

Instructions for testing the RESTful web service for converting "molar" concentrations to "mass" concentrations and vice versa using UCUM units and LOINC codes.

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Introduction

Converting lab values representing "molar" concentrations to values representing "mass" concentrations and vice versa in an automated way is not an easy task. Reason is that the molecular weight of the analyte is required to do such a conversion.

REMARK: In clinical research, and especially at the FDA, "molar" concentration units are often named "*SI units*" and "mass" concentration units are often named "*US Conventional units*" although such a designation is essentially incorrect.

Essentially, the CDISC "LBTESTCD" value is nothing else than the analyte, but CDISC does not provide any molecular weights (MWs) for them, so the value of "LBTESTCD" is not of any help here.

Things are different when LOINC is used. For many LOINC codes that represent quantitative laboratory test, the molecular weight is (although indirectly) available from the LOINC database.

Therefore, we developed a RESTful web service that allows to do conversions from "molar" concentrations to "mass" concentrations using UCUM notation for the units and using the LOINC code of source executed test.

Example: we executed the LOINC test 14749-6: "Glucose [Moles/volume] in Serum or Plasma" with a test value of 7.1 mmol/L, and want to convert the value to mg/dL.

REMARK: UCUM is considerably broader than CDISC units, as it is a system, not a list, so such conversions are not limited to "CDISC units". For example, if you would like to convert the above molar concentration to cg/L (centigrams per liter), which is not in the CDISC controlled terminology list, this is perfectly possible using UCUM notation. Also remark that for "liter", as well "L" (uppercase) as well as "l" (lowercase) are valid in UCUM.

The RESTful web service

RESTful web services are meant for machine-machine communication. This has the advantage that they can be implemented (usually requiring a few lines of code only) into your own programs, be it SAS code, R code, Java software, Python code, etc..

Usually (but not always), such RESTful web services can also be tested/used just using a web browser. In the following, we will explain how to use the RESTful web service in a web browser, and give a code snippet for use in Java code.

The base of the RESTful web service is:

<http://xml4pharmaserver.com:8080/UCUMService2/rest/>

The method called is:

ucumtransform

The parameters to be provided are:

- *source_quantity*: the quantity (numeric value) to be converted from, e.g. "7.1"
- *source_unit*: the source unit in UCUM notation, e.g. "mmol/L"
- *target_unit*: the target unit to which the source quantity need to be converted to, e.g. "mg/dL"
- *loinc_code*: the LOINC code of the source lab test, e.g. "14749-6"

The construct for the RESTful Web Service request is then:

[base]/ucumtransform/{source_quantity}/from/{source_unit}/to/{target_unit}/LOINC/{loinc_code}

For example:

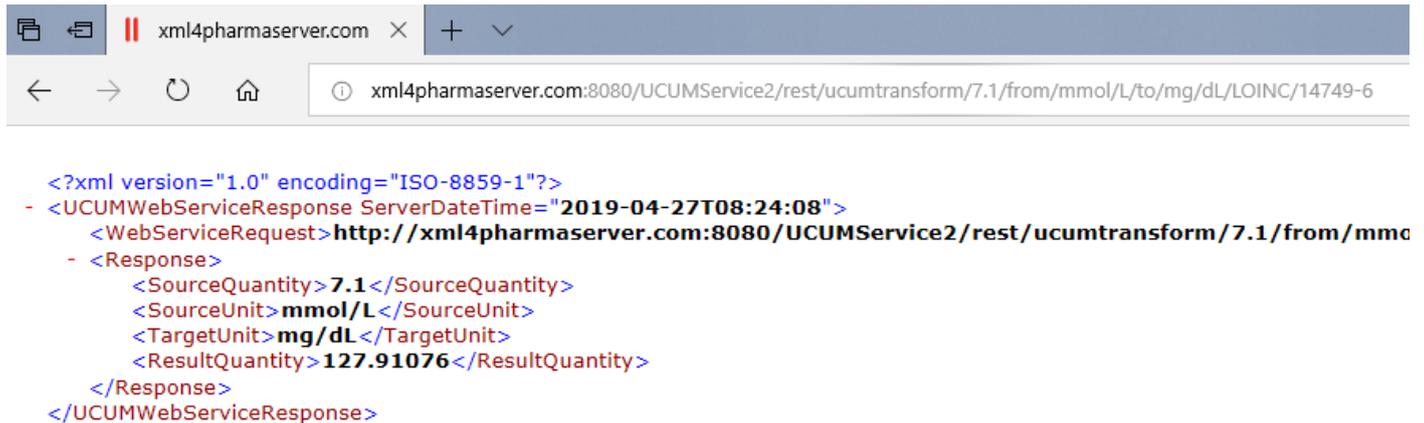
<http://xml4pharmaserver.com:8080/UCUMService2/rest/ucumtransform/7.1/from/mmol/L/to/mg/dL/LOINC/14749-6>

Note the keywords "from", "to" and "LOINC" in the request.

