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# Molecular sonification for molecule to music information transfer†

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Organic chemical structures encode information about a molecule's atom and bond arrangement. The most established way to encode a molecular structure is through line drawing, although other representations based on graphs, strings, one–hot encoded labels, or fingerprint arrays are critical to the computational study of molecules. Here we show that music is a highly dimensional information storage medium that can be used to encode molecular structure. The resultant method allows a molecular structure to be heard as a musical composition, where the key of the music is based on the molecular properties and the melody is based on the atom and bond arrangement. This allows for a molecular generation approach that leverages modern artificial intelligence tactics for music generation.

## Introduction

The representation of chemical structures is critical to the study and invention of functional molecules. Organic molecules are classically described as line drawings,[1] where all atoms and their corresponding bonds are drawn on paper or on a computer. Other simple molecular representations or identifiers include molecular formulae, IUPAC names or CAS numbers, which require little memory and are machine readable, but carry minimal information. Molecules can also be represented as graphs, with atoms as nodes and bonds as edges. By encoding atomic coordinates and connectivities line by line, the topology of molecules can be embedded as a graph on a computer for rendering, editing and analysis. The transmission of molecular information into machine-readable formats has invited new molecular structure representations, such as SMILES,[2] SMARTS,[3] InChI keys,[4] Deep-SMILES,[5] and SELFIES.[6] These representations are cheap to store in memory and provide valuable structural information for rapid lookup and comparison. While these aforementioned representations have been useful for inputting molecules into computers, and encoding structural and stereochemical information, they are one-dimensional string representations that are more difficult for human users to interpret and interact with than the classic line drawing representation of molecules. To adapt them for machine learning and data science algorithms, SMILES and other strings are typically converted to vector representations *via* molecular

fingerprints such as Extended Connectivity Fingerprints (ECFP),[7] Morgan Fingerprints,[8] atom-pair fingerprints,[9] and others. This dimensionality expansion is a core tactic in the analysis of virtual chemical libraries or predictions of molecular properties. Other high-dimensionality fingerprint representations, such as physics-based descriptors[10] or physicochemical descriptors,[11,12] are also common. While computers can easily parse molecular information from these representations, interactivity with human users is difficult with the fingerprint-based information media. In addition, once converted to such a fingerprint, the molecule is typically no longer uniquely revertible to its atom-bond representation.[13]

Music is a high-dimensional information storage medium that maximizes both human and computer interactivity, interpretability, and creativity. We considered that music could be used for storage of molecular information. While many aspects of a molecule are readily visible to the trained eye, a soundbite may be able transmit more information about the molecule into the mind. The encoding of molecules as music is particularly intriguing since the multiple dimensions of music can allow encoding of many molecular properties.[14] Music is also highly interactive both for humans and for computers. Musicians can control many parameters that can embed information about a molecule, such as tempo, rhythm, notes, key, instrument, effects, *etc.* If molecules could be encoded as music, opportunities would emerge for visual-to-audio sensory substitution, for instance providing blind chemists new ways to interact with molecules.[15] Contemporary chemistry and drug discovery leverage artificial intelligence[16] (AI) and there has meanwhile been an explosion of AI methods in the study and creation of music,[17] so we were excited by the prospects of merging modern chemistry machine learning (ML) techniques with recent ML techniques for music. Our initial impetus was to explore how music could be used as a creative medium to generate new molecules, but in the course of our studies we have

