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REGULAR PAPER

Detection of biological contamination protozoa in drinking water using surface plasmon resonance-based technique

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Abstract

Water is one of the fundamental needs for human life on earth. Different kinds of contaminants that exist in the drinking water may cause serious health issues, affect body organs, or may cause mortality. One of the main sources of biological contaminants in the water is protozoan parasites, which are normally transmitted through the oral-fecal route. Two frequently water born protozoan parasites are *C. parvum* and *G. lamblia*. Both of these parasites have different values of refractive index and size. Using these biophysical parameters, the new detection system may be developed for real-time and on-site measurement. In this paper surface plasmon resonance (SPR) technique is utilized for theoretical investigation of biological contamination protozoa in drinking. Based on angle interrogation, the Kretschmann configuration is used to elaborate the concept of the setup. The performance is analysed on the basis of incident light wavelength in visible region and radiative properties of a multi-layered structure are studied using the transfer Metrix method.

Keywords Biological and nonbiological contamination · Drinking water · SPR sensor · Nanomaterials · Performance parameter. Kretschmann configuration

1 Introduction

Water is a fundamental need of all living organism on earth. As it's a basic need of life so it should be pure, non-contaminated, and hygienic [1]. Many commercial companies are offering different types of water purification systems, government and non-government oranizations are continuously awaring contryment to use safe drinking water.. Water contamination is of two types biological and non-biological. Numerous non-biological contaminants like silica, sodium, sulfur, ammonia, and chlorine existed in the water. Heavy metals such as cadmium (Cd), lead (Pb), arsenic (As), mercury (Hg), and nickel (Ni) are also found in water as contaminant agents [2]. Benzene, toluene, ethylbenzene, and xylenes are found in water as chemical contamination so they need to be investigated. Boiling, filtering, disinfection with iodine, chlorine, and chlorine dioxide are some common processes to remove bacteria from water [3]. Unfortunately, these processes are not in practice in large section of population. There are a lot of chances for spreading various kinds of contaminated water-generated diseases like asymptomatic infections, nausea, diarrhea, anorexia, uneasiness in the upper intestine, malaise, occasionally low-grade fever and Jaundice, etc. An on-chip immersion refractometer used by Chin et.al. [4] in the year 2011 for biophysical measurement of protozoa. He observed that *Cryptosporidium parvum* oocysts and *Giardia lamblia* are two commonly found waterborne protozoan parasites. It was found that both types differ from each other by size, shape, and by their refractive index. C. parvum oocyst is spherical in shape with an ovality of 3–7 μm and refractive index of 1.418 while G. lamblia cyst has ovality of 8–12 μm and refractive index of 1.433 [5]. The optical sensor detect light in specific range and convert it into electronic signals. These sensors detect the change in wavelength, frequency, polarization, and intensity of light [6]. In this paper, the author gives a theoretical investigation of biological contamination protozoa in drinking water using a surface plasmon resonance (SPR) based sensor. SPR sensors can identify the change in the refractive index of the sample. This is label-free detection technique and gives a real-time sensing response that makes it extraordinary with respect to other biosensing techniques like ELISA, RTPCR, etc. [7]. We have calculated various performance indicating

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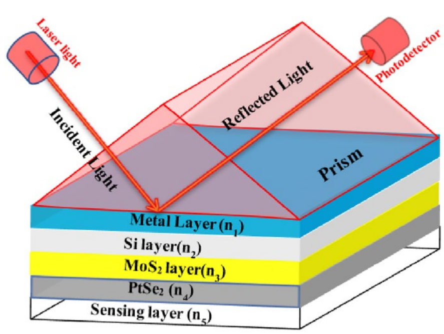
parameters like sensitivity, Figure of Merit (FoM), and Detection accuracy. The mathematical concepts and advantages of this technique is also discussed in brief.