Testing the RESTful web service in the browser

You can easily test the service in your favorite browser. Only limitation is that your browser must support the display of XML. This is usually the case in modern browsers.

So, if you copy-paste the above request string in the browser, you will get:



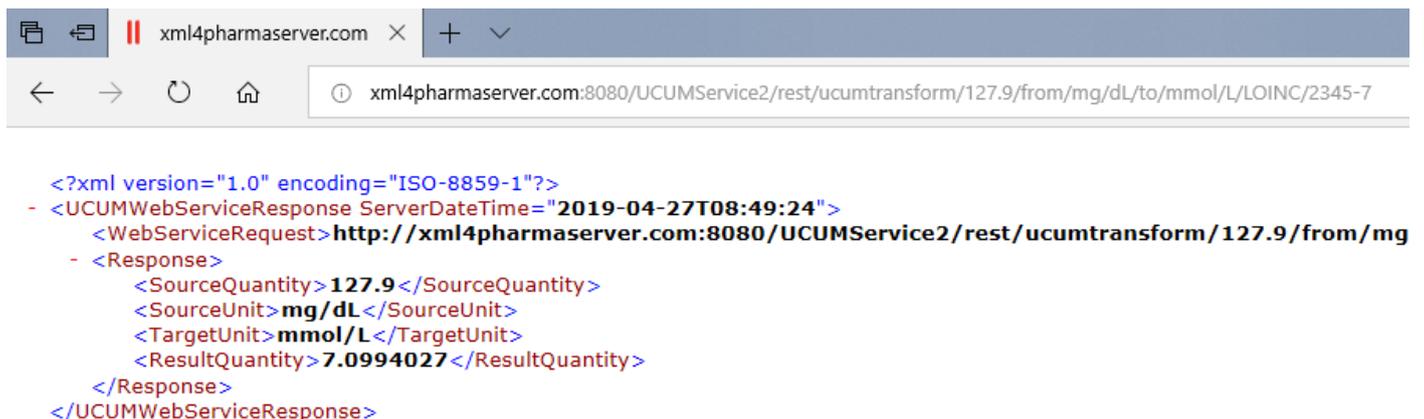
```
<?xml version="1.0" encoding="ISO-8859-1"?>
- <UCUMWebServiceResponse ServerDateTime="2019-04-27T08:24:08">
  <WebServiceRequest>http://xml4pharmaserver.com:8080/UCUMService2/rest/ucumtransform/7.1/from/mmol/L/to/mg/dL/LOINC/14749-6
  - <Response>
    <SourceQuantity>7.1</SourceQuantity>
    <SourceUnit>mmol/L</SourceUnit>
    <TargetUnit>mg/dL</TargetUnit>
    <ResultQuantity>127.91076</ResultQuantity>
  </Response>
</UCUMWebServiceResponse>
```

With the result quantity (in mg/dL) provided in the XML tag "ResultQuantity"

The other way around: we want to convert 127.9 mg/dL, which is a result of the (corresponding) LOINC test 2345-7: "Glucose [Mass/volume] in Serum or Plasma" to mmol/L. The query string then is:

<http://xml4pharmaserver.com:8080/UCUMService2/rest/ucumtransform/127.9/from/mg/dL/to/mmol/L/LOINC/2345-7>

and the result in the browser is:



```
<?xml version="1.0" encoding="ISO-8859-1"?>
- <UCUMWebServiceResponse ServerDateTime="2019-04-27T08:49:24">
  <WebServiceRequest>http://xml4pharmaserver.com:8080/UCUMService2/rest/ucumtransform/127.9/from/mg/dL/to/mmol/L/LOINC/2345-7
  - <Response>
    <SourceQuantity>127.9</SourceQuantity>
    <SourceUnit>mg/dL</SourceUnit>
    <TargetUnit>mmol/L</TargetUnit>
    <ResultQuantity>7.0994027</ResultQuantity>
  </Response>
</UCUMWebServiceResponse>
```

Working with "equivalents"

For some tests, people use the "eq" unit, for example for the test "Magnesium in stool" (LOINC code 26708-8), which is usually measured in "meq/kg" (milli-equivalents per kg).

