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Data Article

Women with temporomandibular disorders: Untargeted proton nuclear magnetic resonance spectroscopy-based metabolomics of saliva and psychological instruments dataset

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ABSTRACT

This article introduces the first dataset of 1H- nuclear magnetic resonance - based metabolomic spectroscopy of saliva samples from women with temporomandibular disorders (TMD) of muscular origin. Our data generated a metabolomic profile for TMD of muscular origin. The samples were separated in two groups: Experimental Group (EG) represented by women with TMD who were submitted to a conservative treatment compared with a Control group (CG) of women without TMD. These data also include information about time of onset the pain, measures of pain obtained before and after the treatment by the visual analogic scale. Information about some psychological instruments as pain

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catrastophizing scale, hospital anxiety and depression, and oral health impact profile-14 were also obtained in the CG and in the EG before submitted to the conservative treatment (EG-pre) and at the end of the treatment (EG-post). Those instruments help differentiate the groups, due to the psychosocial impact that TMD has on their lives perpetuating the physiological imbalance of the stomatognathic system. Raw data are available at: https://data.mendeley.com/datasets/wys5xd2vfg/1. It's published on mendeley, the DOI is DOI:10.17632/wys5xd2vfg.1. The data presented in this article are related to the research article entitled "1H–NMR-Based salivary metabolomics from female with temporomandibular disorders – a pilot study" (Lalue Sanches et al. 2020, https://doi.org/10.1016/j.cca.2020.08.006).

Specifications Table

Subject	Biological Sciences / Orofacial Pain and Psychology
Specific subject area	Saliva ^{1}H NMR spectroscopy-based metabolomics / Pain intensity, Catastrophizing, Anxiety, Depression, Quality of life
Type of data	Tables
How data were acquired	^{1}H NMR spectra using a Varian Inova® spectrometer (Agilent Technologies Inc., Santa Clara, CA, USA) equipped with a triple-resonance cold probe and operating at a ^{1}H resonance frequency of 600 MHz / Visual analogic scale (VAS), Pain Catastrophizing Scale (PCS), Hospital Anxiety and Depression Scale (HAD) and The Oral Health Impact Profile - 14(OHIP-14).
Data format	Raw Analyzed
Parameters for data collection	Collection of unstimulated saliva samples from participants in the control group (CG) ($n = 27$) and the experimental group before being submitted to conservative treatment (EG-pre) ($n = 26$) and at the end of conservative treatment (EG -post) ($n = 26$). The psychological instruments were also applied in the CG and in the EG-pre and EG-post.
Description of data collection	The collection of saliva and the application of psychological instruments in the experimental group (EG) was carried out twice: 1-during the initial consultation, after the diagnosis of temporomandibular disorder of muscular origin, according to the validated criteria RDC / TMD, and before the prescription of a conservative treatment (EG-pre), and 2- at the end of treatment (EG-post). In the control group (CG), participants collected saliva and responded to psychological instruments on a scheduled day and time.
Data source location	Universidade Federal de São Paulo – UNIFESP Sao Paulo/ Sao Paulo Brazil
Data accessibility	Data are available at: https://data.mendeley.com/datasets/wys5xd2vfg/1 it's published on mendeley, the DOI is DOI:10.17632/wys5xd2vfg.1
Related research article	M. Lalue Sanches, M.L. Sforça, E.G. Lo Turco, J. Faber, R.L. Smith, L.O.C.Moraes, 1H–NMR-Based salivary metabolomics from female with temporomandibular disorders – a pilot study, Clin Chim Acta. 2020, https://doi.org/10.1016/j.cca.2020.08.006.

Value of the Data

- Untargeted ^{1}H – NMR saliva metabolomic data may be used for study in depth temporomandibular disorders in women.

- This data shows that the understanding to find the answers to those cases of temporomandibular disorder with difficult resolution due to the complexity of its ethiopathogenesis, in some way might be achieved in the study of salivary metabolomics.
- Having a metabolic profile of TMD can serve to distinguish it from other conditions with similar symptoms such as headache, otalgias, cervicalgias and others.

1. Data Description

Table 1 performs a descriptive analysis of the sample with respect to age and its painful condition. It reports the average age of the groups studied (CG and EG), the time of pain onset of patients in the experimental group and the mean intensity of pain by the visual analog scale (VAS) of the experimental group before conservative treatment (EG-pre) and at the end of it (EG-post).

