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Data Article

Quantitative proteomic dataset of whole protein in three melanoma samples of 92.1, 92.1-A and 92.1-B

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ABSTRACT

Distant metastasis is common in ocular uveal melanoma (uveal melanoma, UM) [1], with possible identification of relevant protein markers in peripheral blood [2,3]. Proteomics analyses serve as a basis for the screening of new target proteins. However, it is difficult to determine whether the relevant proteins in peripheral blood are the same kinesins as those in primary lesions and metastases. Specially in this study, human UM cells (92.1) [4] were inoculated into the back of the eyeball and the brain of inbred line nude mice transplanted with enhanced green fluorescent protein (EGFP) [5], respectively, to simulate the growth of UM *in situ* and in brain metastases. A database was established as follows: Firstly, the xenograft was taken for monoclonal re-culture and amplification. Then, the cells after amplification (92.1-A in the back of the eyeball and 92.1-B in the brain) and their parent cells (92.1) were subjected to Tandem Mass Tag (TMT)-labeling proteomic analysis and liquid chromatography-mass spectrometry (LC-MS). Covering differential proteomes of three cell lines in a pairwise model, the

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data could be used to further screen the kinesins that play a vital role in regulating the growth of UM.

Specification Table

Subject:	Cancer research
Specific subject area:	Screening of target molecules of uveal melanoma (UM)
Type of data:	Raw data storage Table Figure
How data were acquired:	A quantitative proteomic analysis of melanoma was conducted via a combination of cutting-edge technologies, including Tandem Mass Tag (TMT) labeling, high-performance liquid chromatography (HPLC) classification technology, and the technology of mass spectrometry-based quantitative proteomics.
Data format:	Raw data Analyzed data Screened data
Parameters for data collection:	The 92.1 cell lines were obtained from the Eye and Ear Institute of the University of Pittsburgh Medical Center. The 92.1-B and 92.1-A cell lines were inoculated *via* the 92.1 cell lines into the back of the eyeball and the brain of inbred line nude mice transplanted with enhanced green fluorescent protein (EGFP), respectively, to simulate the grow of UM *in situ* and in metastases, with the xenograft taken for monoclonal re-culture and amplification of cells. The data covered a group of proteomes of three cell lines in a pairwise model.
Description of data collection:	There were 6081 proteins identified, among which 5267 carried quantitative data. Of all the quantified proteins, 302 and 335 proteins were downregulated and upregulated, respectively, in the 92.1-A/92.1 comparison group, provided a 1.2-fold change threshold and a standard of t-test $p < 0.05$, and 160 and 129 proteins were downregulated and upregulated, respectively, in the 92.1-B/92.1 comparison group.
Data source location:	Data were stored in the ProteomeXchange Consortium by virtue of the identifier PXD032215 of the PRIDE repository.
Data accessibility:	Name: PRIDE repository, Code: PXD032215, Link: http://www.ebi.ac.uk/pride/archive/projects/PXD032215
Related research article:	Xifeng Fei, Xiangtong Xie, Ruwei Qin, et al. Proteomics analysis: inhibiting the expression of P62 protein by chloroquine combined with dacarbazine can reduce the malignant progression of uveal melanoma. BMC Cancer. 2022 Apr 14;22(1):408.

Value of the Data

- This dataset covers the information on 5267 proteins in human UM cells and tumor cells developed in the eyeball and the brain of human UM cells-tumor bearing mice that was published for the first time, as well as hundreds of up- and down-regulated proteome groups that are differentially expressed.
- The data can be used as a basis for identification of key regulatory molecules that help distinguish metastatic UM in brain from UM *in situ*, as well as for the screening of target molecules for targeted therapies.
- The data are of great significance for the research of the ophthalmologists, neurosurgeons, graduate students and administrators who are committed to the basic and clinical therapeutic research of UM.

1. Data Description

Human UM cell lines (92.1) were adopted and transplanted into the back of the eyeball and the brain of nude mice, respectively, to simulate the growth of UM *in situ* and in brain metastases. The xenograft was taken for monoclonal culture, and the resulting cells were named 92.1-A and 92.1-B. The data were obtained from a comparative proteomics experiment of the three kinds of cell lines described above. Cells were collected for quantitative proteomic analysis through the combination of cutting-edge technologies, including TMT labeling, HPLC classification technology, and the technology of mass spectrometry-based quantitative proteomics. There were 6081 proteins identified, among which 5267 carried quantitative data(supplementary data 1). Of all the quantified proteins, 302 and 335 proteins were downregulated and upregulated, respectively, in the 92.1-A/92.1 comparison group, provided a 1.2 fold-change threshold and a standard of *t*-test $p < 0.05$, and 160 and 129 proteins were downregulated and upregulated, respectively, in the 92.1-B/92.1 comparison group (Fig. 1 and supplementary data 2). According to these data, bioinformatics analyses of proteins were performed, including functional classification, protein annotation, cluster analysis and functional enrichment. A total of 22 kinesins underwent initial analysis, of which P62 (Sequestosome 1, SQSTM 1) was validated via animal models [6].

