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Data on FTIR spectra of mixtures of sodium valproate (VPA) and histones H1 and H3.

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Benedicto de C. Vidal[1], Maria Luiza S. Mello[*1]

ABSTRACT

Valproic acid/sodium valproate (VPA), a drug primarily used for treatment of seizure disorders, is recognized as an efficient epigenetic agent, inducing inhibition of histone deacetylases, promoting changes in the methylation status of DNA and histones, and affecting chromatin structure. In addition to these epigenetic effects, molecular affinity of VPA for histone H1 has been proposed based on thermal denaturation, fluorescence spectroscopy and circular dichroism assays. VPA interactions with DNA and histones using Fourier transform infrared (FTIR) microspectroscopy and high-performance polarization microscopy that are not related to the effects promoted on epigenetic markers have been recently explored. Data in this article provide supplementary information for a better understanding of the resulting FTIR spectra for mixtures of VPA and histones H1 and H3 and of the potential effect of VPA directly on histones that has been reported in the literature.

Keywords: FTIR; Histones; Pharmacology; Sodium valproate (VPA).

PRIOR PUBLICATIONS

VIDAL, B. C.; MELLO, M. L. S. Sodium valproate (VPA) interactions with DNA and histones. Int J Biol Macromol 163:219-231, 2020. DOI: 10.1016/j.ijbiomac.2020.06.265.

[1] Universidade Estadual de Campinas, Instituto de Biologia, Campinas, SP, Brazil. mlsmello@unicamp.br.

DATA IMPORTANCE

- Present data indicate VPA effects other than those usually affecting epigenetic markers on histones;
- These data provide indication of VPA interaction with histone molecules;
- Present data expand the understanding of the pharmacological potential of VPA;
- Cell Biologists, chemists and pharmacologists can benefit from these data.

MATERIALS AND METHODS

Materials

Valproic acid-sodium salt (VPA) (P4543, Sigma®, St. Louis, MO, USA) and calf thymus H1 (Code 382150, Merck/Millipore, Billerica, MA, USA) and histone H3 (Code 11034758001, Roche, Mannheim, Germany/Sigma-Aldrich®) were used. Ten-µL drops of VPA were dissolved in Milli-Q water at concentrations of 20 mM and 40 mM and then dripped on glass slides. Next, the preparations were left in the refrigerator overnight and then dried at 37 ℃ for one to three hours before examination. Ten-µL drops of a solution of 5 mg of histone H1 dissolved in 84 µL of Milli-Q water and of a solution of 2 mg of histone H3 dissolved in 69 µL of Milli-Q water were treated similarly to the VPA preparations. The same process was applied to VPA-histone H1 and VPA-histone H3 mixtures (5-µL each). The samples dripped on slides formed small dried hemispheres (drop-casting samples) that gradually dried from the periphery to the center of the preparation, forming concentric circles ("the coffee-ring effect") (DEEGAN et al., 1997) and that were examined at an ambient relative humidity <70% at 27 ℃ at their periphery and central region.

Methods

Attenuated total reflectance (ATR) Fourier-transform infrared spectra were automatically obtained using an Illuminat IR II™ microspectroscope (Smiths Detection, Danbury, CT, USA) equipped with a liquid-nitrogen cooled mercury-cadmium-telluride detector and with Grams/AI 8.0 software for spectroscopy (Thermo Electron Corporation, Waltham, MA, USA), and connected to an Olympus BMX-51 microscope (Olympus America, Center Valley, PA, USA). The ATR diamond objective magnification used was equal to 36 x. The equipment resolution was equal to 4 cm^{-1}. The measurement site was a square of 25 µm per side. Each spectral profile was generated from 64 scans over the range of 4000 to 650 cm^{-1}. The baseline correction that used four fitting points and level-plus-zero conditions as applied to each spectral profile was provided following Grams/AI 8.0 software indications. Each raw IR spectrum contains all of the information in one time-domain signal.