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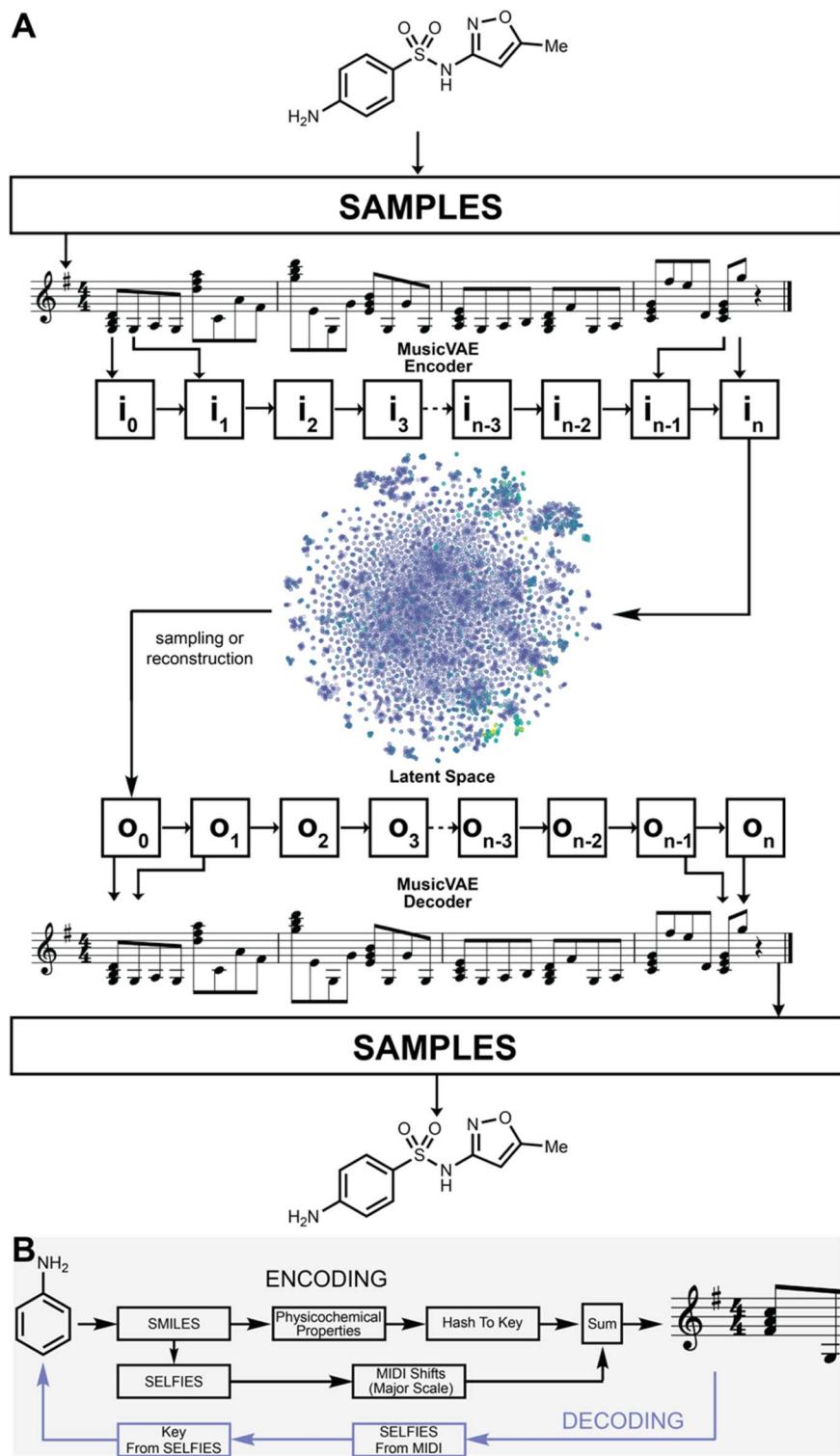
Fig. 1 (A) Workflow for SAMPLES. Molecules are first assigned a musical key based on aggregate chemical properties, then converted into a sequence of notes based on SELFIES encoding. MusicVAE is trained on a collection of sonified molecules to formulate the chemical/musical latent space. The latent embedding of molecular music can then be sampled, for instance through the interpolation between two embedded molecules, decoded by the MusicVAE decoder, then converted back into a molecular structure by SAMPLES. (B) Detailed workflow schematic of SAMPLES. Molecules are binned into base keys based on their physicochemical properties. More druglike molecules correspond to melodies that are more popular as reflected in the distribution of songs listed in Spotify. Specific SELFIES tokens are mapped to MIDI shifts, that result in a final MIDI value when summed with the base key of the molecule, which is hashed from aggregate physicochemical properties. The MIDI shifts correspond to SELFIES tokens as ranked by their popularity in DrugBank. As such, lower MIDI shifts away from the encoded key of the molecule indicate the more popular the SELFIES token. Melodies can then be decoded back into molecules.

learned that molecules likewise can provide an inspiration and creative outlet for the generation of new music.

Sonification is the encoding of non-musical information as music and provides a means to encode information in many musical dimensions, while simultaneously providing a new means of interactivity.[18] A variety of information sources have been sonified, such as visual art,[19] the architecture of spider webs,[20] infrared spectra of chemicals,[21] amino acid sequences,[22] air pollution,[23] fire,[24] and many more.[25–32] The SELFIES representation provided a viable input for molecular sonification, both for the encoding of molecules into a melody and the construction of new molecules *via* performance on a musical instrument such as the piano. We developed a workflow for transferring molecules into music, and *vice versa*, which we call Sonic Architecture for Molecule Production and Live-Input Encoding Software, or SAMPLES (Fig. 1).

