Text2Mol: Cross-modal Molecular Retrieval with Natural Language Queries

Carl Edwards, ChengXiang Zhai, and Heng Ji

Department of Computer Science, College of Engineering, University of Illinois at Urbana-Champaign

MOLECULE MAKER LAB INSTITUTE

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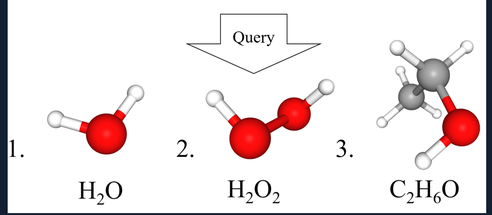
INTRODUCTION

- There are hundreds of millions of molecules, so finding the right molecule for a problem can be challenging.
- Many current information retrieval systems rely only on textual descriptions of molecules, but there are more molecules than can possibly be tested in a lab and then described.
- To address this issue, it is critical to retrieve molecules directly from natural language descriptions.

TASK DEFINITION

- Given a text query and list of molecules with out any reference textual information, retrieve the molecule corresponding to the query.
- We assume there is only one correct (relevant) molecule for each description, so we consider two measures for this task: Hits@1 and mean reciprocal rank (MRR).

Water is an oxygen hydride consisting of an oxygen atom that is covalently bonded to two hydrogen atoms.

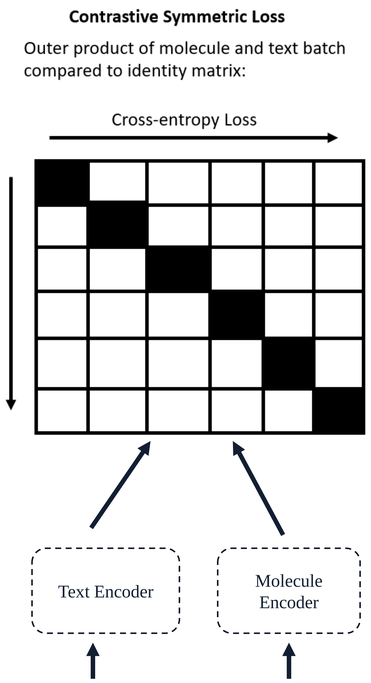


DATA

- We collect ChEBI annotations of compounds scraped from PubChem, which consists of 102,980 compound-description pairs
- Using this data, we create a dataset consisting of 33,010 pairs, which we call **ChEBI-20**, that contains descriptions of more than 20 words.
- The dataset is split into 80%/10%/10% train/validation/test splits. Models are trained on the training data, and queries are performed on all molecules in the entire dataset.

METHOD

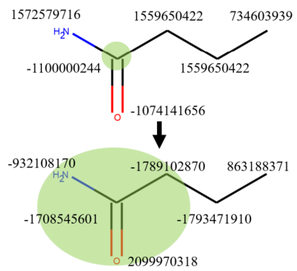
- Molecules and natural language are very different though: how can we combine them?
- In this work, we learned an aligned embedding space between molecules and natural language using symmetric contrastive loss.



Rostratin D is an organic disulfide isolated from the whole broth of the marine-derived fungus Exserohilum rostratum and has been shown to exhibit antineoplastic activity. […] It is a bridged compound, a cyclic ketone, a lactam, an organic disulfide, an organic heterohexacyclic compound, a secondary alcohol, a dithiol and a diol.

Encoding

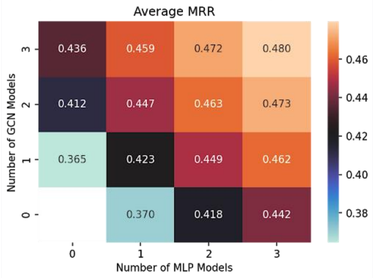
- Descriptions are encoded using SciBERT [1].
- Molecules are encoded with two methods: an MLP and GCN. The MLP builds off Mol2vec [2].
- We introduce a GCN to better incorporate the graph structure of the molecule.



- Mol2vec uses Morgan fingerprints of atoms to turn molecules into "sentences" for the Word2vec algorithm

Ensemble

- The correct molecule was very frequently ranked highly by all models.
- Incorrect molecules ranked highly don't frequently occur in multiple models.
- Averaging ranks improves performance significantly.