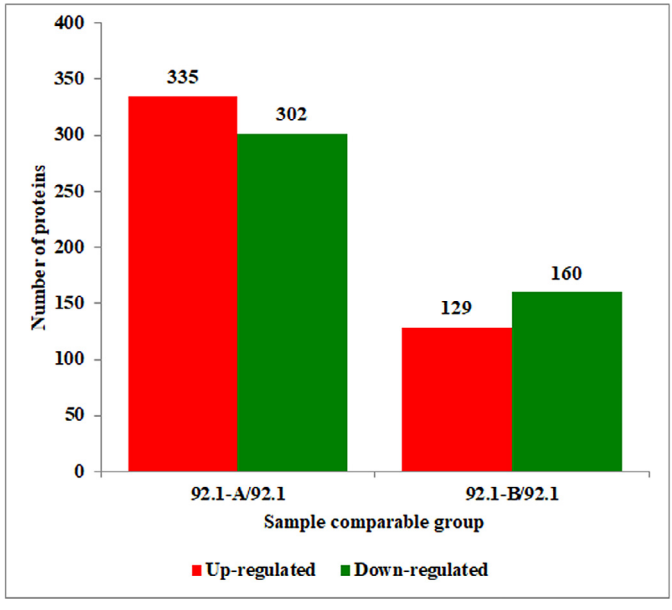

Fig. 1. Differential protein expression. 302 and 335 proteins were downregulated and upregulated, respectively, in the 92.1-A/92.1 comparison group, and 160 and 129 proteins were downregulated and upregulated, respectively, in the 92.1-B/92.1 comparison group.

2. Experimental Design, Materials and Methods

2.1. Cell culture

The 92.1 choroidal melanoma cells were obtained from the same institute mentioned above. The cells were cultured in RPMI1640 (Corning, USA) containing 10% FBS at 5% CO_2 and 37 °C.

2.2. Animals

EGFP transgenic nude mice (4–6-week-old, weighing 25 g) were maintained in our laboratory [7]. All mice were maintained in a Specific-Pathogen-Free facility (Grade = Nasal-1000). The animal experiments were in compliance with the Guide for the Care and Use of Laboratory Animals and ARRIVE guidelines.

2.3. Tumor cells inoculation

2.3.1. Orthotopic transplantation mouse model of human UM

After vortexing, the cell suspension (2.5×10^5 cells in 25 μL) was drawn into an inoculation needle. The animals (five nude mice) were narcotized, and iodophor was used to disinfect the skin surrounding the right orbit. The right eye of each mouse was punctured into the inner side (3 mm) of the orbital rim at 45° using a 27 G needle. The pre-collected cells were slowly inoculated into the retro-ocular soft tissues.

2.3.2. Transplantation mouse model of UM in the brain ventricles

After narcotizing the animals ($n = 5$), a hole was created at 1 mm left of the sagittal suture and 0.22 mm posterior to the bregma using a small-sized cranial drill under the guidance of stereotactic devices [8]. Next, the hole was inserted with a microinjection needle (depth = 2.5 mm), followed by micropump injection of 15μL cell suspension (2×10^5 cells) for 10 min. The needle was allowed to retain in the hole for 5 min. After 3–4 weeks, the tumor-bearing mice ($n = 4$) were killed, and the whole brain was isolated.

2.4. Monoclonal culture of 92.1-A and 92.1-B cells

After micropipette aspiration, the tumor tissues were grown in a 6-well culture plate containing 5 mL 1640 medium. Replacement of the culture medium was carried out every 3 days. After 14 days, the cells were placed into a new culture flask. The limiting dilution method was used to repeatedly perform monoclonal subculture [6].

2.5. Sample preparation

2.5.1. Protein isolation

Cell sample was added in lysis buffer containing Protease Inhibitor Cocktail (1%), urea (8 M), and sonicated 3 times with the Scientz ultrasonic processor. Following centrifugation (12,000 g, 10 min, 4 °C), the supernatant was collected and total protein was detected using the BCA kit using the kit's protocol.

2.5.2. Trypsinization

The protein solution was reduced with dithiothreitol (5 mM) at 56 °C for 30 min and alkylated with iodoacetamide (11 mM) at room temperature for 15 min in the dark. TEAB (100 mM) was then added to urea (2 M) to dilute the protein sample. Lastly, trypsin was added at 50:1 protein:trypsin ratio for overnight, and then at 100:1 protein:trypsin for 4 h.

2.5.3. TMT labeling

After trypsinization, the peptide was desalted with Strata-X C18 SPE column (Phenomenex), and then vacuum-dried. After reconstitution in 0.5 M TEAB, the peptide was processed using the TMT kit. Then, 1 unit of TMT reagent was thawed, followed by reconstitution in acetonitrile. Following incubation at room temperature for 2 h, the peptide mixture was pooled, desalted and vacuum-dried.

2.5.4. HPLC fractionation

High-pH reversed-phase fractionation of the tryptic peptides was carried out with HPLC using the 300Extend-C18 column (Agilent). Acetonitrile (pH 9.0) at a gradient of 8%–32% was used to separate the peptide into sixty fractions over 1 h. Subsequently, the peptides were merged into eighteen fractions, followed by vacuum drying.