# Methods and workflow

### Encoding

To create a melody based on a molecular structure, the key and the sequence of notes are derived from its physicochemical properties and its SELFIES sequence, respectively. To determine the key, the physicochemical properties of a molecule—such as $\log P$, molecular weight, and number of hydrogen bond donors and acceptors—are summed, and the final number is linearly projected into the integer space between 1 and 12 from the minimum and maximum values found in the entire dataset (in this case, DrugBank), with each bin corresponding to a particular key. In our encoding scheme, the projection is largely dictated by the molecular weight due to its magnitude with respect to the other features. Due to low deviation, low mean, and outliers of high molecular weight, most molecules from the
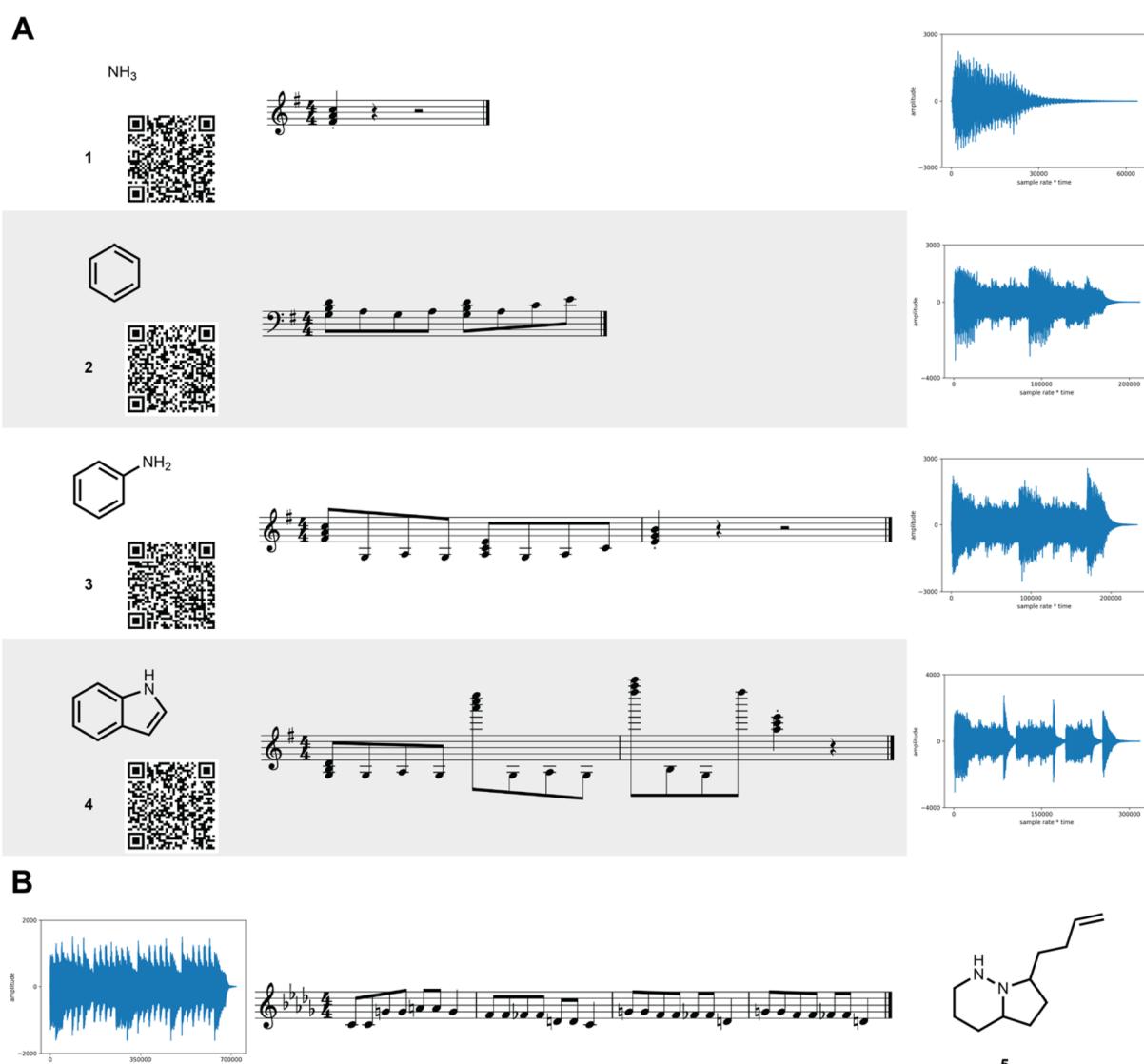


Fig. 2 SAMPLES translates molecules into music. (A) The generation of increasingly complex molecules from **1** through **4** corresponds to increasing musical complexity. Each line shows the molecular structure, the corresponding musical score, and a waveform of the MIDI output. Audio recordings are available in the ESI† and can be quickly retrieved by scanning the QR code with a mobile device. (B) In the reverse direction, the song "Twinkle, Twinkle Little Star" produces molecule **5**.
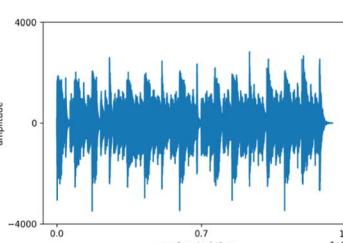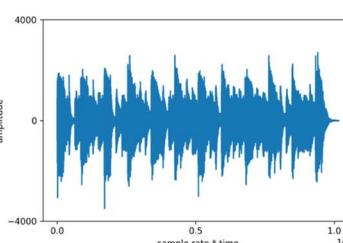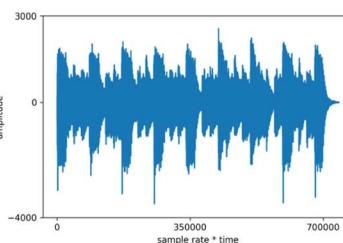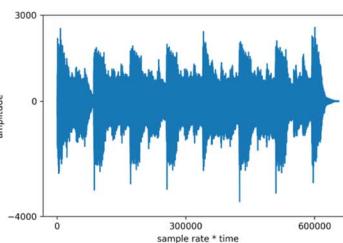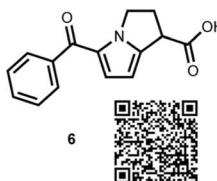
Fig. 3 SAMPLES is amenable to encoding complex molecules. (A) The pair of similar molecules 6 and 7 have SAMPLES compositions that are distinct from another similar pair of molecules 8 and 9. (B) QR codes linking to SAMPLES encodings of select large complex molecules.

DrugBank dataset fall into the first bin. In our scheme, the keys represented by the bins are ordered by the popularity of keys found on Spotify, with the most popular bin being the key of G (see Fig. S1†). As such, most compounds in DrugBank are encoded into G and larger molecules are encoded into the less popular keys. The sequence of notes is determined from a one-to-one mapping between the SELFIES token of the molecule and multi-octave steps in the major scale (see ESI† for the specific mappings and key distribution used in this study). By adding the MIDI value of the melody's key to the MIDI shifts that correspond to notes of the major scale (derived from the SELFIES tokens of the molecule), the final melody is produced.

