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# Study the solvation and slit width changing on properties of some endocrine disrupting agents

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**Abstract**---The spectral characteristics of Bisphenols (BPA, BPS, and BPF) were investigated using room temperature emission and excitation spectroscopy in solvents (n-hexane, ethanol, 1-propanol, and butanol). The slit offers were used in various offers ;The device is set to different slit widths (1.5; 3; 5; 10 and 15 nm) ; The results revealed to us changing the slit width affects the fluorescence signal's FWHM and intensity. Thus, larger slit width gives higher intensity values with lower fluorescence signal detail. The results of the work showed a wide range of differences across different solvents, as these spectral differences are attributed to the differences in different solubility processes when using different types of organic solvents.

**Keywords**---solvents, EDC, metabolite, fluorescence, slit width.

**Introduction**

Fluorescence spectroscopy is a vital technique in biochemistry and molecular physics and is also one of the most popular and widely available., although the fluorescence technique does not give much information, but it is very sensitive to structural and dynamic changes and biomolecular bio complexes. Fluorescence technology can give distinctive features called (fingerprinting) especially for each compound [1-6].Bisphenol compounds, which are called endocrine compounds, and they are pollutants that cause what is called endocrine disruption. One of the main effects of these substances work to confuse the work of hormone receptors, as they either inhibit, stimulate or confuse hormonal messages or signals. BPA can enter the organism through the digestive or respiratory system, or through skin absorption and the greatest source of absorption is the gut system. Blood,

urine, breast milk, fluids, and other tissues can all contain BPA. Estrogen and androgen are two types of hormones that show a great effect with these substances called EDC in terms of secretion and function, where their concentration is small, which causes a toxic effect. This requires the use of highly sensitive technology that has the ability to detect such compounds [7-16]. When considering the spectral profile produced by chemical solution analysis, it was observed that numerous instrumental aspects of fluorescence spectroscopy, such as the influence of different scan velocities, lamp, and slits width changes on the acquired spectrum, were discovered. Fluorescence spectroscopy is an important laboratory method because it provides highly sensitive and precise results. Throughout the course, of these investigations, it was discovered that there is a more widespread issue with determining the impact of various slit width alterations on the spectrum that was recorded. The slit width effect has received minimal attention in the chemistry literature; broader slit widths are utilized narrower slits are utilized For the purpose of qualitative and quantitative analysis where spectrum detail is required, whereas wider slits are employed for quantitative research when exact absorbance measurements are required [17-22]. Three chemical compounds ( Bisphenol a, Bisphenols, and Bisphenol F) were utilized with four different solvents for the aforesaid purpose (ethanol, 1-propanol, butanol and n-hexane) .

### **Materials and Methods**

Solvents of the Aldrich HPLC grade were employed. Chemicals of analytic reagent grade were used without additional purification. Unless otherwise stated, nano-pure grade water was used throughout. Bisphenol A, Bisphenol S, and Bisphenol F were purchased from Sigma Aldrich. The remaining chemicals were purchased commercially.

### **Bisphenols stock solution preparation**

By dissolving 1.0 mg of standards in 10 ml of deionized water, stock solutions of bisphenol A, bisphenols and bisphenol F were generated. All stock solutions were kept at 4 °C in a dark place out of the way. Stock solutions were monitored for possible photo-degradation of Bisphenols using fluorescence spectroscopy at room temperature prior to use. Within 6 months of preparation, all stock solutions had been used. Each day, working solutions of bisphenol A were made by repeated dilution of the stock solutions. Calibration curve generation tests were performed using pure standard solutions containing each bisphenol at different concentrations.

### **Results and Discussions**

#### **Excitation and Emission spectrum**

The commercial spectrometer was used to get the excitation and emission spectra (Shimadzu RF-5301pc). A 150-watt radiating Xenon lamp with a wavelength range of 220 to 900 nm was used as the excitation source. The accuracy reached a color uniformity of 1.5 nm. The wavelength scan was performed at a rate of 5500 nm per minute. By solubilizing each component in a certain amount of

Nano-pure-water, the excitation and emission spectra for bisphenols (endocrine disrupters compounds) were computed. At the maximum emission wavelength, the excitation spectrum was determined. At room temperature, all measurements were taken.

