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Effects of Excitation in Neutron Induced Fissile Isotopes of Uranium Using the OPTMAN Code Up to 20 MeV.

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Abstract

In this work, the effects of neutron-induced fissile isotopes of Uranium, particularly; Uranium-233 and Uranium-235 are studied using the Coupled-Channelled Optical Model code (OPMAN) code up to 20 MeV. The high demand for nuclear reactor fuels has necessitated this research. As one of the major naturally occurring radionuclides with lots of fuel prospect, Uranium-233 occurred in trace while Uranium-235 occur in 0.71%. Two steps process away from Uranium-233 and Uranium-235 on neutron capture can produce fissile materials to be used as reactor fuel. Though, Uranium-233 and Uranium-235 are not by them self a fissile material, but they are breeder reactor fuels. Computations were done for both the Potential Expanded by Derivatives (PED) which account for the Rigid-Rotor Model (RRM) that treat nuclei as rigid vibrating sphere as well as account for nuclear volume conservation and Rotational Model Potentials (RMP) which account for the Soft-Rotator Model (SRM) that treat nuclei as soft rotating spherical deformed shapes. Each of the calculated data was compared with the retrieved data from Evaluated Nuclear Dada File (ENDF) which was found to be in good agreement. The threshold energies in all cases were found to be 4 MeV for both PED (Potential Expanded by Derivatives) and RMP (Rotational Model Potentials). It is observed that results from RMP much better agreed with the retrieved data than one obtained from PED.

1. Flow Injection System(FIA):

1.1 Introduction FIA:

The needs for Fissile isotopes of uranium are due to their practical applications. These isotopes or materials can be used as fuel in nuclear reactors of both power plants and research reactors, as they can be split by neutrons in a self-sustaining nuclear chain reaction. The amount of energy released during these reactions is large enough to generate electricity. Aside from being used as nuclear reactor fuels, fissile materials can undergo fission reaction processes.

They are the key components of nuclear weapons or other nuclear explosives devices. Those mostly used in nuclear weapons are highly enriched uranium (uranium - 235 and plutonium-239). However, this research is for nuclear research reactor application. As such, we shall focus on nuclear reactor fuels [1]. It is pertinent to search for alternative fuel means in some isotopes that are radioactive aside the uranium-235 and plutonium-239. We may recall that the two most important fissile materials normally used as fuels are uranium-235 and Plutonium-239.

These are weapon-grade materials that can also be used

as reactor fuels. Uranium 235 is a natural isotope of uranium with an abundance of 0.72%. This concentration is very small. Nuclear physicists have made efforts to increase this concentration through the enrichment process. But, due to the prevalent need for reactor fuels, we ought to seek alternative isotopes that can be used as fuels [2].

The fissile materials Plutonium-239 and uranium-233, which do not occur in nature, are produced by the transmutation of uranium-238 and thorium-232 respectively. These materials are called fertile materials. For fuel cycles using plutonium-239 and uranium-233 as fuel, irradiation of uranium-238 and thorium-232 in the fuel blanket and reprocessing to extract the plutonium-239 and uranium-233 become important steps in the cycle [3]. Plutonium-239 is not a natural isotope of plutonium. It is bred from the naturally occurring uranium-238 whose natural abundance is 99.9%.

Uranium-238 is irradiated by fast neutrons to produce Uranium-239 and this Uranium-239 can undergo a radioactive decay to produce Plutonium-239. Plutonium-239 just like Uranium-235 is a fissile material. The Plutonium-239 can then be bombarded with high-speed neutrons. When a Plutonium nucleus absorbs one such free neutron, it splits into two fission fragments. This fissioning releases heat as well as neutrons, which in turn splits other plutonium nuclei present, freeing still more neutrons. As this process is repeated again and again, it becomes a self-sustaining chain reaction, yielding a steady source of energy, chiefly in the form of heat which is transported from the reactor core by a liquid sodium coolant to a system of heat exchange. This system utilizes heat to produce steam for a turbine that drives an electric generator [4], [5].

