***Journal of Proteome Data and Methods* Template forData Descriptor Article**

*Version 0.3*

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This document contains the template for the Data Descriptor article.

Please note:

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* A Data Descriptor article should **describe data. It should not provide** conclusions or interpretive descriptions. As such, words like ‘study’, ‘results’ or ‘conclusions’ are not relevant.
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Reminder: A Data Descriptor article **describes data**. **It should not provide** conclusions or interpretive descriptions.

Data Descriptor

[https://doi.org/10.14889/jpdm.2020.xxxx](https://dx.doi.org/10.14889/jpdm.2020.xxxx)

**Data for proteomic analysis of XXXXXX**

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[Title: The article title must include the word ‘data’ or ‘dataset’. The title should describe the content of the article briefly but clearly and is important for search purposes by third-party services. Do not use the same main title with numbered minor titles, even for a series of papers by the same authors. Do not use abbreviations in the title, except those used generally in related fields. Max 120 characters including spaces.]

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**Keywords**

[Include up to 5 keywords (or phrases) to facilitate others finding your article online. Tip: Try Google Scholar to see what terms are most common in your field. In biomedical fields, MeSH terms are a good ‘common vocabulary’ to draw from.]

Interactome, GTP-binding proteins, GTPome, Kinase

**Dataset summary**

[Every section of this table is mandatory. Please enter information in the right-hand column]

|  |  |
| --- | --- |
| **Specific subject area** | [Briefly describe the narrower subject area. Max 150 characters]  ATP-binding proteins and mass spectrometry (MS) |
| **Data acquisition** | [Instruments: e.g. hardware, software, program, model and make of the instruments used:]  MS: Data-dependent acquisition acquired on Q-Exactive (Thermo) |
| **Dataset repository** | [State here the name of a public repository.]  jPOST |
| **Dataset identifiers** | [State data set identification number used in the public repository, PXD no., JPST no., etc.]  JPST9000100 |

**Abstract**

[The Abstract should clearly express the basic content of the paper in a single paragraph, including the purpose of acquiring the data and a brief description of the experimental approach. Abstracts must not exceed 250 words. Avoid using acronyms or abbreviations that are not commonly understood outside your field. If it is essential to refer to a previous publication, omit the article title (e.g. Ogata, K.; Krokhin, O. V.; Ishihama, Y. *Anal. Sci.*, **2018**, *34 (1)*, 1037-1041).]

Interactions between ATP and ATP-binding proteins (ATPome) are common and are required for most cellular processes. Thus, it is clearly important to identify and quantify these interactions for understanding basic cellular mechanisms and the pathogenesis of various diseases….

1. **Materials and Methods**

[The data acquisition or newly proposed methods should be described in sufficient detail to allow the experiments to be repeated. In addition, the sources of unusual chemicals, animals, microbial strains or equipment should be described, and the location (city, state, country) of the manufacturer or supplier should be provided in parentheses. If hazardous materials or dangerous procedures are used in the experiments and the precautions related to their handling are not widely recognized, the authors should provide the necessary details.

The authors should provide detailed information about the data deposited and registered in the data repository, using the sections below.]

**1.1. Samples**

[The source of origin of the samples and their culture conditions should be described. The authors should provide relevant details not only of the species but also of the tissues, cell types and disease conditions.]

Table 1 shows sample information.

Table 1. Information of sample.

|  |  |
| --- | --- |
| **Sample related item** | **Information** |
| Sample type | Cultured cell |
| Cell name | HEK293T |
| Species | Human |
| Medium | DMEM-10% FBS |
| Stimulation | None |

**1.2. Sample pretreatment for MS analysis**

[The sample processing methods and conditions should be described. For example, the extraction of sub-organelles, enrichment processes, separation of proteins or peptides, fractionation of the samples, and the enzymatic digestion conditions.]

Details of sample pretreatment were described in the report by Kawashima *et al*1. Table 2 shows important details in sample pretreatment.

Table 2. Information of sample pretreatment.

|  |  |  |
| --- | --- | --- |
| **Sample pretreatment related item** | **Method/Reagent** | **Reaction condition** |
| Sample pretreatment method | SP32 | - |
| Protein lysis buffer | 100 mM Tris-HCl (pH 8.5) containing 2% SDS | - |
| Protein extraction method | Sonication | - |
| Amount of protein used | 20 µg | - |
| Reduction | 20 mM TCEP | 10 min, 80 °C |
| Alkylation | 35 mM iodoacetamide | 30 min, room temperature |
| Protease | 1 µg of Trypsin/Lys-C Mix (Promega, Madison, WI, USA) | Overnight, 37 °C |
| Desalting of peptide sample | GL-Tip SDB (GL Sciences Inc., Tokyo, Japan) | - |
| Peptide lysis solution | 2% ACN containing 0.1% TFA | - |

**1.3. MS analysis**

[The following must be provided: mass spectrometer model name, instrument mode (e.g. DDA-high resolution), and the detailed parameters of the operations.]