### **The effect of the type of solvent on the signal of the fluorescence spectrum**

Excitation and Emission spectrum were produced by dissolving Bisphenol A, Bisphenol S and Bisphenol F in different solvents (hexane, propanol, butanol and ethanol). Excitation-emission spectra were obtained by dissolving BPA, BPA-S and BPA-F in several solvents (hexane, propanol, butanol and ethanol), as shown in the data shown in Table 1. When the compounds were excited, the excitation and emission spectra were not identical. As in Bisphenol A (fig. 1.), where there is a difference in intensity and width of the top. When using propanol, the width was less than butanol and hexane, while we find that the intensity of butanol is not related to the excitation spectrum.

Table 1  
Bisphenols FWHM value in organic solvents

	BPA		BPS		BPF	
	intensity	FWHM	intensity	FWHM	intensity	FWHM
1-propanol	75	32	95	13	1016	-
ethanol	1016	-	520	54	562	66
butanol	511	54	247	90	77	100
n-hexane	470	46	191	20	547	40

For BPS (fig. 2) The emission-excitation spectra did not have the same structure, FMHMs were lower when 1-propanol was used as a solvent, and intensity was highest when ethanol was used as a solvent. The band's shape and position are discovered to be independent of ex-wavelength., suggesting that in any solvent occurred the transition of between the comparable electronic states, Introducing of more polar solvents resulted in improved fluorescence with a reduced FWHM value. For BPF (fig. 3.) The em-ex spectra did not have the same structure; FMHMs were lower when butanol was used as a solvent, and intensity was highest when ethanol was used. The structure and position of the band was shown to be independent of ex-wavelength. The form and position of the band was found to be independent of ex-wavelength, indicating that the BPF molecule transitioned between similar electronic states in every solvent. The inclusion of higher polarity liquids resulted in improved fluorescence and a reduced FWHM value.

