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Perspective

Pseudo-Resonance Structures: Potential Functional Materials and/or Pharmaceutical Applications

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Introduction

Pseudo-Resonance Structures (PRS) have been reported recently [1]. These structures have two sets of physical data-for instance, dual NMR spectra in solution (e.g., compound **1** in Figure 1), or two distinct structural forms observed in X-ray crystallography, even two sets of ^{13}C Cross-Polarized Magic Angle Spinning (CP-MAS) NMR spectra in the solid state (as in compound **2**), including separate IR absorption bands for the same >C=O group (**2**). In some cases, both solution and solid-state data show such duality, as exemplified by compound **3** (Figure 1). Notably, several natural products, such as **4** and **5**, have also been re-identified as belonging to the PRS category [2,3].

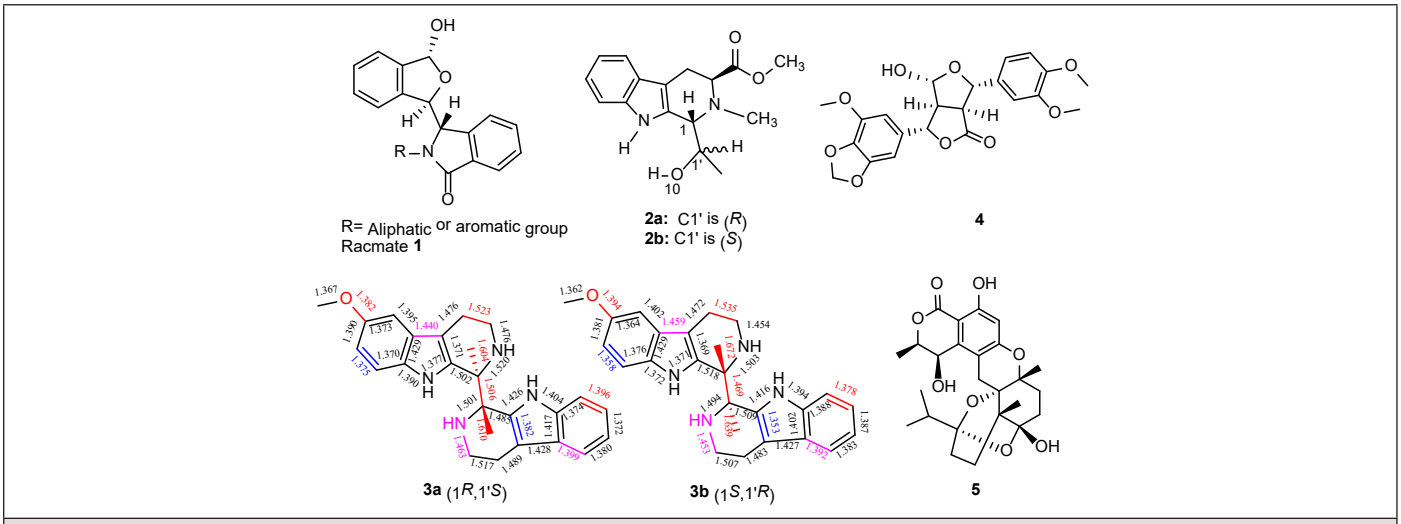

Figure 1: The three compounds 1 to 5.

It is hypothesized that the observation of dual NMR signals for PRS in solution may reflect alternating bond-length changes, similar to those documented for compound **3**. These systems exist as dimers in solution-a structure that remains remarkably stable even at elevated temperatures up to 350 K in DMSO-d_6. [2b]The possible distinct bond lengths between the two forms necessarily lead to separate sets of physical data, as the electron density distribution differs in each structure. A representative example is