In our case, the MIDI shifts correspond to SELFIES tokens as ranked by their popularity in DrugBank. As such, lower MIDI shifts away from the encoded key of the molecule indicate the more popular the SELFIES token. Every fourth note, starting from the first note, was converted to a major chord to increase the texture of the music. We envision polyphony as a potential avenue to encode atomic features. This algorithm could be extended by including more descriptors in the encoding and assigning distinct keys to clusters. As well, mapping more elements or structural subgroups to MIDI shifts or other musical parameters can enable the encoding of proteins, inorganic molecules, and other chemical phenomena.
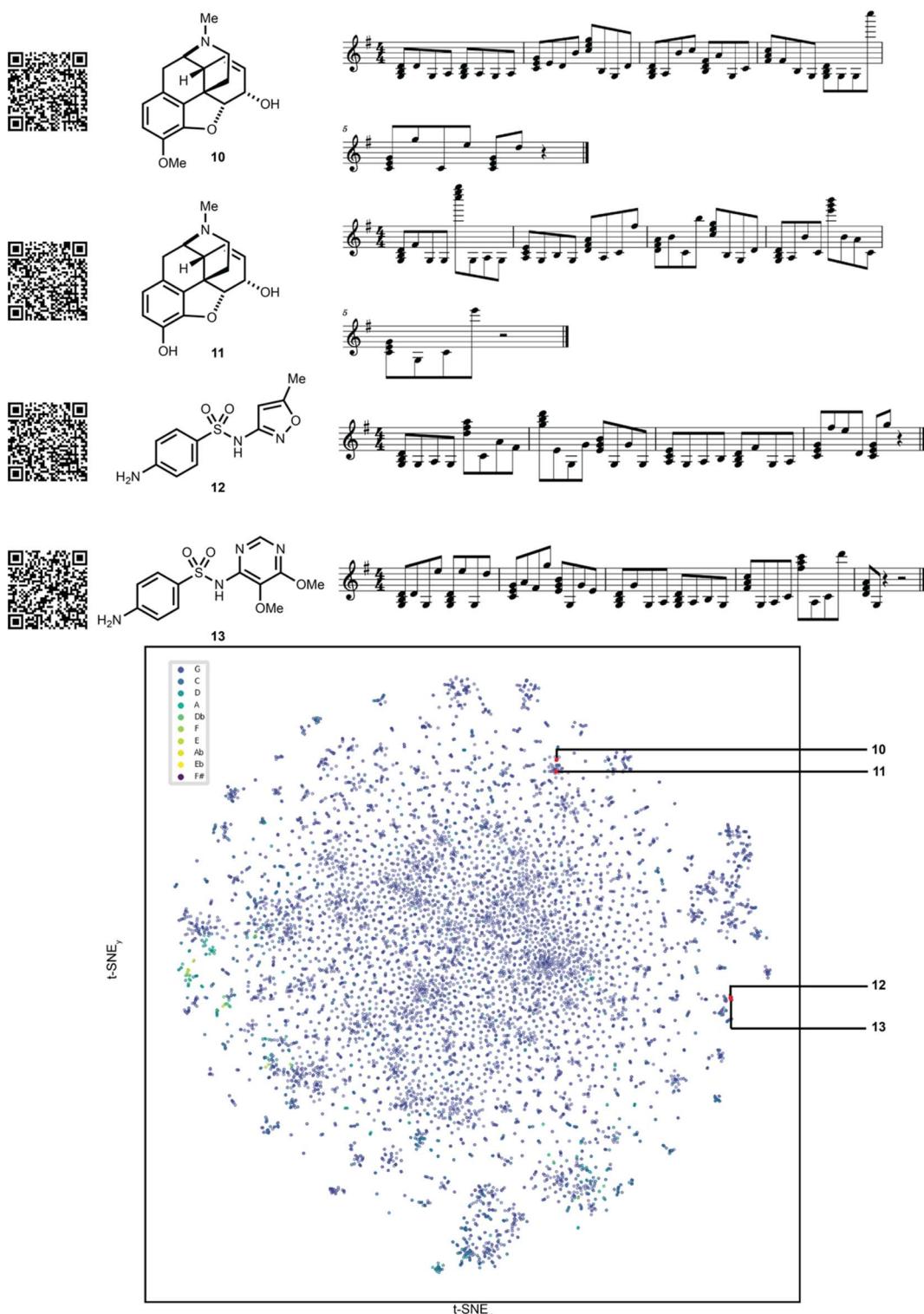
**Fig. 4** tSNE embedding of 11 159 drugs from DrugBank (2048 bit Morgan Fingerprints of radius 2), coloured by their SAMPLES musical key. Similar molecules **10** and **11** have SAMPLES outputs that are distinct from other similar molecules **12** and **13**. The music encoded by the score adjacent to the molecules can be listened to by following the QR code. It can be heard that these similar molecules have similar musical encodings when using our algorithm.