The value of "eq" however depends on the properties or charge of the molecule. In cases of non-ionic molecules, usually, 1 eq = 1 mol. For ions however, the value of 1 eq depends on the charge of the molecule. For example:

Molecule or ion	Charge	Value of 1 eq
Sodium	+1	1 eq = 1 mol
Magnesium	+2	1 eq = 2 mol
Calcium	+2	1 eq = 2 mol
Sulfate	-2	1 eq = 2 mol
Phosphate	-3	1 eq = 3 mol

i.e. the value of 1 eq equals the absolute value of the charge of the ion.

The RESTful web service now also allows conversions for that involve "eq" units. Also in this case, the LOINC code of the analyte is necessary, not only for the molecular weight, but also as the analyte name needs to be looked up, which is then compared with a list of charges.

At the moment, this list comprises: Lithium, Magnesium, Potassium, Zinc, Sodium, Calcium, Sulfate, Chloride, Phosphate.

Example: For the test "Magnesium in stool", the request may be:

<http://xml4pharmaserver.com:8080/UCUMService2/rest/ucumtransform/1/from/meq/kg/to/mg/g/LOINC/26708-8>

Leading to the result:

```
▼ <UCUMWebServiceResponse ServerDateTime="2019-05-26T16:36:09">
  ▼ <WebServiceRequest>
    http://xml4pharmaserver.com:8080/UCUMService2/rest/ucumtransform/1/from/meq/kg/to/mg/g/LOINC/26708-8
  </WebServiceRequest>
  ▼ <Response>
    <SourceQuantity>1.0</SourceQuantity>
    <SourceUnit>meq/kg</SourceUnit>
    <TargetUnit>mg/g</TargetUnit>
    <MolecularWeightUsed>24.3</MolecularWeightUsed>
    <ResultQuantity>0.01215</ResultQuantity>
  </Response>
</UCUMWebServiceResponse>
```

Stating that 1 meq/kg Magnesium in stool is 0.0125 mg/g in stool.

Essentially the request could also be (shortened here)

.../ucumtransform/1/from/meq/kg{stool}/to/mg/g{stool}/LOINC/26708-8

demonstrating the use of [UCUM annotations](#).

Also the more simple conversion from "eq" to "mol" is supported, also such a conversion would probably be more seldom. For example, for Calcium in stool again:

<http://xml4pharmaserver.com:8080/UCUMService2/rest/ucumtransform/1/from/meq/kg/to/mmol/g/LOINC/26708-8>

leading to the (to be expected) result:

```

▼<UCUMWebServiceResponse ServerDateTime="2019-05-26T16:38:12">
  ▼<WebServiceRequest>
    http://xml4pharmaserver.com:8080/UCUMService2/rest/ucumtransform/1/from/meq/kg/to/mmol/g/LOINC/26708-8
  </WebServiceRequest>
  ▼<Response>
    <SourceQuantity>1.0</SourceQuantity>
    <SourceUnit>meq/kg</SourceUnit>
    <TargetUnit>mmol/g</TargetUnit>
    <MolecularWeightUsed>24.3</MolecularWeightUsed>
    <ResultQuantity>0.001</ResultQuantity>
  </Response>
</UCUMWebServiceResponse>

```

If the component (obtained from the LOINC code) is NOT in the list of ions, one could assume that 1 eq = 1 mol. This is however potentially dangerous. So, we decided to then return an error message. For example, when wanting to convert from "eq" to "g" for Albumin in Serum/Plasma (LOINC code 1751-7), one will get:

```

▼<UCUMWebServiceResponse ServerDateTime="2019-06-19T10:07:30">
  ▼<WebServiceRequest>
    http://www.xml4pharmaserver.com:8080/UCUMService2/rest/ucumtransform/1/from/meq/dL/to/mg/dL/LOINC/1751-7
  </WebServiceRequest>
  ▼<Response>
    ERROR: Invalid UCUM Transformation Expression - No charge found for Compound of LOINC code 1751-7
  </Response>
</UCUMWebServiceResponse>

```

Alternative when the LOINC code is not available

In case the LOINC code is not available, but the molecular weight of the analyte is available, there is an alternative, that still allows to use the advantages of the UCUM system. The query string then becomes:

