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

*Version 0.2*

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Data Descriptor

<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**

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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.]

HeLa-S3 cells were grown in DMEM with 10% fetal bovine serum plus antibiotics in 10% CO2 at 37 °C. For SILAC labeling, HeLa-S3 cells were cultured in DMEM supplemented with 10% dialyzed fetal bovine serum and either 28.0 mg/L normal isotopic abundance arginine and 48.7 mg/L normal isotopic abundance lysine (Light) or 28.0 mg/L arginine with six 13C and four 15N atoms and 48.7 mg/L lysine with six 13C and two 15N atoms (Heavy).

**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, and fractionation of the samples.]

Proteins from cell lysates were dried and resuspended in 50 mM Tris-HCl buffer (pH 9.0) containing 8 M urea. These mixtures were subsequently reduced, alkylated, and digested with Lys-C (Wako, Osaka, Japan) and trypsin (Promega, Madison, WI). Digested solutions were acidified with TFA and desalted and concentrated using C18 StageTips...

**1.3. MS analysis**

[The enzyme (e.g. trypsin) and both fixed and variable modifications used for mass spectrometric measurement should be described in detail, along with the reaction conditions.]

All nanoflow LC/MS/MS experiments were performed on a Q-Exactive mass spectrometer (Thermo Fisher Scientific). Data were acquired in data-dependent mode using Xcalibur software. The precursor ion scan MS spectra (m/z 350–1800) were acquired in the Orbitrap with 70,000 resolution...

**1.4. Data analysis**

[The following must be provided: mass spectrometer model name, instrument mode (e.g. DDA-high resolution), purpose of measurements (e.g. relative quantification), quantitation method (e.g. spectral counting, SILAC, and TMT), and the detailed parameters of the operations.]

All raw files were processed by MaxQuant software suite (version 1.3.0.5) supported by the Andromeda search engine for peptide identification [4]. MaxQuant was used to score peptides for identification based on a search with an initial allowed mass deviation of the precursor ion of up to 7 ppm....

**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.]

In the present work, we provide the ATP binding protein catalog generated by ATP competition assay including kinases and other ATP binding proteins [1]. We extracted qualitative and quantitative information about ATP-binding proteins (Supplementary Table 1) and mapped all identified kinases (Supplementary Figure 1).

**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. DOI:10.1021/pr5012685.
[2] Ong, S.; Blagoev, B.; Kratchmarova, I.; Kristensen, D. B.; Steen, H.; Pandey, A.; Mann, M., *Mol. Cell. Proteomics* **2002,** *1*, 376–86. DOI:10.1074/mcp.m200025-mcp200.

[3] Rappsilber, J.; Mann, M.; Ishihama, Y., *Nat. Protoc.* **2007**, *2 (8)*, 1896-1906. DOI:10.1038/nprot.2007.261.
[4] Cox, J.; Neuhauser, N.; Michalski, A.; Scheltema, R. A.; Olsen, J. V.; Mann, M., *J. Proteome Res.* **2011**, *10*, 1794–1805. DOI:10.1021/pr101065j.

**Supporting Information**

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