

重水素学：重水素が示す特性の理解と活用

領域番号 20B204

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研究成果報告書

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研究成果の概要：

本領域の目的は、重水素が示す特性を深く理解し、物質の機能を精密な重水素化により最大限に引き出す研究領域「重水素学」の創成である。本領域研究を通じて、医薬品をはじめ幅広い材料に重水素を導入する基礎を構築し、重水素化で物質の機能をデザインする次の時代のスタンダード「Deut-Switch」を提案した。近年、重水素化物質は重医薬品として脚光を浴びるようになったが、重水素化された物質の応用は、医農薬品に留まらず、エネルギー・通信、分子イメージング、中性子分光のような産業的な応用分野にまで拡大していくと考えられる。研究領域「重水素学」の構築ならびに重水素に関する研究および技術の発展は、物質科学の水準を格段に向上させ、社会を一步前に進める鍵となり得る。本研究活動により「重水素学」はその普及に向けて意義深い一步を踏み出した。

研究組織

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交付決定額 (配分額)

	合計 (千円)	直接経費 (千円)	間接経費 (千円)
令和 2 年度	55,900	43,000	12,900
令和 3 年度	51,220	39,400	11,820
令和 4 年度	51,220	39,400	11,820
総計	158,340	121,800	36,540

研究発表

○原著論文

A01

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A04 該当なし

○総説

A01

- 澤間善成. 重水素標識機能性材料の網羅的合成を目指して. *YAKUGAKU ZASSHI.* **2022**, *142*, 139–144. DOI: 10.1248/yakushi.21-00173-2 (査読有)
- 澤間善成. 重水素化体の合成と重水素学(Deut-Switch)としての歩み. *生産と技術*, **2022**, *74*, 55–58. (査

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A02 該当なし

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A04 該当なし

○受賞

2022	糸賀萌子 (京大院薬)	第 42 回有機合成若手セミナー 優秀研究発表賞
2022	今井啓介 (阪大院薬)[26PO8-pm1-12S]	日本薬学会第 142 年会 学生優秀発表賞
2022	森山将吾 (阪大院薬)[28PO8-pm1-09S]	日本薬学会第 142 年会 学生優秀発表賞
2023	小笠原陸 (阪大院薬)[28B1-pm08S]	日本薬学会第 143 年 学生優秀発表賞
2023	前光結 (阪大院薬)[26P1-am1-028S]	日本薬学会第 143 年 学生優秀発表賞
2023	小林文音 (同志社女大薬)[27P2-pm2-007S]	日本薬学会第 143 年 学生優秀発表賞
2023	阪一穂 (阪大院薬)[P7-036]	第 13 回 CSJ フェスタ 2023 優秀ポスター発表賞
2024	清水彪雅 (阪大院薬)[29P-pm055S]	日本薬学会第 144 年 学生優秀発表賞

○その他

- ・重水素化医薬品の情報について領域内で情報源を整理し、領域ウェブサイトに掲載.
- ・提供可能な重水素化合物を領域ウェブサイトに掲載.
- ・重水素に関連する基礎的な専門用語の解説を用語集として領域ウェブサイトで共有.

領域ウェブサイト：<https://deut-switch.pharm.kyoto-u.ac.jp/>

成果一覧：<https://deut-switch.pharm.kyoto-u.ac.jp/results/>

それぞれの研究の成果報告 (KAKEN)：<https://kaken.nii.ac.jp/ja/grant/KAKENHI-AREA-20B204/>

International Review

Advisor: Dr. Tamim Darwish (NDF, ANSTO)

Due Feb 22, 2022. 17:00–19:00 JST (online)