2.6. LC-MS/MS assays

After dissolving in formic acid (0.1%, solvent A), the tryptic peptides were injected into a reversed-phase column. The solvent B (0.1% formic acid in 98% acetonitrile) was elevated from 6% to 23% over 26 min, 23% to 35% over 8 min, aroused to 80% over 3 min, and then held at 80% for 3 min. LC-MS/MS analysis was conducted using the EASY-nLC 1000 UPLC system at 400 nL/min.

The peptide was analyzed by MS/MS using the UPLC coupled with Orbitrap Fusion™ Lumos™ Tribrid™ (Thermo) in NSI source. The Orbitrap was employed to detect intact peptides at 60,000 resolution. The peptides with NCE setting of 32 were subjected to MS/MS analysis. The Orbitrap was also employed to detect ion fragments at 15,000 resolution. MS/MS analysis was conducted in data-dependent acquisition mode with 1 MS scan and then 20 MS/MS scans for the precursor ions with a cut-off value of >5E3. The voltage of electrospray was 2.0 kV. To avoid overfilling, automatic gain control was implemented. The accumulation of 5E4 ions was selected for generating MS/MS spectral data. The range of *m/z* scan was 350–1550, and the fixed first mass was 100 *m/z*.

2.7. Database search

The obtained MS/MS data were processed with Maxquant 1.5.2.8. All MS/MS spectral data were searched against the human Swissprot database (20,130 sequences), mouse Swissprot database (16,839 sequences) and their combined libraries concatenated with reverse-decoy database. Cleavage enzyme with maximum 2 missed cleavages was defined as Trypsin/P. The mass tolerance for fragment ions was 0.02 Da, while those for precursor ions were 5 and 20 ppm in Main and First searches, respectively. The oxidation on Met-and carbamidomethyl on Cys-were described as variable and fixed modifications, respectively. The minimum score for peptides and FDR rate were set as >40 and <1%, respectively.

2.8. Bioinformatic analyses

2.8.1. Annotation methods

2.8.1.1. Functional annotation. UniProt-GOA database was utilized to retrieve Gene Ontology (GO) annotation proteome. First, the identified protein identity was converted to UniProt identity and then mapped to GO identity based on the protein identity. When the identified protein was not annotated by UniProt-GOA, the functional annotation of that protein was conducted using the InterProScan software according to the amino acid sequence alignment approach. All proteins were then classified into 3 groups: molecular function, cellular component and biological process.

2.8.1.2. Domain annotation. Annotation of protein domains (PDs) was carried out using the InterProScan software that integrates different information regarding protein families, PDs and functional sites.

2.8.1.3. Pathway annotation. KAAS was employed to annotate the protein pathways. KEGG mapper was then used for mapping the annotation data on KEGG pathway database.

2.8.1.4. Subcellular localization. Wolfpsort was used for predicting the subcellular localization of eukaryotic sequences, which represents a newer version of PSORT/PSORT II.

2.8.2. Functional enrichment

GO enrichment. Proteins were classified based on the above-mentioned GO groups. The GO enrichment of differentially expressed proteins (DEPs) was compared using a 2-tailed Fisher exact. The GO terms with $p<0.05$ are deemed statistically significant.

2.8.2.1. KEGG enrichment. KEGG pathways were assigned into hierarchical groups using the KEGG database. The KEGG enrichment of DEPs was compared using a 2-tailed Fisher exact. The pathways with $p<0.05$ are deemed statistically significant.

2.8.2.2. PD enrichment. InterPro was used to enrich each PD. The PD enrichment of DEPs was compared using a 2-tailed Fisher exact. The domains with $p < 0.05$ are deemed statistically significant.

2.8.3. Hierarchical clustering

For hierarchical clustering, the enrichment data were collated according to their p-values, and the categories enriched in $\geq$1 clusters ($p < 0.05$) were filtered. All the *p*-values were transformed using the formula (−Log10 p-value)) into enrichment scores. The obtained z-cores were subjected to hierarchical clustering (average linkage, Euclidean distance) using the Genesis software. Finally, a heatmap was constructed by "heatmap.2″ function using the "gplots" R-package.

Ethics Statement

Animal experiments were approved by Animal Experimentation Ethics Committee at Genepharma company(approval number 2,022,539).

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships, which have or could be perceived to have influenced the work reported in this article.

Data Availability

Quantitative proteomic analysis of whole protein in three melanoma samples of 92.1, 92.1-A and 92.1-B (Original data) (PRIDE repository).

CRediT Author Statement

Xifeng Fei: Writing – original draft, Methodology, Software, Investigation; **Xiangtong Xie:** Methodology, Software, Investigation; **Xiaoyan Ji:** Methodology, Investigation; **Haiyan Tian:** Software; **Fei Sun:** Software, Methodology, Resources; **Dongyi Jiang:** Resources; **Zhimin Wang:** Conceptualization; **Qiang Huang:** Conceptualization, Writing – original draft, Methodology.

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Supplementary Materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.dib.2022.108592.

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