様　式　Ｃ－１９、Ｆ－１９－１、Ｚ－１９　（共通）

科学研究費助成事業　　研究成果報告書

令和　５ 年　 ６ 月 １２ 日現在

機関番号：８２１０８
研究種目：基盤研究(C)（一般）
研究期間：2019～2022
課題番号：１９Ｋ０５２２９

研究課題名（和文）3D spatial imaging of chirality using nuclear magnetic resonance (NMR)

研究課題名（英文）3D spatial imaging of chirality using nuclear magnetic resonance (NMR)

研究代表者
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研究者番号：００７２０６９０

交付決定額（研究期間全体）：（直接経費）　　3,300,000円

研究成果の概要（和文）：一連のポルフィリン型化合物を合成した。これらの化合物は、陰イオン結合性が向上し、触媒活性が向上することが検討された。これらの材料は一重項酸素を発生させることができ、治療応用（光線力学的療法など）に重要である。我々は、NMRスペクトル交換ラインシェイプを解析的に計算する方法を開発しました。この方法は、ホスト-ゲスト複合体、互変異性体過程、局所的な分子回転など、幅広い系における分子動力学の解析に用いることができる。また、適切なポルフィリン型分子検出器を用いることで、NMRマイクロイメージング法により、キラル環境（エナンチオマー過剰）をサブミリメートルの分解能で空間的にモニターできることも証明した。

研究成果の学術的意義や社会的意義
Most drugs currently in use are chiral compounds. In situ or in vivo chirality imaging would be helpful in drug development. We have shown that the NMR microimaging technique can achieve this using an appropriate molecular detector.

研究成果の概要（英文）：A series of porphyrin- or oxoporphyrinogen-type compounds were synthesized. Namely, β-functionalized, non-planar N-heterocycle-fused, and star-shaped water-soluble porphyrins. These compounds were studied for their improved anion-binding properties and catalytic activity. Some of the compounds can form porous coordination polymers. These materials are also capable of singlet oxygen generation and therefore are interesting for therapeutic applications, especially photodynamic therapies.
We have developed a method for analytical calculation of NMR spectral exchange lineshapes. The method can be used to analyze molecular kinetics in a wide range of systems, such as host-guest complexes, tautomeric processes, or local molecular rotations. We have also proven that by using a suitable porphyrin-type molecular detector, a sub-millimetre resolution of chiral environment (i.e. enantiomeric excess) can be spatially monitored by NMR microimaging method.

研究分野：物理化学

キーワード：Porphyrin　Chirality　NMR lineshape　Phase Separation　pH-responsiveness　Chemical kinetics　NMR microimaging

様　式　Ｃ－１９、Ｆ－１９－１、Ｚ－１９（共通）

１．研究開始当初の背景

Chirality is a critical feature in many biological events. The two enantiomers of the same molecule differ when interacting with other chiral species. This is especially important in the development of new pharmaceuticals where their pharmacological effect depends on the identity of the enantiomer. More than half of the drugs currently used are chiral compounds, and nearly 90% of the latest ones are marketed as racemates (consisting of an equimolar mixture of both enantiomers, usually due to a costly separation process). Although they have the same chemical structure, most isomers of chiral drugs exhibit differences in biological activities such as pharmacology, toxicology, pharmacokinetics, metabolism etc. Therefore, it is essential to promote the chiral separation and analysis (monitoring) of chiral drugs in the pharmaceutical industry and clinical use to eliminate the adverse effects of unwanted enantiomers and improve the patient treatment process. Therefore, chirality imaging which can be performed *in situ* or *in vivo* can be a useful tool for drug development and analysis of effects of new drugs. There is also a need to monitor and separate individual enantiomers in industrial and research applications.

Previously we have developed a novel Nuclear Magnetic Resonance (NMR) chirality detection mechanism, which is *not based on* the formation of *diastereomeric complexes*. More specifically, the method can determine enantiomeric excess (*ee*), a quantity usually used to assess the enantiopurity of the sample (*Acc. Chem. Res.*, 2015; *Nat. Commun.*, 2013; *Chem. Eur. J.*, 2011, *patents in* 2017, 2014). In this method, the chiral information is transferred in the formed host-guest complex from *chiral* analyte to *achiral* detector molecule (porphyrin-type macrocyclic compound) and subsequently read out using NMR. Therefore, the detector molecule is called a pro-chiral solvating agent (pro-CSA). This method has a good potential for further improvements and applications.

