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Dibenzothiazepine Based MCR Chemistry

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Privileged scaffolds which can unveil unknown territories of the chemical space are constantly prominent. As such, 1,5-dibenzothiazepines not only offer structural diversification but also a very unique binding mode due to their "butterfly" conformation. We provide MCR-based annulations of this scaffold towards three different tetracycles in a straightforward, two-step procedure. We synthesize a library of 30 tetracyclic 1,5-tetrazolo-, fused imidazo- and lactam-1,5-dibenzothiazepines with scalable and one-pot procedures. In addition, we obtained single crystal structures of certain derivatives, demonstrating the conformational behavior of the scaffold.

Introduction

As a continuation of the quest for exploring different areas of the chemical space[1] for novel entities with interesting dynamic properties, we spot the 1,5-dibenzothiazepine (Figure 1A). It constitutes a privileged scaffold with unique properties and conformations (Figure 1B).[2,3] Three features of the dibenzothiazepine scaffold renders it a prime hub for further elaboration and medicinal chemistry strategic syntheses: a secondary amine, an oxidizable sulfur atom embedded in a tricyclic ring system and a unique "butterfly" conformation (Figure 1A, Figure 1B).[4,5] Many commercial drugs consist of a benzothiazepine core, including quetiapine, metiapine and clotiapine with an antipsychotic mechanism of action[6–9] and bioactive compounds[2,3] such as Ca^{2+} channel blockers,[10] antiviral,[11,12] antimicrobial,[13] antifungal,[14] histone deacetylase 6 (HDAC6) inhibitors[15] and even molecules with interesting electronic properties (Figure 1C).[16]

The unusual conformational equilibrium, which has been reported multiple times,[4,5,17–19] affords atropisomers. Those atropisomers, which depend on the substitution pattern can have high energy interconversion and can be separated, are non-superimposable mirror images thus, enantiomers. The addition of extra rings restricts the inversion of the seven membered ring which improves the thermodynamic profile of the scaffold.[2] In addition, it offers a very specific binding mode in various targets (Figure 2).[11,14] Atropisomers are becoming more and more important in medicinal chemistry and are challenging to selectively construct.[20]

Although there are quite a few sequential approaches towards 1,5-dibenzodiazepine derivatives, divergent approaches which allow the rapid synthesis of versatile libraries for screening docks are scarce.[2,3,21,22] Multicomponent reactions chemistry (MCRs)[23] is one of the tools that allows for fast and convergent access on polycyclic (more than three rings), diverse

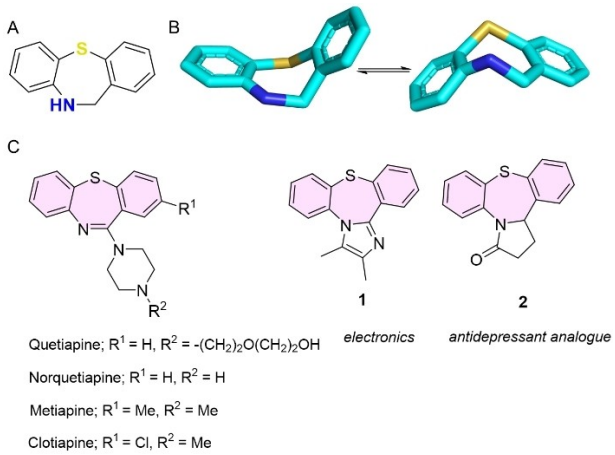

Figure 1. A. The privileged structure of the tricyclic dibenzothiazepine with the secondary NH and the oxidizable sulfur atom; B. The "butterfly" conformation of the ring with the isomer interconversion; C. Examples of molecules of interest based on the specific dibenzothiazepine core.

