The effects of baffle configuration and number on inertial mixing in a curved serpentine micromixer: Experimental and numerical study

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Abstract

Recently, the application of micromixers in microfluidic systems including chemical and biological assays has been widely accomplished. Passive micromixers, benefitting from the low-cost and a less-complex fabrication process, rely solely on their geometry. In particular, Dean vortices generated in curved microchannels enhance the mixing performance through chaotic advection. To improve the mixing performance at relatively low Reynolds numbers (i.e., $1 \leq \text{Re} \leq 50$), this study introduces baffles into the side walls of curved serpentine micromixers with curvature angles of $280^\circ$, which constantly agitate, stretch and fold the fluids streams. Six different baffle configurations were designed and the effects of geometry and the number of baffles were investigated both experimentally and numerically. According to the experimental results, while the maximum outlet mixing index of the micromixer with no baffles was 0.61, that of the micromixer with quasi-rectangular baffles was 0.98 at a low Reynolds number of 20, indicating the major contribution of the generated chaotic advection by baffles. Furthermore, numerical results, which were in good agreement with experimental results, shed more light onto the mechanisms involved in micromixing in terms of the flow behavior and mixing index.

1. Introduction

Over the past two decades, microfluidic devices housing geometries with dimensions varying from ten micrometers to few hundred micrometers have attracted great attention in the fields of medicine, biotechnology, and various engineering disciplines. Exceptional advantages of these microfluidic tools such as high throughput, small sample usage, rapid response time, low cost, easy fabrication, and portability have led to the developments of Lab-On a Chip (LOC) and micrototal analysis devices (μTAS) as remarkable examples of microfluidics.

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Micromixer designs

The effect of curvature angle on mixing in curved serpentine micromixers was investigated in our previous study (Aljani et al., 2019). Accordingly, the higher curvature angle leads to a higher mixing efficiency at lower Reynolds numbers. The obtained results are utilized in this study. By introducing baffles into the side walls of the micromixers with a higher curvature angle (i.e. 280°), we aim to enhance the mixing performance. The reason why we cannot go beyond the 280° is the fabrication limitations. For curve angles close to 360°, the curves contact each other (Aljani et al., 2019).

The inner radius of curvature of the inner arcs is 500 μm, and the width and height of the micromixers are 300 μm and 100 μm, respectively. Three different baffle configurations including quasi-rectangular, forward triangular, and backward triangular are designed. Table 1 includes the geometrical parameters of the micromixer designs. The width of the baffles in all designs is kept as 150 μm, which is half of the micromixers’ widths. As Fig. 1 shows, all the micromixers consist of six mixing segments. Accordingly, there are five baffles in each curve in micromixers M2, M4, and M6, while
cally studied the Dean vorticities and velocity maxima shift in these curved micromixers. Clark et al. (2018) numerically investigated the serpentine curved microchannels having non-circular cross-sections with a curve angle of 180°. This type of micromixers operates well at flows with moderate Reynolds numbers (i.e. a few hundred) (Capretto et al., 2011) but they have a low performance at low Reynolds numbers (Re = 1–40) (Telemann, 2004; Hessel et al., 2005; Marques and Fernandes, 2011). To further enhance the performance, obstacles are embedded to curvilinear microchannels for low Reynolds numbers. Such barriers can be placed either on channel sidewalls (Wang et al., 2003) or on the center of the channels (Bhagat and Papautsky, 2008; Bhagat et al., 2007). As an example, Bhagat et al. (2007) conducted an experimental and numerical study over a wide range of flow rates on passive micromixers with obstructions. Wang et al. (2002) obtained the optimum design parameters such as the layout and number of obstacles in Y-channels to improve the mixing performance.