The data were collected during 2019-2020. The data source location was at the University of Campinas (Unicamp), Institute of Biology, Campinas, Brazil (latitude: -22.8203482; longitude: -47.0700119).

DATA DESCRIPTION

The information here presented contains FTIR data (Figures 1-4) supplementing a report on interactions of sodium valproate (VPA) with DNA and histones that were studied using high-performance polarization microscopy and ATR FTIR microspectroscopy (VIDAL; MELLO, 2020). All the spectral curves shown in Figures 1-4 are furnished as raw spectra that were provided directly by the equipment using the Fourier transform mathematical process. Raw FTIR spectra of VPA (Figures 1a, b), VPA-histone H1 mixtures and respective histone control (Figures 2a-e, 3a-e) and of a VPA-histone H3 mixture and respective histone control (Figures 4a-c) are shown to demonstrate overall consistency in spectral signature profiles but variability in band

peak intensities and in some band peak frequencies within each group under consideration. The band peak component at ~1550 cm^{-1} is the frequency of the maximal band peak of VPA (Figure 1). Absorbances at this frequency contributes to a band contained within the wavenumber edges 1580 cm^{-1} and 1480 cm^{-1} in histone H1 and H3 controls (Figures 2 and 4). The frequency variability detected in the raw spectra of films of VPA-histone H1 and VPA-histone H3 mixtures and respective histone controls is especially evident in the band peaks assigned to amide I and amide II (Figures 2a-e, 4a-c). Frequency variability is also evident in the most intense band peak of the spectra of the VPA-histone H1 mixtures and histone H1 control, that is positioned at 1088-1078 cm^{-1} (Figures 3a-c, e). All these pure raw FTIR spectral curves were used for the estimation of the averaged spectral profiles reported elsewhere.

Figure 1. Raw FTIR spectral curves of VPA in drop-casting preparations. A detail from (a) at the 1700-1250 cm^{-1} wavenumber window is shown in (b).