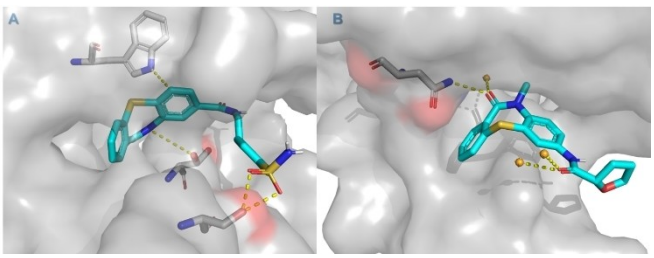

Figure 2. Dibenzothiazepine-receptor bind modes. A. The antiviral activity of the dibenzothiazepine DBT1 against the capsid protein of Hepatitis B Virus (HBV) (PDB ID 6WFS). A NH-π interaction of Trp102 (grey sticks) with the aromatic ring of 3.4 Å along with hydrogen bonds with Thr128 (grey sticks) and Ser121 (grey sticks) can be observed; B. The antifungal activity of a dibenzothiazepinone against the BET protein Bdf1. A hydrogen bond network between the carbonyl groups of the small molecule with Asn291 (gray sticks) and certain molecules of water (orange spheres) of 3.0 Å, 2.8 Å, 3.3 Å and 3.1 Å, respectively is revealed (PDB ID 5N17).

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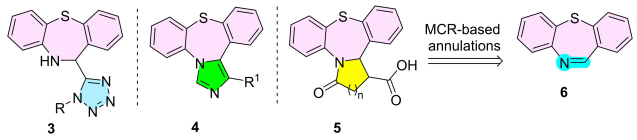
and complex adducts.[24–28] In general, MCRs have been utilized towards the 1,5-dibenzothiazepine core, e.g. Ugi-Joullie three-component reaction (UJ-3CR),[29] Mannich,[30] Strecker,[31] Pudovik reaction[32] and aza-Henry.[33,34] However, there is only one report of an MCR-based annulation of this scaffold towards polycyclic and rigid derivatives.[35]

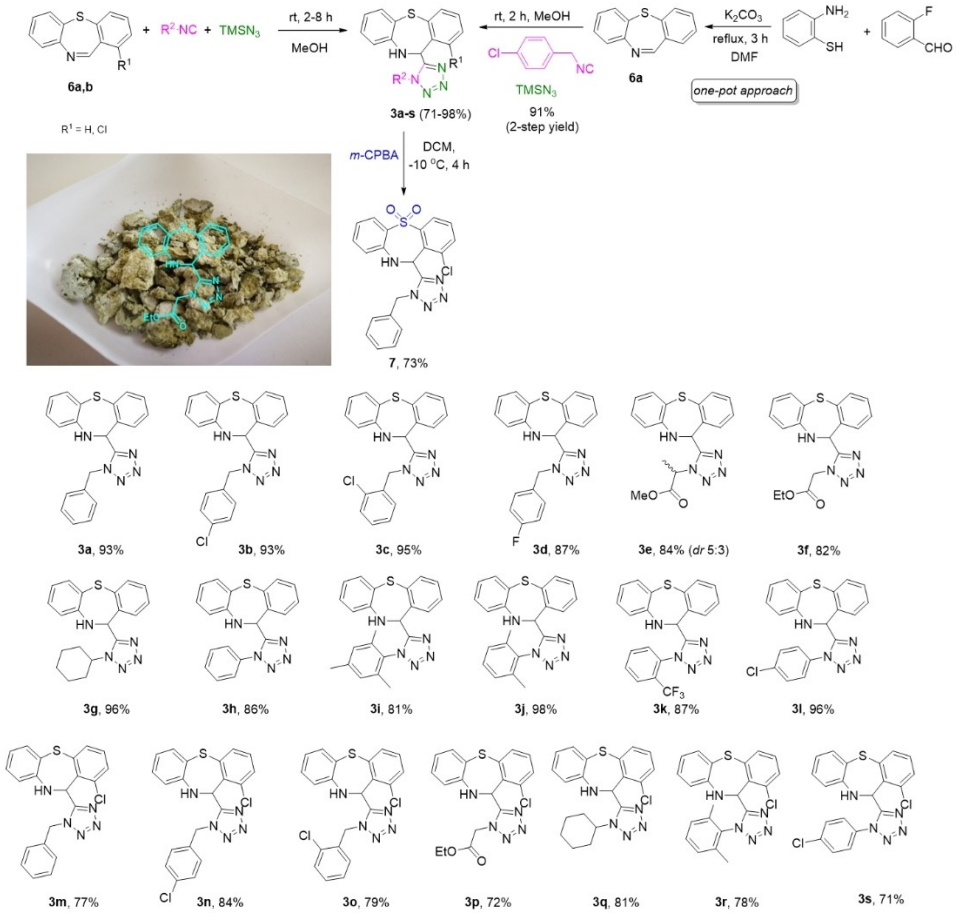
Specifically, the tetracyclic benzothiazepine scaffolds **3**–**5** are prevalent motifs encountered in synthetic pharmaceuticals, bioactive analogues[36–39] and in material science.[16] Our retro-synthetic plan towards distinct cycles such as the tetrazole, imidazole, γ- and δ-lactams rings consists of MCR-based annulations, starting from the versatile building block **6** and targeting the imine bond (Scheme 1).[40]



