO_000300 (has value)
  Object: double (identity threshold for BLAST hit regions)

<sio:SIO_000230>
<aistls:BlastSearch>
<sio:SIO_000216>
<aistls:identity>
<sio:SIO_000300>35.0</sio:SIO_000300>
</aistls:identity>

```
            </sio:SIO_000216>
        </aistls:BlastSearch>
    </sio:SIO_000230>
```

- Triple for a minimum sequence length threshold of BLAST hit regions:

  Subject: ModellingInput

  Predicate: SIO_000230 (has input)

  Object (Subject): BlastSearch

  Predicate: SIO_000216 (has measurement value)

  Object (Subject): minSequenceLength

  Predicate: SIO_000300 (has value)

  Object: integer (minimum sequence length threshold of BLAST hit regions)

```
    <sio:SIO_000230>
        <aistls:BlastSearch>
            <sio:SIO_000216>
                <aistls:minSequenceLength>
                    <sio:SIO_000300>31</sio:SIO_000300>
                </aistls:minSequenceLength>
            </sio:SIO_000216>
        </aistls:BlastSearch>
    </sio:SIO_000230>
```

- Triple for a coverage threshold for selecting template sequences:

  Subject: ModellingInput

  Predicate: SIO_000230 (has input)

  Object (Subject): templateSearch

  Predicate: SIO_000216 (has measurement value)

  Object (Subject): coverage

  Predicate: SIO_000300 (has value)

  Object: double (coverage threshold for selecting template sequences)

```
    <sio:SIO_000230>
        <aistls:templateSearch>
            <sio:SIO_000216>
                <aistls:coverage>
                    <sio:SIO_000300>96.0</sio:SIO_000300>
                </aistls:coverage>
```

```
            </sio:SIO_000216>
        </aistls:templateSearch>
    </sio:SIO_000230>
    <aistls:setupTemplateCoverageThreshold>90.0
    </aistls:setupTemplateCoverageThreshold>
```

- Triple for an identity threshold for selecting template sequences:

  Subject: ModellingInput

  Predicate: SIO_000230 (has input)

  Object (Subject): templateSearch

  Predicate: SIO_000216 (has measurement value)

  Object (Subject): identity

  Predicate: SIO_000300 (has value)

  Object: double (identity threshold for selecting template sequences)

```
    <sio:SIO_000230>
        <aistls:templateSearch>
            <sio:SIO_000216>
                <aistls:identity>
                    <sio:SIO_000300>96.0</sio:SIO_000300>
                </aistls:identity>
            </sio:SIO_000216>
        </aistls:templateSearch>
    </sio:SIO_000230>
```

- Triple for MODELLER license key:

  Subject: ModellingInput

  Predicate: SIO_000230 (has input)

  Object (Subject): modeller

  Predicate: SIO_0000008 (has attribute)

  Object (Subject): LicenseKey

  Predicate: SIO_000300 (has value)

  Object: string (MODELLER license key)

```
    <sio:SIO_000230>
        <aistls:modeller>
            <sio:SIO_000008>
                <aistls:LicenseKey>
                    <sio:SIO_000300>****</sio:SIO_000300>
```

```
                </aistls:LicenseKey>
            </sio:SIO_000008>
        </aistls:modeller>
    </sio:SIO_000230>
```

*Modelling execution needs MODELLER license key. Please visit a MODELLER registration site (http://saliab.org/modeller/registration.html).

- Triple for a threshold of number of models generated by MODELLER:

  Subject: ModellingInput

  Predicate: SIO_000230 (has input)

  Object (Subject): modeller

  Predicate: SIO_000216 (has measurement value)

  Object (Subject): numberOfModel

  Predicate: SIO_000300 (has value)

  Object: integer (threshold of number of models generated by MODELLER)

```
<sio:SIO_000230>
    <aistls:modeller>
        <sio:SIO_000216>
            <aistls:numberOfModel>
                <sio:SIO_000300>3</sio:SIO_000300>
            </aistls:numberOfModel>
        </sio:SIO_000216>
    </aistls:modeller>
</sio:SIO_000230>
```

Sample input RDF file is as follows:

```
<rdf:RDF
    xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
    xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#"
    xmlns:sio="http://semanticscience.org/resource/">
    <aistls:ModellingInput rdf:about="http://www.molprof.jp/ontologies/modelling.rdf#1">
        <sio:SIO_000230>
            <sio:SIO_010015>
                <sio:SIO_000300>
>sp|P04156|PRIO_HUMAN Major prion protein OS=Homo sapiens GN=PRNP PE=1 SV=1
MANLGCWMLVLFVATWSDLGLCKKRPKPGGWNTGGSRYPGQGSPGGNRYPPQGGGGWGQP
HGGGWGQPHGGGWGQPHGGGWGQPHGGGWGQGGGTHSQWNKPSKPKTNMKHMAGAAAAGA
VVGGLGGYMLGSAMSRPIIHFGSDYEDRYYRENMHRYPNQVYYRPMDEYSNQNNFVHDCV
NITIKQHTVTTTTKGENFTETDVKMMERVVEQMCITQYERESQAYYQRGSSMVLFSSPPV
ILLISFLIFLIVG
                </sio:SIO_000300>
            </sio:SIO_010015>
        </sio:SIO_000230>
        <sio:SIO_000230>
            <aistls:BlastSearch>
                <sio:SIO_000008>
                    <aistls:BlastProgram rdf:about="#PSI-BLAST"/>
                </sio:SIO_000008>
            </aistls:BlastSearch>
        </sio:SIO_000230>
        <sio:SIO_000230>
            <aistls:BlastSearch>
                <sio:SIO_000216>
                    <aistls:iteration>
                        <sio:SIO_000300>2</sio:SIO_000300>
                    </aistls:iteration>
                </sio:SIO_000216>
            </aistls:BlastSearch>
        </sio:SIO_000230>
        <sio:SIO_000230>
            <aistls:BlastSearch>
                <sio:SIO_000216>
                    <sio:SIO_001021>
                        <sio:SIO_000300>0.00005</sio:SIO_000300>
                    </sio:SIO_001021>
                </sio:SIO_000216>
            </aistls:BlastSearch>
        </sio:SIO_000230>
……
……
……
        <sio:SIO_000230>
            <aistls:modeller>
                <sio:SIO_000008>
                    <aistls:LicenseKey>
                        <sio:SIO_000300>****</sio:SIO_000300>
                    </aistls:LicenseKey>
                </sio:SIO_000008>
            </aistls:modeller>
        </sio:SIO_000230>
        <sio:SIO_000230>
            <aistls:modeller>
                <sio:SIO_000216>
                    <aistls:numberOfModel>
                        <sio:SIO_000300>3</sio:SIO_000300>
                    </aistls:numberOfModel>
                </sio:SIO_000216>
            </aistls:modeller>
        </sio:SIO_000230>
    </aistls:ModellingInput>
</rdf:RDF>
```