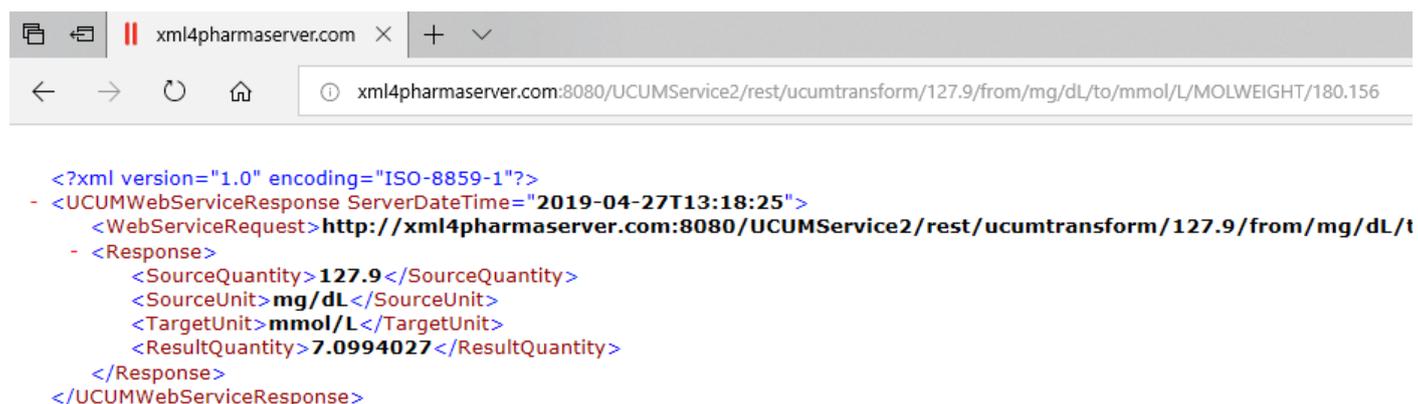
[base]/ucumtransform/{source_quantity}/from/{source_unit}/to/{target_unit}/**MOLWEIGHT**/{molecular_weight}

Note the keyword "MOLWEIGHT" (uppercase).

For our glucose example (MW=180.156), the request then becomes

http://xml4pharmaserver.com:8080/UCUMService2/rest/ucumtransform/127.9/from/mg/dL/to/mmol/L/**MOLWEIGHT**/180.156

When tested in the browser, we get:



The screenshot shows a web browser window with the address bar containing the URL: `xml4pharmaserver.com:8080/UCUMService2/rest/ucumtransform/127.9/from/mg/dL/to/mmol/L/MOLWEIGHT/180.156`. The browser displays the following XML response:

```

<?xml version="1.0" encoding="ISO-8859-1"?>
- <UCUMWebServiceResponse ServerDateTime="2019-04-27T13:18:25">
  <WebServiceRequest>http://xml4pharmaserver.com:8080/UCUMService2/rest/ucumtransform/127.9/from/mg/dL/t
  - <Response>
    <SourceQuantity>127.9</SourceQuantity>
    <SourceUnit>mg/dL</SourceUnit>
    <TargetUnit>mmol/L</TargetUnit>
    <ResultQuantity>7.0994027</ResultQuantity>
  </Response>
</UCUMWebServiceResponse>

```

Just as a demo of the power of the use of UCUM, we can also set the source unit to kg/m3 (kilogram per cube meter), which is of course also a concentration, giving:

```
xml4pharmaserver.com x + v
xml4pharmaserver.com:8080/UCUMService2/rest/ucumtransform/127.9/from/kg/m3/to/mmol/L/MOLWEIGHT/180.156

<?xml version="1.0" encoding="ISO-8859-1"?>
- <UCUMWebServiceResponse ServerDateTime="2019-04-27T13:23:20">
  <WebServiceRequest>http://xml4pharmaserver.com:8080/UCUMService2/rest/ucumtransform/127.9/from/kg/m3/to/mmol/L/MO
  - <Response>
    <SourceQuantity>127.9</SourceQuantity>
    <SourceUnit>kg/m3</SourceUnit>
    <TargetUnit>mmol/L</TargetUnit>
    <ResultQuantity>709.94027</ResultQuantity>
  </Response>
</UCUMWebServiceResponse>
```

Please be aware that this method does not work for "eq" units, as the LOINC code must be known in order to retrieve the charge of the molecule or ion.

Running the RESTful web service in Java programs

When using the service in Java software, you will probably want to use existing Java libraries such as Jersey-2 (<https://jersey.github.io/>). The following snippet assumes that your Java software has the necessary Jersey-2 libraries on the classpath.

