Performance evaluation of side-by-side optically coupled monolithic LYSO crystals

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Abstract
Background: Significant interest has been recently shown for using monolithic scintillation crystals in molecular imaging systems, such as positron emission tomography (PET) scanners. Monolithic-based PET scanners result in a lower cost and higher sensitivity, in contrast to systems based on the more conventional pixellated configuration. The monolithic design allows one to retrieve depth-of-interaction information of the impinging 511 keV photons without the need for additional hardware materials or complex positioning algorithms. However, the so-called edge-effect inherent to monolithic-based approaches worsens the detector performance toward the crystal borders due to the truncation of the light distribution, thus decreasing positioning accuracy.

Purpose: The main goal of this work is to experimentally demonstrate the detector performance improvement when machine-learning artificial neural network (NN) techniques are applied for positioning estimation in multiple monolithic scintillators optically coupled side-by-side.

Methods: In this work, we show the performance evaluation of two LYSO crystals of $33 \times 25.4 \times 10$ mm$^3$ optically coupled by means of a high refractive index adhesive compound (Meltmount, refractive index $n = 1.70$). A $12 \times 12$ silicon photomultiplier array has been used as photosensor. For comparison, the same detector configuration was tested for two additional coupling cases: (1) optical grease ($n = 1.46$) in between crystals, and (2) isolated crystals using black paint with an air gap at the interface (named standard configuration). Regarding 2D photon positioning (XY plane), we have tested two different methods: (1) a machine-learning artificial NN algorithm and (2) a squared-charge (SC) centroid technique.

Results: At the interface region of the detector, the SC method achieved spatial resolutions of $1.7 \pm 0.3, 2.4 \pm 0.3,$ and $2.6 \pm 0.4$ mm full-width at half-maximum (FWHM) for the Meltmount, grease, and standard configurations, respectively. These values improve to $1.0 \pm 0.2, 1.2 \pm 0.2,$ and $1.2 \pm 0.3$ mm FWHM when the NN algorithm was employed. Regarding energy performance, resolutions of $18 \pm 2\%$, $20 \pm 2\%$, and $23 \pm 3\%$ were obtained at the interface region of the detector for Meltmount, grease, and standard configurations, respectively.

Conclusions: The results suggest that optically coupling together scintillators with a high refractive index adhesive, in combination with an NN algorithm, reduces edge-effects and makes it possible to build scanners with almost no gaps in between detectors.
1 | INTRODUCTION

The two most prevalent geometry configurations of scintillation crystals used on conventional gamma-ray scanners are the pixelated and the monolithic.\(^1\) Pixelated crystal configurations are the most extended configuration in positron emission tomography (PET) scanners, since it allows for a relatively easy pixel identification. Nevertheless, monolithic scintillators offer lower cost, higher sensitivity, and provide intrinsic depth-of-interaction (DOI) information of the gamma-ray interaction within the scintillator, thus enabling the possibility to correct for parallax errors.\(^2\) Moreover, monolithic-based designs allow one to accurately characterize the scintillation light distributions (LDs) and, thus spatial resolutions of 1 mm have already been obtained.\(^3\) As a consequence of all these features, a significant interest has grown over the recent years for using gamma-ray scanners based on monolithic crystals for both academic and commercial purposes.\(^4\)–\(^11\)

In both the pixelated and monolithic approaches, the gaps in between detectors decrease system sensitivity. Moreover, the performance of monolithic scintillators tends to be compromised toward the crystal edges (border effect)\(^12\) due to the strongest truncation of the LD in these areas. Therefore, data recorded at the edges have a poorer performance and are eventually discarded,\(^13\)–\(^15\) thus, reducing the useful detector volume and consequently decreasing the system sensitivity.