Modelling 用入力 RDF

2.2.2. Execution command

% curl --data-binary @"input RDF file"
http://semantic.medals.jp:8090/sadi-services/Modelling

Modelling is an asynchronous SADI service, and first an RDF stored a URL polling for the SADI server is displayed in command lines as below. Next, the user asks to the SADI server using the URL defined in "isDefinedBy" tag whether Modelling execution is completed or not.

```
<rdf:RDF
    xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
    xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#">
    <aistls:ModellingOutput rdf:about="http://www.molprof.jp/ontologies/modelling.rdf#1">
        <rdfs:isDefinedBy
rdf:resource="http://semantic.medals.jp:8090/sadi-services/Modelling?poll=10"/>
    </aistls:ModellingOutput>
</rdf:RDF>
```

RDF stored the URL to poll for the SADI server

% curl http://semantic.medals.jp:8090/sadi-services/Modelling?poll=10 (in this case)
%

If Modelling execution is completed, the URL of an output RDF file stored Modelling results is displayed in command lines.
% curl http://semantic.medals.jp:8090/sadi-services/Modelling?poll=10
COMPLETE: http://semantic.medals.jp/tmp/xxx/yyyy/modellingResult.rdf
%

The user can get the RDF file as follows:
% curl http://semantic.medals.jp/tmp/xxx/yyyy/modellingResult.rdf -o "output RDF name"

2.2.3. Execution result

Modelling output RDF format is as follows:

- RDF header:
  <rdf:RDF
  xmlns:rdf “http://www.w3.org/1999/02/22-rdf-syntax-ns#”
  xmlns:aistls “http://www.molprof.jp/ontologies/aistlssio.owl#”
  xmlns:sio “http:://semanticscience.org/resource/”>
- Subject: ModellingOutput, rdf:about: the string as same as specifying in the input RDF
  <aistls:ModellingOutput
  rdf:about=”http://www.molprof.jp/ontologies/modelling.rdf#1”>
- Triple for a protein sequence:
  Subject: ModellingOutput
  Predicate: SIO_000229 (has output)
  Object (Subject): SIO_010015 (protein sequence)
  Predicate: SIO_000300 (has value)
  Object: string (protein sequence)

```
<sio:SIO_000229>
    <sio:SIO_010015>
        <sio:SIO_000300>
            Protein sequence
        </sio:SIO_000300>
    </sio:SIO_010015>
</sio:SIO_000229
```

- Triple for BLAST results:
  Subject: ModellingOutput
  Predicate: SIO_000229 (has output)
  Object (Subject): BlastHit
  Predicate: SIO_000673 (has unique identifier)
  Object (Subject): SIO_000729 (record identifier)
  Predicate: SIO_000300 (has value)
  Object: string (hit sequence ID)

Predicate: SIO_000216 (has measurement value)
Object (Subject): SIO_000794 (count)
Predicate: SIO_000300 (has value)
Object: integer (hit count)
Predicate: SIO_000008 (has attribute)
Object (Subject): BlastAlignment
Predicate: SIO_000008 (has attribute)
Object (Subject): query
Predicate: SIO_000216 (has measurement value)
Object (Subject): SIO_000792 (sequence end position)
Predicate: SIO_000300 (has value)
Object: integer
Predicate: SIO_000216 (has measurement value)
Object (Subject): SIO_000791 (sequence start position)
Predicate: SIO_000300 (has sequence)
Object: integer
Predicate: SIO_000216 (has measurement value)
Object (Subject): coverage
Predicate: SIO_000300 (has value)
Object: double (%)
Predicate: SIO_000216 (has measurement value)
Object (Subject): sequenceLength
Predicate: SIO_000300 (has sequence)
Object: integer
Predicate: SIO_000008 (has attribute)
Object (Subject): subject
Predicate: SIO_000216 (has measurement value)
Object (Subject): SIO_000792 (sequence end position)
Predicate: SIO_000300 (has value)
Object: integer
Predicate: SIO_000216 (has measurement value)
Object (Subject): SIO_000791 (sequence start position)
Predicate: SIO_000300 (has sequence)
Object: integer
Predicate: SIO_000216 (has measurement value)
Object (Subject): coverage

Predicate: SIO_000300 (has value)

Object: double (%)

Predicate: SIO_000216 (has measurement value)

Object (Subject): sequenceLength

Predicate: SIO_000300 (has sequence)

Object: integer

Predicate: SIO_000216 (has measurement value)

Object (Subject): SIO_001021 (expected value)

Predicate: SIO_000300 (has value)

Object: double (e.g. 10e-30)

Predicate: SIO_000216 (has measurement value)

Object (Subject): identity

Predicate: SIO_000300 (has value)