Scheme 1. Retrosynthetic plans towards the privileged tetracyclic scaffolds of **3**, **4** and **5** bearing a tetrazole (cyan), imidazole (green) and lactam (yellow) ring, respectively based on the dibenzothiazepine imine **6**.

Results and Discussion

We investigated the synthetic access of the unprecedented scaffold of the 1,5-tetrazolo dibenzothiazepines **3**. It is known that the tetrazole ring not only offers significant improvements of the physicochemical properties of the synthesized libraries[41] but it also serves as a bioisostere to carboxylic acids and cis-amides.[42,43] Noteworthy, fused tetracyclic tetrazolo dibenzothiazepine derivatives have demonstrated mild analgesic activity.[44] Thus, the reaction of the imines **6a**,**b** with TMS-azide and a range of different isocyanides afforded the desired 1,5-tetrazolodibenzothiazepines under very mild conditions in good to excellent yields (Scheme 2, 71–98%). The reaction proceeded smoothly with all the different isocyanides e.g. benzylic (**3a**–**d**, **3m**–**o**), aliphatic (**3e**–**g**, **3p**–**q**) and aryl (**3h**–**l**, **3r**–**s**) bearing both electron withdrawing (EWG) and donating groups (EDG). Amino acid-based isocyanides afforded the desired adducts as well, where the alanine gave expectedly a mixture of diastereomers (*dr* 5:3). The imine **6b**, bearing a chlorine on the 1-position of the aromatic ring, afforded the targeted library in slightly lower yields, probably due to solubility issues.



Scheme 2. The Ugi tetrazole reaction of the imines **6** towards the tetracyclic tetrazolo dibenzothiazepines **3**. An example of the one-pot approach is also shown. The scale-up of the reaction (left picture) and the oxidation of **3m** to the dioxide derivative **7** are shown.

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The reaction is scalable (Scheme 2, left image) as we synthesized **3f** on a 5 mmol scale (81% yield, 2.97 g).

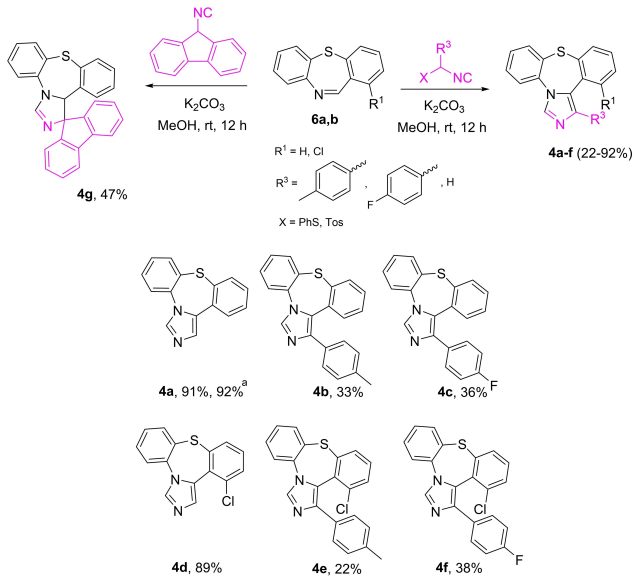
Attempting to first react the components in the UT-4CR followed by cyclization to the dibenzothiazepine failed: the reaction of *o*-aminothiophenol, *o*-fluorobenzaldehyde, the corresponding isocyanide and $TMSN_3$ afforded a complex mixture of products, despite attempts to optimize the reaction conditions. However, a sequential one-pot approach without purifying the intermediate imine, afforded the desired adduct (**3b**) in 91% yield. The imine **6a** can be simply synthesized by refluxing *o*-fluorobenzaldehyde and *o*-aminothiophenol in the presence of K_2CO_3[45] without the need of stronger bases and additives (Scheme 2).[29]