Several methods have been developed to mitigate border effects, some of them are based on weighted centroid methods\(^16\) or squared-charge (SC) centroids.\(^17\) Recently, the development of multichannel photosensor-readout application-specific integrated circuits combined with silicon photomultipliers (SiPMs) enabled the possibility to build highly granular, scalable, and large arrays for position sensitive gamma-ray detectors.\(^18\)–\(^20\)

These developments allowed for an exhaustive characterization of the 3D spatial detector response, paving the way for new positioning algorithms, such as maximum-likelihood (ML) methods,\(^21\),\(^22\) nonlinear data fit,\(^23\) k-NN technique,\(^24,25\) Voronoi-based calibration methods,\(^26\) and machine-learning artificial neural-network (NN) algorithms.\(^27\)–\(^29\) However, these new algorithms only partially alleviate edge-artifacts and, thus, these effects are still present,\(^30\) particularly when using thick scintillators. The use of bigger monolithic crystals would be a good approach; however, this presents some limitations in crystal growth size and geometrical flexibility in ring construction. A proposed solution is to optically couple side-by-side monolithic crystals.\(^31\),\(^32\)

A previous simulation study demonstrated that using optical coupling compounds with refractive index approaching the refractive index of the scintillation crystal allows the scintillation light to spread through the crystal junctions almost preserving the shape of the LD and, therefore, reducing substantially edge-artifact.\(^31\) In addition to this, optically coupling monolithic crystals reduces the gaps in between detectors, thus increasing sensitivity; and overcomes the challenges in using large scintillator volumes. Other authors have experimentally evaluated the use of optical adhesive to couple LYSO monolithic blocks, and generated look up tables followed by a least-squares minimization and ML methods for event positioning.\(^32\) They have also concluded that the adoption of optically coupled monolithic crystals can be a useful and feasible method to improve the uniformity of performances in the whole sensitive area.\(^32\)

In this work, we have experimentally evaluated, as a proof-of-concept, the performance of a detector based on a 12 × 12 SiPM array and two LYSO crystals of 33 × 25.4 × 10 mm\(^3\) optically coupled by means of a high refractive index compound (refractive index \(n = 1.70\)). This configuration was compared to two additional coupling methods, namely: (1) optical grease (refractive index \(n = 1.46\)) between crystals and (2) isolated blocks using black paint and air interface. For XY event positioning, we have tested two different methods: (1) SC centroid technique, which is a modified Anger logic procedure that has demonstrated enhanced linearity and spatial resolution,\(^16\) and (2) machine-learning artificial NN algorithm. The performance of the optically coupled system was evaluated in terms of spatial linearity and resolution (including DOI determination) as well as energy performance.

2 | MATERIALS AND METHODS

For the experimental setup, two \((\text{LuY})_2\text{SiO}_5\) (LYSO) crystals of 33 × 25.4 × 10 mm\(^3\) with refractive index of 1.81 from EPIC Crystals Co., Ltd, China, were used. All crystal faces were polished and black painted except one of 33 × 10 mm\(^2\) that was rough. The two crystals were coupled along this face.

Three configurations were tested; in the first one, a high refractive index compound named “Cargille Meltmount” \((n_{\text{Meltmount}} = 1.70)\) was used.\(^33\) Meltmount is a thermal plastic material, thus its viscosity is inversely dependent on the temperature. Therefore, it was heated to 70°C on a hotplate to decrease its viscosity. The two sides of the crystals to be glued were also heated to avoid sudden temperature changes when applying the
Meltmount compound. When the targeted temperature was reached, the Meltmount compound was spread in the side of one of the crystals using a spatula and was immediately attached to the side of the other crystal. Then, the coupled crystals cooled down to room temperature. For the second configuration, named optical grease, the crystals were coupled together using “SS-988 Non-Curing Optical Coupling Gel - V-788 Offset” ($n_{\text{grease}} = 1.46$) from Silicone Solutions. For the third configuration, named standard configuration, these side faces of the crystal were black painted and placed together letting an air gap between them. For all cases, the gap between the two faces was 0.5 mm (Figure 1).

Table 1 summarizes the refractive index and optical properties of the different used compounds.

![Figure 1](image.png)

**Figure 1** Detector configurations used in this work. (a) Meltmount or grease configuration, where all lateral faces were painted black except the interface one that was used to coupled crystals. (b) Standard configuration, where all the lateral faces of the crystal were painted black.