Object: double (%)

```
<sio:SIO_000229>
    <aistls:BlastHit>
        <sio:SIO_000008>
            <aistls:BlastAlignment>
                <sio:SIO_000008>
                    <aistls:subject>
                        <sio:SIO_000216>
                            <sio:SIO_000792>
                                <sio:SIO_000300>117</sio:SIO_000300>
                            </sio:SIO_000792>
                        </sio:SIO_000216>
                        <sio:SIO_000216>
                            <sio:SIO_000791>
                                <sio:SIO_000300>1</sio:SIO_000300>
                            </sio:SIO_000791>
                        </sio:SIO_000216>
                        <sio:SIO_000216>
                            <aistls:coverage>
                                <sio:SIO_000300>100.00</sio:SIO_000300>
                            </aistls:coverage>
                        </sio:SIO_000216>
                        <sio:SIO_000216>
```

```
                    <aistls:sequenceLength>
                        <sio:SIO_000300>117</sio:SIO_000300>
                    </aistls:sequenceLength>
                </sio:SIO_000216>
            </aistls:subject>
        </sio:SIO_000008>
        <sio:SIO_000008>
            <aistls:query>
                <sio:SIO_000216>
                    <sio:SIO_000792>
                        <sio:SIO_000300>225</sio:SIO_000300>
                    </sio:SIO_000792>
                </sio:SIO_000216>
                <sio:SIO_000216>
                    <sio:SIO_000791>
                        <sio:SIO_000300>119</sio:SIO_000300>
                    </sio:SIO_000791>
                </sio:SIO_000216>
                <sio:SIO_000216>
                    <aistls:coverage>
                        <sio:SIO_000300>42.29</sio:SIO_000300>
                    </aistls:coverage>
                </sio:SIO_000216>
                <sio:SIO_000216>
                    <aistls:sequenceLength>
                        <sio:SIO_000300>107</sio:SIO_000300>
                    </aistls:sequenceLength>
                </sio:SIO_000216>
            </aistls:query>
        </sio:SIO_000008>
        <sio:SIO_000216>
            <sio:SIO_001021>
                <sio:SIO_000300>6.7286e-43</sio:SIO_000300>
            </sio:SIO_001021>
        </sio:SIO_000216>
        <sio:SIO_000216>
```

<aistls:identity>
<sio:SIO_000300>38.46</sio:SIO_000300>
</aistls:identity>
</sio:SIO_000216>
</aistls:BlastAlignment>
</sio:SIO_000008>
<sio:SIO_000673>
<sio:SIO_000729>
<sio:SIO_000300>1u3mA</sio:SIO_000300>
</sio:SIO_000729>
</sio:SIO_000673>
<sio:SIO_000216>
<sio:SIO_000794>
<sio:SIO_000300>17</sio:SIO_000300>
</sio:SIO_000794>
</sio:SIO_000216>
</aistls:BlastHit>
</sio:SIO_000229>

- Triple for hit region information for modelling:
  Subject: ModellingOutput
  Predicate: SIO_000229 (has output)
  Object (Subject): TemplateHit
    Predicate: SIO_000673 (has unique identifier)
    Object (Subject): SIO_000729 (record identifier)
      Predicate: SIO_000300 (has value)
      Object: string (hit sequence ID)
    Predicate: SIO_000216 (has measurement value)
    Object (Subject): SIO_000794 (count)
      Predicate: SIO_000300 (has value)
      Object: integer (hit count)
    Predicate: SIO_000008 (has attribute)
    Object (Subject): query
      Predicate: SIO_000216 (has measurement value)
      Object (Subject): SIO_000792 (sequence end position)
        Predicate: SIO_000300 (has value)
        Object: integer

Predicate: SIO_000216 (has measurement value)
Object (Subject): SIO_000791 (sequence start position)
Predicate: SIO_000300 (has sequence)
Object: integer
Predicate: SIO_000216 (has measurement value)
Object (Subject): coverage
Predicate: SIO_000300 (has value)
Object: double (%)
Predicate: SIO_000216 (has measurement value)
Object (Subject): sequenceLength
Predicate: SIO_000300 (has sequence)
Object: integer
Predicate: SIO_000008 (has attribute)
Object (Subject): subject
Predicate: SIO_000216 (has measurement value)
Object (Subject): SIO_000792 (sequence end position)
Predicate: SIO_000300 (has value)
Object: integer
Predicate: SIO_000216 (has measurement value)
Object (Subject): SIO_000791 (sequence start position)
Predicate: SIO_000300 (has sequence)
Object: integer
Predicate: SIO_000216 (has measurement value)
Object (Subject): coverage
Predicate: SIO_000300 (has value)
Object: double (%)
Predicate: SIO_000216 (has measurement value)
Object (Subject): sequenceLength
Predicate: SIO_000300 (has sequence)
Object: integer
Predicate: SIO_000008 (has attribute)
Object (Subject): BlastAlignment
Predicate: SIO_000216 (has measurement value)
Object (Subject): SIO_001021 (expected value)
Predicate: SIO_000300 (has value)
Object: double (e.g. 10e-30)

Predicate: SIO_000216 (has measurement value)
Object (Subject): identity
Predicate: SIO_000300 (has value)
Object: double (%)

```
<sio:SIO_000229>
    <aistls:templateHit>
        <sio:SIO_000008>
            <aistls:subject>
                <sio:SIO_000216>
                    <sio:SIO_000792>
                        <sio:SIO_000300>111</sio:SIO_000300>
                    </sio:SIO_000792>
                </sio:SIO_000216>
                <sio:SIO_000216>
                    <sio:SIO_000791>
                        <sio:SIO_000300>1</sio:SIO_000300>
                    </sio:SIO_000791>
                </sio:SIO_000216>
                <sio:SIO_000216>
                    <aistls:coverage>
                        <sio:SIO_000300>100.00</sio:SIO_000300>
                    </aistls:coverage>
                </sio:SIO_000216>
                <sio:SIO_000216>
                    <aistls:sequenceLength>
                        <sio:SIO_000300>111</sio:SIO_000300>
                    </aistls:sequenceLength>
                </sio:SIO_000216>
            </aistls:subject>
        </sio:SIO_000008>
        <sio:SIO_000008>
            <aistls:query>
                <sio:SIO_000216>
                    <sio:SIO_000792>
                        <sio:SIO_000300>231</sio:SIO_000300>
                    </sio:SIO_000792>
```

```
            </sio:SIO_000216>
            <sio:SIO_000216>
                <sio:SIO_000791>
                    <sio:SIO_000300>121</sio:SIO_000300>
                </sio:SIO_000791>
            </sio:SIO_000216>
            <sio:SIO_000216>
                <aistls:coverage>
                    <sio:SIO_000300>43.87</sio:SIO_000300>
                </aistls:coverage>
            </sio:SIO_000216>
            <sio:SIO_000216>
                <aistls:sequenceLength>
                    <sio:SIO_000300>111</sio:SIO_000300>
                </aistls:sequenceLength>
            </sio:SIO_000216>
        </aistls:query>
    </sio:SIO_000008>
    <sio:SIO_000008>
        <aistls:BlastAlignment>
            <sio:SIO_000216>
                <sio:SIO_001021>
                    <sio:SIO_000300>5.25043e-64</sio:SIO_000300>
                </sio:SIO_001021>
            </sio:SIO_000216>
            <sio:SIO_000216>
                <aistls:identity>
                    <sio:SIO_000300>90.99</sio:SIO_000300>
                </aistls:identity>
            </sio:SIO_000216>
        </aistls:BlastAlignment>
    </sio:SIO_000008>
    <sio:SIO_000673>
        <sio:SIO_000729>
            <sio:SIO_000300>1xyuA</sio:SIO_000300>
        </sio:SIO_000729>
```

```
            </sio:SIO_000673>
            <sio:SIO_000216>
                <sio:SIO_000794>
                    <sio:SIO_000300>1</sio:SIO_000300>
                </sio:SIO_000794>
            </sio:SIO_000216>
        </aistls:templateHit>
    </sio:SIO_000229>
```

