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DATA NOTE

A novel dataset of helical twisting powers of chiral dopants in nematic liquid crystals phase

[version 1; peer review: awaiting peer review]

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Abstract

Molecular chirality has a key role in the helical phase structures of some liquid crystals. In particular, the induced nematic helical structure by a chiral dopant provides the macroscopic information of the dopant's chirality at the molecular level. Developed theoretical models relate the dopants molecular chirality to their helical twisting power in a nematic host phase. Furthermore, experiments show that helical twisting power depends on temperature, solvent host, and dopant chirality. In addition, the theoretical measurements highlight a strong linear relationship between experimental helical twisting power and measured molecular chirality of some chiral dopants.

We aim to create a large dataset of experimental helical twisting power measured for a wide range of nematic hosts and chiral dopants at various temperatures. The data points were collected manually using the experimental measurements. Each record consisted of the experimental molar helical twisting power, the nature of the nematic host, the nature of the chiral dopant, the molar concentration, and the temperature. The primary focus of this dataset is its reuse for machine learning predictions of the experimental helical twisting power by generating efficient chiral descriptors of dopant molecules utilised for machine learning models. In addition, the dataset aims to predict the helical twisting power of new chiral dopant molecules in various nematic liquid crystals.

The primary dataset consists of 527 experimental measurements of helical twisting powers. We optimised the three-dimensional geometry of chiral dopant molecules using molecular force fields in RDKit. Then, the bootstrapping method was used to generate about 30 conformers for each primary molecule in the dataset using RDKit.

Open Peer Review

Approval Status *AWAITING PEER REVIEW*

Any reports and responses or comments on the article can be found at the end of the article.

The chiral descriptors were developed for use in machine-learning models for each data entry point.

Keywords
Helical Twisting Power, Molecular Chirality, Machine Learning, Liquid Crystals, Nematic Phase

This article is included in the Data Science gateway.

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Value of the data

The main scientific question is on how the molecular chirality transfers from chiral dopant into supermolecular chirality of the LC nematic phase. This process gives a unique observation on investigation of the relationship between chirality of molecular structure, intermolecular interactions, and bulk chirality.[1–4]

The key values of the data include the following.

- This is the first available dataset of the helical twisting power (HTP) of chiral dopants in nematic liquid crystals.
- The dataset can be reused for machine learning predictions of HTP.
- The dataset can be reused for generating efficient chiral descriptors of dopant molecules to be utilised with machine learning models.
- The dataset can be reused for predicting new chiral dopant molecules with specific helical twisting power.
- The dataset can be reused to add new chiral dopant molecules with known experimental helical twisting powers in various nematic liquid crystals.

Background

Molecular chirality plays a key role in the helical structures of nematic liquid crystals.[5–7] The induced helical structure by chiral dopants provides the macroscopic information of the molecular chirality. Theoretical models relate the dopant molecular chirality to its HTP in the nematic host phase.[8–10] The HTP is an experimental measurement quantifying the chirality of nematic phase structure by relating the macroscopic helical structure of the host phase (pitch p), dopant molar concentration (c), and its enantiomeric purity (r).[11,12]

$$\beta_M = \frac{1}{rcp}$$

Experiments highlight the dependence of HTP on the temperature, solvent host, and dopant chirality.[2,13] In addition, the theoretical measurements highlight a strong linear relationship between experimental HTP and measured molecular chirality for some dopants.[3,14]

We aim to create a large dataset of the experimental HTPs for a wide range of nematic hosts and chiral dopants at various temperatures. The data points were collected manually using the experimental HTPs (β_M). The dataset primarily focuses on reuse for machine learning predictions by generating efficient chiral descriptors of dopants. In addition, the dataset aims to predict the HTP of new chiral dopants in various nematic liquid crystals.

Data description

Figure 1 presents a flowchart of the data distribution and the contents of each dataset.