Uranium-233 is a fissile isotope of uranium that is bred from thorium-232 as part of the thorium fuel cycle. Uranium-233 was investigated for use in nuclear weapons and as reactor fuel. It has been successfully used or tested in experimental nuclear reactors and has been proposed for much more or wider use as nuclear fuel. It has a half-life of 160,000 years [3]. Uranium-233 is produced by neutron irradiation of thorium-232. When thorium-232 absorbs a fast neutron, it becomes thorium-233 with a half-life of 22 minutes. After 22 minutes, thorium-233 decay by beta to protactinium 233 with a half-life of 27 days, and beta decays to uranium 233. Just like uranium-235 and plutonium 239, uranium-233 has also been proposed to be used as nuclear fuel as asserted above. The only challenge with uranium-233 is that; its fission on neutron capturing, but, sometimes retain the neutron to become uranium-234 which is a fertile material [6].

Therefore, uranium-233 and uranium-235 are the two fissile isotopes of uranium. Uranium-235 is a naturally occurring isotope while uranium-233 is an artificial isotope irradiated from thorium-232. The computational approach is used in this research to investigate the effects of excitation in neutron-induced fissile isotopes of uranium using the OPTMAN code up to 20 MeV. Since it is for the research reactor application, a 20 MeV range of energy will be good. The calculations and all the simulations will be carried out in the OPTMAN code and each excitation function shall be analysed [7].

Research was conducted by Avrigeanu & Avrigeanu, (2019) [8] on the analysis of neutron bound states of 208Pb by a dispersive optical model potential, in their research, they discussed the effect of dispersive-correction terms on the calculation of the bound-state energies and finally reported that, the derived 208Pb root mean square radius shows good agreement with measured data.

Another research was carried out by Avrigeanu & Avrigeanu et al., (2021) [9] on the dispersive optical model description of nucleon scattering on Pb–Bi isotopes and reported that the new potential is shown to give a very good description of nucleon scattering data on near-magic targets $^{206,207}Pb$ and ^{209}Bi.

This work investigates the effects of excitation in neutron induced fissile isotopes of uranium for 20 MeV using Coupled-Channels Optical Model OPTMAN Code with adjustment for soft and rigid rotation of the nucleus.

2. Theory:

The current optical potential encompasses corrections (relativistic) as reported by Avrigeanu & Avrigeanu (2022) [10] and expanded by Avrigeanu & Avrigeanu et al (2018) [11].

Surface variation W_D (E) and potential for volume absorption W_V (E) can wisely be presented in terms of energy which could be suitable for the dispersive optical model analysis [12], [13]. The most utilized energy (dependence) for the surface (imaginary) term has been pointed out by Avrigeanu & Avrigeanu et al, (2023) [14] as.

$$W_D(E) = A_D\big[\frac{(E-E_F)^{-2}}{(E-E_F)^{-2}+(B_D)^2} - exp(\lambda_D(E-E_F))\big] \quad (1)$$

A_D, B_D and λ_D are constants (undetermined), E and Ef are Proton and fermi energy respectively. Another utilized energy (dependence) for the surface (imaginary) term has been pointed out by Naik et al, (2021) [15] Naik et al, (2020) [16] as follow;

$$A_{D,V} = W_{D,V}^{DISP}\big[1+(-1)^{Z'+1}\frac{C_{wiso,wviso}(N-Z)}{W_{D,V}^{DISP}A}\big] \quad (2)$$

$W_{D,V}^{DISP}$ and $C_{wiso,wviso}$ are constants (undetermined) , A, N and Z are mass, neutron and atomic number respectively. Utilized energy (dependence) for the volume (imaginary) term has been confirmed in studies of nuclear matter theory by Gopalakrishna et al. (2018) [17]

$$W_v(E) = A_V \frac{(E-E_F)^2}{(E-E_F)^2 + (W_v^{DISP})^2} \quad (3)$$

A_V and W_v^{DISP} are constants (undetermined), E and E_f are proton and femi energy respectively [18], [19], [20], [21], [22], [23] and [24].

3. Methodology:

The OPTMAN code for this work was downloaded from the IAEA website at http://nds-IAEA.org. The optical model code OPTMAN was chosen because it can study nucleon interactions with light-mass, medium-mass, and heavy-mass nuclei for a broad range of energy up to 200 MeV. Additionally, it has a Soft-Rotator model in addition to its Rigid-Rotator model, which improves the precision of the even-even nuclide.

The selection of the appropriate record cards and switches determines how the code will run when the software has been successfully installed using the G-FOTRAN compiler. Record cards that describe input data are themselves described by switches for the description of the model. The "va" executable file is used to invoke each calculation's input data and is produced using the Windows command.