- Triple for MODELLER results:

  Subject: ModellingOutput

  Predicate: SIO_000229 (has output)

  Object (Subject): PdbFormatStructureModel

  Predicate: SIO_000300 (has value)

  Object: string (MODELLER execution result)

```
    <sio:SIO_000229>
        <aistls:PdbFormatStructureModel>
            <sio:SIO_000300>
                MODELLER execution result
            </sio:SIO_000300>
        </aistls:PdbFormatStructureModel>
    </sio:SIO_000229>
```

Sample output RDF file is as follows:

```
<rdf:RDF
   xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
   xmlns:sio="http://semanticscience.org/resource/"
   xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#">
  <aistls:ModellingOutput rdf:about="http://www.molprof.jp/ontologies/modelling.rdf#1">
   <sio:SIO_000229>
     <aistls:BlastHit>
       <sio:SIO_000008>
         <aistls:BlastAlignment>
          <sio:SIO_000008>
            <aistls:subject>
              <sio:SIO_000216>
                <sio:SIO_000792>
                  <sio:SIO_000300>117</sio:SIO_000300>
                </sio:SIO_000792>
              </sio:SIO_000216>
              <sio:SIO_000216>
                <sio:SIO_000791>
                  <sio:SIO_000300>1</sio:SIO_000300>
                </sio:SIO_000791>
              </sio:SIO_000216>
              <sio:SIO_000216>
                <aistls:coverage>
                  <sio:SIO_000300>100.00</sio:SIO_000300>
                </aistls:coverage>
              </sio:SIO_000216>
              <sio:SIO_000216>
                <aistls:sequenceLength>
                  <sio:SIO_000300>117</sio:SIO_000300>
                </aistls:sequenceLength>
              </sio:SIO_000216>
……
……
……
    <sio:SIO_000229>
      <sio:SIO_010015>
        <sio:SIO_000300>
&gt;sp|P04156|PRIO_HUMAN Major prion protein OS=Homo sapiens GN=PRNP PE=1 SV=1
MANLGCWMLVLFVATWSDLGLCKKRPKPGGWNTGGSRYPGQGSPGGNRYPPQGGGGWGQP
HGGGWGQPHGGGWGQPHGGGWGQPHGGGWGQGGGTHSQWNKPSKPKTNMKHMAGAAAAGA
VVGGLGGYMLGSAMSRPIIHFGSDYEDRYYRENMHRYPNQVYYRPMDEYSNQNNFVHDCV
NITIKQHTVTTTTKGENFTETDVKMMERVVEQMCITQYERESQAYYQRGSSMVLFSSPPV
ILLISFLIFLIVG
              </sio:SIO_000300>
      </sio:SIO_010015>
    </sio:SIO_000229>
……
……
……
    <sio:SIO_000229>
      <aistls:PdbFormatStructureModel>
        <sio:SIO_000300>MODEL:2     Query hit region:121-231
EXPDTA    THEORETICAL MODEL, MODELLER 9v5 2013/12/26 17:27:52
REMARK   6 MODELLER OBJECTIVE FUNCTION:      629.3421
REMARK   6 MODELLER BEST TEMPLATE % SEQ ID:  90.991
ATOM      1  N   VAL   121     17.477 -11.772  -0.651  1.00 89.30          N
ATOM      2  CA  VAL   121     16.995 -11.872  -2.041  1.00 89.30          C
ATOM      3  CB  VAL   121     17.764 -12.926  -2.780  1.00 89.30          C
ATOM      4  CG1 VAL   121     17.518 -14.283  -2.094  1.00 89.30          C
ATOM      5  CG2 VAL   121     17.351 -12.873  -4.259  1.00 89.30          C
……
……
……
     </sio:SIO_000229>
  </aistls:ModellingOutput>
</rdf:RDF
```

Modelling output RDF

2.3. PoodleL

2.3.1. Preparing input RDF

PoodleL input RDF format is as follows:

- RDF header:
  <rdf:RDF
  xmlns:rdf “http://www.w3.org/1999/02/22-rdf-syntax-ns#”
  xmlns:aistls “http://www.molprof.jp/ontologies/aistlssio.owl#”
  xmlns:sio “http://semanticscience.org/resource/”>
- Subject: PoodleLInput, rdf:about: an arbitrary string
  <aistls:PoodleLInput
  rdf:about=”http://www.molprof.jp/ontologies/poodlel.rdf#1”>
- Triple for a protein sequence:
  Subject: PoodleLInput
  Predicate: SIO_000230 (has input)
  Object (Subject): SIO_010015 (protein sequence)
  Predicate: SIO_000300 (has value)
  Object: string (protein sequence)

```
<sio:SIO_000230>
    <sio:SIO_010015>
        <sio:SIO_000300>
            Protein sequence
        </sio:SIO_000300>
    </sio:SIO_010015>
</sio:SIO_000230>
```