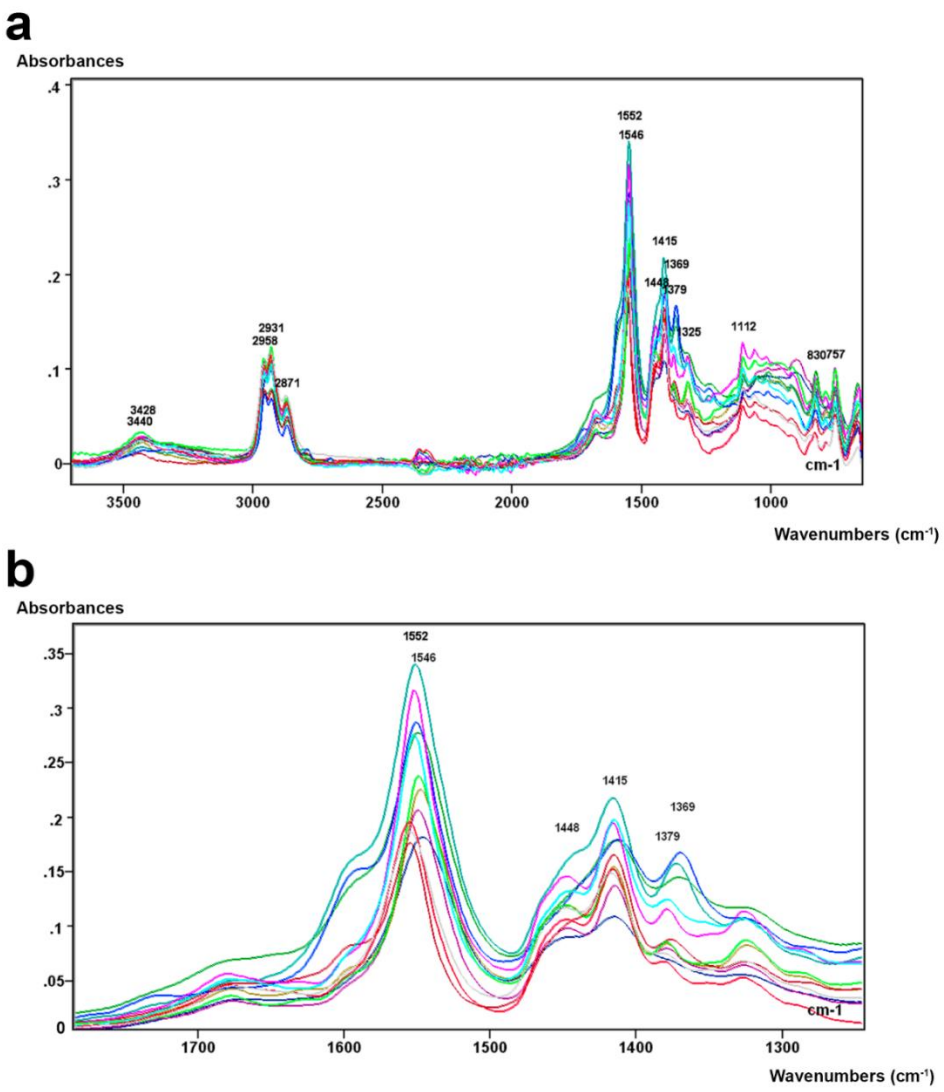


Figure 2. Raw FTIR spectral curves of histone H1 and VPA-histone H1 mixtures. Variability in the frequency of the band peak assigned to amide I (1640-1623 cm^{-1}) is detected in the curves of drop-casting samples of histone H1 (a), and in the curves obtained at the periphery (b) and center (c, e) of the hemispheres formed after drying of the drops of the 20 mM VPA-histone H1 mixture (b, c) and the 40 mM VPA-histone H1 mixture (d, e). Variability is also observed in the band peak frequency assigned to amide II (1529-1527 cm^{-1}) when obtained at the center of the hemispheres formed after drying of the drops containing the 20 mM VPA-histone H1 mixture (b). In a-e, a band peak element (shoulder) is suspected at the 1548-1546 cm^{-1} spectral region.

