NOVÉ TECHNIKY SAMO-KONTROLOVANÉHO UČENIA SA PRE KLASIFIKÁCIU A PREDIKCIU MOLEKULÁRNYCH VLASTNOSTÍ

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MOLEKULÁRNE VLASTNOSTI

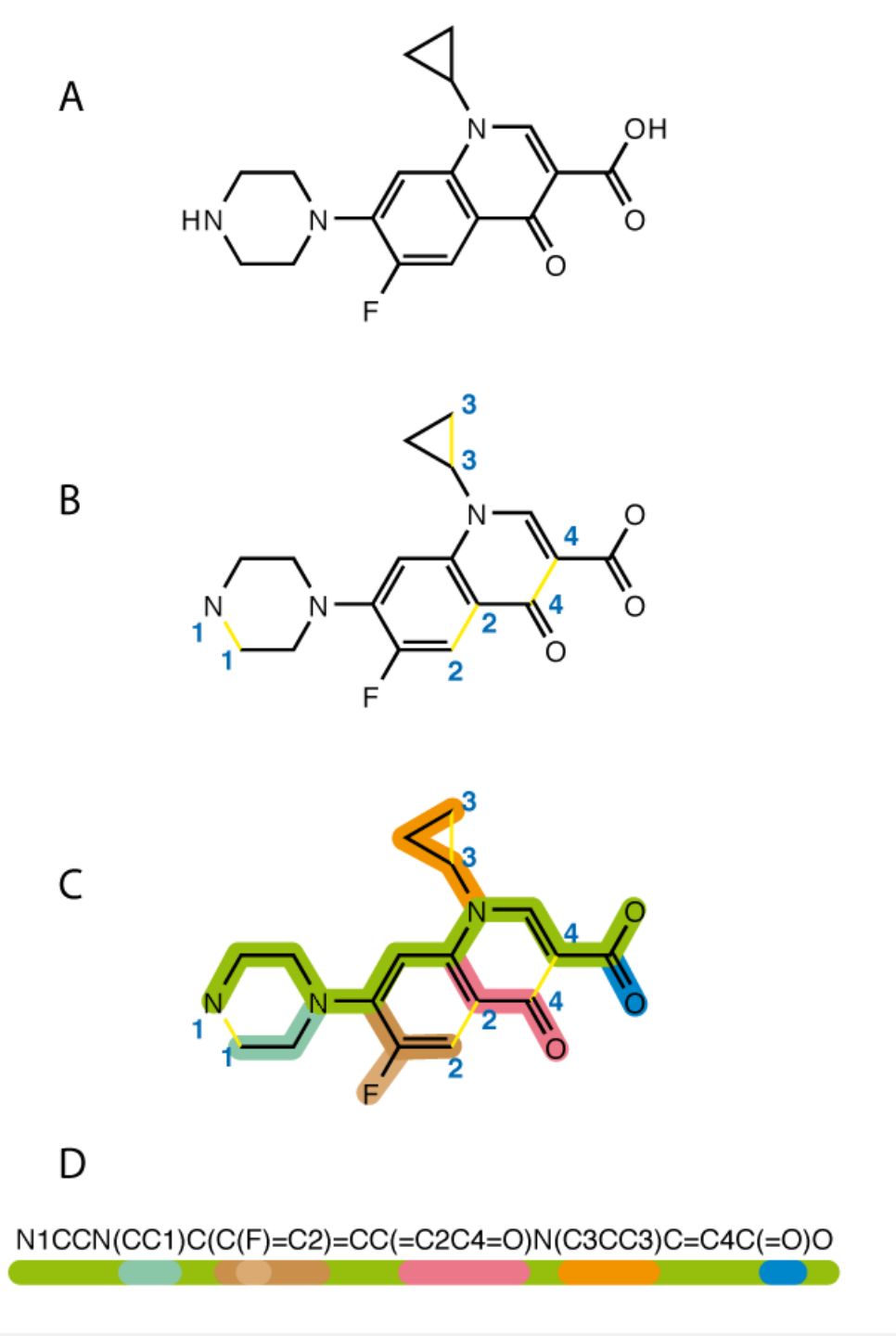
MoleculeNet datasety

- 4 kategórie
  - Kvantová mechanika: QM7, QM7b, QM8, QM9
  - Fyzikálna chémia: ESOL, FreeSolv, Lipophilicity
  - Biofzyika: MUV, HIV, PCBA BACE, PDBind
  - Fyziológia: BBBP, Tox21, ToxCast, SIDER, ClinTox