Sample input RDF file is as follows:

```
<rdf:RDF
    xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
    xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#"
    xmlns:sio="http://semanticscience.org/resource/">

    <aistls:PoodleLInput rdf:about="http://www.molprof.jp/ontologies/poodlel.rdf#1">
       <sio:SIO_000230>
          <sio:SIO_010015>
             <sio:SIO_000300>
>sp|P04156|PRIO_HUMAN Major prion protein OS=Homo sapiens GN=PRNP PE=1 SV=1
MANLGCWMLVLFVATWSDLGLCKKRPKPGGWNTGGSRYPGQGSPGGNRYPPQGGGGWGQP
HGGGWGQPHGGGWGQPHGGGWGQPHGGGWGQGGGTHSQWNKPSKPKTNMKHMAGAAAAGA
VVGGLGGYMLGSAMSRPIIHFGSDYEDRYYRENMHRYPNQVYYRPMDEYSNQNNFVHDCV
NITIKQHTVTTTTKGENFTETDVKMMERVVEQMCITQYERESQAYYQRGSSMVLFSSPPV
ILLISFLIFLIVG
             </sio:SIO_000300>
          </sio:SIO_010015>
       </sio:SIO_000230>
    </aistls:PoodleLInput>
</rdf:RDF>
```

PoodleL input RDF

2.3.2. Execution command

% curl --data-binary @"input RDF file"
http://semantic.medals.jp:8090/sadi-services/PoodleL

PoodleL is an asynchronous SADI service, and first an RDF stored a URL polling for the SADI server is displayed in command lines as below. Next, the user asks to the SADI server using the URL defined in "isDefinedBy" tag whether PoodleL execution is completed or not.

```
<rdf:RDF

    xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"

    xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#">

    <aistls:PoodleLOutput rdf:about="http://www.molprof.jp/ontologies/poodlel.rdf#1">

       <rdfs:isDefinedBy

rdf:resource="http://semantic.medals.jp:8090/sadi-services/PoodleL?poll=21"/>

    </aistls:PoodleLOutput>

</rdf:RDF>
```

RDF stored the URL to poll for the SADI server

% curl http://semantic.medals.jp:8090/sadi-services/PoodleL?poll=21 (in this case)
%

If PoodleL execution is completed, the URL of an output RDF file stored PoodleL results is displayed in command lines.
% curl http://semantic.medals.jp:8090/sadi-services/PoodleL?poll=21
COMPLETE: http://semantic.medals.jp/tmp/xxx/yyyy/poodleLResult.rdf
%

The user can get the RDF file as follows:
% curl http://semantic.medals.jp/tmp/xxx/yyyy/ poodleLResult.rdf -o "output RDF file"

2.3.3. Execution result

PoodleL output RDF format is as follows:

- RDF header:
  <rdf:RDF
    xmlns:rdf “http://www.w3.org/1999/02/22-rdf-syntax-ns#”
    xmlns:aistls “http://www.molprof.jp/ontologies/aistlssio.owl#”
    xmlns:sio “http://semanticscience.org/resource/”>
- Subject: PoodleLOutput, rdf:about: the string as same as specifying in the input RDF
  <aistls:PoodleLOutput
  rdf:about=”http://www.molprof.jp/ontologies/poodlel.rdf#1”>
- Triple for PoodleL results:
  Subject: PoodleLOutput
  Predicate: SIO_000229 (has output)
  Object (Subject): PoodleResult
    Predicate: SIO_000008 (has attribute)
    Object (Subject): disorderPrediction
      Predicate: SIO_000216 (has measurement value)
      Object (Subject): SIO_000765 (probability value)
        Predicate: SIO_000300 (has value)
        Object: double (disorder probability)
      Predicate: SIO_000216 (has measurement value)
      Object (Subject): SIO_000789 (sequence element position)
        Predicate: SIO_000300 (has value)
        Object: double
      Predicate: SIO_000008 (has attribute)
      Object (Subject): SIO_010074 (amino acid residue)
        Predicate: SIO_000300 (has value)
        Object: double
      Predicate: SIO_000008 (has attribute)
      Object: SIO_000758 (disordered)
      Predicate: SIO_000008 (has attribute)

Object: SIO_001093 (rigid)

```
<sio:SIO_000229>
    <aistls:PoodleResult>
        <sio:SIO_000008>
            <aistls:disorderPrediction>
                <sio:SIO_000216>
                    <sio:SIO_000765>
                        <sio:SIO_000300>0.1024</sio:SIO_000300>
                    </sio:SIO_000765>
                </sio:SIO_000216>
                <sio:SIO_000008>
                    <sio:SIO_001093/>
                </sio:SIO_000008>
                <sio:SIO_000008>
                    <sio:SIO_010074>
                        <sio:SIO_000300>T</sio:SIO_000300>
                    </sio:SIO_010074>
                </sio:SIO_000008>
                <sio:SIO_000216>
                    <sio:SIO_000789>
                        <sio:SIO_000300>192</sio:SIO_000300>
                    </sio:SIO_000789>
                </sio:SIO_000216>
            </aistls:disorderPrediction>
        </sio:SIO_000008>
    </aistls:PoodleResult>
</sio:SIO_000229>
```

Sample output RDF file is as follows:

```
<rdf:RDF
    xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
    xmlns:sio="http://semanticscience.org/resource/"
    xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#">
  <aistls:PoodleLOutput rdf:about="http://www.molprof.jp/ontologies/poodlel.rdf#1">
    <sio:SIO_000229>
      <aistls:PoodleResult>
        <sio:SIO_000008>
          <aistls:disorderPrediction>
            <sio:SIO_000216>
              <sio:SIO_000765>
                <sio:SIO_000300>0.9723</sio:SIO_000300>
              </sio:SIO_000765>
            </sio:SIO_000216>
            <sio:SIO_000008>
              <sio:SIO_000758/>
            </sio:SIO_000008>
            <sio:SIO_000008>
              <sio:SIO_010074>
                <sio:SIO_000300>P</sio:SIO_000300>
              </sio:SIO_010074>
            </sio:SIO_000008>
            <sio:SIO_000216>
              <sio:SIO_000789>
                <sio:SIO_000300>76</sio:SIO_000300>
              </sio:SIO_000789>
            </sio:SIO_000216>
          </aistls:disorderPrediction>
        </sio:SIO_000008>
……
……
……
              <sio:SIO_000789>
                <sio:SIO_000300>165</sio:SIO_000300>
              </sio:SIO_000789>
            </sio:SIO_000216>
          </aistls:disorderPrediction>
        </sio:SIO_000008>
        <sio:SIO_000008>
          <aistls:disorderPrediction>
            <sio:SIO_000216>
              <sio:SIO_000765>
                <sio:SIO_000300>0.1024</sio:SIO_000300>
              </sio:SIO_000765>
            </sio:SIO_000216>
            <sio:SIO_000008>
              <sio:SIO_001093/>
            </sio:SIO_000008>
            <sio:SIO_000008>
              <sio:SIO_010074>
                <sio:SIO_000300>T</sio:SIO_000300>
              </sio:SIO_010074>
            </sio:SIO_000008>
            <sio:SIO_000216>
              <sio:SIO_000789>
                <sio:SIO_000300>192</sio:SIO_000300>
              </sio:SIO_000789>
            </sio:SIO_000216>
          </aistls:disorderPrediction>
        </sio:SIO_000008>
      </aistls:PoodleResult>
    </sio:SIO_000229>
  </aistls:PoodleLOutput>
</rdf:RDF>
```