2 Proposed sensing structure

Surface plasmons are like electron clouds at the surface of noble metals like gold(Au), Silver(Ag), Copper(Cu), etc. These plasmon get excited in some particular condition and start to resonate this is called surface plasmon resonance (SPR). SPR provides some significant conditions that are highly useful for a sensing points of view. Plasmon excitation can initiated by various methods like using grating, waveguide, and prism. A traditional Kretschmann configuration [8] is used in this paper where a prism is used as a dielectric substrate and at the base of the prism a thin layer of metal is applied. The proposed sensor structure, optical and physical parameters of each layer are given in Fig. 1. When a p-polarized laser light of any particular wavelength is incident at a metal–dielectric interface with total internal reflection(TIR) condition the surface plasmon gets excited and tends to resonate. This action cause to generate a surface plasmon wave (SPW) along the interface. A non-propagating electromagnetic field known as the evanescent field is observed here and is highly sensitive toward the change in the refractive index of the sample under consideration. The value of the evanescent field is maximum where incident light strikes the metal–dielectric interface and at the same time the reflection intensity of the reflected wave is reported as minimum. This results in sharp dip in resonance angle, known as SPR angle (θ_{spr}). This angle shifts from its position when the incident light angle changes. In general, the prism having a low refractive index like BK7, CaF_2, FK51A is used to get a large shift in SPR angle while high refractive index prism-like SF5, ZnSe, H-ZF62 etc. is used to find large dynamic range. The refractive index of the prism can be calculated using the Sellmeier equation and the refractive index of metal estimate using Drude-Lorentz model. Prism increases the momentum of incident light necessary to with momentum of surface plasmon wave which is a key requirement for plasmon excitation [9]. Nanomaterials(2D material) layering over metal have a significant role in sensor performance. It protects of metal layer from corrosion, provide a high surface-to-volume ratio, less electron scattering, and less toxicity towards biomolecules. The aim of functionalizing the conventional structure of the SPR sensor with 2D material is to enhance the performance of the sensor. The only metal layer based structure or conventional structure is not suitable to attach biomolecules and the stability of the thin metal layer in the ambient environment is also an issue. It's observed that the conventional structure shows a sensitivity of 84°/RIU that is not up to the mark and needs to modify. $PtSe_2$ belongs to the family of Transition metal dichalcogenide (TMDC), its monolayer film thickness is 0.37 nm [10] and monolayer bandgap is 1.2 eV. Similarly, its bilayer (0.74 nm) thickness shows a bandgap of 0.21 eV. This property shows that $PtSe_2$ has thickness-dependent tuneable bandgap properties (exhibit the property of semiconductor to metal). The bandgap modulation property is useful in optoelectronic devices. High electron mobility upto 3000 $cm^2\ V^{-1}\ s^{-1}$, large electrical conductivity (this is much high than well-known TMDC MoS_2, 50–200 $cm^2\ V^{-1}\ s^{-1}$), low toxicity, and air-stablity makes it a suitable candidate to work as a Bio recognition element (BRE) layer [11]. Some biological process are required to immobilize the ligands on sensor surface so that desired biomolecules may be attached (attachment of antigen with antibody). Silicon (Si) is used as an interlayer between the metal and dielectric medium and an additional MoS_2 layer is used before the BRE layer. The aim of including these nanolayers is to enhance the sensitivity by means of increasing the Goos-Hänchen (GH) shift. A 5 nm thick interlayer of silicon (Si) between the metal and dielectric sample work as a nearly guided wave [12] and increases the field intensity of the excitation light at the silicon–sensing layer interface [13]. Enhancement in field intensity helps to enhance the excitation of surface plasmons. The MoS_2 belongs to the TMD materials family also



Layer/ component	Type/ Optimized Thickness (nm)	Refractive index At 633nm wavelength
Prism	SF5	1.6685
Silver layer	40	0.18344+3.4332i
Silicon layer	5	3.8823+0.019589i
MoS_2 layer	0.65	5.08+1.1723i
$PtSe_2$	0.37	2.9029 + 0.8905i
Sensing layer	Protozoan	C.parvum 1.418 G.lamblia 1.433

Fig. 1 schematic diagram of the proposed SPR sensor and physical and optical parameters of each layer

called beyond graphene material. It has high light absorption (≈ 5%) and thickness-dependent tunable bandgap. These layers are used to improve the light absorption of the proposed sensor and provide enough excitation energy for effective charge transfer [14]. Therefore, the multilayered structure (Ag/Si/MoS_2/$PtSe_2$) is used to achieve significant enhancement in performance of the sensor in comparison to conventional SPR sensors[15].