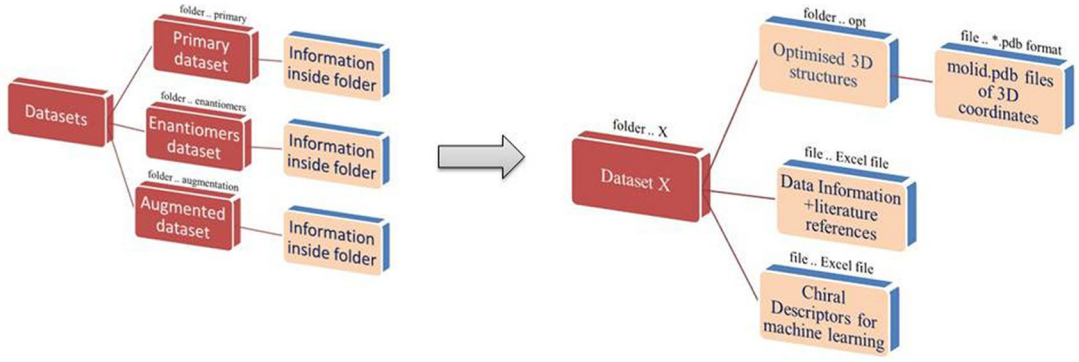


Figure 1. A flowchart of the datasets created in this study including the data information for each dataset and the chiral descriptors for use in machine learning approaches.

Primary data

Figure 2 shows the experimental helical twisting powers (in μm-1) of the primary dataset and the enantiomers of the chiral molecules. In addition, a violin plot of the kernel probability density distribution of HTP is presented in Figure 2B. Figure 2A shows the total chiral volume of the chiral centres of the primary dataset and the enantiomers of the chiral molecules, as computed using the RDKit package (using the ComputeChiralVolume module of the package RDKit. Chem.Pharm3D.EmbedLib). Figure 2B is a violin plot of the kernel probability density distribution of total chiral volume.

Figure 3A presents, graphically, the number of chiral centres for each compound, as defined using the Chem. FindMolChiralCenters module of the RDKit package, while Figure 3B shows the frequency of occurrence of the number of chiral centres in the dataset.

Figure 4A presents the total chiral index,[9] calculated by summing the chiral index of the RS-isomer centre in the structure considered as non-interacting chiral centres. In addition, Figure 4B presents a violin plot of the probability distribution of the total chiral index.

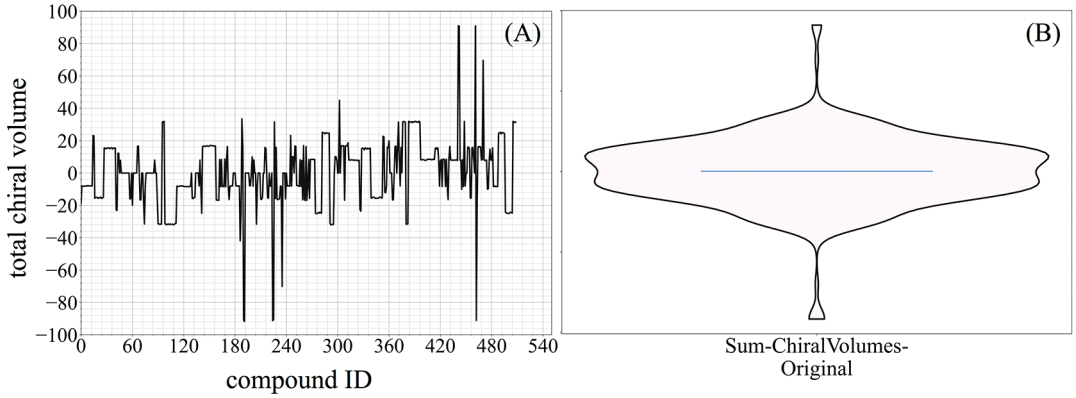


Figure 2. (A) Total chiral volume of the chiral centres of the primary dataset and the enantiomers of the chiral molecules, as computed using the RDKit package (using the ComputeChiralVolume module of the package RDKit.Chem.Pharm3D.EmbedLib). (B) A violin plot of the kernel probability density distribution of total chiral volume.