PoodleL output RDF

2.4. PoodleS

2.4.1. Preparing input RDF

PoodleS input RDF format is as follows:

- RDF header:
  <rdf:RDF
  xmlns:rdf “http://www.w3.org/1999/02/22-rdf-syntax-ns#”
  xmlns:aistls “http://www.molprof.jp/ontologies/aistlssio.owl#”
  xmlns:sio “http://semanticscience.org/resource/”>
- Subject: PoodleSInput, rdf:about: an arbitrary string
  <aistls:PoodleSInput
  rdf:about=”http://www.molprof.jp/ontologies/poodles.rdf#1”>
- Triple for a protein sequence:
  Subject: PoodleSInput
  Predicate: SIO_000230 (has input)
  Object (Subject): SIO_010015 (protein sequence)
  Predicate: SIO_000300 (has value)
  Object: string (protein sequence)

```
<sio:SIO_000230>
    <sio:SIO_010015>
        <sio:SIO_000300>
            Protein sequence
        </sio:SIO_000300>
    </sio:SIO_010015>
</sio:SIO_000230>
```

Sample input RDF file is as follows:

```
<rdf:RDF
    xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
    xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#"
    xmlns:sio="http://semanticscience.org/resource/">

    <aistls:PoodleSInput rdf:about="http://www.molprof.jp/ontologies/poodles.rdf#2">
        <sio:SIO_000230>
            <sio:SIO_010015>
                <sio:SIO_000300>
>sp|P35413|GPR3_MOUSE G-protein coupled receptor 3 OS=Mus musculus GN=Gpr3 PE=2 SV=1
MMWGAGSSMAWFSAGSGSVNVSSVDPVEEPTGPATLLPSPRAWDVVLCISGTLVSCENAL
VVAIIVGTPAFRAPMFLLVGSLAVADLLAGLGLVLHFAADFCIGSPEMSLMLVGVLAMAF
TASIGSLLAITVDRYLSLYNALTYYSETTVTRTYVMLALVWVGALGLGLVPVLAWNCRDG
LTTCGVVYPLSKNHLVVLAIAFFMVFGIMLQLYAQICRIVCRHAQQIALQRHLLPASHYV
ATRKGIATLAVVLGAFAACWLPFTVYCLLGDADSPRLYTYLTLLPATYNSMINPVIYAFR
NQDVQKVLWAICCCCSTSKIPFRSRSPSDV
                </sio:SIO_000300>
            </sio:SIO_010015>
        </sio:SIO_000230>
    </aistls:PoodleSInput>
</rdf:RDF>
```

PoodleS input RDF

2.4.2. Execution command

% curl --data-binary @"input RDF file"
http://semantic.medals.jp:8090/sadi-services/PoodleS

PoodleS is an asynchronous SADI service, and first an RDF stored a URL polling for the SADI server is displayed in command lines as below. Next, the user asks to the SADI server using the URL defined in "isDefinedBy" tag whether PoodleS execution is completed or not.

```
<rdf:RDF

    xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"

    xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#">

    <aistls:PoodleSOutput rdf:about="http://www.molprof.jp/ontologies/poodles.rdf#1">

        <rdfs:isDefinedBy

rdf:resource="http://semantic.medals.jp:8090/sadi-services/PoodleS?poll=3F"/>

    </aistls:PoodleSOutput>

</rdf:RDF>
```

RDF stored the URL to poll for the SADI server

% curl http://semantic.medals.jp:8090/sadi-services/PoodleS?poll=3F (in this case)
%

If PoodleS execution is completed, the URL of an output RDF file stored PoodleS results is displayed in command lines.
% curl http://semantic.medals.jp:8090/sadi-services/PoodleS?poll=3F
COMPLETE: http://semantic.medals.jp/tmp/xxx/yyyy/poodleSResult.rdf
%

The user can get the RDF file as follows:
% curl http://semantic.medals.jp/tmp/xxx/yyyy/ poodleSResult.rdf -o "output RDF file"

2.4.3. Execution result

PoodleS output RDF format is as follows:

- RDF header:
  <rdf:RDF
    xmlns:rdf “http://www.w3.org/1999/02/22-rdf-syntax-ns#”
    xmlns:aistls “http://www.molprof.jp/ontologies/aistlssio.owl#”
    xmlns:sio “http://semanticscience.org/resource/”>
- Subject: PoodleSOutput, rdf:about: the string as same as specifying in the input RDF
  <aistls:PoodleSOutput
  rdf:about=”http://www.molprof.jp/ontologies/poodles.rdf#1”>
- Triple for PoodleS results:
  Subject: PoodleSOutput
  Predicate: SIO_000229 (has output)
  Object (Subject): PoodleResult
    Predicate: SIO_000008 (has attribute)
    Object (Subject): disorderPrediction
      Predicate: SIO_000216 (has measurement value)
      Object (Subject): SIO_000765 (probability value)
        Predicate: SIO_000300 (has value)
        Object: double (disorder probability)
      Predicate: SIO_000216 (has measurement value)
      Object (Subject): SIO_000789 (sequence element position)
        Predicate: SIO_000300 (has value)
        Object: double
      Predicate: SIO_000008 (has attribute)
      Object (Subject): SIO_010074 (amino acid residue)
        Predicate: SIO_000300 (has value)
        Object: double
      Predicate: SIO_000008 (has attribute)
      Object: SIO_000758 (disordered)
      Predicate: SIO_000008 (has attribute)