Motivated by the aforementioned developments in the field, this study includes both experimental and numerical results and aims to enhance the mixing efficiency by introducing baffles into the side walls of micromixers. According to our previous study (Aljani et al., 2019), the optimum micromixer consisted of ten arcs of 280° curve angle. Here, seven micromixers (M1 to M7) were designed, each possessing six mixing segments. In particular, three different baffle configurations including quasi-rectangular, forward triangular, and backward triangular were designed. It was expected that the baffles would generate local small vortices in the laminar flow (Santana et al., 2019; Alam et al., 2014), which would enhance the mixing performance by agitation the flow (Baaz et al., 2018). In this regard, their efficiency in mixing denized (DI) water and diluted Rhodamine B streams at relatively low Reynolds numbers (Re = 1–50) is assessed, and the relevant mechanisms are discussed. This study investigates the mixing capability of each micromixer by obtaining the mixing index along the longitudinal length of the micromixers at various flow rates. Moreover, in order to provide further discussion and better understanding about the mixing capability and mechanisms, this study also presents simulations of flows in the micromixers by using the commercial finite element software COMSOL Multiphysics 5.5. The results of this investigation will be useful to provide better designs for microfluidic devices with curved serpentine microchannel geometries.

2. Materials and methods

2.1. Micromixer designs

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Table 1 – Summarized designs of micromixers.

<table>
<thead>
<tr>
<th>Micromixer types</th>
<th>Baffle geometry</th>
<th>Baffle width (µm)</th>
<th>Baffle length θb (degrees)</th>
<th>Baffle spacing θs (degrees)</th>
</tr>
</thead>
<tbody>
<tr>
<td>M1</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>M2</td>
<td>Quasi-rectangular</td>
<td>150</td>
<td>14</td>
<td>42</td>
</tr>
<tr>
<td>M3</td>
<td>Quasi-rectangular</td>
<td>150</td>
<td>8.75</td>
<td>26.25</td>
</tr>
<tr>
<td>M4</td>
<td>Forward triangular</td>
<td>150</td>
<td>14</td>
<td>42</td>
</tr>
<tr>
<td>M5</td>
<td>Forward triangular</td>
<td>150</td>
<td>8.75</td>
<td>26.25</td>
</tr>
<tr>
<td>M6</td>
<td>Backward triangular</td>
<td>150</td>
<td>14</td>
<td>42</td>
</tr>
<tr>
<td>M7</td>
<td>Backward triangular</td>
<td>150</td>
<td>8.75</td>
<td>26.25</td>
</tr>
</tbody>
</table>

Fig. 1 – The schematics of micromixers (M1 to M7). The green lines demonstrate the location of evaluated mixing indices over the channel length. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article).

There are eight baffles in micromixers M3, M5, and M7. It is expected that the baffles generate local small vortices in the laminar flow, which enhances mixing of two fluids (Santana et al., 2019; Alam et al., 2014). Also, Fig. 1 displays the location of the inlets of the two streams, where the main flow direction is from left to right.

2.2. Micromixers fabrication

The micromixers were fabricated by taking the advantage of the standard soft lithography fabrication techniques (Please refer to ESI for entire steps of fabrication).

2.3. Solution preparation

In order to provide the fluorescent solution observable under the fluorescence microscope, Rhodamine B powder (Merck KGaA, Darmstadt, Germany) was solved in DI water and a 0.5 mM solution was prepared. Then, the mixture was magnetically stirred for 15 min to ensure the uniform distribution of Rhodamine B.

2.4. Experimental procedure

In order to observe the fluid flow and then to obtain the mixing efficiency based on the taken pictures (fluorescence intensity maps), this study utilized an inverted fluorescence microscope (ZEISS Axio Observer Z1 Live Cell Imaging) (Please refer to ESI for detailed information).

2.5. Image processing

The software (ZEN Blue 3.1) of the microscope was utilized to extract the fluorescence intensity for each of the captured images. In this regard, the software provides the intensity versus length profiles at the determined locations (green lines)
in Fig. 1. To quantify the mixing capability, the following expression gives the mixing index, \( M \) (Fan et al., 2017):

\[
M = 1 - \left[ \frac{1}{n} \sum_{i=1}^{n} \left( \frac{l_i}{l} \right)^2 \right]^{\frac{1}{n}}
\]

where \( n \) is the number of pixels, \( l_i \) is the fluorescence intensity of the \( i \)th pixel and \( l \) is the average fluorescence intensity of all pixels. Accordingly, no mixing and perfect mixing conditions occur when the \( M \) value is equal to zero and unity, respectively.