２．研究の目的

The purpose of this project is to develop NMR enantiomeric excess (*ee*) mapping method, which can be used for monitoring local *ee* content, ideally with spatial (i.e. in 3D space) and temporal resolution (i.e. in time). Such a method would allow the investigation of various chiral interconversion, enantioenrichment or racemization reactions (e.g. Soai-type reaction, pharmacokinetics, drug metabolism, etc.) *in situ* or *in vivo*. Part of the aim is also the development of robust NMR techniques, which will be used for the actual spatial *ee* detection.

３．研究の方法

In order to achieve the targets of this proposal, novel porphyrin-type and also other molecules (e.g. metal complexes) were prepared by organic synthetic methods. Some of the molecules were modified in order to achieve water solubility, an essential feature for applications. The aim was to probe a broader set of molecules that can serve as enantiomeric excess (*ee*) detectors. The structure of these compounds was characterized using analytical methods, such as NMR spectroscopy, UV-Vis, FTIR, etc. and, where possible, by X-ray crystallography. In some cases, we employed the DFT calculations and classical molecular dynamics (MD) simulations to closely understand the physical behaviour, kinetics, or inter- and intra-molecular interactions.

We also theoretically and experimentally improved the analyses of NMR spectral patterns (so-called NMR lineshapes) of host-guest systems. The formation of a host-guest complex is essential for the transfer of chiral information (*ee*). The NMR lineshape of the host-guest complex was analyzed based on the temperature and concentration of individual components. These findings are useful for processing data obtained from measurements of the 3D spatial distribution of *ee* by means of NMR micro-imaging techniques.

４．研究成果

The results can be divided into three categories: (a) Synthesis of novel porphyrin-type molecules and basic characterization, (b) Theoretical and experimental analyses

of NMR spectral patterns, and (c) Measurements of 3D spatial distribution of chirality.

(a) Synthesis of novel porphyrin-type molecules and basic characterization.
As a part of this project, a series of compounds were prepared (Figure 1): β-functionalized calix[4]pyrrole derivatives (**1-3**) based on the oxoporphyrinogen (OxP) core chromophore including non-planar saddle-shaped N-heterocycle-fused metallo-porphyrinoids (**2**), star-shaped water-soluble porphyrins containing tetraethylene glycol monomethyl ether chains (**4**) or poly(N-isopropylacrylamide) chains (**5**) at the periphery, and chiral 1,1'-binaphthyl-linked diporphyrin 'tweezers' (**6**) were prepared.

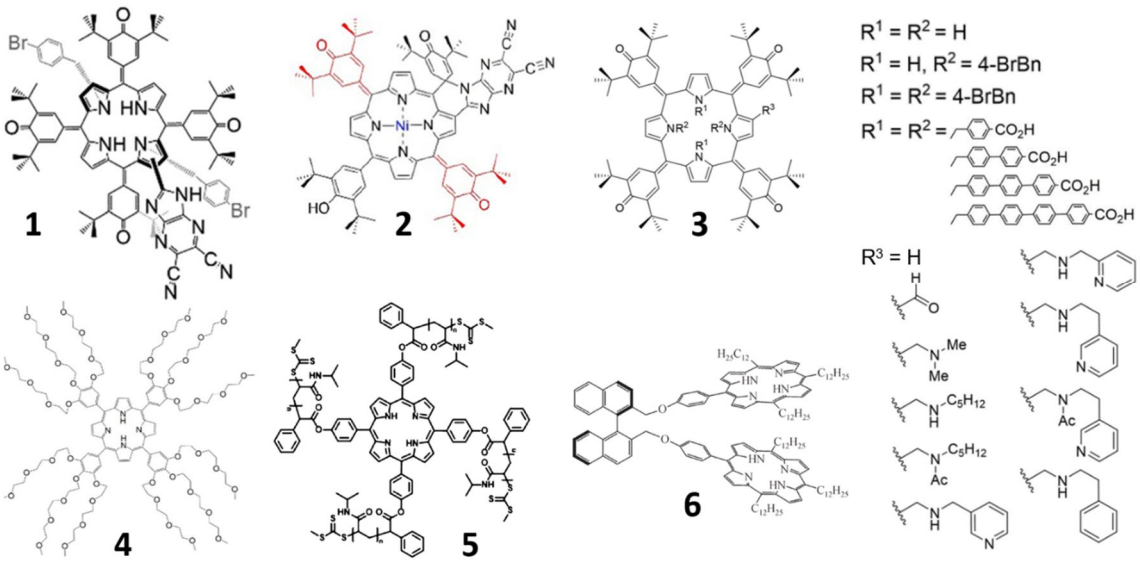

Figure 1. Compounds synthesized in this work.