Table 2 describes the average values found in the responses to the questionnaires to assess the psychological conditions of the groups studied. The questionnaires studied were: pain catastrophizing scale (PCS), hospital anxiety and depression (HAD) and oral health impact profile - 14 (OHIP-14). The analysis of the values between the CG and EG-pre was performed using the t-test. In the EG-pre and EG-post group, the paired t test was applied.

The average values of the concentrations, expressed in millimolar/milliliters (μM/mL), and the standard deviation of the metabolites found in the saliva in the three groups are described in Table 3. The preparation of this table was based on the primary data stored at https://data.mendeley.com/datasets/wys5xd2vfg/1.

Table 1
Analysis of the study sample. Age, pain duration, and pain intensity levels.

	CONTROL GROUP ($n=27$)		EXPERIMENTAL GROUP ($n=26$)		p-values
Mean AGE (years)	39	SD (± 13.09)	42	SD (± 11.66)	0.3651
DURATION OF PAIN (months)			mean 48	SD (± 79.57)	(min - max.) (12 - 360)
Mean VAS score (0–10)			before treatment 6.25 (±1.93)	after treatment 0.9 (± 1.35)	<0.0001

VAS - visual analogic scale (means and standard deviations).
$p<0.05$ = significantly different.

Table 2
Assessment of the modified Oral Health Impact Profile (OHIP-14), Hospital Anxiety and Depression Scale (HAD), and Pain Catastrophizing Scale (PCS) in the groups CG × EG-pre and EG-pre × EG-post. Values correspond to the average total scores of each instrument.

	Control group (CG) $n=27$	Experimental group before treatment (EG-pre) $n=26$	*t*-test	Experimental group before treatment (EG-pre) $n=18$	Experimental group after treatment (EG-post) $n=18$	Paired *t*-test
Psychological Instruments	$\bar{x}$ (±SD)	$\bar{x}$ (±SD)	p	$\bar{x}$ (±SD)	$\bar{x}$ (±SD)	P
OHIP-14 modif.	4 (±5.12)	26 (±12.97)	<0,0001*	23 (±13.80)	15 (±11.80)	0,0013*
HAD - anxiety	7 (±3.49)	10 (±4.91)	0,0039*	10 (±5.25)	8 (±4.52)	0,0052*
HAD - depression	4 (±2.40)	6 (±3.87)	0,032*	6 (±3.53)	6 (±3.48)	0,8731
PCS	11 (±12.03)	24 (±15.11)	0,0007*	21 (±15.39)	12 (±10.81)	0,0092*

* = significantly different at $p<0.05$.

Table 3
Concentrations (μm/mL), average ± SD of salivary metabolites, in Control group (CG), experimental group before treatment (EG-pre) and experimental group after treatment (EG-post).