2.6. Numerical simulations

To better understand the flow behavior and concentration contours of the designed micromixers, the whole domain was simulated using COMSOL Multiphysics 5.5a which is a commercially available software based on finite element methods. Governing equations of this study are continuity, Navier-Stokes, and convection-diffusion:

\[
\nabla \cdot \vec{V} = 0
\]

\[
\frac{\partial \vec{V}}{\partial t} + \rho \left( \vec{V} \cdot \nabla \right) \vec{V} = -\nabla P + \mu \nabla^2 \vec{V}
\]

\[
\frac{\partial C}{\partial t} + \left( \vec{V} \cdot \nabla \right) C = D \nabla^2 C
\]

Here, \( \vec{V} \) represents velocity vector, \( P \) defines the pressure, \( C \) is the concentration of species, and \( D \) is the diffusion coefficient. The fluid behavior inside the channel is characterized using Reynolds number:

\[
Re = \frac{\rho UD_h}{\mu}
\]

where \( \rho \), \( U \) and \( \mu \) are the fluid density, average fluid velocity and viscosity. \( D_h \) is the hydraulic diameter of the channel:

\[
D_h = \frac{4A}{P}
\]

where \( A \) is the channel cross-section area and \( P \) is the wetted perimeter of the cross-section (Bazaz et al., 2020a). In curvilinear channels with laminar flow and low Reynolds numbers, the flow regimes and generation of vortices are dependent on the dimensionless Dean number (De) (Dean and Hurst, 1959), which is defined as:

\[
De = \frac{Re \sqrt{D_h}}{2R}
\]

where \( R \) is the radius of curvature of the microchannel.

In the numerical part, the properties of fluid were considered as Newtonian and incompressible flow with the dynamic viscosity of 0.001 Pa.s and density of 1000 kg/m\(^3\), respectively. When solving the equations, the flow was considered as steady-state. Uniform velocity was applied at the inlets, zero static pressure was set to the outlet, and wall condition was set as the no-slip boundary condition. In these micromixers, each stream was labeled by colored dye. Accordingly, the uniform mixing happens when the molar concentration reaches 0.5. The diffusion coefficient between these two streams was conserved as \( 3.6 \times 10^{-10} \) m\(^2\)/s (Bazaz et al., 2020b) (Please refer to ESI for grid study of numerical simulations).

3. Results and discussion

3.1. Experimental results

Fig. 2 displays the outlet mixing index (M) for all the micromixers (M1 to M7) for Reynolds and Dean numbers (De) ranging from 1 to 50 and 0.39 to 19.36, respectively. Despite the availability of these two dimensionless numbers, for the sake of fair comparison with other types of micromixers in the literature, the results are explained only based on the Reynolds number.

Fig. 2 shows that M1 has the lowest efficiency among the designed micromixers as expected, while M3 is the most efficient one. In addition to M3, the micromixers M7 and M5 exhibit a good mixing performance for high Re, which can be attributed to the higher number of designed baffles in the mentioned micromixers and consequently enhanced chaotic advection. The micromixers M2, M4, and M6 have lower mixing index values compared to their similar counterparts (i.e. M3, M5 and M7) but with more vortex generators (i.e. baffles). The generation of vortices by baffles increases with the fluid velocity (Santana et al., 2019). For low velocity, the molecular diffusion as major mass transfer mechanism results in relatively higher mixing indices as there is a longer time for intermixing water and Rhodamine B (Santana et al., 2019; Bazaz et al., 2018). While the fluorescence intensity maps of M1, M3, and M7 are provided here, those of other micromixers are shown in Fig. A.2 in ESI. Also, the supplementary videos A1–A7 include the consecutive display of the fluorescence intensity maps of the micromixers M1 to M7 at various flow rates.

The outlet mixing index of the micromixer M1 is 0.55 at Re = 1 and remains constant only with slight fluctuations until Re = 15. Then, the mixing efficiency grows with flow rate. The outlet M experiences its largest growth for this micromixer from 0.52 at Re = 15 up to 0.60 at Re = 30. It can be claimed that the induced secondary flows by curved microchannels improves the mixing quality since it generates partially chaotic advection (Xie and Xu, 2017). For Re≥30, outlet M approximately remains unchanged until Re = 50, where the outlet mixing index is equal to 0.61. The poor mixing performance indicates that the chaotic advection (Xie and Xu, 2017) is not initiated for M1 at the tested flow rates and Dean vortices only could mod-
Fig. 3 – The fluorescence intensity maps of micromixer M1 at (a) Re = 1, (b) Re = 25, (c) Re = 50.

derately raise outlet M through the partially chaotic advection. Fig. 3 shows the fluorescence intensity maps of M1 at Re = 1, 25, and 50. It can be inferred that the secondary flows are not sufficiently strong to expand the diffusion layer, which is located at the interface of water and diluted Rhodamine B. That is the reason why it never covers the entire width of the micromixer despite partially widening of the diluted Rhodamine B stream width with the increase in fluid velocity.