The code is executed immediately the command "va" is issued, the input file name is requested and supplied, the output file name is requested and supplied, and the enter key is pushed. The OPTMAN code computation was based on Equation (1) to (3).

4. Results and Analysis

The results obtained from the computer software (OPTMAN Code) based on the Equation (1) to (3) for Rotational Model Potential (RMP) which accounts for Soft-Rotator Model and Potentially Expanded by Derivatives (PED) accounts for Rigid-Rotor Model by calculating the neutron-induced Total Potentially Expanded by Derivatives (TPED) and Total Rotational Model Potential (TRMP), Reaction Potentially Expanded by Derivatives (RPED) and Reaction Rotational Model Potential (RRMP) and Elastic Potentially Expanded by Derivatives (EPED) and Elastic Rotational Model Potential (ERMP) cross section reactions for ^{233}U and ^{235}U are presented in Table 1 and 2 respectively, below:

To compare the obtained results from this study with retrieved data (TENDF), charts for the computation of the excitation function for the cross-section (Total), cross-section (Reaction) and cross-section (Elastic) of ^{233}U and ^{235}U are plotted and presented in Figure 1, 2, 3, 4, 5 and 6.

Based on Figure 1, the excitation function of the neutron-induced total cross section of 233U shows the same trend which increased from 4 – 9 MeV and decreased from 9-20 MeV. The result obtained from Total Rotational Model Potential (TRMP) agrees more with the retrieved data (TENDF) than the Total Potential Expanded by Derivatives (TPED).

Furthermore, the effect of rotational excitation is more obvious and is best accounted for by Rotational Model Potential.

From Figure 2, According to Figure 2, the excitation function of Uranium-233 shows agreement between both RPED and RRMP with the retrieved standard data (RENDF) from 4-6 MeV. This indicates threshold energy for the neutron-induced reaction for both Potential Expanded by Derivatives (RPED) and Rotational Model Potential (RRMP) to be ≤ 4 MeV.

Additionally, there is poor agreement between the calculated PED values with the standard data of ENDF from 6-12 MeV. Results from Rotational Model Potential show better agreement with the retrieved standard data (RENDF) than the Potential Expanded by Derivatives. This shows that the changing nature of the nucleus under rotation is best described by the Rotational Model Potential.

Figure 3 indicated that for the neutron-induced elastic scattering of Uranium-233 in both Potential Expanded by Derivatives (EPED) and the Rotational Model Potential (ERMP) there is an agreement with retrieved data (EENDF) observed between 4 to 6 MeV and 10 to 20 MeV. But no agreement between EPED and the retrieved EENDF standard data from the 6 to 9 MeV. This, indicates that the Rotational model potential which accounts for the soft-Rotor model of the Coupled-channels Optical Model is best used to describe the effect of rotation under excitation on neutron capture and agreed more with the standard data (EENDF).

Referring to Figure 4, the excitation function of the total cross section induced by neutrons in 235U displays a consistent pattern: an escalation from 4 to 9 MeV followed by a decline from 9 to 20 MeV. Notably, the outcomes derived from the Total Rotational Model Potential (TRMP) exhibit a higher degree of concurrence with the data obtained from the Thermal Neutron-Induced Fission Data File (TENDF), in comparison to the outcomes produced by the Total Potential Expanded by Derivatives (TPED).

Additionally, the impact of rotational excitation becomes more conspicuous, with the Rotational Model Potential emerging as the optimal approach for effectively accounting for this phenomenon.

As depicted in Figure 5, the excitation function of Uranium-235 exhibits a noteworthy alignment between the Potential Expanded by Derivatives (RPED) and the Rotational Model Potential (RRMP), particularly within the energy range of 4-6 MeV, as evidenced by the congruence with the established reference data (RENDF). This alignment suggests that the threshold energy for neutron-induced reactions in both RPED and RRMP lies at ≤ 4 MeV.

However, a marked disparity arises between the calculated PED values and the established ENDF standard data within the

Table 1. Results Obtained for Soft and Rigid-Rotor Model for Uranium-233 (^{233}U).