REPREZENTÁCIA DÁT

SMILES

- Simplified molecular-input line-entry system
- textová reprezentácia molekúl (1D)
- spätne rozšíriteľná na 2D reprezentáciu
- konverzia do 3D
  - prístupy minimalizujúce energiu

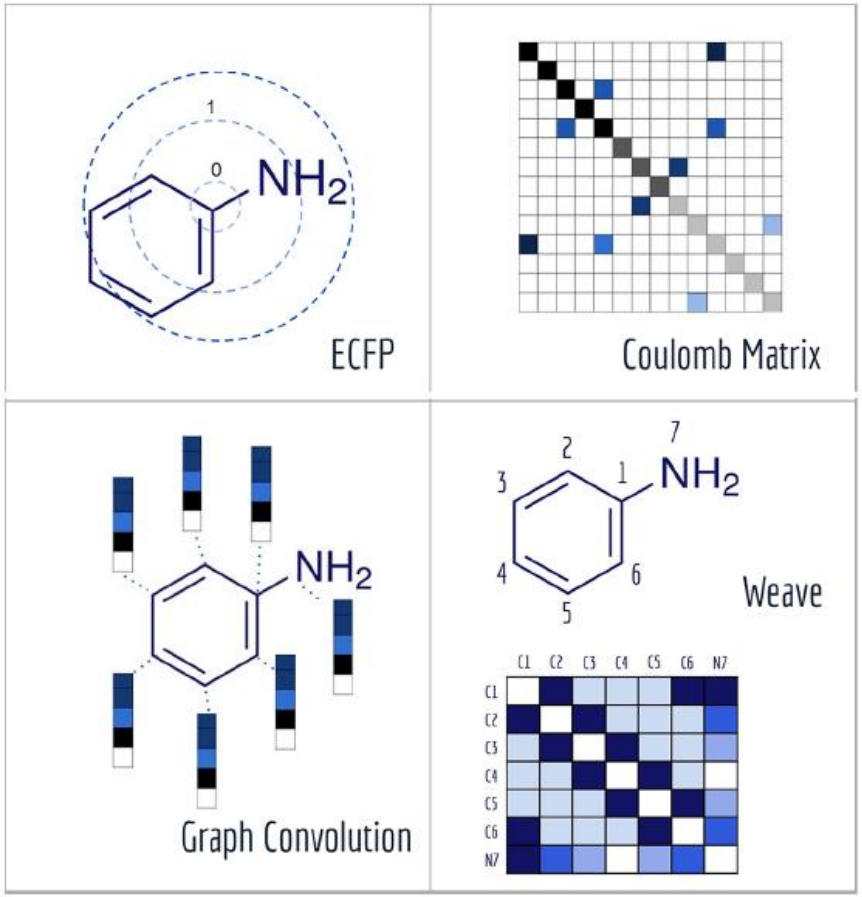


QM8

	A	B	C	D	E
1	Column1	Column2	Column3	Column4	Column5
2	smiles	E1-CC2	E2-CC2	f1-CC2	f2-CC2
3	[H]C([H])([H])[H]	0.43295186	0.43295958	0.24972825	0.24973648
4	[H]N([H])[H]	0.26521952	0.35008064	0.06701544	0.03004918
5	[H]O[H]	0.28653735	0.363579	0.03775532	0
6	[H]C#C[H]	0.35862867	0.35862867	0	0
7	[H]C#N	0.31995762	0.33607406	0	0
8	[H]C([H])=O	0.15391355	0.29123378	0	0.09102332
9	[H]C([H])([H])C([H])([H])[H]	0.37613753	0.37614568	0	0
10	[H]OC([H])([H])[H]	0.26669063	0.33319051	0.0009443	0.07160772
11	[H]C#CC([H])([H])[H]	0.27338914	0.2857496	0	0.0011942
12	[H]C([H])([H])C#N	0.31965511	0.3344136	0.00000001	0.002747