Although the micromixer M2 has the outlet mixing index around 0.70 for Re ≤ 5, it exhibits a rise beyond Re > 1 and reaches its highest efficiency with outlet M of 0.97 at Re = 30. Vortex generation is obviously dependent on the fluid velocity (Santana et al., 2019). Therefore, as Re approaches 30, the generated vortices and subsequent chaotic advection intensify and considerably enhance the mixing performance. Also, secondary vortices start to contribute to the mixing index enhancement and generate partially chaotic advection. For 30 ≤ Re ≤ 50, there is a slight fluctuation, and outlet M is higher than 0.92. Fig. A.2a and Video A2 display that the diffusion layer is eliminated for Re > 25.

The micromixer M3, which has the outlet M of 0.62 at Re = 1, experiences the sharpest increase among the designed micromixers and provides its best performance with a 0.98 mixing index at Re = 20. The initial relatively higher M values are present since the flow requires longer time for low Re to arrive to the channel outlet and the species have more time to diffuse into each other (Santana et al., 2019; Bazaz et al., 2018). With the increase in the stream velocity, the partially chaotic and chaotic advection start to dominate the molecular
diffusion. As an important result, this micromixer is capable of offering the highest mixing efficiency starting from a rather low Re (Re = 20) compared to the other micromixers. Thus, the existence of more quasi-rectangular baffles in M3 compared to M2 (eight baffles compared to five in each arc) obviously promotes the vortex generation for lower Re, which leads to the improvement in the mixing performance. Furthermore, the baffles can agitate the flow, which further enhances the mass transfer rate (Bazaz et al., 2018). Beyond Re = 20, the mixing efficiency remains stable only with negligible changes between 0.98 and 0.97 implying that even low fluid velocities are sufficient for this type of micromixer to provide excellent mixing. The explained trend for M3 can be also observed in the fluorescence intensity maps displayed in Fig. 4a.

The outlet M of the micromixer M4 slightly decreases from 0.71 to 0.66 as Re increases from 1 to 5 and then maintains at the same level until Re = 20. The relatively higher mixing efficiency at the initial flow rates can be explained by the fact that the molecular diffusion is the dominant mass transfer mechanism. In other words, the species have a longer time to move to the opposite side of the channel or to deform the diffusion layer. While there is a plateau for 5 ≤ Re ≤ 20, with the intensified Dean vortices and the resulting chaotic advection, the outlet M significantly increases to 0.96, when Re is raised from 20 to 45. Video A4 shows that there is an obvious difference between Re = 25 and 40, which confirms the mentioned increase within 20 ≤ Re ≤ 45. When Re is lower than 25, the minor widening of the diluted Rhodamine B flow stream is due to the weak Dean vortices.

The micromixer M5, similar to its counterpart (i.e. M4), initially shows a higher outlet M value of 0.64 at Re = 1 and then slowly decreases to 0.60 when Re is 2. It can be inferred that for M4 and M5 with forward triangular baffle configuration, the molecular diffusion mainly contributes to enhance the mixing efficiency at the beginning. Also, the following decrease can be attributed to the reduced diffusion time because of the fluid velocity increase (Santana et al., 2019). Subsequently, the outlet M increases from 0.60 to 0.98 within the range of 2 ≤ Re ≤ 40. Here, with the initiation of the secondary flows effect and chaotic advection, especially for relatively higher Re (i.e. Re ≥ 15), an increase beyond the decreasing region is apparent. The outlet M remains almost unchanged beyond Re = 40, which suggests perfect mixing (Please refer to Video A5).