3 Basic concept of Evanescent wave and transfer matrix method

Let light be launched from one medium to another medium having a refractive index n_1 and n_2 respectively. Some of its part get reflected from the interface and some refracted. let x direction is parallel to the interface and z is normal to the interface as given in Fig. 2.from Snell's law, we have-

$n_1 \sin\theta_I = n_2 \sin\theta_T$

Or $\theta_T = \sin^{-1}\left(\frac{n_1}{n_2}\sin\theta_I\right)$

This shows that $\sin\theta_I > \frac{n_2}{n_1}$, $\theta_I > \theta_C$, where θ_C is a critical angle.

Total internal reflection (TIR) mean incident light beam is completely reflects back into the medium from where it comes. For it, incident light angle must be greater than the critical angle. The ray diagram dictates that:

$$\vec{E}_T = \vec{E}_{\mathrm{OT}} e^{i(\vec{K}\gamma - \omega t)} \tag{1}$$

$\vec{K}$ is propagation vector, ω is the frequency of light, $\vec{E}_T$ is electric field vector amplitude and $\vec{E}_{\mathrm{OT}}$ is a constant and γ is pointing vector. As $\vec{E}_y$ is component coming out from the plane so that it can ignored. Splitting Eq. 1 into x and z components we have:

$$\vec{E}_T = \vec{E}_{\mathrm{OT}} e^{i(k_x x + k_z z - \omega t)} \tag{2}$$

As

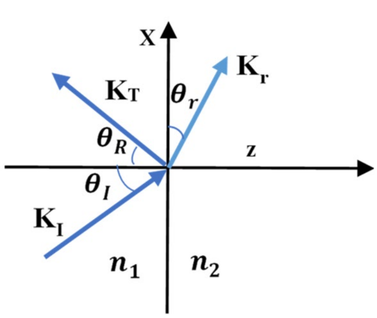


Fig. 2 wavevector presentation

$$k_x = k_T \sin\theta_T \text{and} k_z = k_T \cos\theta_T \tag{3}$$

So, Eq. 2 will be as:

$$\vec{E}_T = \vec{E}_{\mathrm{OT}} e^{i[(k_T \sin\theta_T)x + (k_T\cos\theta_T)z] - \omega t)} \tag{4}$$

Since $\sin\theta_T > 1$ the solution of Eq. 4 gives an imaginary term.

Let $k_T \cos\theta_T = Ai$ then Eq. 4 will be:

$$\vec{E}_T = \vec{E}_{OT} e^{i[(k_T \sin\theta_T)x - \omega t])} \cdot e^{-A_z} \tag{5}$$

From Eq. 5, shows damping nature of the wave in the z direction. Using the Eulers formula we have two components real and imaginary. Considering only real terms we have-

$$Re(\vec{E}_T) = \vec{E}_{OT}\left[\cos\left(k_T \sin\theta_T\right)x - \omega t\right] \cdot e^{-A_z} \tag{6}$$

This is an expression of evanescent wave which shows that this kind of wave has some amplitude and damping nature. The mathematical expression of surface Plasmon resonance generation is given in Eq. 7. Its clear from this equation that the wavevector of incident light must match to wavevector of the SPR wave [16].

$$k_o n_p \sin\theta_{\mathrm{spr}} = Re\left\{k_o \sqrt{\varepsilon_m \varepsilon_s / (\varepsilon_m + \varepsilon_s)}\right\} \tag{7}$$

where $\varepsilon_m and \varepsilon_s$ are the dielectric constants of the metal and the sensing layers respectively. $k_0 = 2\pi/\lambda_0$ is the wavenumber of the incident light in free space and n_p is the refractive index of the prism [17]. For calculating the reflectivity of the reflected light of the multilayer model, the transfer matrix method is used. This method is efficient and no approximations are considered. First boundary tangential fields related to the final boundary by the relation given in Eq. 8.