### Decoding

The MIDI shifts are reverse calculated for each key and converted into a molecular structure. As such, multiple structures are generated (one for each key) for the same MIDI sequence. Each structure is then hashed into a key using the original key encoding algorithm. If the hashed key matches the key used in
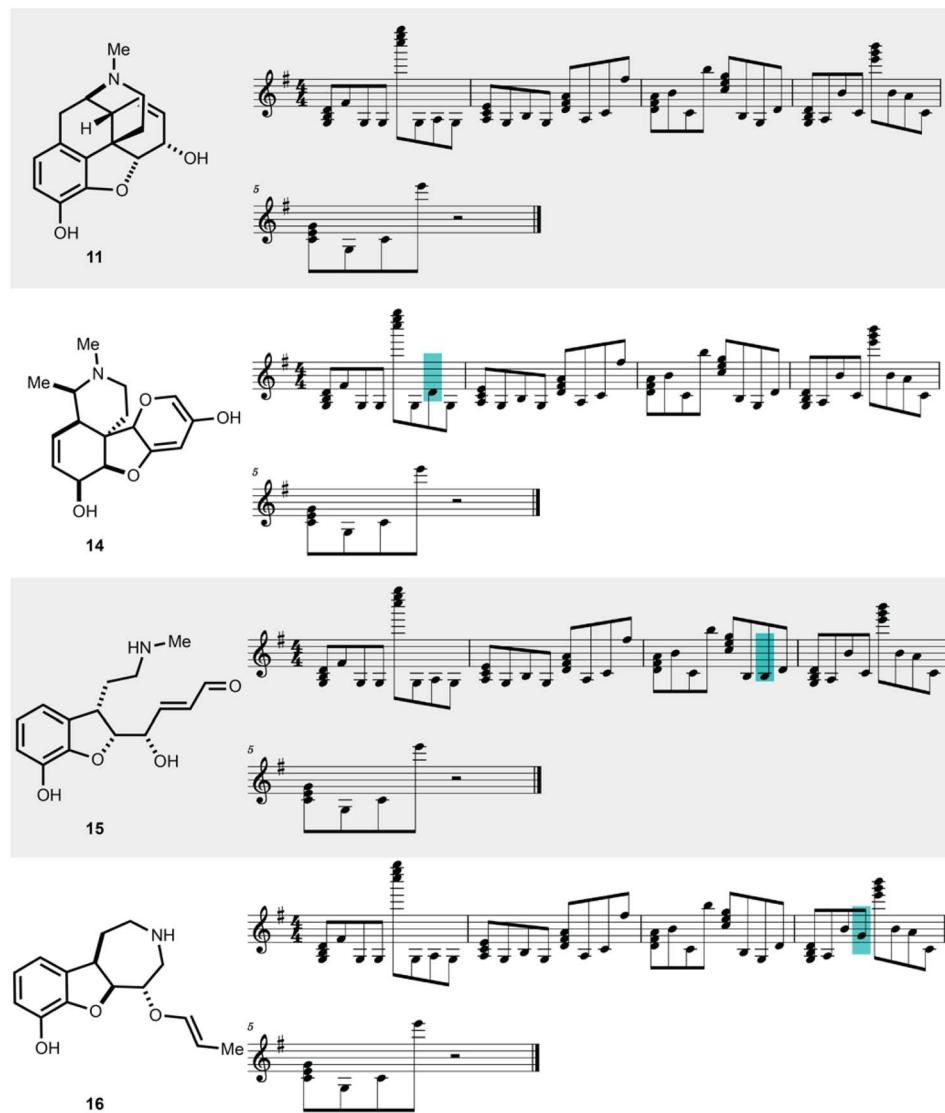
Fig. 5 Molecular editing in SAMPLES generates distinct but related molecules. The manual editing of single notes in the SAMPLES of **11** leads to **14**, **15**, or **16**.

the reverse calculation, the molecular structure is decoded. It is guaranteed that at least one decoding key will match a hashed key for any MIDI generated from SAMPLES.

A demonstration of the SAMPLES encoding function is shown in Fig. 2. Ammonia (**1**) appears as a single note while benzene (**2**) generates a slightly more complex musical composition. The unity of these two molecules produces aniline (**3**) whose musical sequence highly resembles the concatenation of the two musical sequences of **1** and **2**. Expansion of **3** into indole (**4**) creates a slightly more complex melody owing to both the increased molecular size and the additional information content required to describe a ring fusion between the 5- and 6-membered rings. In the reverse direction, songs are readily translated to molecules, such as **5**, which is produced from the song "Twinkle, twinkle little star" when played using D flat as the reference note (the decoding key).

SAMPLES is readily scaled to more complex and drug-like molecules (Fig. 3). Tolmetin (**6**) and ketolorac (**7**) create a rich and textured musical composition. Meanwhile, tabersonine (**8**) and vindoline (**9**) provide complex melodies. Scaling to large complex molecules, such as taxol, oxytocin, or vincristine (see ESI†) required no modifications and generated nuanced euphonic melodies.