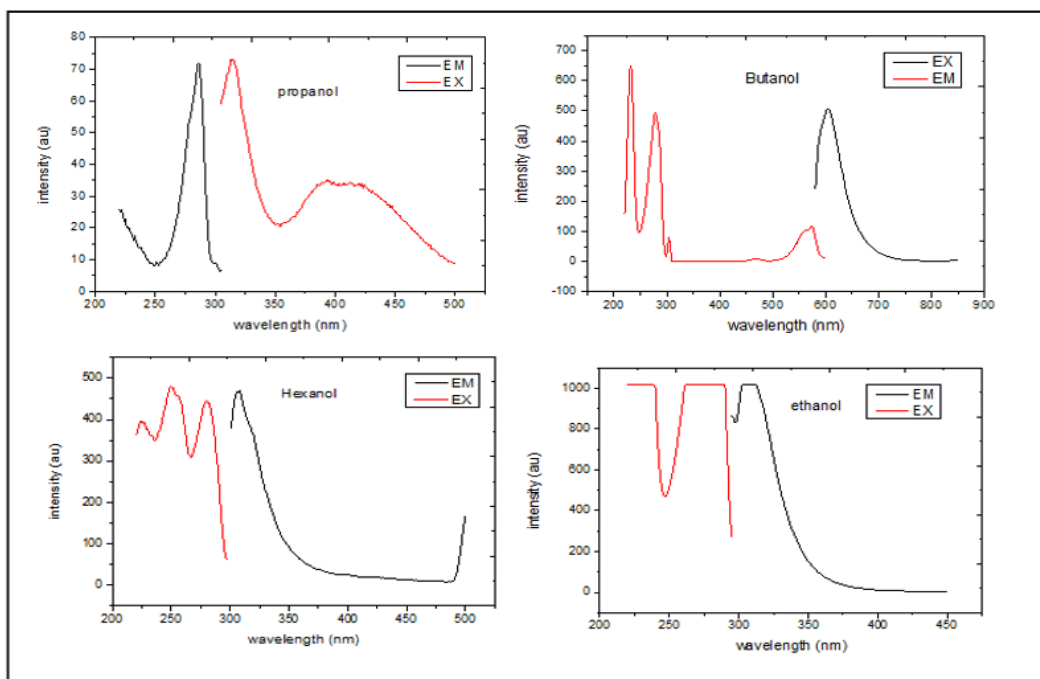


Figure 1. Ex-em spectrum for 2 ppm BPA in different solvents

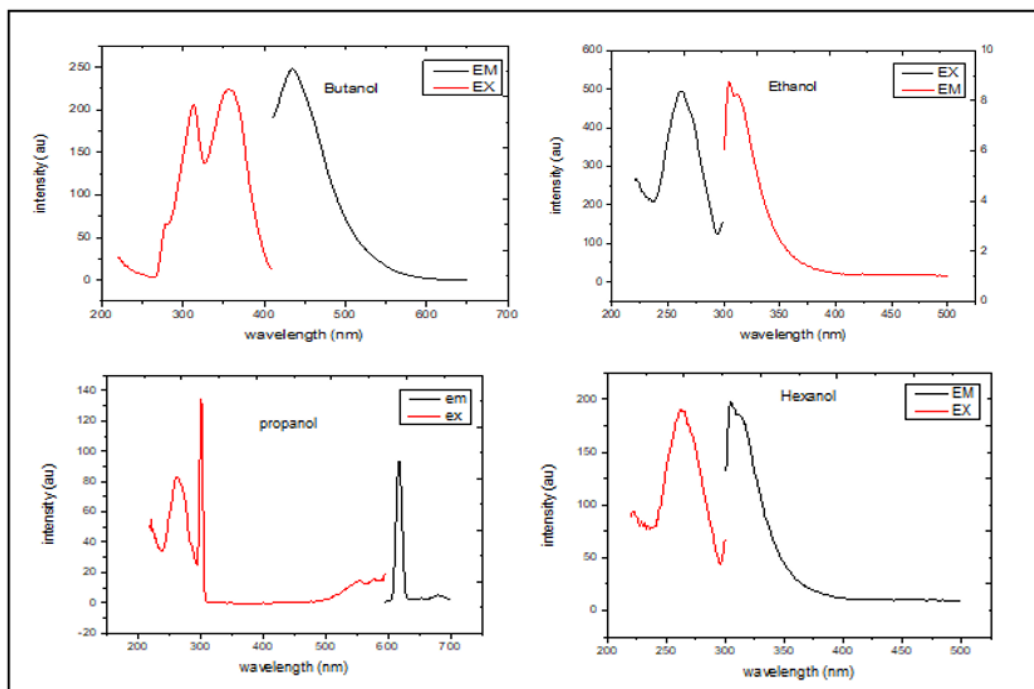


Figure 2. Ex-em spectra for 2 ppm BPS in different solvents

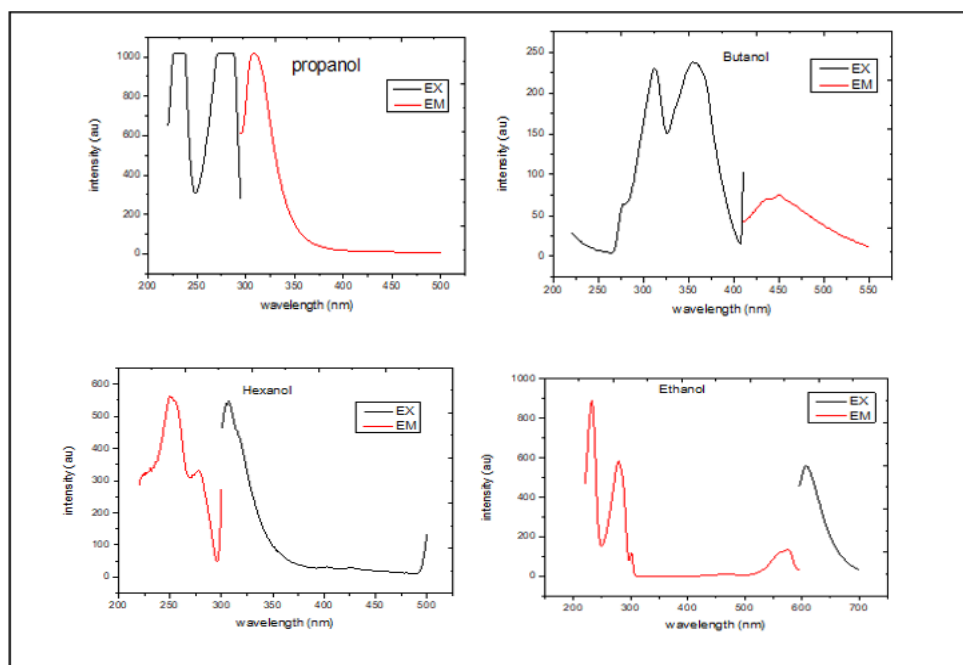


Figure 3. Ex-em spectra for 2 ppm BPF in different solvents

### Effect of slit width

The emission and excitation spectra of selected (BPA, BPS, and BPF) were measured using various slit widths (15, 10, 5, 3, and 1.5 nm) in Figures (2, 3 and 4). Small slit widths provide highly organized spectral patterns With superb spectral resolution and clear signal-to-noise ratio. It was discovered that small slit widths result in finely structured spectral forms in exchange For great spectral resolution and a high signal-to-noise ratio, whereas large emission slit widths result in the opposite. When employing tiny and big excitation slits, the resulting spectral shapes are not similar. The main difference is in the signal-to-noise ratio, which is lower when a wide slit is used, and in the full width at half maximum (FWHM); which is larger. Furthermore, we can observe that increasing the( slit width) has a far bigger influence on the fluorescence intensity level1 that was recorded than decreasing the slit width.

Table 2