13	[H]C(=O)C([H])([H])[H]	0.16572695	0.28555558	0.00004483	0.04090803
14	[H]C(=O)N([H])[H]	0.21631598	0.28221985	0.00093894	0.01318951
15	[H]C([H])([H])C([H])([H])C([H])([H])[H]	0.35880714	0.36925461	0.0015726	0.00298485
16	[H]OC([H])([H])C([H])([H])[H]	0.26669876	0.32436	0.00021511	0.02683589
17	[H]C([H])([H])OC([H])([H])[H]	0.2741024	0.31468983	0.04407212	0.06006052
18	[H]C1([H])C([H])([H])C1([H])[H]	0.32815231	0.3281839	0.00723734	0.00724217
19	[H]C1([H])OC1([H])[H]	0.29635574	0.29981734	0.00682283	0.06824817
20	[H]C([H])([H])C(=O)C([H])([H])[H]	0.17028194	0.2585645	0	0.03421965

DALŠIE REPREZENTÁCIE MOLEKÚL

- OneHotFeaturizer
- Smiles2Vec
- SmilesToImage
- MolGanFeaturizer
- ConvMolFeaturizer
- SmilesTokenizer
- BertFeaturizer



MODELY

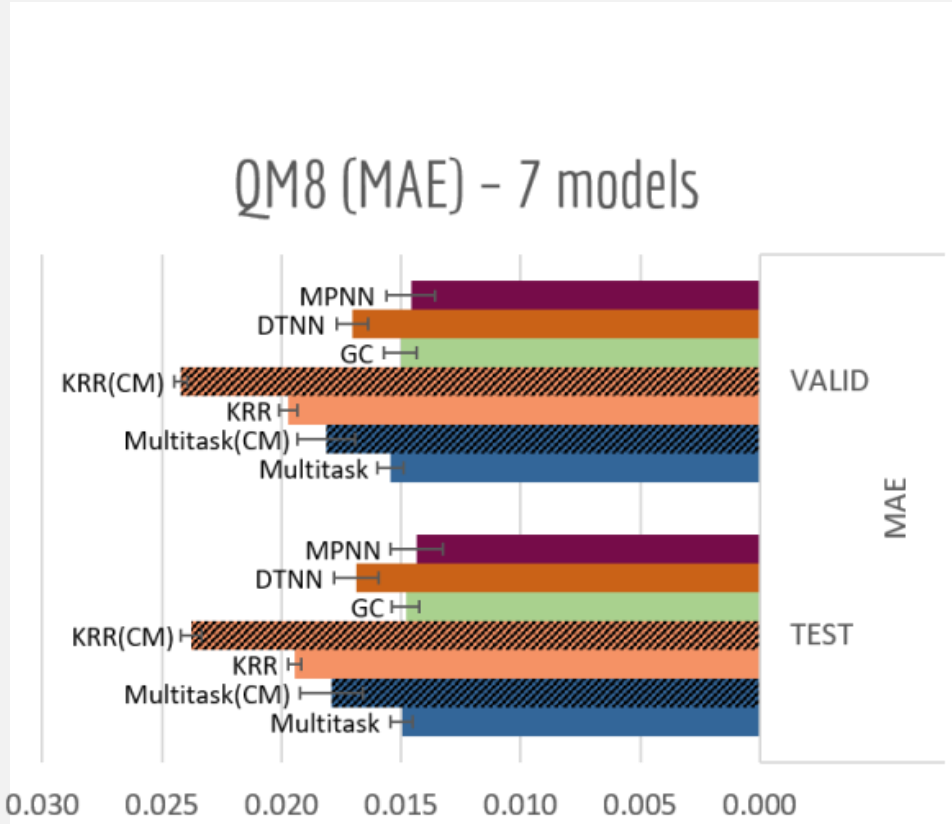
Multitask regressor

Kernel ridge regressor (KRR)