Compounds	CONTROL GROUP Average ± SD	EXPERIMENTAL GROUP before treatment (EG-pre) Average ± SD	EXPERIMENTAL GROUP after treatment (EG-post) Average ± SD
5-Aminopentanoate	112.05 ± 102.02	92.63 ± 87.47	105.75 ± 134.86
AMP	4.48 ± 3.82	3.81 ± 2.51	3.29 ± 1.83
Acetate	297.58 ± 378.96	369.02 ± 590.21	336.40 ± 604.27
Acetoin	0.06 ± 0.34	1.43 ± 3.06	0.10 ± 0.37
Alanine	59.62 ± 43.12	41.68 ± 20.52	52.01 ± 26.39
Arginine	17.40 ± 10.25	11.74 ± 5.19	13.70 ± 8.25
Aspartate	18.62 ± 8.05	15.28 ± 6.28	15.57 ± 7.52
Betaine	4.72 ± 2.92	3.27 ± 1.85	4.02 ± 1.86
Butyrate	5.40 ± 5.91	5.88 ± 7.88	5.39 ± 7.80
Choline	4.71 ± 2.15	3.59 ± 1.49	4.83 ± 3.11
Citrate	48.21 ± 26.53	63.37 ± 42.46	54.22 ± 34.58
Creatine	40.07 ± 25.66	28.85 ± 9.72	30.60 ± 15.07
Creatinine	2.74 ± 1.42	3.51 ± 1.64	2.56 ± 1.30
Dimethylamine	1.70 ± 2.56	0.00 ± 0.00	0.78 ± 1.43
Ethanol	25.60 ± 37.03	54.86 ± 70.88	544.01 ± 2671.93
Ethanolamine	21.90 ± 11.13	18.80 ± 11.48	20.05 ± 20.32
Formate	125.27 ± 103.76	103.34 ± 70.75	74.06 ± 63.31
Fucose	13.82 ± 13.31	14.71 ± 13.34	13.88 ± 19.53
Galactose	14.51 ± 12.15	14.24 ± 14.41	12.13 ± 14.95
Glucose	124.42 ± 84.75	82.00 ± 65.56	73.87 ± 37.82
Glutamate	52.85 ± 29.77	40.25 ± 18.42	37.23 ± 19.43
Glutamine	51.74 ± 41.13	37.16 ± 22.76	35.42 ± 16.45
Glycerol	523.42 ± 495.06	349.13 ± 144.33	235.07 ± 180.68
Glycine	107.04 ± 74.15	84.36 ± 46.76	101.24 ± 90.02
Histidine	9.40 ± 6.82	9.80 ± 7.51	8.76 ± 4.24
Hypoxanthine	6.07 ± 2.87	4.70 ± 2.25	4.95 ± 3.07
Isovalerate	0.25 ± 0.53	0.81 ± 1.39	0.00 ± 0.00
Lactate	660.50 ± 424.11	440.58 ± 194.13	520.01 ± 276.36
Lactose	12.15 ± 7.63	13.46 ± 12.10	12.58 ± 22.51
Leucine	10.33 ± 4.56	10.61 ± 7.77	9.74 ± 3.90
Lysine	25.21 ± 14.85	25.44 ± 13.22	23.96 ± 19.30
Maltose	161.54 ± 128.83	80.19 ± 62.28	75.60 ± 68.10
Methanol	37.87 ± 23.03	49.61 ± 30.46	33.71 ± 23.02
Methionine	3.09 ± 1.86	2.10 ± 1.22	1.78 ± 0.80
Methylamine	3.23 ± 2.01	2.71 ± 2.26	4.29 ± 3.41
O-Acetylcholine	2.62 ± 2.00	1.21 ± 0.64	1.67 ± 1.04
O-Phosphoethanolamine	181.64 ± 119.76	125.03 ± 81.07	122.13 ± 42.16
Ornithine	10.47 ± 8.08	8.25 ± 6.92	6.67 ± 3.52
Phenylacetate	3.88 ± 3.33	0.00 ± 0.00	3.63 ± 5.88
Phenylalanine	15.44 ± 8.32	13.39 ± 7.96	10.85 ± 5.59
Proline	44.13 ± 42.65	40.42 ± 29.65	40.83 ± 35.50
Propionate	27.96 ± 41.96	42.90 ± 71.34	25.11 ± 46.21
Propylene glycol	2.84 ± 2.73	1.00 ± 2.71	1.90 ± 1.86
Putrescine	27.85 ± 26.96	28.45 ± 24.79	25.08 ± 30.12
Pyruvate	18.02 ± 11.56	18.64 ± 11.39	16.35 ± 10.92
Sarcosine	5.95 ± 3.42	5.55 ± 3.57	5.85 ± 4.28
Succinate	55.45 ± 33.20	37.21 ± 23.69	32.78 ± 22.85
Taurine	168.73 ± 104.52	121.23 ± 52.11	136.41 ± 72.07
Threonine	15.11 ± 12.31	12.55 ± 4.90	14.26 ± 7.44
Tyrosine	26.96 ± 11.71	25.37 ± 15.92	20.13 ± 9.11
Uracil	0.43 ± 1.28	0.00 ± 0.00	0.00 ± 0.00
Valine	10.87 ± 7.02	7.99 ± 4.48	9.59 ± 4.89
Xanthine	11.20 ± 8.04	7.00 ± 5.26	6.08 ± 4.45
myo-Inositol	11.75 ± 6.47	12.82 ± 10.52	9.86 ± 3.84
sn-Glycero-3-phosphocholine	14.37 ± 12.36	10.35 ± 5.03	9.33 ± 5.16
π-Methylhistidine	3.50 ± 3.11	2.79 ± 1.69	3.21 ± 2.37

Red highlight; ANOVA One Way Statistically different ($p<0.05$).