Due to the interesting biological activities that benzo[*f*][1,2]thiazepinedioxides possess,[2] we performed a post modification on the initial UT-scaffold. We oxidized the sulfur atom of the thiazepine ring with *m*-CPBA, affording the derivative **7** in 73% yield (Scheme 2).

Next, we investigated the van Leusen imidazole reaction,[46] to synthesize the fused tetracyclic imidazo-1,5-dibenzothiazepines **4**. Fused imidazo-azepines have been reported as selective GABAA receptor antagonist (e.g. Flumazenil),[47] antiviral and antibacterial agents.[48] Satisfyingly, under mild conditions, we were able to get the desired polycyclic thiazepines **4a–g** in good yields (Scheme 3, 22–91%). We employed not only TosMIC and its substituted derivatives (**4b–c**, **4e–f**) but also other acidic isocyanides such as the phenylsulfane (related to AsMIC)[49] and the fluorene isocyanide. Interestingly, the phenylsulfane isocyanide behaves similarly to TosMIC by which the thiophenolate acts as the leaving group (**4a**). Substituted TosMICs (**4b–c**, **4e–f**) led to reduced yields as expected due to their increased instability in the reactions conditions (prone to dimerization).[50] Fluorene isocyanide, which has been recently explored by us,[51] afforded the complex 7-membered spiro thiazepine **4g** (Scheme 3). In all cases, we obtained the imidazole thiazepines compared to the work of Sharma *et al.*[35] who afforded the corresponding imidazoline derivatives under different reaction conditions.

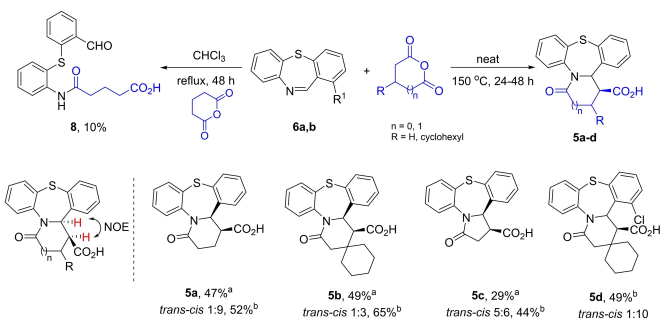
The third type of cycles that we approached are the γ- and δ-lactam carboxylic acids **5**. The reaction between imines and α-C–H cyclic anhydrides which provides the valuable[52,53] polysubstituted lactam carboxylic acids is generally known as the Castagnoli-Cushman reaction (CCR).[54–58] The reaction of the imine **6a–b** with three different cyclic anhydrides provided the desired adducts in good yields. The dibenzothiazepine imine survives the high temperatures and gives access in one-step under neat conditions to otherwise quite difficult to obtain γ- and δ-lactams **5**, as reported previously.[59–61] The reaction proceeds in a relatively diastereoselective way (Scheme 4); Interestingly, the major isomer is the *cis*-isomer as analyzed by both NOE experiments (see supporting information, SI) and the characteristic ^{1}H NMR patterns despite the fact that usually the CCR gives rise to the *trans* isomer in those reaction conditions.[62] However, we were able to obtain the major *cis* isomer (besides the case of **5d**) after recrystallization with EtOH.[56] Surprisingly, prolonged heating in lower boiling point solvents as chloroform or toluene led to ring-opening adducts[55] such as the derivative **8**, whereas refluxing in bromobenzene gave traces of the adducts **5** (Scheme 4).