$$\begin{bmatrix} X_1 \\ Y_1 \end{bmatrix} = A2\ A3\ A4\ A5 \ldots AN - 1 \begin{bmatrix} X_{N-1} \\ Y_{N-1} \end{bmatrix} = A \begin{bmatrix} X_{N-1} \\ Y_{N-1} \end{bmatrix} \tag{8}$$

where X_1 and Y_1 represent the tangential component of electric and magnetic fields respectively at the boundary of the first layer and X_{N-1} and Y_{N-1} are the corresponding field at the nth layer. For p-polarized light the characteristic matrix of the combined structure of the sensor is denoted by $A_{ij.}$

$$Aij = \left(\prod_{q=2}^{N-1} A_k\right)_{ij} = \begin{bmatrix} A_{11}A_{12} \\ A_{21}A_{22} \end{bmatrix} \tag{9}$$

with

$$Ak = \begin{bmatrix} \cos\beta_k - i\sin^{\beta_k/q_k} \\ -iq_k sin\beta_k cos\beta_k \end{bmatrix} \tag{10}$$

where $q_k = \left(\mu_k/\varepsilon_k\right)^{1/2} \cos\theta_k$

$$\beta_k = \frac{2\pi}{\lambda} n_k \cos\theta_k (d_k)$$

One can get the value of reflection coefficient for p polarized light by driving some mathematical steps.

$$r_p = \frac{(A_{11} + A_{12}q_n)q_1 - (A_{21} + A_{22}q_n)}{(A_{11} + A_{12}q_n)q_1 + (A_{21} + A_{22}q_n)} \quad (11)$$

Finally, reflectivity R of given multilayer structure is directly related to reflection coefficient by $R = \left|r_p\right|^2$

4 Result and discussion

An analysis of the performance of the sensor using different kinds of prism with a high refractive index (greater than 1.5) is presented here. Low refractive index prism has the advantage that they are robust, cost-effective, show low scattering behavior and excellent transmission from visible to IR range, but they have a very short dynamic range so it's difficult to analyze the liquid sample which has a high refractive index (RI) [18]. This paper aims to detect protozoan in drinking water which have major differences in refractive index concerning drinking water RI. Therefore prism analysis is intentionally done with prisms having high RI. Sensitivity is a major factor for sensor. Sensitivity is the ratio of a shift in SPR angle concerning a change in refractive index. From the Table 1 and Fig. 3 its concluded that the sensor using SF5 Prism shows a maximum value of sensitivity of 136.31°/RIU. Although detection accuracy (DA) and figure of merit (FoM) is relatively low in comparison to other prism. There are various method like long-range SPR method(LRSPR) [19] to increase the value of these parameters.

Incident light wavelength also influences the performance of the sensor so its analysis using different wavelengths is also important. The refractive index of each layer depends on the incident light wavelength [20] hence we have centralized our analysis in the visible region and varied the incident light wavelength from 550 to 750 nm. The effect on the performance is shown in Fig. 4a, b and Table 2. It's observed that maximum sensitivity is obtained when the incident light wavelength of 550 nm is used, but the minimum reflectance (R_{min}) is obtained at 633 nm wavelength. This shows that at

Table 1 effect of prism on performance parameter of SPR sensor

Type of prism used with High Refractive index	Refractive Index	θ_{spr}	Sensitivity °/RIU	FWHM	DA	FoM
2S2G PRISM	2.358	39.85	46.69	2.8	0.35	16.67
SF11 PRISM	1.7786	57.95	94.56	5.28	0.18	17.90
SF10	1.723	60.93	110.09	5.9	0.16	18.65
SF5	1.6685	64.43	136.31	4.24	0.23	41.58
H-ZF62	1.9141	52.05	73.45	4.3	0.23	17.08