Table 1

| Material          | Optical properties at the interface | Refractive index |
|-------------------|-------------------------------------|------------------|
| LYSO              | Partial transmission                 | $n_{\text{LYSO}} = 1.81$ |
| Black paint       | Absorption                           | -                |
| Grease            | Partial transmission                 | $n_{\text{grease}} = 1.46$ |
| Meltmount         | Partial transmission                 | $n_{\text{Meltmount}} = 1.70$ |
| Air               | Partial transmission                 | $n_{\text{air}} = 1.00$   |

The detector performance was studied through coincidence measurements using a reference detector based on a LYSO crystal of $50 \times 50 \times 15 \text{ mm}^3$. The reference detector was coupled to an identical $12 \times 12$ SiPMs array. Coincidence data were acquired using a $^{22}\text{Na}$ pencil beam (450 $\mu\text{m}$ slit) generated using a $^{22}\text{Na}$ source of 1 mm in diameter with an activity of about 7 $\mu\text{Ci}$, attached to a mechanical collimator composed of two tungsten blocks of $56 \times 56 \times 30 \text{ mm}^3$ separated by the slit (Figure 2). The slit collimator was moved in steps of 0.5 mm along the $x$ and $y$ directions. For the scan along the $y$ direction, the studied detector was rotated 90°. The acquisition time was 1000 s for each slit position. We have scanned the slit along each direction started and ended outside the crystal to ensure that the entire scintillation volume was scanned. Plotting the number of events as a function of the slit position, the borders of the crystals can be found, and the real position of the slit determined. A total of 101 slit positions in $x$ direction and 64 positions in $y$ direction covered the detector under study (Figure 2).

### 2.1 XY positioning, DOI, and energy estimation

For the 2D positioning of the scintillation events in the crystals, the $x$ and $y$ coordinates were calculated using...
both the SC and the NN positioning methods. For the NN method, one multilayer perceptron architecture (MLP) was used for each direction, named x-MLP and y-MLP, respectively (Figure 3). Both MLPs contain five hidden layers and 100 nodes. The inputs of the networks are the digitized SiPM projection signals, thus 12 signals for x projection and 8 signals for y projection were included. The slit measurement along the x and y directions was used to train the x-MLP and y-MLP, respectively. Two filters were applied to the data:

- Energy filter: The energy was calculated for each individual event as the mean of the sum of signals for x and y projections. For each slit position, only the events that fell within ±15% of the energy spectra photopeak were considered.

- Position filter: The coordinates were pre-estimated using the center-of-gravity (CoG) algorithm.\(^{35}\) The CoG\(_x\) and CoG\(_y\) ensemble distribution of each slit position was obtained for the scanning along x and y directions, respectively. Events outside the 10% of the peak ensemble distribution along each direction were removed in order to discard events that have suffered Compton scatter, or other interactions, before photoelectric absorption.\(^{36}\)

After these prefilters, the dataset, that contains about 7k events per slit position, was split into three datasets: train (50%), evaluation (5%), and test (45%). Each MLP was trained using the train dataset by the Adagrad optimizer using rectified linear activation function (RELU) and the root mean squared median (RMSE) loss function:

\[
RMSE = \sqrt{\frac{\sum_{i=1}^{N} (pos_{real}(i) - pos_{pred}(i))^2}{N}},
\]

where \(N\) is the number of events, \(pos_{real}\) is the real position of the slit in mm, and \(pos_{pred}\) is the predicted position also in mm. After training, the MLP was evaluated using the evaluation dataset to avoid overfitting.

In the SC algorithm, the \(x_c\) and \(y_c\) coordinates from the test dataset were first estimated using the following equations:\(^{17}\)

\[
x_c = \frac{\sum_{i=1}^{12} c_i^2 x_i}{\sum_{i=1}^{12} c_i^2},
\]

\[
y_c = \frac{\sum_{i=1}^{8} r_i^2 y_i}{\sum_{i=1}^{8} r_i^2},
\]

where \(c_i\) and \(r_i\) are the digitized signals for the projected columns and rows, respectively, and \(x_i\) and \(y_i\) are the SiPM positions on the detection surface. Acquired data moving the slit along the x and y directions were used...
to calibrate the estimated \( x_c \) and \( y_c \) coordinates into mm units. The position profile was fitted using a Gaussian distribution, and the centroid of each measurement was recorded. The slit real position was plotted versus the estimated centroids and a third polynomial fit was used to convert the measured units to mm (see sketch in Figure 4).