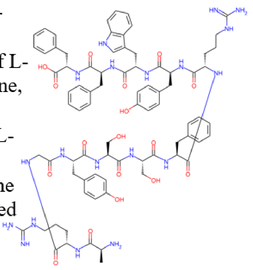


Model	Training Mean Rank	MRR	Hits@1	Hits@10	Test Mean Rank	MRR	Hits@1	Hits@10
MLP1	9.55	0.428	26.5%	77.5%	30.38	0.372	22.4%	68.6%
MLP2	9.82	0.425	26.4%	77.1%	30.72	0.369	22.3%	68.9%
MLP3	9.53	0.431	26.9%	77.8%	36.30	0.372	22.3%	67.9%
GCN1	10.22	0.432	27.2%	76.5%	42.28	0.366	21.7%	68.2%
GCN2	9.67	0.423	26.7%	77.4%	41.90	0.371	22.3%	68.9%
GCN3	10.12	0.420	25.8%	76.7%	39.11	0.366	22.3%	67.9%
MLP-Ensemble	5.81	0.520	35.1%	86.4%	20.78	0.452	29.4%	77.6%
GCN-Ensemble	6.09	0.516	35.0%	86.1%	28.77	0.447	29.4%	77.1%
All-Ensemble	**4.67**	**0.568**	**40.2%**	**89.8%**	**20.21**	**0.499**	**34.4%**	**81.1%**
MLP1+Attn					30.37	0.375	22.8%	68.7%
MLP1+FPGrowth					30.37	0.374	22.6%	68.6%

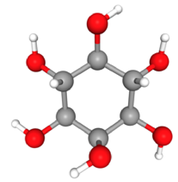
RESULTS

Retrieved Correctly:

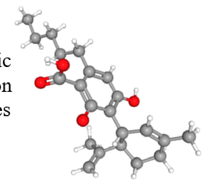
Argyssfrywff: Ala-Arg-Gly-Tyr-Ser-Ser-Phe-Arg-Tyr-Trp-Phe-Phe is an oligopeptide composed of L-alanine, L-arginine, glycine, L-tyrosine, L-serine, L-serine, L-phenylalanine, L-arginine, L-tyrosine, L-trytophan, L-phenylalanine and L-phenylalanine joined in sequence by peptide linkages.



Inositol: Myo-inositol is an inositol having myo-configuration. It has a role as a member of compatible osmolytes, a nutrient, an EC 3.1.4.11 (phosphoinositide phospholipase C) inhibitor, a human metabolite, a Daphnia magna metabolite, …

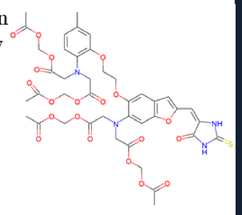


Cannabidiolate is a dihydroxybenzoate that is the conjugate base of cannabidiolic acid, obtained by deprotonation of the carboxy group. It derives from an olivetolate. It is a conjugate base of a cannabidiolic acid.

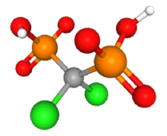


Retrieved Incorrectly:

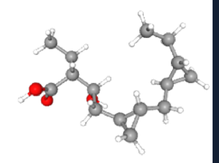
Fura red is a 1-benzofuran substituted at position 2 by a (5-oxo-2-thioxoimidazolidin-4-ylidene)methyl group, and at C-5 and C-6 by heavily substituted oxygen and nitrogen …



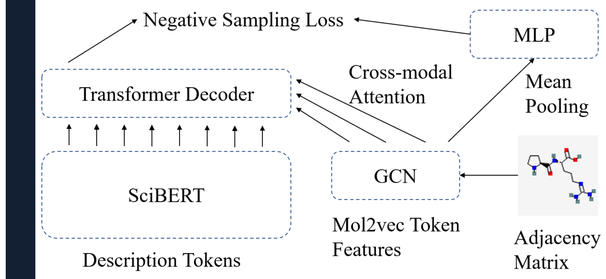
Clondronate(2-) is the dianion resulting from the removal of two protons from clondronic acid. It is a conjugate base of a clodronic acid.



An alpha-mycolic acid is a class of mycolic acids characterized by the presence of two cis cyclopropyl groups in the meromycolic chain. It is an organic molecular entity and a mycolic acid. …



ATTENTION-BASED ASSOCIATION RULES



Token	Substructure	Supp	Conf
Titanium	Ti=O	1.29	0.65
Aluminium	Al^{3+}	4.31	0.23
Manganese	Mn^{2+}	10.08	0.30
Toluene	C – C=C	12.93	0.231
Toluene	C_7H_8	23.79	0.425
##chloro	Cl – C	18.81	0.207
pollutant	F – C	3.097	0.208
chromatography	C – Si	2.976	0.271
acid	C – O – H	2398.7	0.078
crown	C – C – O	4.18	0.325

CONCLUSIONS

We show that it is possible to align molecules and their descriptions for cross-modal retrieval. We argue that natural language and molecules, while very different, are complementary sources of information that can and should be integrated together.

References

[1] Beltagy, Iz, Kyle Lo, and Arman Cohan. "SciBERT: A Pretrained Language Model for Scientific Text." Proceedings of the 2019 Conference on Empirical Methods in Natural Language Processing and the 9th International Joint Conference on Natural Language Processing (EMNLP-IJCNLP). 2019.

[2] Jaeger, Sabrina, Simone Fulle, and Samo Turk. "Mol2vec: unsupervised machine learning approach with chemical intuition." Journal of chemical information and modeling 58.1 (2018): 27-35.

ACKNOWLEDGEMENTS

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