Object: SIO_001093 (rigid)

```
<sio:SIO_000229>
    <aistls:PoodleResult>
        <sio:SIO_000008>
            <aistls:disorderPrediction>
                <sio:SIO_000216>
                    <sio:SIO_000765>
                        <sio:SIO_000300>0.1024</sio:SIO_000300>
                    </sio:SIO_000765>
                </sio:SIO_000216>
                <sio:SIO_000008>
                    <sio:SIO_001093/>
                </sio:SIO_000008>
                <sio:SIO_000008>
                    <sio:SIO_010074>
                        <sio:SIO_000300>T</sio:SIO_000300>
                    </sio:SIO_010074>
                </sio:SIO_000008>
                <sio:SIO_000216>
                    <sio:SIO_000789>
                        <sio:SIO_000300>192</sio:SIO_000300>
                    </sio:SIO_000789>
                </sio:SIO_000216>
            </aistls:disorderPrediction>
        </sio:SIO_000008>
    </aistls:PoodleResult>
</sio:SIO_000229>
```

Sample output RDF file is as follows:

```
<rdf:RDF
    xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
    xmlns:sio="http://semanticscience.org/resource/"
    xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#">
  <aistls:PoodleSOutput rdf:about="http://www.molprof.jp/ontologies/poodles.rdf#2">
    <sio:SIO_000229>
      <aistls:PoodleResult>
        <sio:SIO_000008>
          <aistls:disorderPrediction>
            <sio:SIO_000216>
              <sio:SIO_000765>
                <sio:SIO_000300>0.0209</sio:SIO_000300>
              </sio:SIO_000765>
            </sio:SIO_000216>
            <sio:SIO_000008>
              <sio:SIO_001093/>
            </sio:SIO_000008>
            <sio:SIO_000008>
              <sio:SIO_010074>
                <sio:SIO_000300>G</sio:SIO_000300>
              </sio:SIO_010074>
            </sio:SIO_000008>
            <sio:SIO_000216>
              <sio:SIO_000789>
                <sio:SIO_000300>254</sio:SIO_000300>
              </sio:SIO_000789>
            </sio:SIO_000216>
          </aistls:disorderPrediction>
        </sio:SIO_000008>
……
……
……
            <sio:SIO_000216>
              <sio:SIO_000789>
                <sio:SIO_000300>260</sio:SIO_000300>
              </sio:SIO_000789>
            </sio:SIO_000216>
          </aistls:disorderPrediction>
        </sio:SIO_000008>
        <sio:SIO_000008>
          <aistls:disorderPrediction>
            <sio:SIO_000216>
              <sio:SIO_000765>
                <sio:SIO_000300>0.0347</sio:SIO_000300>
              </sio:SIO_000765>
            </sio:SIO_000216>
            <sio:SIO_000008>
              <sio:SIO_001093/>
            </sio:SIO_000008>
            <sio:SIO_000008>
              <sio:SIO_010074>
                <sio:SIO_000300>D</sio:SIO_000300>
              </sio:SIO_010074>
            </sio:SIO_000008>
            <sio:SIO_000216>
              <sio:SIO_000789>
                <sio:SIO_000300>86</sio:SIO_000300>
              </sio:SIO_000789>
            </sio:SIO_000216>
          </aistls:disorderPrediction>
        </sio:SIO_000008>
      </aistls:PoodleResult>
    </sio:SIO_000229>
  </aistls:PoodleSOutput>
</rdf:RDF>
```

PoodleS output RDF

2.5. Rassie

2.5.1. Preparing input RDF

Rassie input RDF format is as follows:

- RDF header:
  <rdf:RDF
    xmlns:rdf “http://www.w3.org/1999/02/22-rdf-syntax-ns#”
    xmlns:aistls “http://www.molprof.jp/ontologies/aistlssio.owl#”
    xmlns:sio “http://semanticscience.org/resource/”>
- Subject: RassieInput, rdf:about: an arbitrary string
  <aistls:RassieInput rdf:about=”http://www.molprof.jp/ontologies/rassie.rdf#1”>
- Triple for an RNA secondary structure:
  Subject: RassieInput
  Predicate: SIO_000230 (has input)
  Object (Subject): secondaryStructureModel
    Predicate: SIO_000300 (has value)
    Object: string (RNA secondary structure)

```
<sio:SIO_000230>
    <aistls:secondaryStructureModel>
        <sio:SIO_000300>
            RNA secondary structure
        </sio:SIO_000300>
    </aistls:secondaryStructureModel>
</sio:SIO_000230>
```

- Triple for command options:
  Subject: RassieInput
  Predicate: SIO_000230 (has input)
  Object (Subject): SIO_000144 (parameter)
    Predicate: SIO_000300 (has value)
    Object: string (Rasssie options)
  <sio:SIO_000230>

<sio:SIO_000144>
<sio:SIO_000300> -q 100 -ins 100 -clst -outclst 10 -ins_chain</sio:SIO_000300>
</sio:SIO_000144>
</sio:SIO_000230>

Sample input RDF file is as follows:

```
<rdf:RDF
   xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
   xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#"
   xmlns:sio="http://semanticscience.org/resource/">

   <aistls:RassieInput rdf:about="http://www.molprof.jp/ontologies/rassie.rdf#1">
      <sio:SIO_000230>
         <aistls:secondaryStructureModel>
            <sio:SIO_000300>
>1CQ5
GGCGUUUACCAGGUCAGGUCCGGAAGGAAGCAGCCAAGGCGCC
(((((((....(((....(((....)))....))).))))))) (g=4,th=0.2)
            </sio:SIO_000300>
         </aistls:secondaryStructureModel>
      </sio:SIO_000230>
      <sio:SIO_000230>
         <sio:SIO_000144>
            <sio:SIO_000300> -q 100 -ins 100 -clst -outclst 10 -ins_chain</sio:SIO_000300>
         </sio:SIO_000144>
      </sio:SIO_000230>
   </aistls:RassieInput>
</rdf:RDF>
```

Rassie input RDF

2.5.2. Execution command

% curl --data-binary @"input RDF file"
http://semantic.medals.jp:8090/sadi-services/Rassie