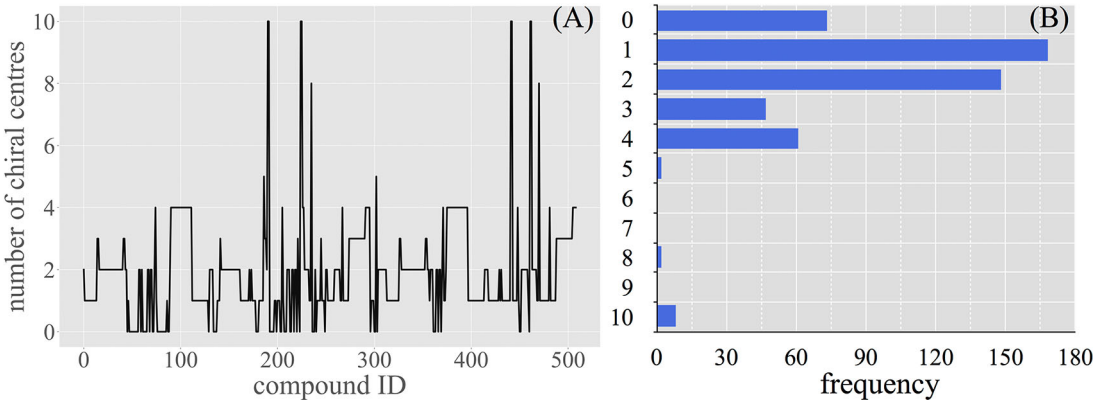


Figure 3. (A) Number of chiral centres for each compound, as defined using the module, Chem.FindMolChiralCenters of the RDKit package. (B) The frequency of occurrence of the number of chiral centres in the dataset.

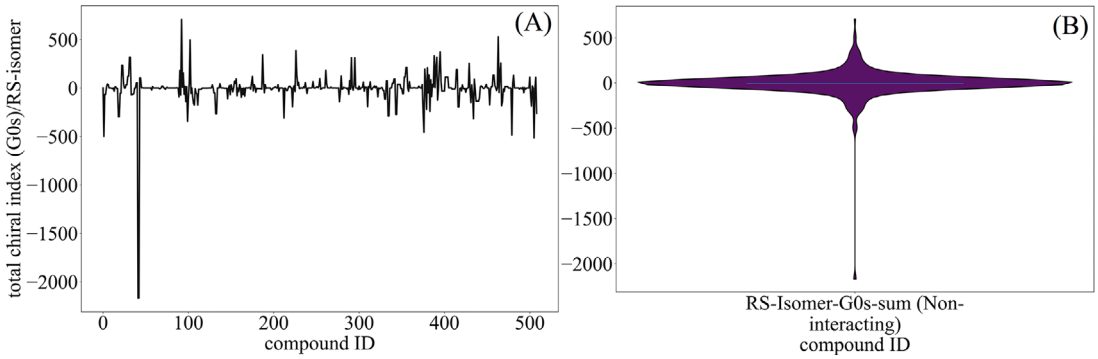


Figure 4. (A) Total chiral index,[9] calculated by summing the chiral index of the RS-isomer centre in the structure considered as non-interacting chiral centres. (B) A violin plot of the probability distribution of the total chiral index.

Bootstrapping data augmentation

Next, we generated 30 conformers for each primary data using the RDKit tools.[15] Then, we calculated the scaled chiral index for each conformer of the RS isomer for each chiral centre.

Figure 5 shows the scaled chiral index for each conformer of the RS isomer for chiral centres. In addition, the moving averages over the conformers for each primary data are shown in red (see also the inset graph).

Experimental design, materials and methods

This dataset consists of data points collected manually using the experimental values of molar helical twisting power, nematic host, chiral dopant, molar concentration of the dopant, and the temperature. The primary dataset is a set of 527 experimental measurements of helical twisting powers for a wide range of dopants in nematic liquid crystal phases. The helical pitch p is typically determined by the Grandjean-Cano technique.[16] The ability of a chiral dopant to induce bulk helical structure in LC host is experimentally measured by HTP,[17] which leads to an amplification of molecular chirality.[18]

First, the dopant molecules are designed using JMOL[19] and MOLVIEW[20] packages in two-dimensional (2D) space, as a SMILES format. Then, the three-dimensional (3D) coordinates of the molecules are obtained using MOLVIEW and initially optimised using molecular mechanics force fields of this package. In addition, the stereoisomers of the chiral centres are defined using JMOL.