Table 3 shows LC-MS setting information.

Table 3. Information of LC-MS analysis.

|  |  |  |
| --- | --- | --- |
|  | | |
| **LC-MS analysis related item** | | **Information** |
| **LC** | NanoLC instrument | UltiMate 3000 RSLCnano LC system (Thermo Fisher Scientific) |
| Pre-column (Trap column) | None |
| Analytical column size | 75 μm × 40 cm |
| Analytical column particles | CAPCELL CORE MP C18, 2.7 μm, 160 Å material (Osaka Soda) |
| LC solvent | A: 0.1% formic acid in water, B: 0.1% formic acid in 80%ACN |
| Gradient time | 120 min (B%: 5-40) |
| Flow rate | 100 nL/min |
| **MS** | MS instrument | Orbitrap Exploris 480 mass spectrometer (Thermo Fisher Scientific) |
| MS data acquisition method | Overlapping window DIA3-5 |
| Polarity | Positive |
| Spray voltage | 2,300 V |
| Ion transfer tube temperature | 275 °C |
| Default charge state | 3 |
| RF Lens | 40% |
| MS1 scan range | *m/z* 495-745 |
| MS1 resolution | 15,000 |
| MS1 automatic gain control target | 3 × 106 |
| MS1 maximum injection time | Auto |
| Precursor *m/z* range for overlapping window DIA | *m/z* 500-740 and *m/z* 498-742 |
| Isolation window width | *m/z* 4 |
| Window placement optimization tool | Skyline v4.16 |
| MS2 scan range | *m/z* 200-1,800 |
| MS2 resolution | 45,000 |
| MS2 automatic gain control target | 3 × 106 |
| MS2 maximum injection time | Auto |
| Collision energy mode | Stepped |
| Collision energy type | Normalized |
| Collision energy | 22, 26, and 30% |

**1.4. Data analysis**

[The software and search engine, including the detailed parameters, should be provided. The author also should describe purpose of measurements (e.g. relative quantification) and quantitation method (e.g. spectral counting, SILAC, and TMT)]

Table 4 shows information of data analysis parameters.

Table 4. Information of data analysis.

|  |  |
| --- | --- |
| **Data analysis related item** | **Information** |
| **Predicted spectral library** | |
| Software/tool | Prosit6,7 |
| Protein sequence database (FASTA) | UniProt (human, proteome ID UP000005640, reviewed, canonical, 20,381 entries) |
| Enzyme | Trypsin/P |
| Charge range | 2-4 |
| Maximum missed cleavage sites | 1 |
| *m/z* range | 490-750 |
| Static modification | Cysteine carbamidomethylation |
| **Protein identification** | |
| Software/tool | Scaffold DIA v3.0.0 |
| Spectral library | Predicted spectral library generated under the above parameters |
| Protein sequence database (FASTA) | UniProt (human, proteome ID UP000005640, reviewed, canonical, 20,381 entries) |
| Precursor mass tolerance | 10 ppm |
| Fragment mass tolerance | 10 ppm |
| Protein FDR | < 1% |
| Peptide FDR | < 1% |
| PSM FDR |  |

**2. Data description**

[The relationships between samples and data files must be described in detail. Authors should take special care to accurately describe the correspondence between samples and labels such as SILAC and TMT. Make sure you refer to each one specifically. No insight, interpretation, background or conclusions should be included in this section.]

**Acknowledgments**

[This section should be brief. Authors should list all funding sources for their work.]

This work was supported by Grants-in-Aid....

**References**

[References should be cited by number in their order of appearance in the text, using square brackets (e.g. [1]). Links to web sites should be cited in the main text but not the References section. The style of the reference should be according to ACS style (no title) as shown here.

[1] Suzuki, T.; Baker, A., *J. Proteome Res.* **2014**, *13 (2)*, 5461–70.   
[2] Ong, S.; Blagoev, B.; Kratchmarova, I.; Kristensen, D. B.; Steen, H.; Pandey, A.; Mann, M., *Mol. Cell. Proteomics* **2002,** *1*, 376–86.

[3] Rappsilber, J.; Mann, M.; Ishihama, Y., *Nat. Protoc.* **2007**, *2 (8)*, 1896-1906.   
[4] Cox, J.; Neuhauser, N.; Michalski, A.; Scheltema, R. A.; Olsen, J. V.; Mann, M., *J. Proteome Res.* **2011**, *10*, 1794–1805.

**Supporting Information**

Supporting information is available online at https://xxxxxxxx.