The micromixer M6 has the lowest mixing performance for the studied flow rates, when M1, the base of comparison, is excluded. The outlet M value of M6 starts from 0.55 and grows to 0.64 when Re is 10. Most probably, for this micromixer, the molecular diffusion is dominant for Reynolds numbers lower than smallest Reynolds number value in this study, and its effect decreases with the flow velocity at low range of Re (Santana et al., 2019). The outlet mixing index remains almost unchanged with a small fluctuation until Re of 35. It can be deduced that the partially chaotic advection (Xie and Xu, 2017) is not noticeably influential for the mentioned range. Subsequently, owing to the chaotic advection impact, there is an upward trend up to the end of experiment (Re = 50) where M = 0.90. Actually, there is a similar trend between M6 and M4; however, the delay in chaotic advection affects the mixing efficiency of M6. Fig. A.2d and Video A6 prove that the diffusion layer remains until the highest flow rate (Re = 50), and only minor widening occurs for lower fluid velocities.

The micromixer M7 has the best performance among the designed micromixers for the lowest flow rates (i.e. Re = 1 and 2) with the corresponding outlet M values of 0.78 and 0.80,
respectively. For $1 \leq \text{Re} \leq 35$, the outlet M experiences an upward trend (from 0.78 into 0.98). Interestingly, the lowest mixing index of 0.78 at Re = 1 is related to the vortex generation at a wide range of Re and consequently enhanced mixing performance. When comparing M6 to M7 both with backward triangular baffles, it can be concluded that the number of baffles is an important parameter since the baffles accelerate chaotic advection through the constantly folding and stretching the fluid. Eventually, for Re $\geq 35$, there is not any significant change. Accordingly, at Re = 25, where M = 0.97, the diluted Rhodamine B stream uniformly covers the channel outlet region as shown in Fig. 4b.

Overall, the designed baffles continuously decrease the stream width over the channel, which results in enlarged contact between the fluids and enhanced mixing (Santana et al., 2019). The generated secondary flow in serpentine micromixers intensifies with an increase in Re. Also, vortex generation by designed baffles and chaotic advection depend on the fluid velocity. The effect of baffle number is obvious for all similar cases, particularly for M6 and M7. Table A.1 in ESI summarizes the mixing efficiency for all the micromixers.

Fig. 5 presents the mixing behavior along the micromixers by supplying M values at four different locations along their longitudinal length, which is 22.64 mm. The measured locations (i.e., 3.38, 9.73, 16.08, and 22.64 mm) correspond to the first, third, and fifth segments as well as the channel outlet (as marked by green lines in Fig. 1). Fig. 5 shows the obtained results for Re = 25 (Please refer to ESI and Fig. A.3 for Re = 1, 10, 20 and 50). Overall, as the fluid moves from the inlet to the outlet, M values experience an increasing trend implying that chaotic advection increases from inlet to outlet, which is also proven with the numerical simulations included in the next section. The micromixer M3 with quasi-rectangular baffles (from the first measurement location) has the best mixing performance compared to others. It can be inferred that the quasi-rectangular baffles properly contribute to stretching and folding of the fluid. Among the presented cases, the mixing index of M2 at the first transition (from first to third segment) possesses the largest increase with 58%, from 0.58 to 0.91.

3.2. Numerical simulations

To provide further insights about the performance of the designed micromixers, numerical simulations corresponding to the experimented baffles configurations were performed. Therefore, this part not only includes the comparison with the experimental results, they (but?) also present(s?) the velocity profiles along with Dean arrows and concentration contours for some selected cases.