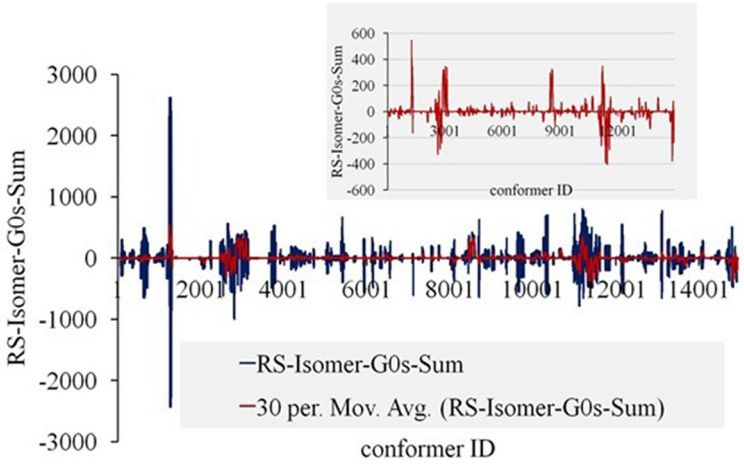


Figure 5. The calculated scaled chiral index for each conformer of the RS isomer for each chiral centre. The moving averages over the conformers for each primary data are shown in red.

Next, the chiral dopant molecules 3D structures are optimised using molecular mechanics force fields in RDKit package, such as MMFF94s. The bootstrapping method was employed to generate of about 30 conformers for each dopant using RDKit. In total, the database has about 15000 data points. The chiral descriptors were developed for use in machine learning models for each data entry point.

Chiral descriptors

The chiral descriptors, in this study included some basic descriptors and the 3D descriptors, as described in the following.

The set of some basic descriptors

1. Number of atoms in molecule
2. Number of bonds
3. Number of rotational bonds
4. Type of the chiral centres, such as a ring
5. Maximum path length in the molecule from the chiral centre
6. Mean pairwise distance of all atom pairs from the chiral centre
7. Number of neighbours per shell distance level
8. The levels until a path length of 10
9. Number of nitrogen and oxygen atoms for each level around the chiral centre
10. Number of aromatic atoms for each level around the chiral centre
11. The size of descriptors for each substituent, sort them from smallest to largest
12. Combination of substituent sizes

3D chiral descriptors

1. Chiral moment
2. Chiral volume
3. Chiral indices
4. Chiral optical gyration tensor elements

Limitations

The limitations faced during this study include the following.

1. The missing significant amount of the experimental data with high values of the helical twisting powers, typically larger than 100 μm^{-1}.
2. Missing the three-dimensional structures of the dopants.
3. Use of high-level quantum mechanics methods to optimize molecular geometries is quite costly from the computational viewpoint.
4. Absence of other existing datasets of the experimental helical twisting values for the sake of comparison.

Conclusions

In this study, we reported a dataset of the chiral dopant molecules, collected manually using the experimental molar helical twisting power, nematic host, chiral dopant, molar concentration of the dopant, and temperature. It consists of 527 experimental values of helical twisting powers, optimised using MMFF94s molecular force fields in RDKit. In addition, a bootstrapping approach was employed to generate of about 30 conformers for each dopant using RDKit. The augmented dataset has about 15000 data points. The chiral descriptors were developed for use in machine learning models for each data entry point.

Software availability

- Software used for analysis is shared through the Github repository, following the link https://github.com/kamberaj/ChiralDopantsDescriptors
- Data identification number: https://doi.org/10.5281/zenodo.22012234[22]
- Direct URL to software: https://zenodo.org/records/22012234
- License: GPL-3.0 license

Ethics and consent

Ethical approval and consent were not required.

Data availability statement

Data are available through the Zenodo repository. Data identification number: https://doi.org/10.5281/zenodo.20688776.[21]

The database consists of three folders:

1) Folder *primary*: This folder contains two subfolders:
    a. *3Dstructures*: It contains the optimized three-dimensional structures of the molecules.
    b. *datadescription*: It contains information about the chiral dopants and their chiral descriptors as a Microsoft Excel Worksheet file “primary_dataset_chiral_descriptors.xlsx”.
2) Folder *enantiomers*: This folder also contains two subfolders:
    a. *3Dstructures*: It contains the optimized three-dimensional structures of the enantiomers of primary chiral dopant molecules.
    b. *datadescription*: It contains information about the enantiomers chiral dopants and their chiral descriptors as a Microsoft Excel Worksheet file “primary_dataset_chiral_descriptors.xlsx”.
3) Folder *augmenteddata*: This folder contains two subfolders:
    a. *3Dstructures*: It contains the optimized three-dimensional structures of the 30 conformers for each primary and enantiomers chiral dopant molecule.
    b. *datadescription*: It contains information about the chiral dopants and their chiral descriptors as a Microsoft Excel Worksheet file “primary_dataset_chiral_descriptors.xlsx”.

Data is available under the terms of the Creative Commons Attribution 4.0 International.

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