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Fourier Transform Infrared Spectroscopic Characterisation of Some Common Antidepressans in Pharmaceutical Preparations

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Abstract

The objective of this study was to analyse some common antidepressants in pharmaceutical preparations. The antidepressants taken for analysis were Selective Serotonin Reuptake Inhibitors [SSRIs]. SSRIs were associated with the significantly lower risk of toxicity, but large number of deaths from SSRIs has occurred in combination with other drugs specifically tricyclic and tetracyclic antidepressants. There has been a lot of work in the characterisation of antidepressants in pharmaceutical preparations but still a rapid and reliable positive qualitative identification of SSRIs needs to be developed. In the present investigation, Fourier Transform Infra Red [FTIR] spectrophotometer in transmission and Attenuated Total Reflectance [ATR] mode was used to qualitatively identify pharmaceutical preparation consisting of Proxetine, Sertraline, Escitalopram, Fluvoxamine. The results suggested that both the modes provided greater sensitivity but the ATR mode has great potential for the characterisation of SSRIs.

Keywords: Pharmaceutical; Selective Serotonin Reuptake Inhibitors [SSRIs]; Attenuated Total Reflectance [ATR].; Fourier Transform Infra Red [FTIR]; Antidepressants.

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Introduction

The SSRIs block neuronal transport of 5-HT (Serotonin) both immediately and chronically, leading to complex secondary responses. Increased synaptic availability of 5-HT results in stimulation of a large number of postsynaptic 5-HT receptor types, which may contribute to adverse effects characteristic of this class of drugs, including GI effects (nausea and vomiting) and sexual effects (delayed or impaired orgasm). Stimulation of 5-HT_{2C} receptors may contribute to the agitation or restlessness sometimes induced by SSRIs.[1]

Several techniques like ultraviolet/visible spectrophotometry, fluorimetry, electroanalytical techniques, chromatographic methods (thin- layer chromatography, gas chromatography and high-performance liquid chromatography), capillary electrophoresis and vibrational spectroscopies are the main techniques that have been used for the quantitative and qualitative analysis of pharmaceutical compounds (like antidepressants). Although simple techniques such as UV/VIS spectrophotometry and TLC are still extensively employed, HPLC is the most popular instrumental technique used for the analysis of pharmaceuticals. In the area of pharmaceutical analysis is showed a trend in the application of techniques increasingly rapid such as ultra performance liquid chromatography and the use of sensitive and specific detectors as mass spectrometers.[2]

Materials and Methods

Collection of Samples

All the samples of drugs were purchased from the medical store in the form of pharmaceutical preparations. The description of the samples analyzed is given in Table 1.

Sample Preparation

About 2 mg of the finely powdered dry material was mixed with 200 mg of KBr, the same was grounded manually in an agate mortar and pressed into a thin disc the idea was to produce a disc as nearly transparent as possible. Small amount of the powdered sample was placed on the ZnSe atr ptalform of the FTIR spectrometer.

Experimental

FTIR and ATR Spectroscopy: The drugs mentioned in table 1 were analyzed with FTIR spectrophotometer, spectrum 2 Perkin Elmer; over the region of mid IR 4000-400 cm^{-1} at transmission mode using standard KBr pellet method. The ATR spectra was recorded with UATR (with ZnSe crystal) over the region of mid IR 4000-200 cm^{-1}.

Results and Discussion

Qualitative analysis using FTIR and ATR spectroscopy

By observing the position and shape of the vibrational bands in FTIR and ATR spectra of the drugs Proxetine, Sertraline, Escitalopram and Fluvoxamine a satisfactory vibrational band assignment has been made. They are summarized in Tables 2, 3 and 4.