Synthesized molecule **1** was studied for improved anion binding properties compared to the parent oxoporphyrinogen (OxP) due to the tritopic interaction point with anion. Molecule **2** forms a persistently microporous crystalline material, which can be prepared directly from the solution without loss of microporosity. A series of molecule **3** were investigated for their activity as H-bond donor catalysts, which operate at low catalysts loadings (≤ 1 mol-%). The beta-substitution is essential to establish catalytic activity. The catalysts exhibit activity in the Michael addition reactions, sulfa-Michael additions, and Henry and aza-Henry reactions. Some of the compounds **3** were also used to synthesize porous coordination polymers with pseudotetrahedral structures using well-known oxo-Zr(IV)$_6$ cluster chemistry. These materials are capable of singlet oxygen generation and therefore are interesting for therapeutic applications, especially photodynamic therapies, oncological treatments and photodynamic inactivation of pathogens.

Also, water-soluble star-shaped porphyrins **4** and **5** were synthesized. Highly soluble, nonionic porphyrin **4** possesses excellent singlet oxygen ($^1O_2$) quantum yield (QY) in a wide variety of common solvents, including water. Its $^1O_2$ QYs in the different solvents studied were found to be 0.86 (acetone), 0.59 (acetonitrile), 0.66 (chloroform), 0.85 (methanol), 0.45 (toluene) and 0.51 (water). Compound **4** can also be used as a reliable and easy-to-implement reference compound to estimate the $^1O_2$-generating activities of new materials. Porphyrin with four poly(N-isopropylacrylamide) chains (**5**) was investigated for its temperature-induced phase separation behaviour. It exhibits lower critical solution temperature (LCST) type II phase behaviour (the experimental data were modelled using Flory–Huggins theory). Various temperature–pH reversible and irreversible "cross-effects" between phase separation and protonation were observed. Below phase-separation temperature (T_p), **5** behaves as a 1D supramolecular polymer with a concentration-dependent length, while above T_p, **5** adopts large spherical globular structures.

Chiral 1,1'-binaphthyl-linked diporphyrin 'tweezers' **6** were prepared as chiral host molecules, and their utility for chiral analyses (especially enantiomeric excess (*ee*) determinations) were evaluated. The host molecules could be used as multichannel probes

of *ee* by using UVvis, circular dichroism (CD), fluorescence emission and ^{1}H nuclear magnetic resonance (^{1}H-NMR) methods.

All these properties are closely related to the formation of host-guest complexes, which is the key concept for chirality sensing. We used the most promising compounds for NMR micro-imaging (see below).

(b) Theoretical and experimental analyses of NMR spectral patterns.
We have developed a method for analytical calculation of NMR spectral exchange lineshapes for general N-state spin kinetics (in the absence of J-coupling) (Figure 2a). Several special cases of two-state, three-state and four-state spin kinetics and their relevance to host-guest binding or isomerization processes, including examples from literature, have been investigated in detail. These examples illustrate the importance of differentiating between ‘reaction rate coefficients’, which describe chemical kinetics, and ‘transition rate coefficients’, which describe spin kinetics. We also introduced the concept of ”reduced equivalent schemes” for spin kinetics containing a fast-exchanging state. These schemes contain fewer states with modified transition rate coefficients, which still contain a physical meaning and allow for the contractions of “expanded chemical kinetics” schemes.

The method can be used to describe molecular kinetics in a wide range of interesting systems with a variety of intra- or intermolecular processes, such as host-guest complexation of oxoporphyrinogen+acid (Figure 2b), tautomeric processes in protonated tetraphenylporphyrin (TPP) (Figure 2c), ligand exchange in Zn_2 coordination complexes (Figure 2d), rotation of phenol meso-substituents in oxidized resorcinarene (Figure 2e) or kinetics of meso-chiral (cis-trans) interconversion in a butterfly-shape overcrowded alkene rotor (Figure 2f).