## Case studies

To showcase the utility of this novel algorithm, four experimental case studies are presented. Using our approach, molecular properties can be heard. For instance, the songs generated from molecules that pass the Lipinski rules[33] can be auditorily distinguished from those that fail the Lipinski rules based on the musical key. This is largely because the molecule's aggregate physicochemical properties were hashed to the musical key, with the most popular physicochemical property fingerprints from the pharmaceutical database DrugBank hashing to the most popular song keys from the music database Spotify.[34] The concept of
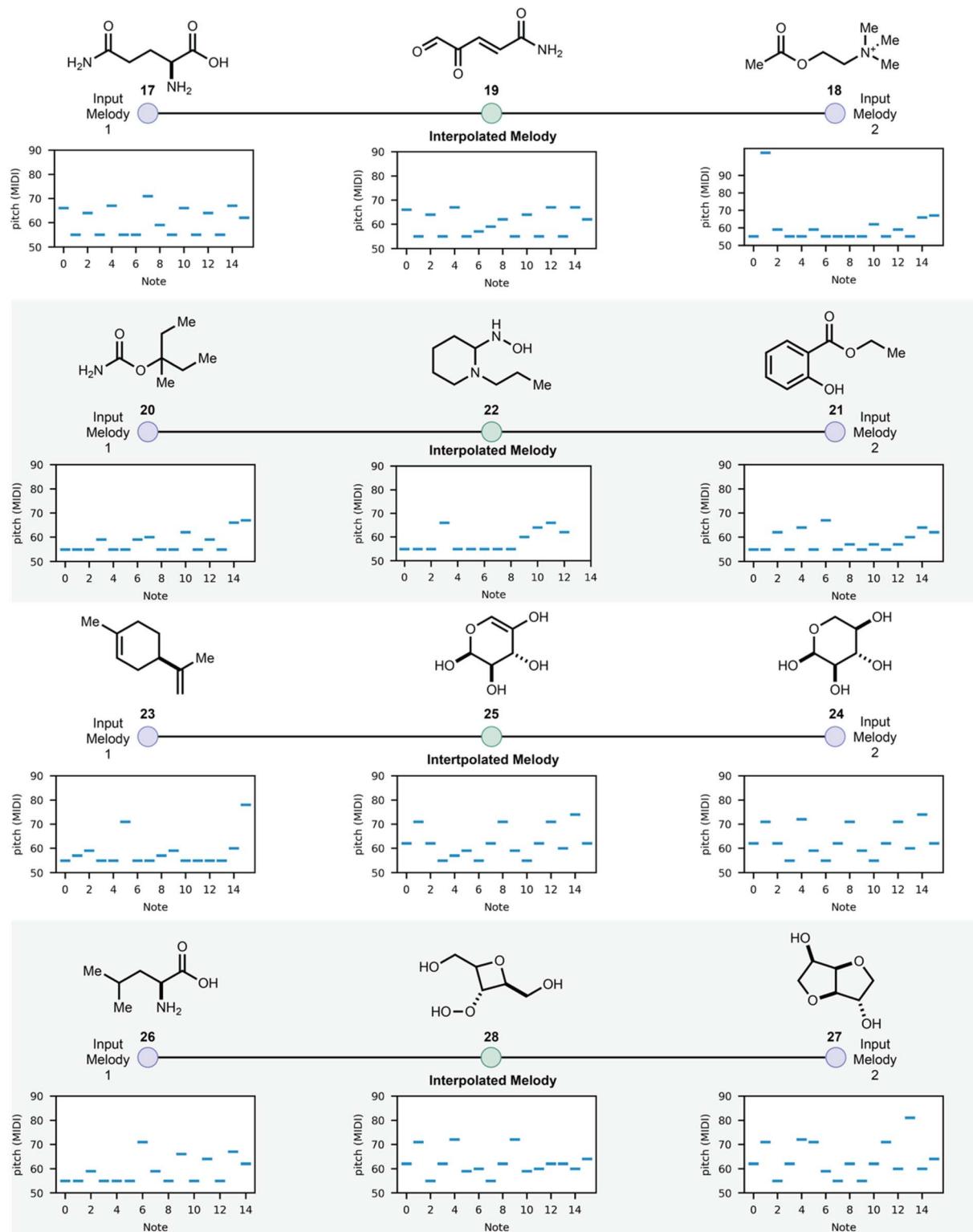
Fig. 6 CROSSFADE merges SAMPLES with the melody mixing function of MusicVAE to create interpolated molecules based on two input molecules.

molecular similarity is of high importance to molecular invention, such as in selecting molecules with comparable functional properties for drug discovery. We were curious to explore if SAMPLES generated from molecules with high Tanimoto similarity[35] (fingerprint based) would sound similar, appreciating that both molecular similarity and musical similarity are difficult to define.[36] Molecules represented in the t-SNE in Fig. 4 are more similar if closer to each other on the plot. Indeed, we deemed the

Fig. 7 A human created music composition leading to **29**.

SAMPLES of codeine (**10**) and morphine (**11**) to sound similar to each other while the SAMPLES of sulfamethoxazole (**12**) and sulfadoxin (**13**) likewise sound similar, while the pair of **10** and **11** sounded distinct from the pair of **12** and **13** (Fig. 4).

Our second experiment investigates the generation of molecules *via* modification of the music domain. A key motivator for our research was the ability to generate new molecules through the interactivity of a piano keyboard, or other musical hardware or software. This was made possible in SAMPLES through the application of SELFIES, which enable editing of string bits while consistently producing valid molecular structures. Thus, starting from morphine (**11**), the musical score could be modified one note at a time (Fig. 5) to generate new chemical structures **14–16** bearing a clear relationship to **11** but with noticeably modified bond and atom architecture. Due to our encoding scheme, shifts further away from the melody's key result in SELFIES being modified into to atoms less commonly found in the DrugBank database. Random modification of SELFIES can result in drastic changes to molecular structure as seen in Fig. 5, due to the non-atom encoding SELFIES tokens that dictate the size of features such as branches and rings. Note that SAMPLES may generate undefined stereocenters.