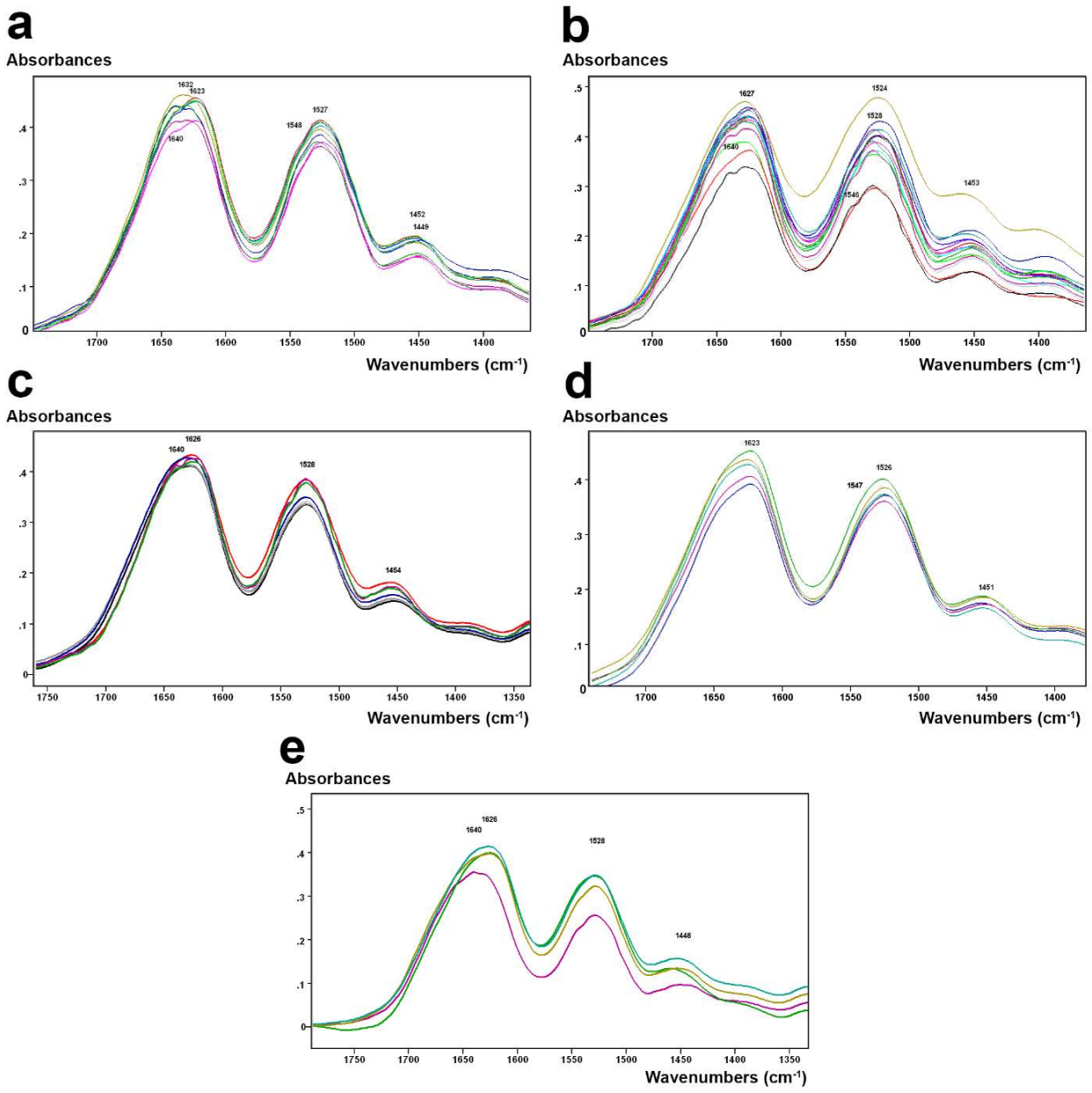


Figure 3. Raw FTIR spectral curves of histone H1 and VPA-histone H1 mixtures. Details at the ~1350-800 cm^{-1} spectral range are shown for curves of histone H1 (a) and at the periphery (b, d) and center (c, e) of hemispheres formed from dried drops of 20 mM VPA- (b, c) and 40 mM VPA-histone H1 mixtures (d, e).