The gamma-ray energy (\( E \)) was calculated as the mean of the sum of signals for \( x \) and \( y \) projections. The gamma-ray impact DOI was estimated by using its correlation with the width of the LD profiles and a model of the light transport in the crystal. It is calculated as the average of the ratio of the energy to the maximum signal value (\( E / I_{\text{max}} \)) for \( x \) and \( y \) projections.\(^{37}\)

### 2.2 Spatial and energy performance

For each tested configuration, the \( x \) and \( y \) coordinates from the test dataset along the \( x \)- and \( y \)-axis (containing the LD profiles after energy and position filter) were calculated using the two studied positioning methods (see sketch in Figure 4). The following parameters along each direction were calculated for each slit measurement:

- Bias\(_x\) and Bias\(_y\), calculated as the difference between the estimated position, \( x_{\text{estimated}} \) or \( y_{\text{estimated}} \), and the known position, \( x_{\text{real}} \) or \( y_{\text{real}} \):

\[
\text{Bias}_{x} = \frac{1}{N} \sum_{i=1}^{N} (x_{\text{estimated}}(i) - x_{\text{real}}(i)) \quad (4)
\]

\[
\text{Bias}_{y} = \frac{1}{N} \sum_{i=1}^{N} (y_{\text{estimated}}(i) - y_{\text{real}}(i)) \quad (5)
\]

- Mean average error, MAE\(_x\) and MAE\(_y\), was calculated following the equations:

\[
\text{MAE}_{x} = \frac{1}{N} \sum_{i=1}^{N} |x_{\text{estimated}}(i) - x_{\text{real}}(i)| \quad (6)
\]

\[
\text{MAE}_{y} = \frac{1}{N} \sum_{i=1}^{N} |y_{\text{estimated}}(i) - y_{\text{real}}(i)| \quad (7)
\]

where \( N \) is the number of events for each slit measurement.

- Spatial resolution, FWHM\(_x\) and FWHM\(_y\), calculated as the FWHM of the Gaussian fit to the \( x_{\text{estimated}} \) and \( y_{\text{estimated}} \) distribution, respectively.

Regarding the DOI performance, we have plotted the \( E/I_{\text{max}} \) histograms for each slit measurement of the dataset along \( x \)-axis (with only energy filter applied) and fitted them using the following analytical expression:\(^{38}\)

\[
\text{DOI}(z) = A \times e^{-ax} \left[ \text{erf} \left( \frac{b - z}{\sqrt{2} \sigma_{\text{int}}} \right) - \text{erf} \left( \frac{a - z}{\sqrt{2} \sigma_{\text{int}}} \right) \right], \quad (8)
\]

where \( a \) is the attenuation coefficient of the material, \( A \) is the amplitude, \( \sigma_{\text{int}} \) is the standard deviation of the distribution which relates to the DOI FWHM as 2.35\( \times \sigma_{\text{int}} \), erf is the Gaussian error function, and \( a \) and \( b \) are the lower and upper limits of the distribution.

Regarding energy performance, a Gaussian fit to the energy spectra (without any filter) was applied to the data at each slit position of the dataset along \( x \)-axis to obtain the photopeak position (\( E_{\text{photopeak}} \)) in energy channels. The photopeak position value corresponding to the slit at the center crystal (\( E_{\text{photopeak,center}} \)) was used to calculate the energy fraction parameter for each slit position, as \( E_{\text{photopeak}} / E_{\text{photopeak,center}} \). Notice that this parameter was calculated for each side of the interface separately. The energy resolution was obtained as \( \Delta E_{\text{FWHM}} / E_{\text{photopeak}} \).

For each configuration, the average and standard deviation of the parameters described in this section were also calculated.

### 3 RESULTS

#### 3.1 Light distribution

The shape of the measured LD varies depending on the detector configuration.\(^{31}\) For the standard configuration (see experimental examples for one gamma-ray impact at 0.5 mm to the left of the interface in Figure 5a), most of the generated scintillation light is absorbed by the black paint and, therefore, the LD is truncated. When the crystals were coupled using the high refractive index compound, the light can travel to the neighbor crystal and be collected by the SiPMs located at the right of the interface (Figure 5b). However, there is not glue compound, to our knowledge, perfectly matching the refractive index of the LYSO scintillator and, therefore, some scintillation light is still reflected at the interface by
this index unmatching. The amount of light transmitted to
the neighbor crystal depends on the difference of such
refractive indexes between the crystal and the coupling
compound. The outcome of this reduced transmission is
a discontinuity in the LDs (Figure 5b) that needs to be
modeled in the detector calibration.