Graph convolution (GC)

Message-passing neural network (MPNN) typ GNN

Deep tensor neural networks (DTNN)



https://moleculenet.org/full-results

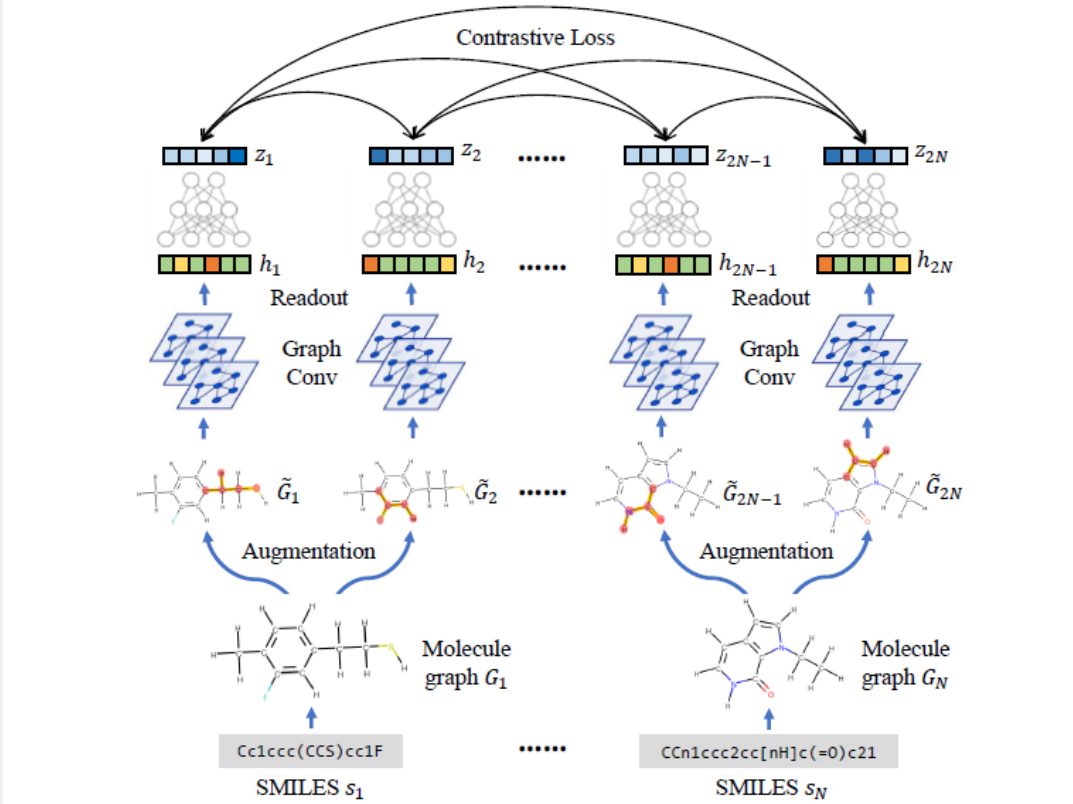
SAMO-KONTROLOVANÉ MODELY

MolCLR

- kontrastívne učenie (SimCLR)
- GNN

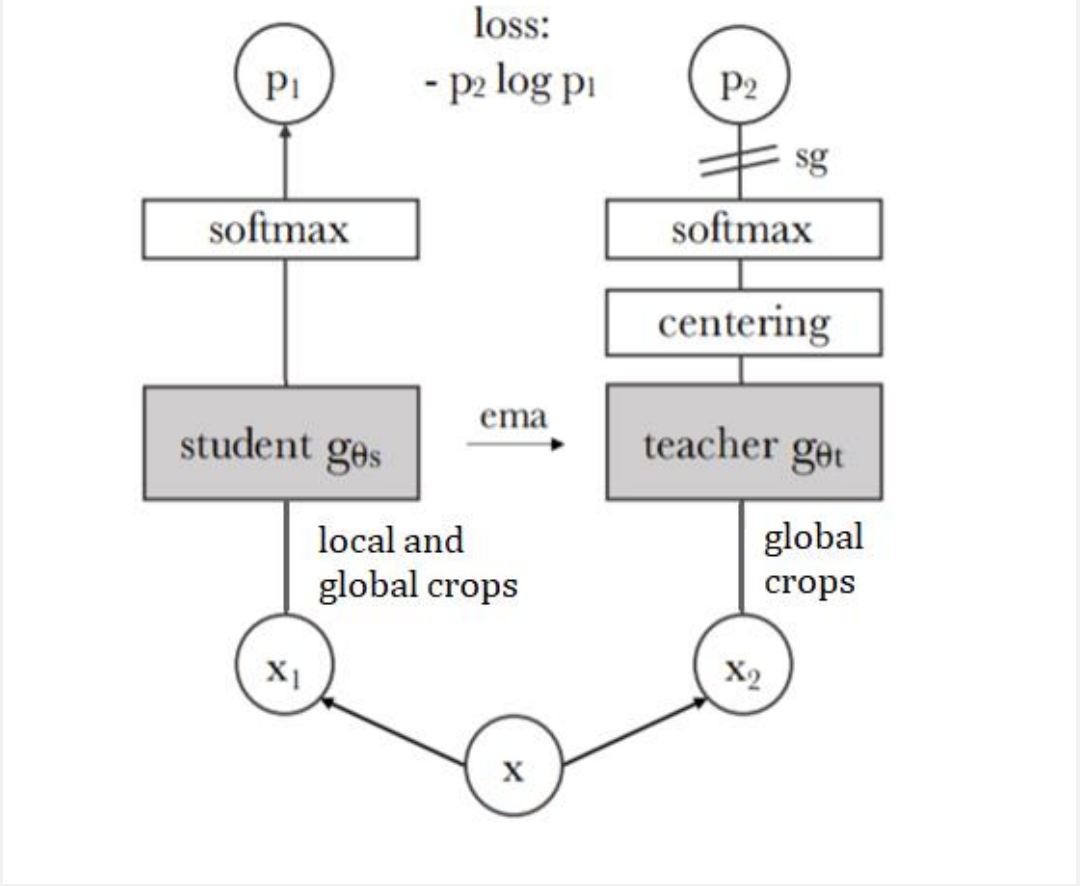