The influence of slit width on fluorescence spectrum of Bisphenols (A, F, S)

Comp.	slit width1.5		slit eidth3		slit width5		slit width10		slit width15	
	intensity	FWHM	intensity	FWHM	intensity	FWHM	intensity	FWHM	intensity.	FWHM
bpa	21	-	30	-	72	31	140	32	280	30
bps	97	60	198	-	514	28	1016	-	1016	-

bpf	-	-	57	-	237	48	513	46	1016	
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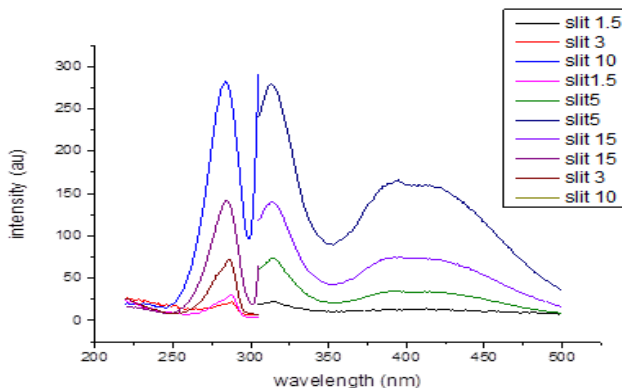


Figure. 4. The effect of varying slit widths on fluorescence spectrum of BPA dissolved in 1-propanol

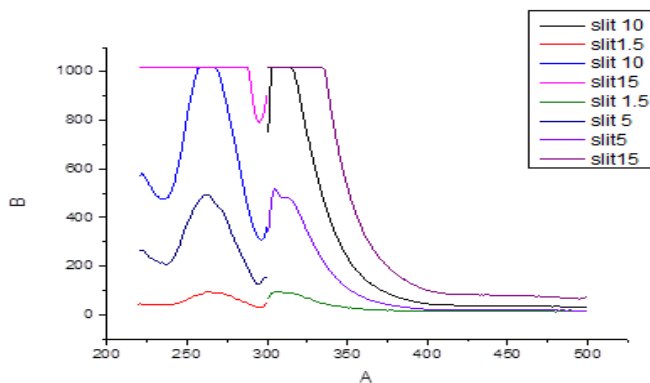


Figure 5. impact slit width change on fluorescence spectrum on fluorescence spectrum of BPS dissolved in ethanol

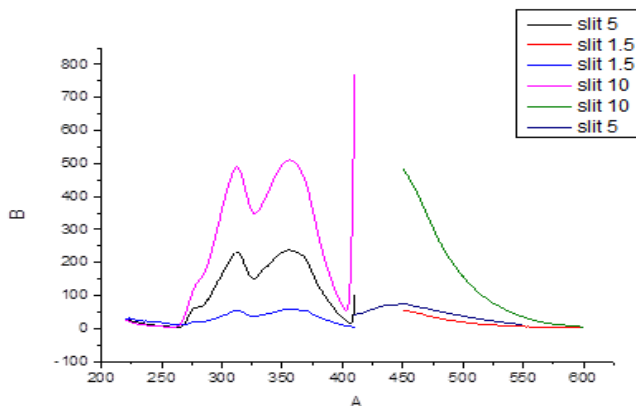


Figure 6. impact Slit width change on fluorescence spectrum of BPF in butanol

## Conclusion

When BPA, BPS, and BPF are mixed into various solvents, the assessment of spectral parameters of Bisphenols (EDC) such as intensity and FWHM could provide a valuable tool for studying its spectroscopic features. In this work, when compared to altering the slit width, solvation was shown to have a considerable influence on fluorescence. According to the findings, a wider slit lowers spectral resolution

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