Data Article

Proteome data of whole saliva which are associated with development of oral mucositis in head and neck cancer patients undergoing radiotherapy

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Abstract

Saliva as major human body fluid may act as an indicator of oral disease status. Oral mucositis is a common and often treatment-limiting side effect of radiotherapy for head and neck cancer patients. In this dataset, we provide the complete proteome dataset (raw and search files) of the patients at baseline of radiotherapy treatment in patients undergoing radiotherapy analyzed by nano liquid chromatography coupled to mass spectrometry (LC–MS/MS). In the data set, 5323 tryptic peptides were identified which can be assigned to 487 distinct proteins (≥ 2 peptides). The MS data have been deposited to the ProteomeXchange ("ProteomeXchange provides globally coordinated proteomics data submission and dissemination" [1]) via the PRIDE partner repository with the dataset identifier PRIDE: PXD003230. The data are associated with the previously published work, "Differences in the whole saliva baseline proteome
profile associated with development of oral mucositis in head and neck cancer patients undergoing radiotherapy” [2].
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Specifications Table

| Subject area          | Biology                  |
|-----------------------|--------------------------|
| More specific subject area | Clinical Proteomics |
| Type of data          | Table                    |
| How data was acquired | Data were recorded using nano-liquid chromatography coupled to an LTQ Orbitrap Velos mass spectrometer |
| Data format           | 1) raw (Thermo instrument output files) |
|                       | 2) .msf (Proteome Discoverer output files) |
| Experimental factors  | Patients received Intensity-modulated radiation (IMRT). Whole saliva was collected from patients at least three days before the radiotherapy started. |
| Experimental features | 1) Whole saliva collection |
|                       | 2) Protein precipitation |
|                       | 3) Proteolytic digestion using trypsin |
|                       | 4) LC–MS/MS analysis |
| Data source location  | Greifswald, Mecklenburg – West Pomerania, Germany |
| Data accessibility    | Data are within this article and deposited to the ProteomeXchange Consortium via the PRIDE partner repository with the dataset identifier PRIDE: PXD003230. |

Value of the data

- Protein signatures of whole saliva from head and neck cancer patients are useful to differentiate between healthy and disease subjects screening for signatures of radiation associated oral mucositis (OM).
- Proteomics revealed correlation of the abundance of 48 of the 488 proteins identified with the risk of developing OM which allow further investigations towards biomarker assays.
- Whole saliva protein profiles at baseline of radiotherapy might allow identification of patients prone to adverse reactions.

1. Data

In this dataset, we measured the whole saliva proteome of patients for differences related to the development of oral mucositis. The data present here are (i) LC–MS/MS raw data and (ii) database search files of 50 head and neck cancer patients.

2. Experimental design, materials and methods

We collected unstimulated whole saliva of 50 patients before receiving radiotherapy. After treatment, 41 out of 50 patients developed oral mucositis (grade III) during radiotherapy, of which 14
patients even displayed an early oral mucositis (grade III) at low radiation dose of 30 Gy. Nine patients did not develop OM (grade III). The whole set were prepared for LC–MS/MS analysis and the acquired data are provided.

Table 1
Proteome data that are provided at PRIDE.