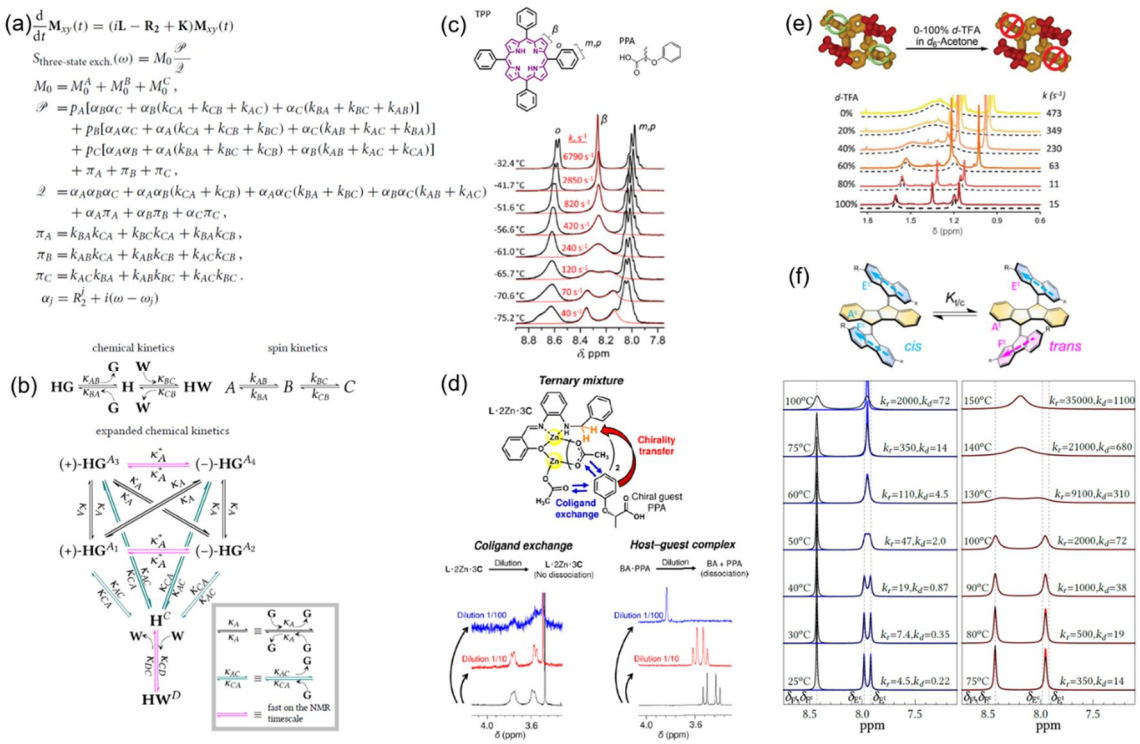

Figure 2. (a) Equation governing evolution of transverse magnetization M_{xy} under chemical exchange of non-*J*-coupled spins modelled classically using Bloch-McConnel equation. An exact solution for NMR spectral lineshape for three-state chemical exchange is shown. (b) Consecutive three-state exchange in 1:1 host-ligand competitive binding: chemical kinetics model and corresponding spin kinetics model. An expanded chemical kinetics scheme is also shown. (c) Tautomerism processes in protonated tetraphenylporphyrin (TPP) and its temperature dependence as obtained by NMR measurements. (d) Ligand exchange in Zn_2 coordination complex and chirality detection of a guest. (e) Rotation of phenol meso-substituents in oxidized resorcinarene affected by solvent composition. (f) Kinetics of meso-chiral (cis-trans) interconversion in a butterfly-shaped overcrowded alkene molecule.

(c) Measurements of 3D spatial distribution of chirality.
The 3D NMR microimaging measurements were performed at the wide-bore NMR device equipped with special probes (Figure 3a) located at Charles University, Prague, Czech Republic. To achieve the ultimate goal (Figure 3b), firstly, we prepared a series of test samples with defined and spatially well-resolved enantiomeric excess (*ee*). Figure 3c shows the result of the NMR microimaging measurement of the sample cross-section with contrast dependent on the local *ee* value.

Due to the Covid-19 travel restrictions, we could not perform all necessary NMR experiments at Charles University, Czech Republic, as initially planned in the proposal. Therefore, at this stage, we cannot disclose the exact molecular detector and conditions (spectra processing method and contrast generating algorithm) used in these NMR imaging studies. However, the concept of spatial enantiomeric excess detection at a sub-millimetre scale using NMR microimaging was proven possible. In the future, detailed experimental conditions will be published.