	Cross Section (Reaction)			Cross Section (Elastic)			Cross Section (Total)		
Energy (MeV)	PED	RMP	ENDF	PED	RMP	ENDF	PED	RMP	ENDF
4.00	1.81	1.76	1.69	1.78	1.87	4.71	3.67	3.63	6.40
5.00	1.66	1.62	1.57	1.95	2.07	4.51	3.68	3.69	6.08
6.00	1.63	1.59	1.64	2.14	2.29	4.18	3.85	3.88	5.82
7.00	1.65	1.61	2.07	2.32	2.48	3.63	4.05	4.09	5.70
9.00	1.65	1.61	2.28	2.52	2.68	2.86	4.24	4.29	5.14
10.0	1.63	1.58	2.26	2.53	2.67	2.67	4.22	4.26	4.93
12.0	1.58	1.53	2.18	2.41	2.50	2.70	4.05	4.04	4.88
14.0	1.56	1.52	2.33	2.19	2.24	2.82	3.80	3.76	5.15
16.0	1.57	1.54	2.45	1.94	1.97	3.02	3.56	3.51	5.47
18.0	1.58	1.56	2.36	1.72	1.73	3.32	3.35	3.29	5.68
20.0	1.57	1.56	2.29	1.53	1.54	3.55	3.15	3.10	5.84

Table 2. Results Obtained for Soft and Rigid-Rotor Model for Uranium-233 (^{235}U).

	Cross Section (Reaction)			Cross Section (Elastic)			Cross Section (Total)		
Energy (MeV)	PED	RMP	ENDF	PED	RMP	ENDF	PED	RMP	ENDF
4.00	1.81	1.76	1.14	1.78	1.87	4.39	3.59 3.63	5.53	
5.00	1.66	1.62	1.07	1.95	2.07	4.21	3.61	3.69	5.28
6.00	1.63	1.59	1.09	2.14	2.29	3.83	3.77 3.88	4.92	
7.00	1.65	1.61	1.54	2.32	2.48	3.31	3.97	4.09	4.85
9.00	1.66	1.62	1.78	2.45	2.62	2.65	4.11	4.24	4.43
10.0	1.63	1.58	1.76	2.53	2.67	2.54	4.16	4.25	4.30
12.0	1.56	1.52	1.72	2.36	2.38	2.61	3.92	3.90	4.33
14.0	1.56	1.52	2.08	2.19	2.24	2.68	3.75	3.76	4.76
16.0	1.57	1.54	2.15	1.94	1.97	2.84	3.51	3.51	4.99
18.0	1.58	1.56	2.06	1.72	1.73	3.13	3.30	3.29	5.19
20.0	1.57	1.56	2.02	1.53	1.54	3.22	3.10	3.10	5.24

energy span of 6-12 MeV. Notably, the results derived from the Rotational Model Potential exhibit superior accord with the reference data (RENDF) when contrasted with the outcomes obtained from the Potential Expanded by Derivatives. This underscores the capacity of the Rotational Model Potential to effectively characterize the dynamic alterations in the nuclear structure brought about by rotation.

As outlined in Figure 6, a noteworthy correspondence is evident in neutron-induced elastic scattering between the Potential Expanded by Derivatives (EPED) and the Rotational Model Potential (ERMP), specifically within the energy intervals of 4 to 6 MeV and 10 to 20 MeV, where alignment with the retrieved reference data (EENDF) is observed. However, a lack of consensus emerges between EPED and the established EENDF standard data within the energy span of 6 to 9 MeV. This discrepancy underscores the efficacy of the Rotational Model Potential, which incorporates the soft-Rotor model of the Coupled-channels Optical Model, in effectively elucidat-

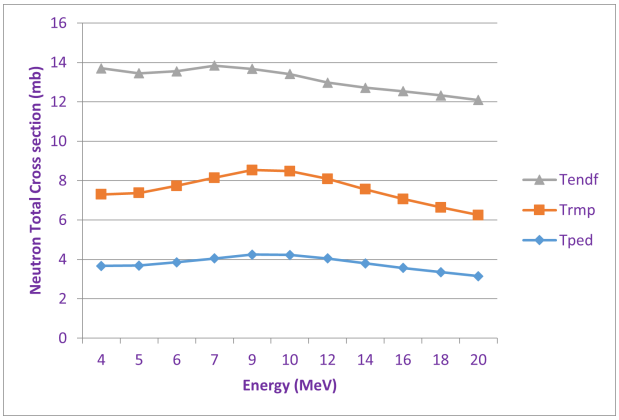

Figure 1. Cross Section (Total) of ^{233}U.