In Table 2 there is description of the FTIR spectra of drugs Proxetine, Sertraline, Escitalopram and Fluvoxamine. In case of Proxetine [sample code A], considering the N-H group of proxetine the vibrational modes of N-H stretching occurs at 3469 cm^{-1}. The aromatic ring [C=C] stretch occur at frequency 1662 cm^{-1} and the C-H stretch and C-H bend of aromatic ring occur at frequency 2915.8 cm^{-1} and 889.23 cm^{-1} respectively. The vibration modes of C-F stretch occurs at 1442.4 cm^{-1}. The ether group [C-O-C] vibrates at frequency 1031cm^{-1}. In case of sertraline [sample code B], the N-H group stretch occurs at frequency 3413 cm^{-1}. The aromatic ring [C=C] stretch occur at frequency 1648.2 cm^{-1} and the C-H stretch and C-H bend of aromatic ring occur at frequency 2921.4 cm^{-1} and 883.67 cm^{-1} respectively. The aliphatic C-H stretch occurs at frequency 1467.5 cm^{-1}. N-C stretch occurs at frequency 1031 cm^{-1}. In case of Escitalopram [sample code C], N:::C stretch occur at 2229.2 cm^{-1} frequency. The aromatic ring [C=C] stretch occur at frequency 1648.2cm^{-1} and the C-H stretch and C-H bend of aromatic ring occur at frequency 2904.2 cm^{-1} and 764.13 cm^{-1} respectively. The C-F bond stretch occurs at frequency 1428.5 cm^{-1}. The ether group [C-O-C] in escitalopram stretch at frequency 1336.8 cm^{-1}. N-C bond stretches at frequency 1022.7 cm^{-1}. In last case of fluvoxamine [sample code D], N-H bond stretches at 3396.8 cm^{-1}, aromatic ring [C=C] stretch occur at frequency 1620.4 cm^{-1}, N-C stretches at frequency 1081 cm^{-1} and the ether group [C-O-C] stretch occur at frequency 1017 cm^{-1}.

In Table 3 there is description of the ATR spectra of drugs Proxetine, Sertraline, Escitalopram and Fluvoxamine. In case of Proxetine [sample code A], considering the N-H group of proxetine the vibrational modes of N-H stretching occurs at 3285.63 cm^{-1}. The aromatic ring [C=C] stretch occur at frequency 1650.03 cm^{-1} and the C-H stretch and C-H bend of aromatic ring occur at frequency 2916.87 cm^{-1} and 892.1 cm^{-1} respectively. The vibration modes of C-F stretch occur at 1418.4 cm^{-1}. The ether group [C-O-C] vibrates at frequency 1032.4 cm^{-1}. In case of Sertraline [sample code B], the N-H group stretch occurs at frequency 3318.3 cm^{-1}. The C-H stretch and C-H bend of aromatic ring occur

Table 1: Description of the drugs analyzes

Sample Code	Generic Name	Category	Composition	Manufacturer
A	Proxetine	Anti- depressant	Anhydrous Proxetine Hydrochloride, 12.5 mg	Zentiva pharmasecutic-al
B	Sertraline	Anti- depressant	Sertraline Hydrochloride, 50 mg	Ranbaxy laboratory limited
C	Escitalopram	Anti- depressant	Escitalopram Oxalate, 10 mg	Akums drugs and pharmaceutical ltd. Haridwar
D	Fluvoxamine	Anti- depressant	Fluvoxamine Malate, 50 mg	Sunpharma Sikkim, Sikkim

at frequency 2856 cm^{-1} and 1018.6 cm^{-1} respectively. N-C stretch occurs at frequency 1137.8 cm^{-1}. In case of Escitalopram [sample code C], the aromatic ring [C=C] stretch occur at frequency 1631.23 cm^{-1} and the C-H stretch of aromatic ring occurs at frequency 2900.44 cm^{-1}. The C-F bond stretch occurs at frequency 1424 cm^{-1}. The ether group [C-O-C] in escitalopram stretch at frequency 1336.63 cm^{1} N-C bond stretches at frequency 1018.01 cm^{-1}. In last case of fluvoxamine [sample code D], N-H bond stretches at 3393.5 cm^{-1}, aromatic ring [C=C] stretch occur at frequency 1619.5 cm^{-1}, N-C stretches at frequency 1075.6 cm^{-1} and the ether group [C-O-C] stretch occur at frequency 1013.4 cm^{-1}.

In Table 4 there is description of comparison of transmission mode and the ATR mode spectra of drugs Proxetine, Sertraline, Escitalopram

Table 2: FTIR spectral readings of drugs Proxetine, Sertraline, Escitalopram, Fluvoxamine.