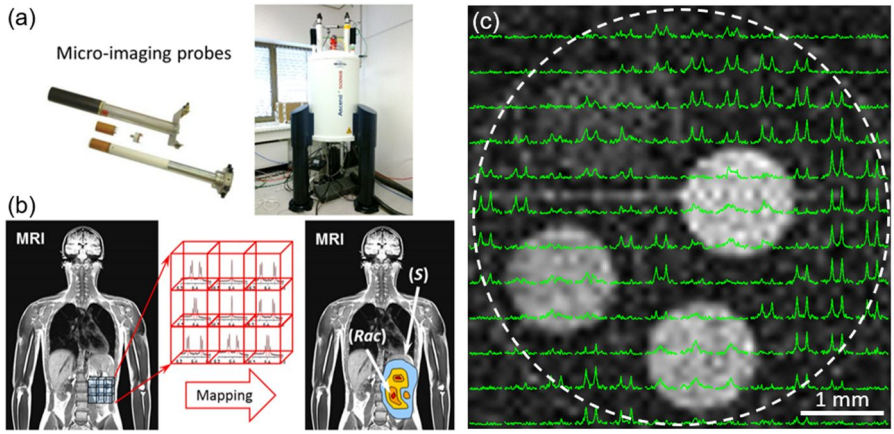

Figure 3. (a) NMR microimaging instrument with special probes. (b) Schematic visualization of in vivo enantiomeric excess (*ee*) mapping of chiral metabolites using MRI. (c) Sample cross-section obtained on specimen consisting of five areas with different *ee* (four small circles and surrounding within a dashed white circle). A dashed white circle denotes the sample border. The brightest area has *ee* = 0 %, and the black (dark) area has *ee* = 100 %. Actual NMR spectra, as obtained from individual voxels, are overlaid.

５．主な発表論文等

〔雑誌論文〕　計15件（うち査読付論文　15件／うち国際共著　15件／うちオープンアクセス　2件）

１．著者名 Labuta Jan、Ishihara Shinsuke、Payne Daniel T.、Takimoto Kazuyoshi、Sato Hisako、Hanykova Lenka、Ariga Katsuhiko、Hill Jonathan P.	４．巻 9
２．論文標題 Estimation of Enantiomeric Excess Based on Rapid Host-Guest Exchange	５．発行年 2021年
３．雑誌名 Chemosensors	６．最初と最後の頁 259～259
掲載論文のDOI（デジタルオブジェクト識別子） 10.3390/chemosensors9090259	査読の有無 有
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２．論文標題 Molecular rotor based on an oxidized resorcinarene	５．発行年 2022年
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2．論文標題 meso-Tetraphenylporphine as a prochiral solvating agent (pro-CSA): A physicochemical study	5．発行年 2020年
3．雑誌名 J. Porphyrins Phthalocyanines	6．最初と最後の頁 320-329
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2．論文標題 Knock-on synthesis of tritopic calix[4]pyrrole host for enhanced anion interactions	5．発行年 2019年
3．雑誌名 Dalton Trans.	6．最初と最後の頁 15583-15596
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1．著者名 Chahal Mandeep K.、Maji Subrata、Liyanage Anuradha、Matsushita Yoshitaka、Tozman Pelin、Payne Daniel T.、Jevasuwan Wipakorn、Fukata Naoki、Karr Paul A.、Labuta Jan、Shrestha Lok Kumar、Ishihara Shinsuke、Ariga Katsuhiko、D ' Souza Francis、Yoshikawa Genki、Yamauchi Yusuke、Hill Jonathan P.	4．巻 7
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2．論文標題 NMR lineshape analysis using analytical solutions of multi-state chemical exchange with applications to kinetics of host-guest systems	5．発行年 2022年
3．雑誌名 Scientific Reports	6．最初と最後の頁 1～15
掲載論文のDOI（デジタルオブジェクト識別子） 10.1038/s41598-022-20136-4	査読の有無 有
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1．著者名 Hill Jonathan P.、Karr Paul A.、Zuniga Uy Roxanne A.、Subbaiyan Navaneetha K.、Futera Zdenek、Ariga Katsuhiko、Ishihara Shinsuke、Labuta Jan、D ' Souza Francis	4．巻 26
2．論文標題 Analyte Interactions with Oxoporphyrinogen Derivatives: Computational Aspects	5．発行年 2022年
3．雑誌名 Current Organic Chemistry	6．最初と最後の頁 580～595
掲載論文のDOI（デジタルオブジェクト識別子） 10.2174/1385272826666220208101325	査読の有無 有
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2．発表標題 Thermal treatment of phase-separable polymers as a possible route to functional porous heterostructures
3．学会等名 International Conference on Materials Science and Engineering 2021（国際学会）
4．発表年 2021年

１．発表者名
Jan Labuta

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2021年

１．発表者名
Jan Labuta

２．発表標題
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３．学会等名
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Jan Labuta

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〔図書〕　計0件

〔産業財産権〕

〔その他〕

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６．研究組織

	氏名 （ローマ字氏名） （研究者番号）	所属研究機関・部局・職 （機関番号）	備考

７．科研費を使用して開催した国際研究集会

〔国際研究集会〕　計0件

８．本研究に関連して実施した国際共同研究の実施状況

共同研究相手国	相手方研究機関