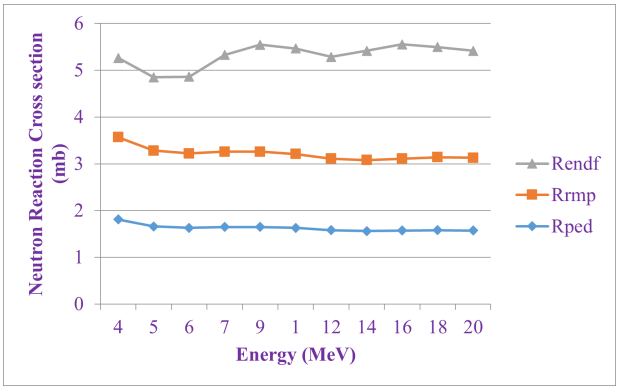

Figure 2. Cross Section (Reaction) of ^{233}U.

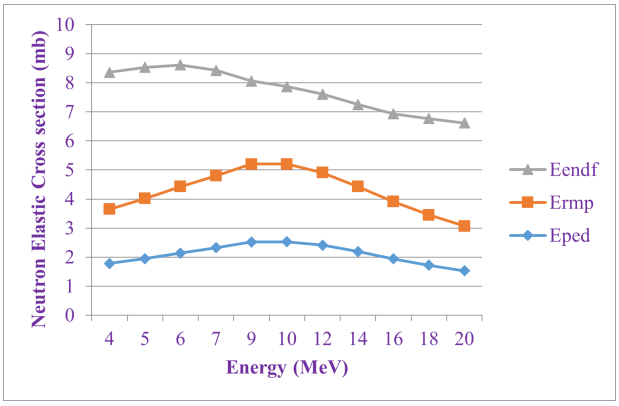

Figure 3. Cross Section (Elastic) of ^{233}U.

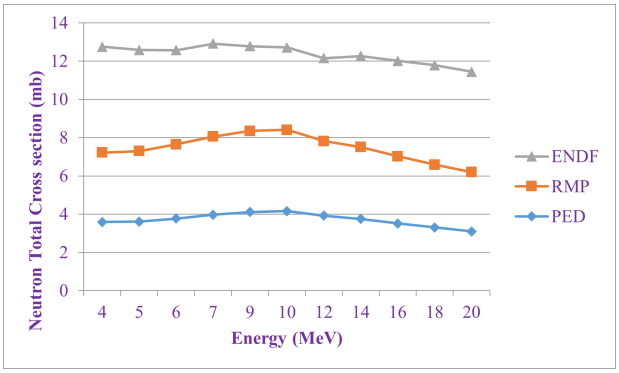

Figure 4. Cross Section (Total) of ^{235}U.

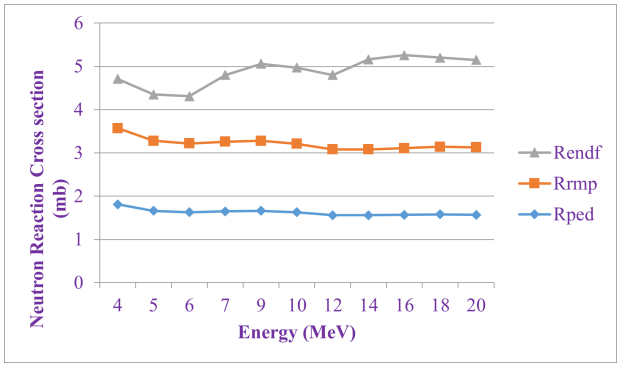

Figure 5. Reaction Cross Section of ^{235}U.

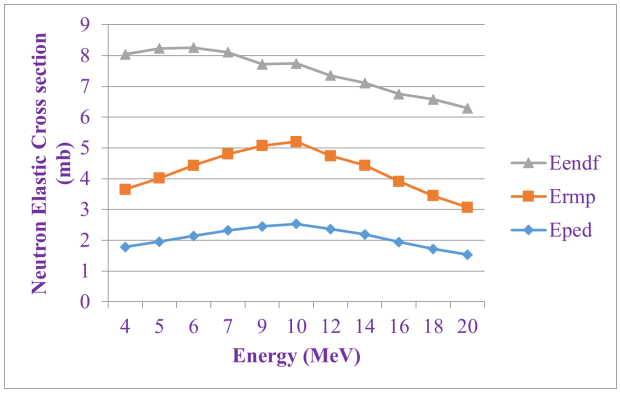

Figure 6. Elastic Cross Section of ^{235}U.

ing the impact of excitation-induced rotation on neutron capture. Notably, this approach exhibits a stronger concurrence with the reference data (EENDF), solidifying its suitability for describing the intricate interplay between rotation and neutron interactions.