Sample Code	Generic Name	FTIR Frequency cm-1	Vibrational band assignment
A	Proxetine	3469	N-H stretch
		2915.8	C-H stretch aromatic
		1662	C=C stretch
		1442.4	C-F stretch
		1031	C-O-C stretch
		889.23	C-H bend aromatic
B	Sertraline	3413	N-H stretch
		2921.4	C-H stretch aromatic
		1648.2	C=C stretch aromatic
		1400.7	C-H bend aliphatic
		883.67	N-C stretch
		675.18	C-H bend aromatic
C	Escitalopram	2904.7	C-H stretch aromatic
		2229.2	N:::C stretch
		1648.2	C=C stretch aromatic
		1428.5	C-F stretch
		1336.8	C-O-C stretch
		1022.7	N-C stretch
		764.13	C-H bend aromatic
D	Fluvoxamine	3396.8	N-H stretch
		1620.4	C=C stretch aromatic
		1081	N-C stretch
		1017	C-O-C stretch

Table 3: ATR spectral readings of drugs Proxetine, Sertraline, Escitalopram, Fluvoxamine.

Sample Code	Generic Name	ATR Frequency cm-1	Vibrational band assignment
A	Proxetine	3285.63	N-H stretch
		2916.87	C-H stretch aromatic
		1650.03	C=C stretch
		1418.67	C-F stretch
		1032.40	C-O-C stretch
		892.1	C-H bend aromatic
B	Sertraline	3318.3	N-H stretch
		2856	C-H stretch aromatic
		1469.3	C-H bend aliphatic
		1018.6	N-C stretch
		829.51	C-H bend aromatic
C	Escitalopram	2900.44	C-H stretch
		1631.23	C=C stretch aromatic
		1424	C-F stretch
		1336.63	C-O-C stretch
		1018.01	N-C stretch
D	Fluvoxamine	3393.5	N-H stretch
		1619.5	C=C stretch aromatic
		1075.6	N-C stretch
		1013.4	C-O-C stretch

Table 4: FTIR and ATR spectrum comparison of drugs Proxetine, Sertraline, Escitalopram, Fluvoxamine.

Sample Code	Generic Name	FTIR Frequency cm^{-1}	ATR Frequency cm^{-1}	Vibrational band assignment
A	Proxetine	3469	3285.63	N-H stretch
		2915.8	2916.87	C-H stretch aromatic
		2648.9		
		1662	1650.03	C=C stretch
		1442.4	1418.67	C-F stretch
		1031	1032.40	C-O-C stretch
		889.23	892.1	C-H bend aromatic
B	Sertraline	3413	3318.3	N-H stretch
		2921.4	2856	N^+H_2 stretch
		2685	2679	
		2473.8	2451.4	
		2364.6		
		1648.2		C=C stretch aromatic
		1681.4		C-H bend aliphatic
		1467.5	1469.3	
		1400.7		
		1133.8	1137.8	N-C stretch
		1031	1018.6	C-H bend aromatic
		883.67	829.51	
		675.18		
C	Escitalopram	3385.6	3266.43	C-H stretch
		2904.7	2900.44	N:::C stretch
		2229.2		C=C stretch aromatic
		1648.2	1631.23	C-F stretch
		1428.5	1424	C-O-C stretch
		1336.8	1336.63	N-C stretch
		1022.7	1018.01	C-H bend aromatic
		764.13		
D	Fluvoxamine	3396.8	3393.5	N-H stretch
		2145.6		
		1695.4		
		1620.4	1619.5	C=C stretch aromatic
		1081	1075.6	N-C stretch
		1017	1013.4	C-O-C stretch

and Fluvoxamine, the basic difference is that in transmission mode there was intense region at higher wavenumbers but at lower wavenumbers the intensity was not found to be good. But while working with UATR, the peaks at lower wavenumbers are more intense as compared to the higher wavenumbers.

It is concluded from the present study that FTIR spectroscopy has great potential as an analytical tool for the characterisation of SSRIs in pharmaceutical preparations. Spectrum in Transmission and ATR modes can be very well assigned to different functional groups present in to the samples. Recording of the spectra in to the ATR mode was found to be much more beneficial because of the presence of more intense peaks at lower wavelengths. Another added advantage in this mode was no sample preparation required.

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