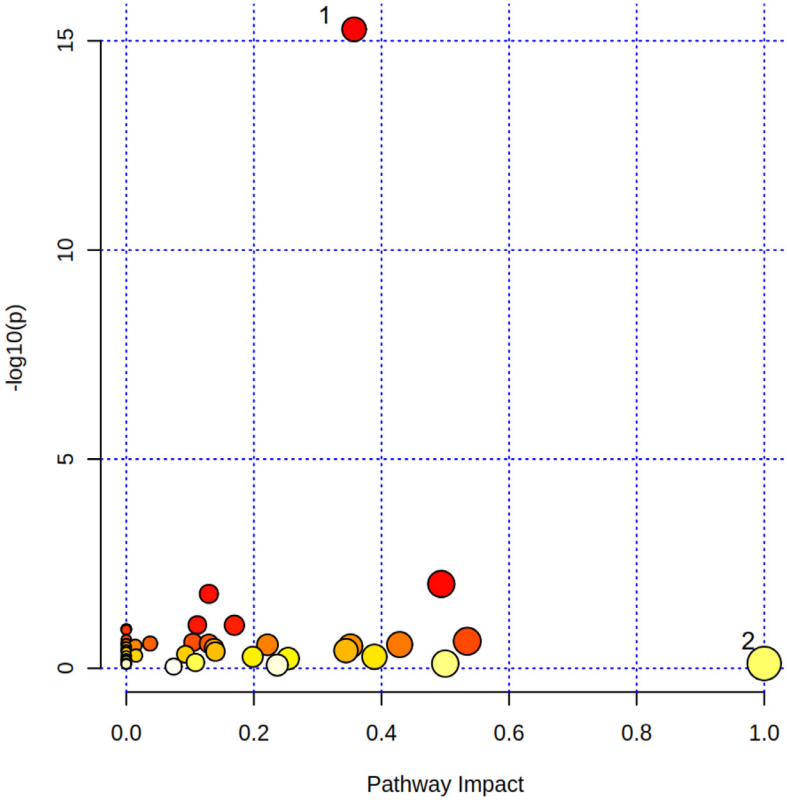

Fig. 1. Metabolic pathway analysis between Control group (CG) and Experimental Group before treatment (EG-pre). 1-Phenylalanine metabolism. 2- Starch and sucrose metabolism.

Fig. 1 shows the metabolic pathway analysis achieved using MetaboAnalyst 4.0 for the 57 quantified and identified metabolites. Paths with $p \leq 0.05$ and impact (PI) ≥ 0.2 were considered responsible for leading to the differences between saliva of control group (CG) and experimental group before treatment (EG-pre). Thus, 1-Phenylalanine metabolism and 2-starch and sucrose metabolism were selected as the most significant.

2. Experimental Design, Materials and Methods

2.1. Participants

This prospective case-control study evaluated data of 53 women aged 21 to 68 years, including 26 women with muscular TMD (experimental group [EG]) and 27 normal women (control group [CG]). The EG comprised patients from the Temporomandibular Disorder and Orofacial Pain Outpatient Clinic of the Escola Paulista de Medicina da Universidade Federal de São Paulo/Hospital São Paulo (EPM-UNIFESP/HSP) between May 2017 and July 2018, diagnosed using the Research Diagnostic Criteria for Temporomandibular Disorders (RDC/TMD) [1]. The EG participants were subjected to conservative treatment and follow-up. This group was subdivided into patients evaluated before (EG-pre) and after (EG-post) conservative treatment. The participants were informed about the study protocols and provided written informed consent. This project complied with STROBE guidelines [2] and was approved by the Research Ethics Committee of the UNIFESP/HSP under CAAE No. 78,339,817.9.0000.5505.

2.2. Assessment of psychological function

Specific and validated instruments were used to assess psychosocial changes. The Pain Catastrophizing Scale (PCS) [3] is a questionnaire containing 13 items with five possible answers for each question as follows: 0, never; 1, rarely; 2, sometimes; 3, usually; and 4, always, and the maximum score was 52. Higher values represented worse results, and a score of 30 was the cut-off value for catastrophizing.