3.2 Spatial and energy performance

The bias$_X$, MAE$_X$, and FWHM$_X$ values along the x-axis
are shown in Figure 6 for both the SC and NN positioning
estimation methods. The values corresponding to slit
positions belonging to the range between −3 and 3 mm,
named the interface region, are shown in Figure 7. It can
be observed that bias$_X$, MAE$_X$, and FWHM$_X$ are signifi-
cantly improved near the optical coupling interface when
using Meltmount compound.

Figure 8 shows the average values of the $|\text{bias}_X|$, 
MAE$_X$, and FWHM$_X$ for the slit positions at the inter-
face region (3 mm from the optical coupling to each side)
as well as their standard deviation (error bars) for each
configuration. Using the SC method, a spatial resolution
of $1.7 \pm 0.3$, $2.4 \pm 0.3$, and $2.6 \pm 0.4$ mm FWHM was
obtained for the Meltmount, grease, and standard con-
figurations, respectively. Lower values are found when
the impact positions are estimated using the NN and
when the crystals are optically coupled using Meltmount,
achieving a FWHM$_X$ of $1.0 \pm 0.2$ mm.

The bias$_Y$, MAE$_Y$, and FWHM$_Y$ values for the slit
position along the y-axis are plotted in Figure 9.
The mean values of the parameters for all slit posi-
tions along y-axis and their standard deviations are
shown in Figure 10. Best values were found for NN
method for all the configurations, as it occurs along x-axis.

The left panel in Figure 11 shows the DOI histograms
(in arbitrary DOI units) measured for one slit position at
the crystal center (15 mm from the optical coupling) and
other at the interface (1 mm from the optical coupling)
for the Meltmount, grease, and standard configurations.
The profiles were fitted using Equation (8), see green
lines.

Figure 12a shows the energy spectra (normalized
to the maximum value) corresponding to one slit posi-
tion at the center region as well as at the interface
region for the three studied configurations, in ADC units.
The energy fraction and resolution are also shown in
Figure 12b. For all configurations near the coupling inter-
face, more energy losses are observed compared to
the center of each crystal (energy fraction values close
to 1). However, for the Meltmount configuration, these
losses are lower compared to the other configurations.
Moreover, better energy resolution values were obtained
at the interface region for the Meltmount configuration.
Figure 12c shows the average and standard deviation
values for slit positions at the interface region. The stan-
dard configuration exhibited lower (20% on average)
photopeak values. These differences are reduced when
using grease as optical coupling and are almost van-
ished using Meltmount. Average energy resolutions at
the interface region of $18 \pm 2\%$, $20 \pm 2\%$, and $23 \pm 3\%
were measured for the Meltmount, grease, and standard
configurations, respectively.
FIGURE 6  Bias$_X$, MAEx$_X$, and FWHM$_X$ as a function of the slit position along the $x$-axis for the three configurations, using SC (a) and NN (b) position estimation methods.

FIGURE 7  Bias$_X$, MAEx$_X$, and FWHM$_X$ as a function of the slit position at the interface region along the $x$-axis for the three configurations, using SC (a) and NN (b) position estimation methods.

FIGURE 8  Average and standard deviation (error bars) values of the $|\text{bias}_X|$, MAE$_X$, and FWHM$_X$ corresponding to the slit positions at the interface region for each position estimation method.
4 | DISCUSSION

In this work, we have experimentally evaluated the performance achieved when coupling two monolithic LYSO crystals using Meltmount ($n_{\text{Meltmount}} = 1.7$), optical grease ($n_{\text{grease}} = 1.46$), and air (standard configuration) between them, in terms of spatial (including DOI) and energy performance. In all cases, the crystals were
coupled to a 12 × 12 SiPMs array and read out with a circuit that provides each row and column signals of the photosensor.