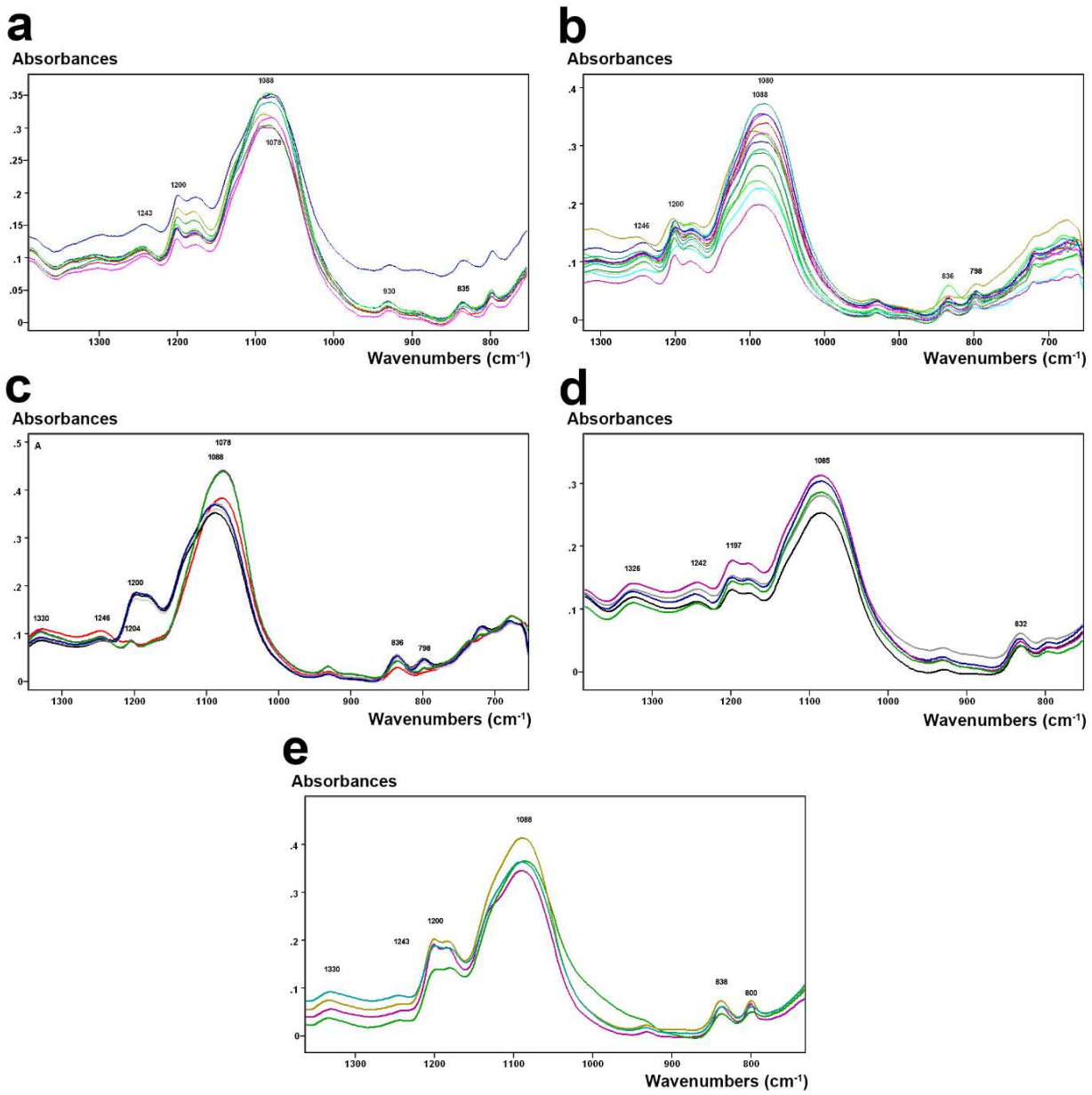
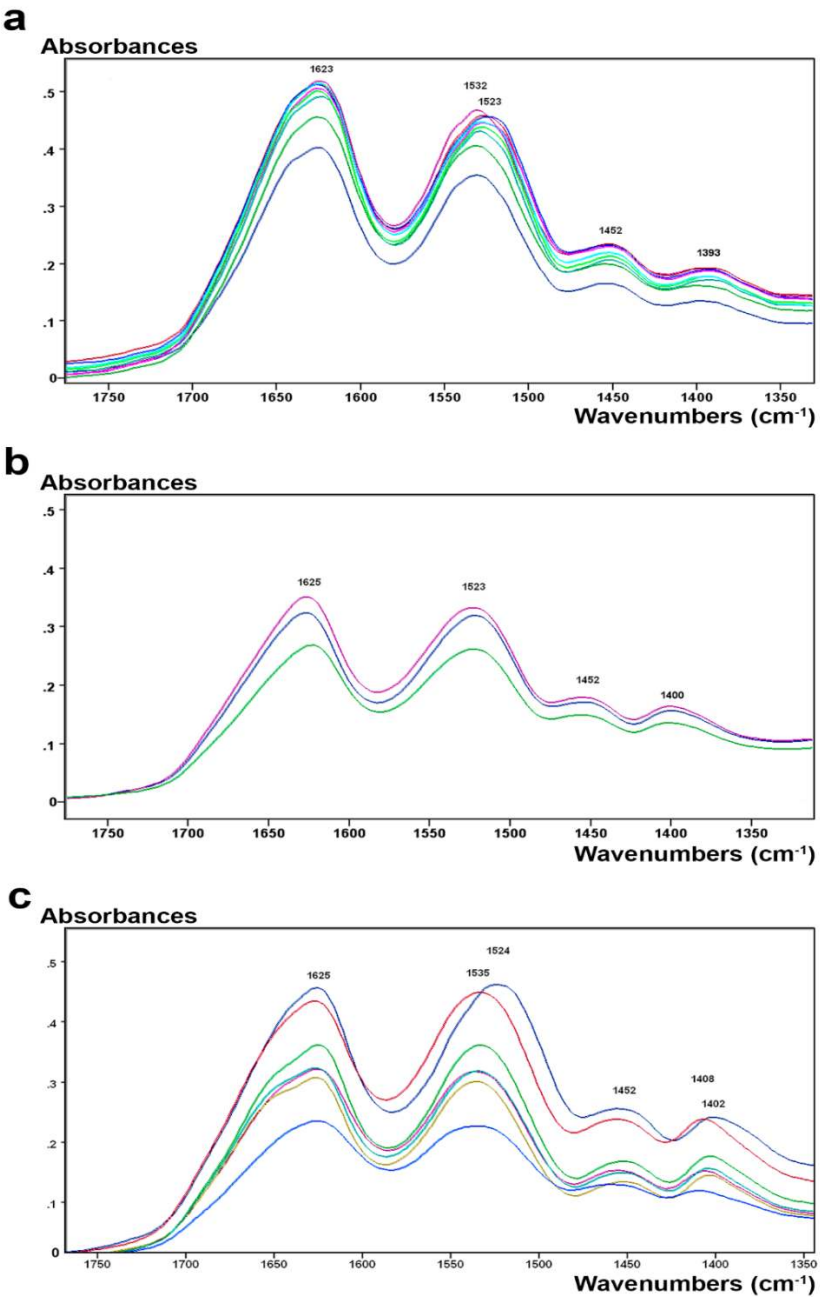