| Sample number | LC–MS/MS file available | Database search file available | Localization | Tumor stage | Oral mucositis developed |
|---------------|-------------------------|-------------------------------|--------------|-------------|--------------------------|
| 1             | x                       | x                             | Oropharynx   | IVa         | yes                      |
| 2             | x                       | x                             | Oropharynx   | IVa         | no                       |
| 3             | x                       | x                             | Hypopharynx  | IVa         | yes                      |
| 4             | x                       | x                             | Hypopharynx  | IVa         | yes                      |
| 5             | x                       | x                             | Larynx       | IVb         | yes                      |
| 6             | x                       | x                             | Hypopharynx  | IVa         | yes                      |
| 7             | x                       | x                             | Oropharynx   | III         | yes                      |
| 8             | x                       | x                             | Oropharynx   | IVa         | yes                      |
| 9             | x                       | x                             | Oropharynx   | IVa         | yes                      |
| 11            | x                       | x                             | Oropharynx   | IVb         | yes                      |
| 12            | x                       | x                             | Hypopharynx  | IVa         | yes                      |
| 13            | x                       | x                             | Oropharynx   | IVa         | no                       |
| 14            | x                       | x                             | Larynx       | 0           | no                       |
| 15            | x                       | x                             | Larynx       | IVa         | yes                      |
| 16            | x                       | x                             | Hypopharynx  | IVa         | no                       |
| 17            | x                       | x                             | Larynx       | IVb         | yes                      |
| 18            | x                       | x                             | Hypopharynx  | IVa         | yes                      |
| 19            | x                       | x                             | Hypopharynx  | IVa         | no                       |
| 20            | x                       | x                             | Oropharynx   | IVa         | yes                      |
| 21            | x                       | x                             | Oropharynx   | IVa         | yes                      |
| 22            | x                       | x                             | Oropharynx   | IVa         | yes                      |
| 23            | x                       | x                             | Oropharynx   | IVa         | yes                      |
| 24            | x                       | x                             | Oropharynx   | IVa         | yes                      |
| 25            | x                       | x                             | Larynx       | IVa         | yes                      |
| 26            | x                       | x                             | Hypopharynx  | IVa         | yes                      |
| 27            | x                       | x                             | Oropharynx   | IVa         | yes                      |
| 28            | x                       | x                             | Oropharynx   | IVa         | no                       |
| 29            | x                       | x                             | Oral cavity  | IVa         | yes                      |
| 31            | x                       | x                             | Oropharynx   | IVa         | yes                      |
| 33            | x                       | x                             | Oropharynx   | IVa         | yes                      |
| 34            | x                       | x                             | Larynx       | IVa         | yes                      |
| 48            | x                       | x                             | Nasopharynx  | II          | yes                      |
| 49            | x                       | x                             | Hypopharynx  | IVa         | yes                      |
| 51            | x                       | x                             | Hypopharynx  | IVb         | yes                      |
| 52            | x                       | x                             | Larynx       | IVa         | yes                      |
| 53            | x                       | x                             | Oral cavity  | III         | yes                      |
| 62            | x                       | x                             | Oropharynx   | IVa         | yes                      |
| 64            | x                       | x                             | Hypopharynx  | IVa         | yes                      |
| 65            | x                       | x                             | Hypopharynx  | IVa         | yes                      |
| 66            | x                       | x                             | Oropharynx   | IVa         | yes                      |
| 67            | x                       | x                             | Oropharynx   | IVa         | yes                      |
| 68            | x                       | x                             | Oral cavity  | I           | yes                      |
| 70            | x                       | x                             | Hypopharynx  | IVa         | yes                      |
| 71            | x                       | x                             | Larynx       | IVa         | no                       |
| 72            | x                       | x                             | Oropharynx   | IVa         | yes                      |
| 73            | x                       | x                             | Oropharynx   | II          | yes                      |
| 74            | x                       | x                             | Maxillary antrum | III        | yes                      |
| 75            | x                       | x                             | Oropharynx   | IVa         | no                       |
| 77            | x                       | x                             | Larynx       | IVb         | no                       |
| 78            | x                       | x                             | Oropharynx   | III         | yes                      |
3. Sample preparation for proteome characterization

The volume of whole saliva ranged from 0.2 to 1.7 mL (average 0.9 ± 0.3 mL). To acquire this proteome dataset, 0.5 mL aliquots of whole saliva proteins were precipitated using trichloroacetic acid (TCA) at a final concentration of 10% (v/v) and dithiothreitol (0.12% w/v) as described [3]. Briefly, protein pellets were resuspended in 8 M urea/ 2 M thiourea buffer. For MS-analysis, 4 μg of protein lysate were reduced (2.5 mM DTT for 1 h at 60 °C) and alkylated (10 mM iodoacetamide for 30 min at 37 °C). Proteolysis was performed overnight using trypsin (Promega, Madison, WI, USA). Tryptic cleavage was stopped by adding 1% acetic acid followed by desalting and purification using ZipTip-μC18 tips (Millipore, Billerica, MA, USA).

4. Mass spectrometric analysis

The 50 patient samples were measured in a randomized design. Proteolytically cleaved peptides were separated prior to MS analyses by reverse phase nano HPLC on a 15 cm Acclaim PepMap100-column (C18, 3 μm, 100 Å) using an EASY-nLC Proxeon system (Thermo Scientific, Waltham, MA, USA) at a constant flow rate of 300 nL/min. The LC separation was achieved using a linear gradient of buffer B from 5% up to 25% within 63 min with 0.1% acetic acid, 2% acetonitrile in water (solvent A) and 0.1% acetic acid in 100% acetonitrile (solvent B). Peptides were measured using an LTQ Orbitrap Velos instrument (Thermo Scientific) equipped with a nano electrospray ion source operated with PicoTip Emitters (New Objective, Woburn, MA, USA). After a first survey scan with a resolution of 30,000, the MS/MS data were measured for the top 20 mass peaks in the linear ion trap at collision induced energy (CID) of 35%. The raw MS-data were processed using the Refiner MS v7.5 module (Genedata, Basel, Switzerland). Peak lists were searched against a human FASTA-formatted database containing 20,268 unique entries (human_uniprot_swissprot_2011_10.fasta) using an in-house Mascot server v2.3.2 (Matrix Science, London, GB). Database searches were performed with carbamidomethyl on cysteine as fixed modification and oxidation on methionine as variable modification. Enzyme specificity was selected to trypsin with up to two missed cleavages allowed using 10 ppm peptide ion tolerance and 0.6 Da MS/MS tolerances. Only ranked 1 peptide hits and a Mascot ion score > 23 were considered as identified (Table 1).

Acknowledgments

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Transparency document. Supplementary material

Transparency document associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.dib.2016.05.053.

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