Here is a Java snippet:

Imports:

```
import java.io.*;
import com.sun.jersey.api.client.*;
```

variable definitions

```
private String base =
"http://xml4pharmaserver.com:8080/UCUMService2/rest/ucumtransform/";
private Client client;
```

Client setup:

```
// create a RESTful-WS client
client = Client.create();
```

Example code for above conversion:

```
String fromQuantity = "7.1";
String fromLOINCCode = "14749-6";
String fromUnit = "mmol/L";
String toUnit = "mg/dL";
String fromLOINCCode = "14749-6";
String path = fromQuantity + "/from/" + fromUnit + "/to/" + toUnit + "/LOINC/" +
fromLOINCCode;
```

```
WebResource resource = client.resource(base + path);
String responseXML = resource.accept("application/xml").get(String.class);
System.out.println("response = " + responseXML);
```

The string "responseXML" contains the XML that is returned (essentially the same as displayed in the browser), and can be parsed using either SAX or DOM to retrieve the value of "ResultQuantity". As the XML is pretty simple, also simple string manipulation can be used to do this extraction.

Running the RESTful web service in Oracle PL/SQL

I was asked how to run the RESTful web service in Oracle PL/SQL. I am not a specialist in PL/SQL at all, the last time I used it was more than 20 years ago ..., but I did find a few articles about how to implement RESTful web services in PL/SQL. Here are some useful links:

- https://technology.amis.nl/2015/05/11/invoke-a-rest-service-from-plsql-make-an-http-post-request-using-utl_http-in-oracle-database-11g-xe/
- <https://sonra.io/2009/03/12/consuming-a-rest-web-service-with-oracle/>

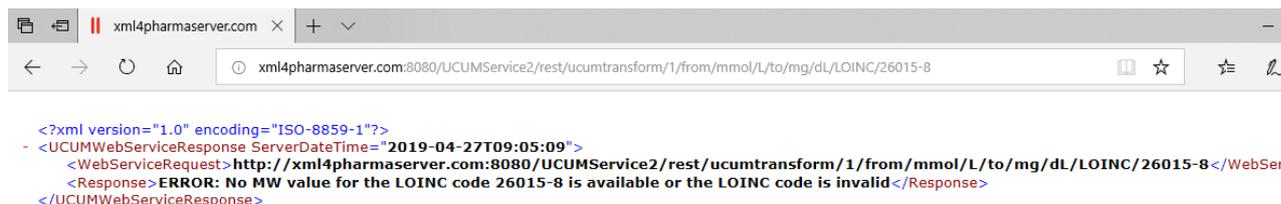
And if you google for "call restful web service from within PL/SQL" you will find much more. Our RESTful web service uses simple "HTTP GET" without authentication necessary, which is the easiest for the "consumer" to implement, so implementing our service in PL/SQL should not be too difficult for experienced PL/SQL developers.

Limitations

The web service currently has the following limitations:

- In either the source or target unit, the term "mol" may only occur once. So, the service cannot be used for conversions that contain ratios, e.g. from "mmol/mol" to "g/kg"
- Though we currently do have a broad coverage of molecular weights from the LOINC codes, the coverage from the LOINC database is not complete. For example, for LOINC test 26015-8: "Cholesterol in HDL 2 [Moles/volume] in Serum or Plasma", the molecular weight cannot yet be retrieved correctly. Reason is that the "analyte" part of the LOINC code is: "Cholesterol.in HDL 2" and not "Cholesterol". The LOINC database does contain a molecular weight for the latter, but not for "Cholesterol.in HDL 2".

In such a case, the XML returned (here in the browser) is like:



```
<?xml version="1.0" encoding="ISO-8859-1"?>
- <UCUMWebServiceResponse ServerDateTime="2019-04-27T09:05:09">
  <WebServiceRequest>http://xml4pharmaserver.com:8080/UCUMService2/rest/ucumtransform/1/from/mmol/L/to/mg/dL/LOINC/26015-8</WebSer
  <Response>ERROR: No MW value for the LOINC code 26015-8 is available or the LOINC code is invalid</Response>
</UCUMWebServiceResponse>
```

We are currently working on solutions for such cases.

Final WARNING

This RESTful web service is "work in progress". It has not been well tested yet. We do know it is not perfect either. **We do not accept any responsibility for incorrect results generated by the web service.**

DO NOT USE FOR PRODUCTION!

Please inform us about problems you encountered when testing the web service, or when you got incorrect results. Of course any other comments are highly appreciated. Please send them to Jozef.Aerts@XML4Pharma.com.

If you want to perform other UCUM unit conversions that are not "molar" concentration to "mass" concentration or vice versa conversions in production, please use the similar RESTful web service from the National Library of Medicine (originally also developed by us). You can find all necessary information at:

<https://ucum.nlm.nih.gov/ucum-service.html>