Evaluation and Suggestions

1. Research Overview

The Deuterium Science Project (or Deut-Switch) that is led by A/Prof Naka from Kyoto University is encompassing 4 subprojects (or project pillars) that are interconnected and contribute to the main project which is aimed at widening the knowledge of deuteration and the use of the deuterium isotope in academic research as well as in industrial applications. The project is well connected domestically with multiple institutes and researchers who are pioneer in their research domains. The theoretical and computational studies group (A02) is a great asset to the research and it is able to support and engage quickly in the development of new ideas in the project. This is a unique component of a project of this kind which is difficult to find in similar research groups. The synthesis group is coming from a well established and productive catalysis group. The metabolic studies group is critical in the investigations of the kinetic isotope effect of deuterium on new lead compounds that are related to biological applications. The analytical group is fundamental to the above three pillars of the projects since it is needed in nearly every component. Therefore, I believe the project has all the necessary components to deliver success and innovation into the field of deuterium science. I believe there has been significant progress since last year in terms of the number of publications and the number of projects initiated. The project is now connected internationally through its membership on the Board of DEUNET which is a deuteration network that joins most if not all the deuteration facilities and groups around the globe. The presence of A/Prof Naka on the Communication Committee of this network is a great opportunity to enhance the outreach activity of the group internationally. The project still have 1 year of funding and I believe the focus now should be on the following areas:

- Articulate the uniqueness of capabilities in this group and what they can contribute to the international deuteration research community. While synthesis or deuterium analysis is available in other deuteration facilities and groups, skills and knowledge developed in theoretical studies, metabolic studies, and analysis are unique when they work together.
- International outreach and collaboration with international groups
- Communicate the value and impact of deuteration research in simple language
- Provide their unique research capability to other deuteration groups and formalize research agreements with national and international partners. For example, the theoretical and computational group is unique on its own whilst other deuteration facilities and groups don't have this specialized skill that would complement many deuteration research projects.
- Produce a white paper presenting the research capabilities of the group that can be used to attract funding from industry
- Utilize their position in academia to work on postgraduate programs for training the next generation deuteration scientists. The field lacks this training and will benefit greatly from such program. This can be performed in association with other domestic and international deuteration facilities.

- Attract PhD students who can work on some of the objectives of the project to alleviate capacity issue in the project.

2. Individual Research: Projects and Achievements

A01: New deuteration methods have been established in this subgroup of the project. This team is well established and very productive. It would be great for the Deuterium Science project to advertise for this research capability within the DEUNET to attract more international collaboration.

A02: This is a unique capability in this project that is not available elsewhere in the deuteration groups and facilities. It is highly recommended for the project to continue forming research collaborations with international groups by providing this capability. This is currently happening as evident by the paper published by Udagawa et al. Theoretical studies on the deuteration of surfaces is another novel area that this group can contribute to if possible. Deuteration of surfaces has potential applications in the electronic and semi-conductor industries.

A03: Research capability in the area of metabolism of deuterated compounds is a great advantage for this project. Further international collaboration with synthetic groups will bring more ideas and research projects. The challenge is to identify the projects that will have the highest impact if successful. Drug companies can be consulted, and partnership can be established to maximize the research outcome.

A04: The analysis group and the knowledge that can be developed in the area of deuterium level calculation is fundamental in almost all areas of this project.

3. Managements of the Research Area

The project has advisory committee that is composed of national and international advisors. Coordinating projects seems to happen through A/Prof Naka based on the strategic objectives of the project. There is limitation in capacity and resources in the project which forms a bottle neck in advancing quickly research ideas. As a result the recommended approach, if possible, would be to consider the value and impact in choosing the research projects in the group and try to involve PhD students to alleviate capacity issues. A science advisory group is an option to consider which could help in advising on science impact of projects to focus the efforts for better outcomes.

4. Support for Young Researchers; Public and International Engagement; Enhancing Diversity

Over the last year, the project has been developing its website and the outreach strategy with some good activities so far, e.g., the young scientists meeting and the strong presence in DEUNET. The project has very good networks domestically and is advocating for their capabilities internationally. The latter is where the focus is believed should be taking place in the next stage of this project.

Other Comments and Suggestions

None.