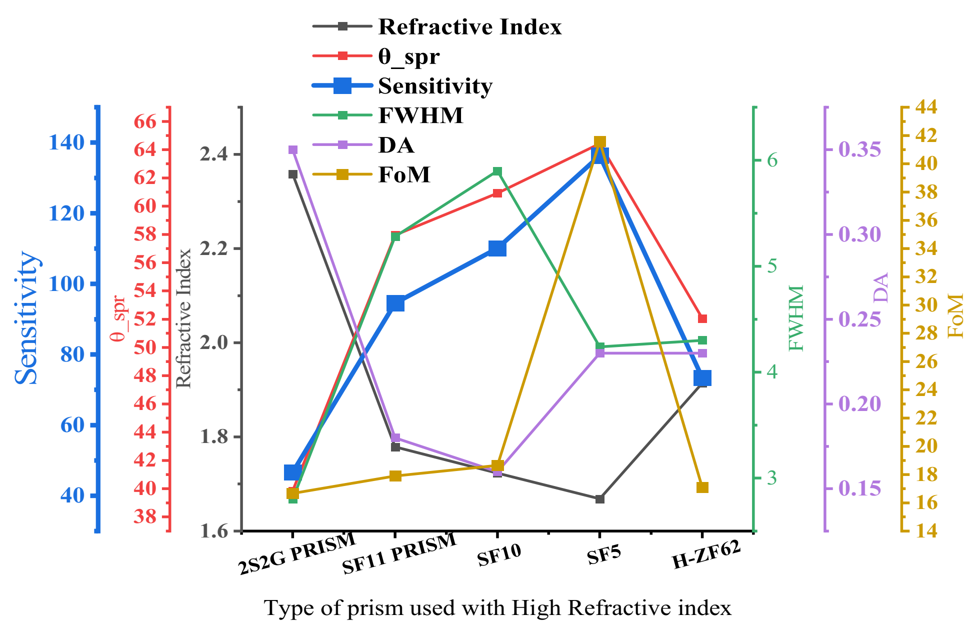
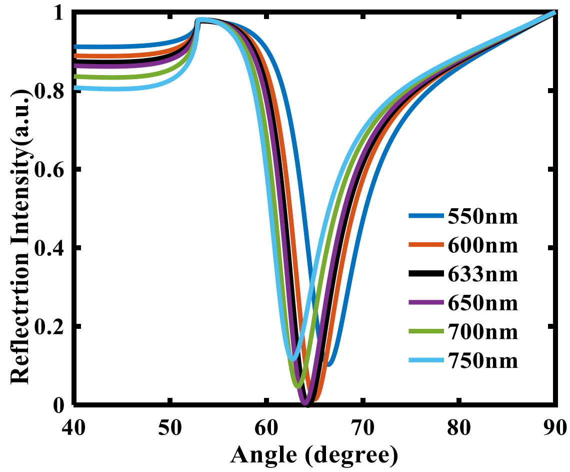
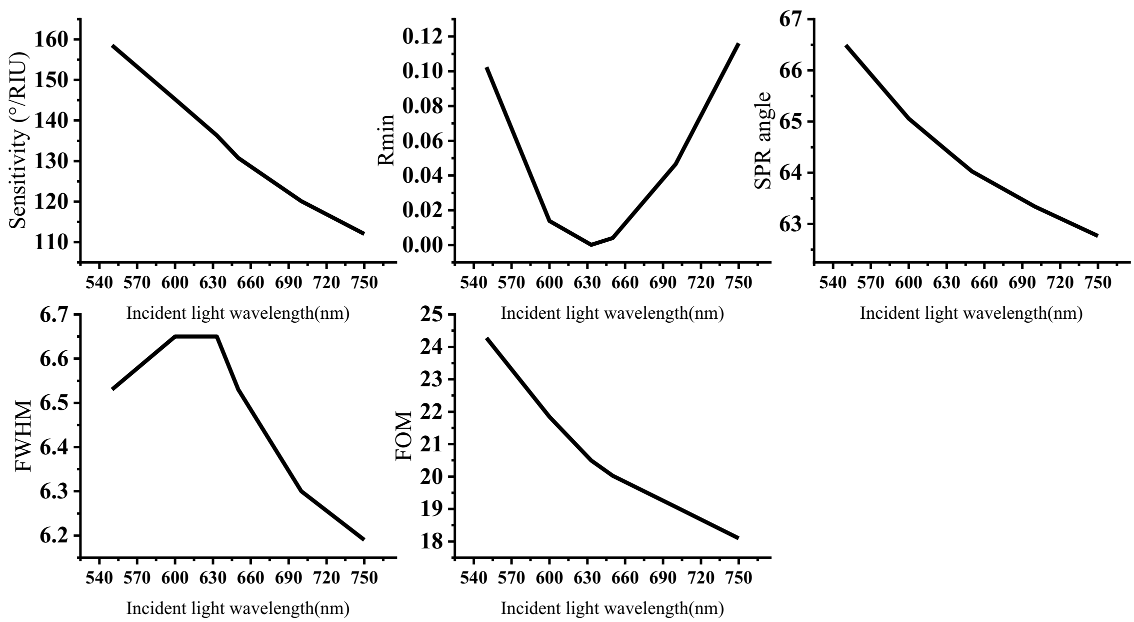