compound **6** (Figure 2), which displays four sets of NMR spectra due to the presence of atropisomers in solution [4]. A strong hydrogen bond forms between molecules **6A** and **6B**, which is the key point for formation of a dimer of PRS, the positive proton of the –OH group in molecule **6A** moves closer to the carbonyl oxygen of molecule **6B**. Therefore, the C=O bond in molecule **6B** becomes longer, and the O–C bond in molecule 6A likely becomes shorter. Through combined conjugative and inductive effects, this leads a partial negative charge to molecule 6A and a partial positive charge to molecule 6B (Figure 2A). Such electronic asymmetry is responsible for the appearance of multiple NMR signal sets. This non-uniform charge distribution further suggests that the dimer may exhibit optical or electronic properties distinct from those of the monomer. Structurally, the aromatic substituent on the nitrogen atom can be varied; for example, the 1 naphthalenyl group in 6 could be replaced by larger conjugated systems such as a pyren 2 amine moiety or even bulkier aromatic units. These aromatic systems can readily stack via π–π interactions and electrostatic attractions, leading to the formation of layered architectures. Owing to their tunable electronic asymmetry, such materials may exhibit different conductivity or other desirable traits relevant to functional materials research, such as in OLEDs and/or related technologies.

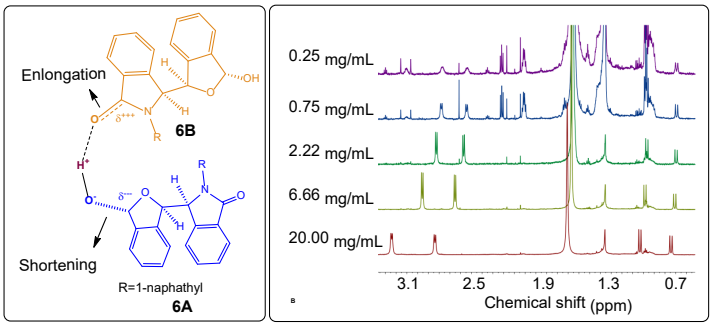

Figure 2: (A) The proposed dimer structure 6 in solution. (B) Concentration-dependent 1H NMR signals for racemic 6.

In addition, the dimer structures remain stable even in methanolic solution. Interestingly, when compound **6** is diluted to 25μg/mL, [4] it exhibits complex ^{1}H NMR signals in the range of 0-4ppm (Figure 2B). This suggests the emergence of multiple new structural forms in the diluted solution. Under such conditions, if a more suitable aromatic substituents or a less bioactive groups were used to replace the 1 naphthalenyl group in **6**, the various dimers may play a significant role in bioactivity studies, as dimeric structures generally exhibit stronger biological effects-such as antitumor activity-compared to their monomeric counterparts [5]. If these two structural forms can dock with corresponding target sites within an enzyme or protein, they may exert more pronounced bioactive roles. Notably, a relevant example has been reported in which structure 7 binds to the enzyme in two distinct orientations (Figure 3) [6]. Importantly, these two forms of structure 7 display alternating bond-length changes similar to those observed in compound **3**.

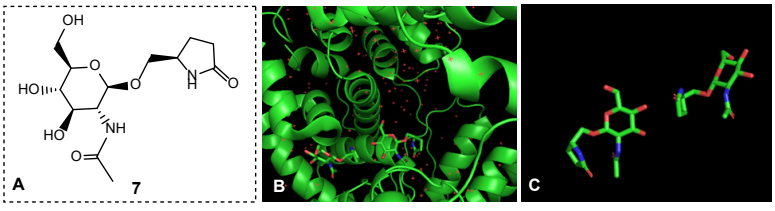

Figure 3: (A) Structure of compound 7. (B) The docking sites and orientations of compound 7. (C) The 3D structure and relative orientation of 7 isolated from the sites.

Summary

In summary, as a novel structural type, PRS display characteristics that depart from the conventional understanding that a single compound typically corresponds to one set of physical data-such as a single NMR or IR spectrum. Grounded in the fundamental principle that structure determines function, PRS may offer a promising platform for the rational design of some kinds of functional materials and/or pharmaceuticals in the synthetic fields.

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