Figure 4. Raw FTIR spectral curves of histone H3 and VPA-histone H3 mixture at the 1750-1350 cm^{-1} spectral range. The curves were obtained at drop-casting samples of histone H3 (a) and at the periphery (b) and center (c) of hemispheres formed from dried drops of a 20 mM VPA-histone H3 mixture. Variability in the frequency of the band peaks assigned to amide I (1626-1623 cm^{-1}) and amide II (1535-1521 cm^{-1}) is observed.



In Tables 1 and 2, comparison of the absorbance values of band peaks assigned to amide groups is shown between the spectra of the VPA-histone H3 mixture and respective histone control. These data were obtained in the peripheric and central areas of the preparations which consisted of dried drop hemispheres dripped on glass slides.

Table 1. Absorbance values for the amide A and I band peaks calculated from raw FTIR spectra for dried drops of 20 mM VPA-histone H3 mixtures.

Samples	n	Amide A absorbances			Amide I absorbances		
		X	S	Md	X	S	Md
Histone H3	8	0.2206	0.0174	0.2166* ◆	0.4893	0.0406	0.5086* ◆
Histone H3 + VPA (hemisphere periphery)	3	0.1692	0.0138	0.1698*	0.3154	0.0405	0.3243*
Histone H3 + VPA (hemisphere center)	7	0.1626	0.0230	0.1583 ◆	0.3498	0.0764	0.3231 ◆

*, ◆, differences significant at the $P_{0.05}$ level (Mann-Whitney test); Md, median; n, number of spectral curves; S, standard deviation; X, arithmetic means.