Fig. 3 Performance parameter analysis using various high refractive index prism



(a) Shift in SPR angle concerning incident light wavelength (wavelength span from 550 to 750 nm)



(b) graphical analysis of performance parameters utilizing different wavelengths of incident light

Fig. 4 **a** Shift in SPR angle concerning incident light wavelength (wavelength span from 550 to 750 nm). **b** graphical analysis of performance parameters utilizing different wavelengths of incident light

Table 2 effects of different incident light wavelengths and their effect on the performance parameter

Incident light wavelength (nm)	Sensitivity (°/{\ mathrm{RIU}})	R_{min}	SPR angle	FWHM	FOM
550	158.543	0.10231	66.49175	6.53	24.27917
600	145.24	0.01384	65.05936	6.65	21.8406
633	136.31	0.00005	64.37181	6.65	20.49774
650	130.77	0.004	64.02803	6.53	20.02603
700	120.09	0.04652	63.34	6.3	19.0619
750	112	0.11614	62.76753	6.19	18.0937

Table 3 effect of an increasing number of $PtSe_2$ layers on performance parameters

Number of $PtSe_2$ layer	Sensitivity (1.33–1.433)	R_{min}	FWHM	Detection accuracy	Figure of merit (FoM)
1	136.31	0.00005	6.59	0.15	20.68
2	138.99	0.00796	7.79	0.12	17.84
3	141.84	0.02808	9	0.11	15.76
4	142.42	0.05484	10.09	0.09	14.11
5	139.61	0.08511	11.85	0.084	11.78

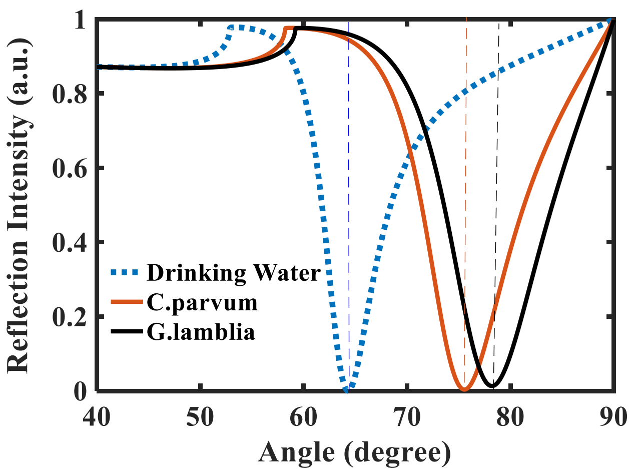


Fig. 5 Reflectance angle analysis for protozoan detection concerning drinking water

633 nm wavelength, maximum light is utilized for surface plasmon generation. Moreover, the 633 nm wavelength has the advantage that it shows minimum optical nonlinearity and minimum Kerr effect hence more advantageous for an efficient sensing point of view [7].

Another analysis is given in Table 3. It shows that by increasing the number of layers of $PtSe_2$ up to four layers the maximum sensitivity of 142.42°/RIU obtained but at the same time value of R_{min} increase. The resonance angle becomes more shallow hence FWHM value increases.

It observed from theoretical analysis that the drinking water having G.Lamblia protozoan shows 142.42°/RIU sensitivity concerning pure water (RI = 1.33) while water contaminated with Cryptosporidium parvum type protozoan exhibit the sensitivity of 117.96°/RIU. The graphical representation of the reflectance curve is shown in this Fig. 5. The work is theoretical and its expected that in future this can help in the area of optical sensing. At the end of this paper authors want to acknowledge some recent and notable waork related to optical sensing [21–24].

5 Conclusion

Theoretical study and numerical simulation of SPR based sensor for protozoan detection in drinking water carried out. Two different types of protozoan G. Lamblia and C. Parvum is detected and for each case sensitivity is calculated.An angle interrogation based on Kretschmann configuration is used for plasmon excitation and some additional nanolayer of Si, MoS_2 and $PtSe_2$ is used with conventional structure for performance enhancement. The proposed sensor is driven by different incident light wavelengths and at each wavelength performance is analyzed. Several types of high refractive index prism are taken and for each case performance parameters are estimated. Maximum sensitivity obtained as 142.42°/RIU and 117.96°/RIU for G. Lamblia and C. Parvum respectively.

Declarations

Conflict of interest The author has no conflict of interest.

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