Having demonstrated the feasibility of molecular generation using SAMPLES, we explored the ability of modern machine learning methods developed for music generation as tools for molecule generation. In this third case study, we applied the melody mixing function of MusicVAE[37] using MIDI melodies derived from SAMPLES as inputs. Using MusicVAE, two melodies could be blended to generate an interpolated melody, and that new melody could be translated back to a molecular structure using SAMPLES, thus creating a new molecule that was a "blend" of the two input molecules (Fig. 6). We call this function CROSSFADE. The blending of musical compositions is an established practice, with considerable hardware and software to support the musical blending process. While algorithms that generate new molecules by blending the structures or properties of input molecules are known,[38] we are intrigued by the interactivity offered by CROSSFADE. As an example, glutamic acid (**17**) and acetylcholine (**18**) were CROSSFADEd to produce **19**, **20** and **21** CROSSFADE to **22** and similar results are obtained for **23–28**. A four-step interpolation is shown in the ESI.†

As a final experiment, to take the editing of the molecules on the keyboard a step further, and to demonstrate the human-interactivity enabled by the SAMPLES algorithm, a human created a monophonic composition inspired by SAMPLES-generated music (Fig. 7), which was decoded to molecule **29**. It was necessary to exert some human bias into the musical composition, based on the composer's knowledge of chemistry and SAMPLES, since generating a molecule that is as carboniferous as most drugs and natural products requires bias towards the key's tonic note, in this case C, since that is mapped to the carbon atom. In other words, the song was written to ensure that the most played note corresponded to the carbon atom to reflect the nature of organic molecules. This required a basic understanding of organic chemistry and musical theory. While this implementation of SAMPLES focuses on major scale notes, the embedding algorithm can be easily modified to include mappings for minor scale notes or accidentals.

One goal of this embedding algorithm was to show that music can be used as a medium to encode molecular information and that similar molecules can produce similar sounding melodies. While this is largely dependent on the featurization and encoding of the molecules into music, our algorithm seemed to perform well for some druglike molecules as tested by the human ear. We surveyed 75 participants from a senior level undergraduate medicinal chemistry course with a blind multiple-choice poll. Students were given four questions, each of which asking the student to compare the melody of four encoded molecules to the melody of an encoded molecule given in the question. The student is prompted to select the melody that they believe to sound most similar to the given sample for each question without being shown any structures. In the first question, **10** was given to the student and the student was given a choice between the melodies of **11**, **30**, **31**, and **32**. In this case, despite the high Tanimoto similarity between codeine **10** and morphine **11**, most students did not recognize similarity between the two encodings, instead hearing **30** and **31** to sound more like **10**. However, in question two where **12** was compared to **13**, **33**, **34**, and **35**, most students correctly identified the melodies of sulfamethoxazole (**12**) and sulfadoxin (**13**) to be most similar. Students were also able to identify the most similar melodies and molecules as described by Tanimoto similarity in questions three and four, where melodies of **7** and **9** were correctly chosen to be similar to **6** and **8** over **36–38** and **39–41**, respectively. Puzzlingly, question one had the highest similarity between the test molecule and correct answer molecule compared to the other question pairs (Fig. 8).
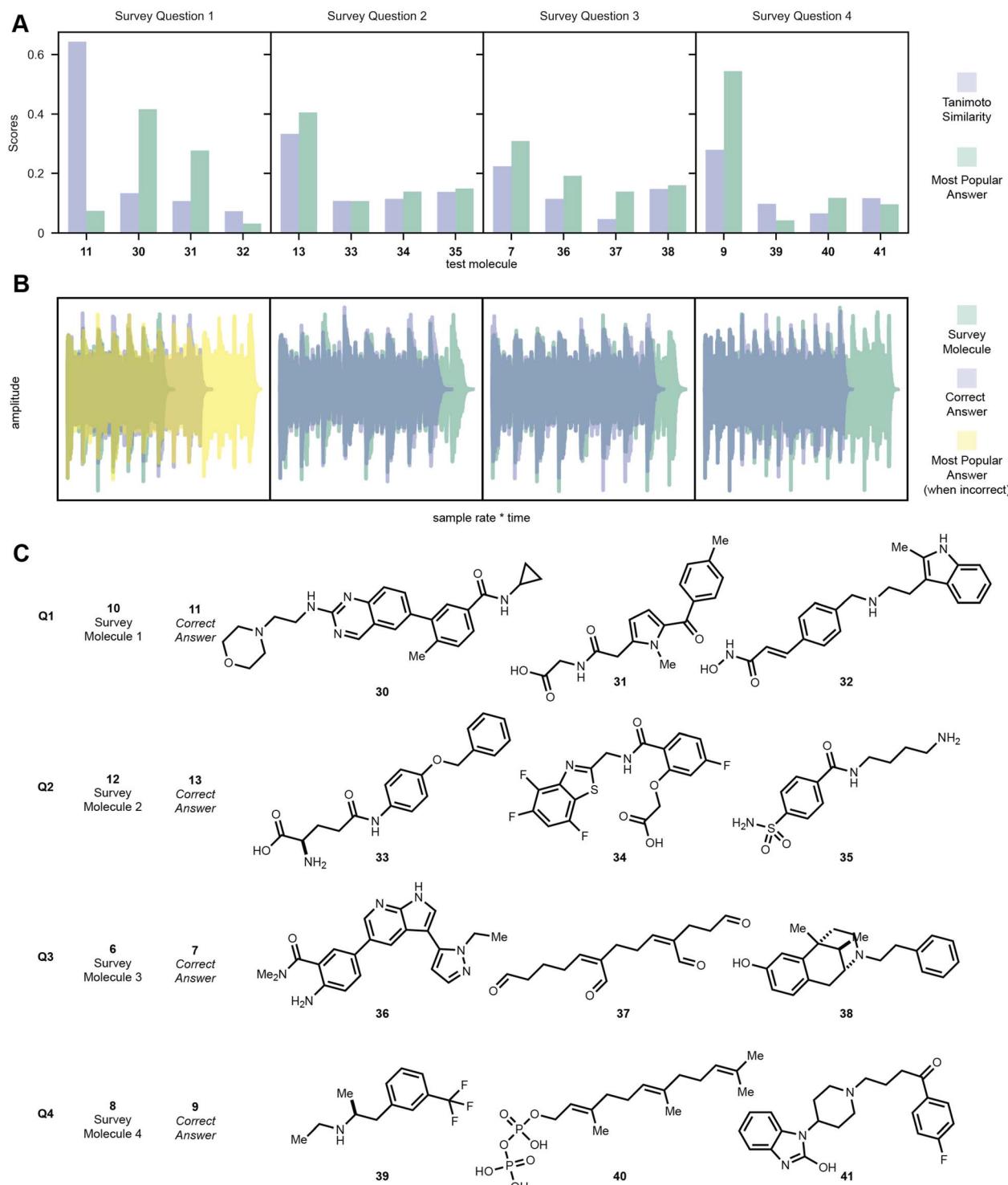
Fig. 8 (A) Survey results from 75 participants. Each participant was given the SAMPLES encoded melody of four survey molecules. For each survey molecule, without knowledge of the name or structure of any molecule, each participant was asked to choose the most similar melody from a selection of four other SAMPLES encoded drugs. Survey responses are cross examined against the Tanimoto similarity between each test molecule and survey molecule for each question. (B) Superimposed waveforms, for each question, of the survey molecule, the molecule most structurally similar to survey molecule, and the most popular answer if the majority response in incorrect. (C) Structures of survey and test molecules for each question. One structure for each set of test molecules was chosen to have high similarity to the respective question's survey molecule to serve as the 'correct answer'.