5. Conclusion:

The two uranium isotopes, uranium-233 and uranium-235, are fissile materials with good cross sections through careful investigation of the excitation functions of their cross sections. While uranium-233 is not frequently utilized as reactor fuel, uranium-235 has historically been the most frequently used fissile element. When thermal neutrons are absorbed or captured, they both start to fission. But one of the main problems with uranium-233 is that it might wind up creating uranium-234, which is a fertile substance when it captures thermal neutrons. This indicates that it has a lower fission probability than uranium-235. This obvious fact is further demonstrated by the excitation functions examined previously. Because of this, uranium-233 is still not used as much as uranium-235 in comparison, even though it has been frequently recommended for use as reactor fuel. Uranium-233 should be considered as a nuclear reactor fuel in the meantime. It is a secure alternative fuel for reactors and is advised.

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تأثيرات الإثارة في النظائر الانشطارية لليورانيوم المستحثة بالنيوترونات باستخدام كود *OPTMAN* لغاية 20 *MeV*

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الخلاصة

في هذا العمل، تمت دراسة النظائر الانشطارية المستحثة بالنيوترونات لليورانيوم، على وجه الخصوص؛ اليورانيوم ـ 233 واليورانيوم ـ 235 باستخدام كود النموذج البصري ذي القنوات المزدوجة (*OPMAN*) حتى 20 إلكترون فولت. استلزم الطلب الكبير على وقود المفاعلات النووية إجراء هذا البحث. كواحد من النويدات المشعة الرئيسية التي تحدث بشكل طبيعي مع وجود الكثير من التنقيب عن الوقود، حدث اليورانيوم ـ 233 في أثر بينما ظهر اليورانيوم ـ 235 في 0.71% . يمكن أن تؤدي العملية بخطوتين بعيدًا عن اليورانيوم ـ 233 واليورانيوم ـ 235 عند التقاط النيوترونات إلى إنتاج مواد انشطارية لاستخدامها كوقود للمفاعلات. على الرغم من أن اليورانيوم ـ 233 واليورانيوم ـ 235 ليسا في حد ذاتها مادة انشطارية، لكنهما وقود مفاعل التوليد. تم إجراء الحسابات لكل من المشتقات المحتملة الموسعة (*PED*) والتي تمثل نموذج الدوار الصلب (*RRM*) الذي يعامل النوى على أنها كرة اهتزازية صلبة بالإضافة إلى حساب الحفاظ على الحجم النووي وإمكانات النموذج الدوراني (*RMP*) التي تمثل نموذج دوار ناعم (*SRM*) يتعامل مع النوى كأشكال كروية مشوهة دوارة ناعمة. تمت مقارنة كل من البيانات المحسوبة بالبيانات المسترجعة من ملف *Dada* النووي المقيَم (*ENDF*) والذي وجد أنه في توافق جيد. تم العثور على طاقات العتبة في جميع الحالات لتكون ≥ 4 *MeV* لكل من *PED* (توسع المحتمل بواسطة المشتقات) و *RMP* (إمكانات النموذج الدوراني). ويلاحظ أن النتائج من خطة إدارة المبردات تتفق بشكل أفضل مع البيانات المسترجعة من تلك التي تم الحصول عليها من *PED*.

الكلمات الدالة: التقنية الالية؛ منظومة حقن الجريان؛ نهج الاقتران منظومة الحقن مع الايون الانتقائي للأيونات؛ القطب الانتقائي للأيونات .

التمويل: لايوجد.

بيان توفر البيانات: جميع البيانات الداعمة لنتائج الدراسة المقدمة يمكن طلبها من المؤلف المسؤول.

اقرارات:

تضارب المصالح: يقر المؤلفون أنه ليس لديهم تضارب في المصالح.

الموافقة الأخلاقية: لم يتم نشر المخطوطة أو تقديمها لمجلة أخرى، كما أنها ليست قيد المراجعة.