Rassie is an asynchronous SADI service, and first an RDF stored a URL polling for the SADI server is displayed in command lines as below. Next, the user asks to the SADI server using the URL defined in "isDefinedBy" tag whether Rassie execution is completed or not.

```
<rdf:RDF
    xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
    xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#">
    <aistls:RassieOutput rdf:about="http://www.molprof.jp/ontologies/rassie.rdf#1">
        <rdfs:isDefinedBy
rdf:resource="http://semantic.medals.jp:8090/sadi-services/Rassie?poll=30"/>
    </aistls:RassieOutput>
</rdf:RDF>
```

RDF stored the URL to poll for the SADI server

% curl http://semantic.medals.jp:8090/sadi-services/Rassie?poll=30 (in this case)
COMPLETE: http://semantic.medals.jp/tmp/xxx/yyyy/rna3dResult.rdf
%

If Rassie execution is completed, the URL of an output RDF file stored Rassie results is displayed in command lines.
% curl http://semantic.medals.jp:8090/sadi-services/Rassie?poll=30
COMPLETE: http://semantic.medals.jp/tmp/xxx/yyyy/rna3dResult.rdf
%

The user can get the RDF file as follows:
% curl http://semantic.medals.jp/tmp/xxx/yyyy/ rna3dResult.rdf -o "output RDF file"

2.5.3. Execution result

Rassie output RDF format is as follows:

- RDF header:
  <rdf:RDF
  xmlns:rdf “http://www.w3.org/1999/02/22-rdf-syntax-ns#”
  xmlns:aistls “http://www.molprof.jp/ontologies/aistlssio.owl#”
  xmlns:sio “http://semanticscience.org/resource/”>
- Subject: RassieOutput, rdf:about: the string as same as specifying in the input RDF
  <aistls:RassieOutput
  rdf:about=”http://www.molprof.jp/ontologies/rassie.rdf#1”>
- Triple for Rassie results:
  Subject: RassieOutput
  Predicate: SIO_000229 (has output)
  Object (Subject): PdbFormatStructureModel
  Predicate: SIO_000300 (has value)
  Object: string (Rassie execution result)

```
<sio:SIO_000229>
    <aistls:PdbFormatStructureModel>
        <sio:SIO_000300>
            Rassie execution result
        </sio:SIO_000300>
    </aistls:PdbFormatStructureModel>
</sio:SIO_000229>
```

Sample output RDF file is as follows:

```
<rdf:RDF
    xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
    xmlns:sio="http://semanticscience.org/resource/"
    xmlns:aistls="http://www.molprof.jp/ontologies/aistlssio.owl#">
  <aistls:RassieOutput rdf:about="http://www.molprof.jp/ontologies/rassie.rdf#1">
    <sio:SIO_000229>
      <aistls:PdbFormatStructureModel>
        <sio:SIO_000300>MODEL 6
ATOM      1 P      G X   1      -5.811  -0.107   0.010
ATOM      2 O5'    G X   1      -4.838  -1.143   0.726
ATOM      3 C5'    G X   1      -3.724  -0.694   1.493
ATOM      4 C4'    G X   1      -2.458  -0.946   0.723
ATOM      5 C3'    G X   1      -1.340  -1.526   1.580
ATOM      6 O3'    G X   1      -1.452  -2.938   1.663
ATOM      7 O4'    G X   1      -1.910   0.339   0.313
ATOM      8 C2'    G X   1      -0.093  -1.133   0.801
ATOM      9 C1'    G X   1      -0.501   0.232   0.241
ATOM     10 N9     G X   1       0.158   1.395   0.842
ATOM     11 C4     G X   1       1.521   1.457   0.889
ATOM     12 C8     G X   1      -0.294   2.576   1.393
ATOM     15 N7     G X   1       0.629   3.367   1.803
ATOM     16 C5     G X   1       1.819   2.702   1.505
ATOM     17 C6     G X   1       3.160   3.093   1.733
ATOM     18 N1     G X   1       4.061   2.116   1.279
ATOM     19 C2     G X   1       3.696   0.918   0.680
ATOM     20 N3     G X   1       2.443   0.552   0.475
ATOM     21 O2'    G X   1      -0.659  -2.130   0.294
ATOM     22 O6     G X   1       3.590   4.130   2.242
ATOM     23 N2     G X   1       4.712   0.130   0.323
ATOM     24 P      G X   2      -1.513  -3.641   3.101
……
……
……
ATOM    907 O2'    C X  42       1.150   0.253  -8.802
ATOM    908 N4     C X  42       5.681   3.921  -4.083
ATOM    909 P      C X  43       3.185   0.660 -11.758
ATOM    910 O5'    C X  43       2.379   1.987 -11.301
ATOM    911 C5'    C X  43       0.972   2.127 -11.562
ATOM    912 C4'    C X  43       0.451   3.512 -11.167
ATOM    913 C3'    C X  43       1.156   4.609 -11.935
ATOM    914 O3'    C X  43       0.484   4.915 -13.168
ATOM    915 O4'    C X  43       0.669   3.787  -9.764
ATOM    916 C2'    C X  43       1.161   5.780 -10.999
ATOM    917 C1'    C X  43       1.061   5.177  -9.610
ATOM    918 N1     C X  43       2.353   5.287  -8.898
ATOM    919 C2     C X  43       2.503   6.326  -7.995
ATOM    920 C6     C X  43       3.366   4.397  -9.135
ATOM    923 C5     C X  43       4.549   4.501  -8.481
ATOM    924 C4     C X  43       4.684   5.584  -7.541
ATOM    925 N3     C X  43       3.686   6.447  -7.321
ATOM    926 O2     C X  43       1.561   7.102  -7.815
ATOM    927 O2'    C X  43      -0.524   6.471 -10.816
ATOM    928 N4     C X  43       5.808   5.737  -6.865
TER
END
</sio:SIO_000300>
      </aistls:PdbFormatStructureModel>
    </sio:SIO_000229>
  </aistls:RassieOutput>
</rdf:RDF>
```

Rassie output RDF

Contact

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Molecular Profiling Research Center for Drug Discovery of AIST plans to listen to user's requests positively, and to make the system better.

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