Table 2. Absorbance values for the amide II and III band peaks calculated from raw FTIR spectra for dried drops of 20 mM VPA-histone H3 mixtures.

Samples	n	Amide II absorbances			Amide III absorbances		
		X	S	Md	X	S	Md
Histone H3	8	0.4335	0.0367	0.4449*	0.1637	0.0175	0.1681* ◆
Histone H3 + VPA (hemisphere periphery)	3	0.3052	0.0382	0.3210*	0.1092	0.0112	0.1157*
Histone H3 + VPA (hemisphere center)	7	0.3496	0.0832	0.3210	0.1105	0.0327	0.1030 ◆

*, ◆, differences significant at the $P_{0.05}$ level (Mann-Whitney test); Md, median; n, number of spectral curves; S, standard deviation; X, arithmetic means.

Data set

The dataset deposited in the repository of the University of Campinas (https://doi.org/10.25824/redu/OSK2UP) shows infrared microspectroscopical absorbances (FTIR) that permit construction of spectral signatures like those shown in Figures 1-4 of this study and statistical analysis like that shown in Tables 1 and 2 of this study. The dataset comprises nine tables detailing in each of their columns, infrared absorbance values estimated at wavenumbers (in cm^{-1}) concerned with the spectral windows for amide A, I, II, and III bands obtained for dried preparations of histones H1 and H3 and mixtures of these histones with VPA. Absorbances at wavenumbers assigned to ν_{as} C=O groups and C-O stretching were plotted for histone H1 and VPA-histone H1 mixtures.

The absorbances concerned with the amide A band for the histone H3 and the 20 mM VPA-histone H3 mixture were plotted at the wavenumbers 3283, 3277, 3275, 3273, 3271, 3269, 3267, 3266, 3265, 3264, 3263, 3261 and 3259 cm^{-1}. Regarding the amide I band for the histone H1 and the 20 mM and 40 mM VPA-histone H1 mixtures, the absorbances were plotted at 1640, 1626 and 1623 cm^{-1}, and for the histone H3 and the 20 mM VPA-histone H3 mixture, at 1626, 1625, 1624 and 1623 cm^{-1}. The absorbances concerned with the amide II band for the histone H1 and the 20 mM and 40 mM VPA-histone H1 mixtures were plotted at the wavenumbers 1536, 1526, 1524 and 1350 cm^{-1}, and those for the histone H3 and the 20 mM VPA-histone mixture were plotted at 1536, 1535, 1534, 1533, 1531, 1530, 1529, 1527, 1524, 1523, 1521

and 1516 cm^{-1}. The absorbances concerned with the amide III band for the histone H3 and the 20 mM VPA-histone H3 mixture were evaluated at the wavenumbers 1259, 1258, 1254, 1253, 1251, 1250, 1247, 1246 and 1245 cm^{-1}.

The absorbances assigned to ν_{as} C=O groups for the histone H1 and the 20 mM and 40 mM VPA-histone H1 mixtures were evaluated at 1550 and 1546 cm^{-1}, and those assigned to C-O stretching for the same samples were evaluated at 1090, 1088 and 1080 cm^{-1}. Absorbances estimated at 2960, 2934, 2931, 2871, 1550, 1546, 1415, 1380 and 1360 cm^{-1} were also plotted for dried drops of VPA (control).

The columns presented in Tables 1 and 2 of this work identify arithmetic means and respective standard deviations and medians calculated from the absorbances concerned with the amide A, I, II, and III band peaks for histone H3 (control) and VPA-histone H3 mixtures identified in the Tables 6, 7, 8, and 9, respectively, of the dataset.

SUPPLEMENTARY MATERIALS

Repository name: REDU, University of Campinas
DOI of the dataset (when available): DOI:10.25824/redu/OSK2UP
Link to access the data: https://doi.org/10.25824/redu/OSK2UP

ACKNOWLEDGEMENTS

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