## Conclusions

We report an alternative means of encoding organic molecules through music. The resultant melodies allow a human to interact with molecular structures through musical hardware and software *via* note editing, insertion and deletion, as well as produce molecular structures through original compositions. We note that far more molecular features can be encoded into a melody or even a short soundbite than can be visually represented by the 2D or 3D structure. Indeed, many richer possibilities can be enabled by encoding more features into musical elements such as other scales, chord compositions, rhythms, timings, timbres, *etc.* One transfer learning application for which the current study may be used is music generation. The motivation for machine learning for content generation is its generality, that is no formal grammar or rules must be specified for such a model to generate content.[17] Transforming molecules into music provides a rich collection of musical data that can be used to train music generation models, as seen with MusicVAE. Particularly, sequence to sequence (seq2seq) models, such as recurrent neural networks,[39] allow for the interconnection of domains containing data signals with variable lengths such as text, music, and machine-readable molecular representations based on structure. Seq2seq models can learn a fixed length embedding of variable length signals that can be used for classification tasks and direct mathematical comparison. For instance, word2vec[40] and GloVe[41] provide pretrained word embeddings that have been learned from massive text corpuses such as Wikipedia or Twitter. In a molecular context, variational autoencoders have been used to learn the distribution of molecular features, such as SELFIES tokens, to provide a continuous embedding of molecular space.[42] SAMPLES provides an avenue to directly connect molecules to content-generating machine learning models in the music domain. Computational exploration and interpolation within the melodies described herein is possible, generating new molecules that sound and look similar to existing molecules. This highlights the possibility of leveraging music-based artificial intelligence for molecular design. An online implementation of the encoding portion of the SAMPLES algorithm can be accessed at http://samples.cernaklab.com.

## Materials

Sonification and visualization code was written in Python (version 3.7.12). All Python dependencies were installed using pip, version 21.1.3. SELFIES (version 1.0.0) was utilized to encode molecules into string format. RDKIT (version 2021.9.2.1) was utilized to calculate physicochemical properties of molecules for key hashing. Magenta (version 2.1.3) provided tools to manipulate MIDI files and train MusicVAE. Fluidsynth (version 2.2.3, installed *via* apt-get) was used to convert MIDI into wav format. Music21 (version 5.5.0) was used to create and read MIDI files. Matplotlib (version 3.2.2) was used to create plots and graphs. Sklearn was used to calculate the tSNE dimensionality reduction. Drug structures were collected from DrugBank Release Version 5.1.8 (2021-01-03).

## Data availability

Code to run the algorithm can be found here: https://github.com/cernaklab/samples. Trained VAE model can be downloaded from here: https://doi.org/10.5281/zenodo.6391612. Webapp of the algorithm can be used at: http://samples.cernaklab.com/

## Author contributions

All authors performed computational experiments and wrote the manuscript. T. C. supervised the work.

## Conflicts of interest

The Cernak Lab has received research funding or in-kind donations from MilliporeSigma, Relay Therapeutics, Janssen Therapeutics, Entos, Inc., SPT Labtech and Merck & Co., Inc. T. C. holds equity in Scorpion Therapeutics, and is a co-Founder and equity holder of Entos, Inc.

## Acknowledgements

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