Understanding the conformational behavior of the dibenzothiazepines is the key to clarify the way that these species behave on a molecular level and subsequently to better understand their interactions with a biological target.[18] We performed a data mining on the Cambridge Structural database (CSD)[63] on the solid-state characterization of this tricyclic scaffold, demonstrating that its overall shape is defined by both the conformation of the seven-membered ring and the relative arrangement of the fused aromatic rings.[17,18] In addition, we noticed that the tricyclic ring folding is influenced by the atom X (Figure 3, X = C, N, O, S).[5] Finally, dihedral angles R^{1}16–N14–C13–C12 and R^{2}17–C15–C3–C2 were taken into account revealing a relative planar conformation (see SI).



[a] *The first yield refers to the reaction with TosMIC, whereas the second yield refers to the reaction with phenylsulfane*

Scheme 3. The van Leusen reaction of the imines **6** with various acidic isocyanides towards the fused polycyclic dibenzothiazepines **4**.



[a] *Isolated yield of the cis-isomer;* [b] *Yield of the mixture trans-cis isomers*

Scheme 4. The Castagnoli-Cushman reaction of the imines **6** towards the γ- and δ-lactams **5**. In most of the cases the major cis-isomer was isolated.

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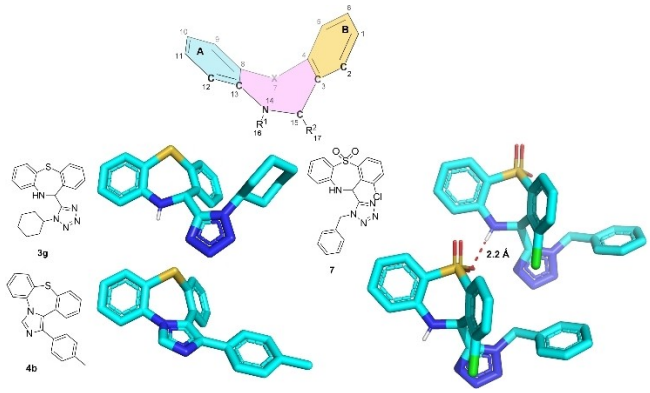

Figure 3. General structure of the dibenzothiazepine scaffold and crystal structures of the **3 g** (CCDC 2123183), **4 b** (CCDC 2123182) and **7** (CCDC 2123184).

In support of the aforementioned conformational behavior of the current scaffolds, we solved the crystal structures of the **3 g**, **7** and **4 b** (Figure 3). In all cases, both atropisomers are present in the unit cell.[19] The dibenzothiazepine ring adopts both the expected butterfly conformation and the geometrical features of this scaffold (*verified by "Mogul geometry check" of the CCDC suite*). Compound **7** possess an intramolecular hydrogen bond of 2.2 Å between the oxygen of the $-SO_2$ group and the polar hydrogen atom of the N–H. In comparison of the **3 g** and **7** with the fused bicyclic compound **4 b**, we can observe the increased rigidity that the fused ring offers to the system. We performed a generation of conformers via the CCDC suite for each of the three different 3D structures we managed to solve (see SI and movies). It is calculated that compound **4 b** has only six different conformers compared with the thirty-one and fifteen of compounds **3 g** and **7**, respectively.

Conclusion

Our disclosed MCR approach is a useful addition to the dibenzothiazepine syntheses toolbox due to both the mildness of the reaction conditions and the easy access to polycyclic, rigid derivatives. Thirty-one derivatives have been synthesized, whereas the reactions described are readily scaled-up and applicable to one-pot approaches. Importantly, over 70% of our library obeys to the rule of 5 (Ro5) and in general our synthesized compounds have a spherical, rigid shape with high complexity (see SI for analysis).

Experimental Section

General procedures, characterization data of all compounds, NMR spectra, single crystal structure analysis, analysis and data mining in CSD. Media files of the generated conformers.

Deposition Numbers 2123183 (for **3 g**), 2123182 (for **4 b**), and 2123184 (for **7**) contain the supplementary crystallographic data for this paper. These data are provided free of charge by the joint Cambridge Crystallographic Data Centre and Fachinformationszentrum Karlsruhe Access Structures service www.ccdc.cam.ac.uk/structures.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords: Atropisomerism · Dibenzothiazepines · Multicomponent reactions · Privileged scaffolds · Ugi reaction

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