The Hospital Anxiety and Depression Scale (HAD) [4] is a questionnaire widely used in primary centers to measure discomfort or psychological changes in patients with physical pain by assessing the effect of psychological pain on somatic symptoms. The HAD is divided into two subcategories—anxiety and depression—and each subcategory contains seven multiple-choice questions with values ranging from zero to three. The following scoring system for anxiety or depression was used: ≤ 7, absent, 8–11, likely present; and >11, definitely present.

The Oral Health Impact Profile (OHIP-14) [5] is composed of 14 questions in seven domains: functional limitation, physical pain, psychological discomfort, physical disability, psychological disability, social disability, and handicap. Each question was scored as follows: 0, never; 1, almost never; 2, sometimes; 3, usually; and 4, very often/every day. The maximum score was 56, and higher values represented worse results. The modified OHIP-14 was used because participants with TMD were analyzed. In the modified OHIP-14 the words “your teeth and dentures,” were replaced with “your joints,” and the word “mouth” was maintained to indicate pain in chewing muscles [6].

2.3. Measurement of pain

The Visual Analog Scale (VAS) was used to assess pain, which was the variable indicative of clinical improvement. The VAS consists of a 10-cm line, where the extreme left corresponds to the “absence of pain,” and the extreme right, to the “highest level of pain” [7]. The participants were asked to mark a point on the line that best represented their pain level. Measurements were obtained before, during, and after treatment.

2.4. Conservative treatment

The treatment program was applied to the EG and involved two stages: the beginning of treatment (T0), and the end of the treatment (days 80 to 90 days after the initiation of treatment) (T1). The Visual Analog Scale (VAS) was used to assess pain, which was the variable indicative of clinical improvement. Measurements were obtained before, and after treatment.

2.5. Saliva samples:collection, storage, preparation for spectra aquisition and metabolites quantification

The participants were instructed not to ingest food or drink (except water) for at least 1 hour before collection (between 8:30 a.m. and 10:30 a.m.). The participants were asked to rinse the mouth with distilled water. After 5 min, a synthetic cotton roll from the Salivette® saliva collection kit (Sarstedt Ltda^{TM}) was placed and remained in the mouth for 5 to 10 min. The participants were asked not to swallow or talk during the procedure to ensure that the produced saliva was absorbed by the cotton roll. The Salivette® tubes were centrifuged at $15{,}000 \times g$ for 10 min. The pellet containing the saliva was transferred to 0.5 mL autoclaved test tubes and stored at $-80\,^{\circ}C$.

^{1}H NMR spectra were acquired using a Varian Inova® spectrometer (Agilent Technologies Inc., Santa Clara, CA, USA) equipped with a triple-resonance cold probe and operating at a ^{1}H resonance frequency of 600 MHz [8]. The lock procedures were performed manually to avoid

fluctuations in the magnetic field and shimming, and to ensure that the magnetic field intensity was the same in the X, Y, and Z axes. Spectra acquisition was performed with 1024 scans collected with 32 K data points over a spectral width of 8000 Hz. A 1.5-s relaxation delay was incorporated between scans, during which a continual water pre-saturation radio frequency (RF) field was applied to eliminate residual water signal. The metabolites were processed and quantified using NMR Suite software version 7.5 (Chenomx Inc^{TM}, Edmonton, AB, Canada). A total of 56 metabolites were identified and their concentrations were measured and normalized, when necessary.

2.6. Statistical analysis

A descriptive analysis of the average and standard deviation of the 56 metabolites concentrations was made [9]. The unpaired *t*-test was used to compare paired mean values between CG and EG, assuming equal variances. The analyzed variables were the age of the participants and psychological test scores in CG and EG-pre. A paired *t*-test was used to compare the average psychological test scores between EG-pre and EG-post [9]. Data on pain duration and intensity in the EG-pre were also analyzed.

Ethics Statement

The participants were informed about the study protocols and provided signed informed consent. This project complied with STROBE guidelines and was approved by the Research Ethics Committee of the Universidade Federal de Sao Paulo/ Hospital Sao Paulo (UNIFESP/HSP) under CAAE No. 78,339,817.9.0000.5505.

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.

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