Fig. 6 demonstrates the comparison of the outlet experimental and numerical M of all the micromixers (M1 to M7) at the Reynolds number of 25. At the first glance, this figure confirms that the corresponding experimental and numerical profiles follow the same trend, and the numerical model mostly agrees with the experimental results. Accordingly, the experimental results could be predicted by the numerical model within approximately ±10%, for all micromixers excluding M2 and M6, which slightly more deviate. These deviations can be attributed to the microfabrication process.
Furthermore, the obtained numerical results match favorably with the literature as well as explanations about the experimental results in the previous section. As mentioned before, the Dean vortices generated in serpentine micromixers enhance chaotic advection and increase with Re (Alijani et al., 2019; Jiang et al., 2004; Santana et al., 2019; Kockmann et al., 2006). Fig. 7 shows the overview of the micromixer M1 and cross-sectional velocity profile along with the Dean vortices for three Re values (1, 25, and 50). As shown in Fig. 7a, the taken cross-sectional velocity profile belong to the first segment. It can be observed that the secondary flow does not form at Re = 1 (Fig. 7b), which is the main reason for low mixing indices in the experimental results at this Re. However, the Dean vortices start to intensify as the Re becomes 25 and 50 (Fig. 7c and d, respectively). Dean flow vectors are directed towards the outer wall along the channel mid-height and towards the inner wall at the top and bottom of the channel. The ESI version provides the detailed information on how the secondary flow gets intense along the micromixer (Fig. A.4). Also, the shape and number of baffles are discussed taking advantage of fluid velocity streamlines (Fig. A.5 and A.6).

For further evaluation, Fig. 8 presents the obtained concentration maps of numerical simulations for the micromixers M1 to M7 at Re = 50 (Please refer to ESI and Fig. A.7 for Re = 25 as well as the concentration streamlines, Fig. A.8 and A.9). The molar concentrations of water and Rhodamine B were set to 0 and 1, respectively, and uniform mixing is achieved when the concentration value of intermixed species reaches to 0.5. Considering this point, among the presented contours, while M1 shows the lowest mixing performance along and at the micromixer outlet, M3 and M7 have a superior mixing performance. Moreover, there is an obvious enhancement in M values when the number of baffles increases, which is also confirmed in the experimental results. Comparing this figure with the given equivalent fluorescence intensity maps also exhibits a close agreement between the numerical and experimental results. For instance, both of these results demonstrate that the micromixers M3 and M7 achieve uniform mixing after first segment. Similar to the experimental results, the forward triangular baffles have a relatively lower performance compared to the other two designs. In addition, the mixing indices along the longitudinal length of the channel in Fig. A.3d validate this claim. Similarly, there is an agreement for other contours in Fig. 8 with the corresponding experimental results.

4. Conclusion

In this study, it was aimed to enhance the mixing performance by introducing baffles into the side walls of curved serpentine micromixers. The effects of configuration and number of baffles were experimentally and numerically investigated. The micromixer M1 with no baffles was the base of comparison. The designed baffle geometries were quasi-rectangular (M2, M3), forward triangular (M4, M5), and backward triangular (M6, M7), where only the number of baffles increased between the similar counterparts. These baffles generated vortices to enhance chaotic advection and consequently mixing index. According to the experimental results for 1 ≤ Re ≤ 50, the maximum outlet M for the micromixer M1 at the tested flow rates was 0.61. Accordingly, Dean vortices could moderately raise the outlet M through partially chaotic advection. How-
ever, due to existence of constantly fluid folding and stretching in micromixers with baffles, the mixing index values could be significantly increased. The micromixer M3 provided highest outlet mixing index (M) of 0.98 at Re = 20, implying that chaotic advection could enhance the mixing efficiency even at low Re. Also, the same outlet M was obtained for the micromixers M5 and M7 at Re = 40 and 35, respectively. Even though the similar counterparts of these micromixers (i.e. M2, M4, and M6) could provide high outlet M, for instance 0.97 at Re = 30 for the micromixer M2, the chaotic advection contributed at rather higher fluid velocities. The prediction of numerical simulations for the flow behavior and outlet M were in close agreement with the experimental results. Overall, the micromixers M3 and M7 had the best mixing performances among others. For future studies, the impact of other parameters such as micromixer hydraulic diameter, aspect ratio, and inner and outer radii will be considered.

**Authors contributions**

V.E., R.A., İ.B., H.A. and A.K. designed the experiments. V.E., R.A., İ.B. and S.Ç. fabricated the device, performed the experiments, and prepared the figures. S.R.B., H.A and M.E.W. performed numerical simulations. All the authors reviewed the manuscript.

**Declaration of interests**

The authors declare no conflicts of interest.

**Declaration of Competing Interest**

The authors report no declarations of interest.

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**Appendix A. Supplementary data**

Supplementary material related to this article can be found, in the online version, at doi:https://doi.org/10.1016/j.chedr.2021.02.028.

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