For the planar coordinates (XY), two positioning estimation methods were compared, named SC and NN. Figure 8 shows that the $|\text{bias}_X|$, $\text{MAE}_X$, and $\text{FWHM}_X$ improved near the interface for the case with smaller mismatch with the refractive index of the crystal, that is, Meltmount configuration. In this case, the total internal reflection is minimal, allowing a better LD characterization and thus, reducing the edge-effect, as expected. Moreover, the NN technique improves the spatial performance along x- and y-axis compared to the SC method (Figures 8 and 10). The NNs are able to learn the LD shapes from all the samples of the training data, and thus, a higher spatial accuracy is expected in contrast to SC method (Figures 8 and 10). The NNs are able to learn the LD shapes from all the samples of the training data, and thus, a higher spatial accuracy is expected in contrast to SC method. However, quite similar performance in terms of bias$_X$, MAE$_X$, and FWHM$_X$ has been obtained for the grease and standard configuration at the interface region (Figure 6). We hypothesize that such a similar behavior is explained by the filter of 10% in positions that may be masking the differences of these two configurations. Higher LD truncation in the interface region for standard configuration should produce a deterioration of spatial parameters with respect to the grease configuration. The best values (lowest mean and standard deviation) were reported for the Meltmount configuration and NN method, obtaining a $|\text{bias}_X|$ of 0.2 ± 0.2 mm and a FWHM$_X$ of 1.0 ± 0.2 mm at the interface region; thus, achieving a uniform spatial resolution. In other experimental work, a $|\text{bias}|$ of 0.4 mm and a FWHM of 2.1 mm was obtained at the transition region between four LYSO crystals glued together with Meltmount and applying both ML and least-squares minimization positioning estimation methods. In other study, a $|\text{bias}|$ of 0.5 mm and a FWHM of 1.5 mm near the optical coupling ($n_{\text{grease}} = 1.7$) was reported using the ML positioning estimation and simulated data. We assume that the improvement in spatial performance obtained in our work is due to the use of machine-learning artificial NN techniques for positioning estimation.

Concerning DOI performance at the interface region, narrower DOI histograms were obtained for grease and standard configurations (Figure 11), because in these...
cases, the LD is no longer preserved, either by internal reflections or its truncation. However, for the Meltmount configuration, the LD is almost preserved and, therefore, the measured DOI histogram follows the shape of the theoretical DOI distribution.\(^2\) Out of the scope of this work, lateral incident experiments would be required to accurately estimate the DOI resolution for each configuration.

Regarding energy performance, Figure 12 shows that in the Meltmount and grease configurations, some optical photons will be collected by the neighbor crystal, thus reaching an energy fraction closer to the unit. However, it is unclear the origin of the observed asymmetric behavior around the interface region for the standard configuration (Figure 12b). Probably, some inhomogeneities on the crystal and/or on the SiPM array could explain this behavior. For instance, an electronic read-out or paint coupling problem for column 9 of the SiPM array (Figure 5) could explain the asymmetric energy performance behavior we have observed for the standard configuration. Moreover, the best average energy resolution value was obtained for Meltmount configuration, improving the energy performance at the interface region.

Table 2 summarizes the obtained spatial and energy parameter values for each configuration at the interface region. Overall, the Meltmount configuration and NN technique allow to reduce border effects in terms of an improved spatial and energy performance.

### 5 | CONCLUSIONS

We have experimentally studied the effect of gluing two monolithic LYSO crystals of 33 × 25.4 × 10 mm\(^3\) using a high refractive index compound. We have demonstrated the edge-effect reduction when optically coupling side-by-side scintillation crystals using a compound with a refractive index \(n_{\text{Meltmount}} = 1.7\). We have also shown that compression effects are further reduced when using NN techniques for the gamma-ray impact position estimation in contrast to analytical methods.

It can be concluded that this approach helps increasing the light transfer between adjacent crystals in monolithic detectors, improving the uniformity of spatial and energy performance. In this way, the design and implementation of molecular imaging scanners with minimum gaps among detector blocks would be possible, enhancing the system sensitivity and performance.

In order to extrapolate this approach to PET systems, monolithic crystals that are curved could be glued together, ensuring no gaps between blocks in the transaxial axis. Our team is currently building a dedicated breast PET system based on a ring made out of 14 monolithic curved surface LYSO crystals glued together using Meltmount and read out using flexible Printed Circuit Boards (PCBs) coupled to SiPM photosensors.

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### CONFLICTS OF INTEREST

The authors have no relevant conflicts of interest to disclose.

### DATA AVAILABILITY STATEMENT

The data supporting the results of this study are available upon reasonable request to the corresponding author.

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