ChemBERTa

- RoBERTa →
  BERT →
  language representation model



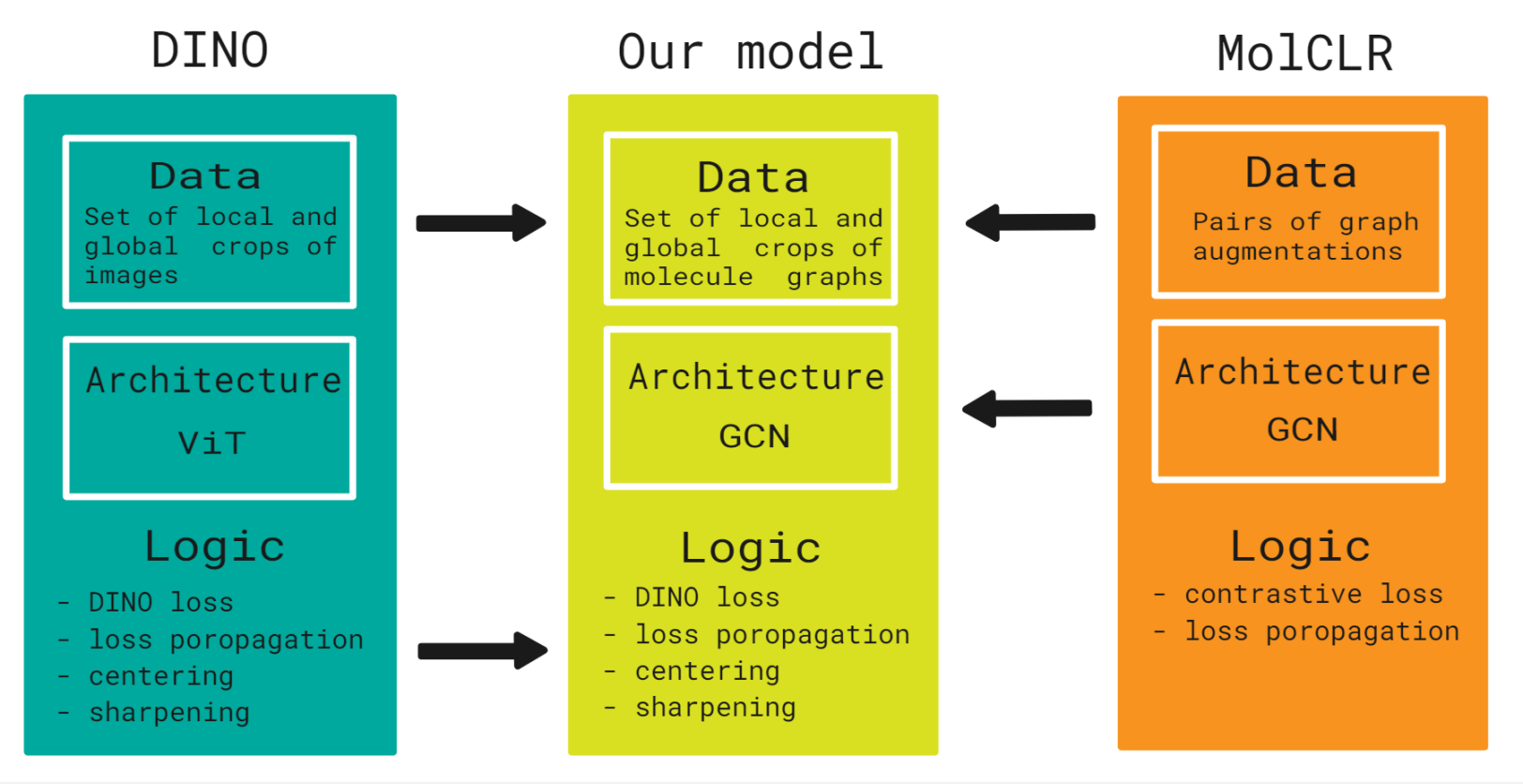
DINO ARCHITEKTÚRA

- DINO: Self-**Di**stillation with **no** labels
  - samo-kontrolovaná metóda
- študent a učiteľ – rovnaká architektúra
- vstupy – výseky obrázkov
- chyba:
  - contrastive loss
  - spätne šírená len v študentskej sieti
- váhy učiteľa – ema (exponential moving average) $W_t = \lambda W_t + (1 - \lambda) W_s$

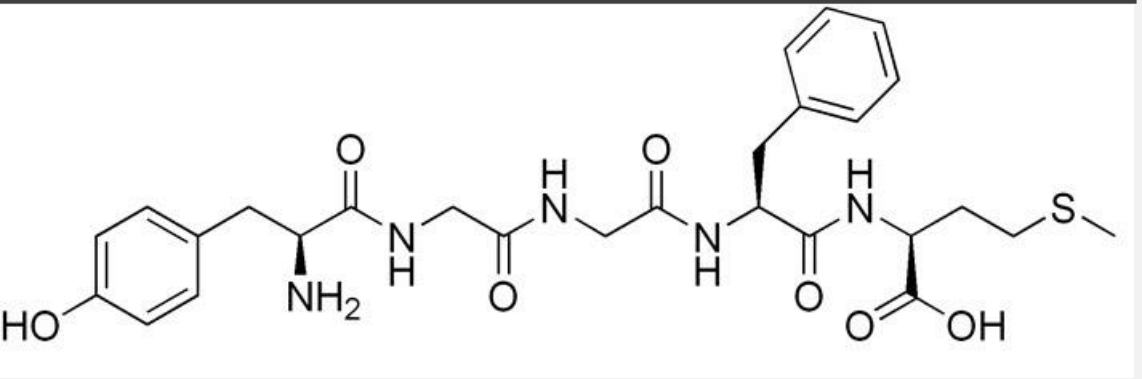


Emerging Properties in Self-Supervised Vision Transformers (2021, Facebook)
https://arxiv.org/abs/2104.14294

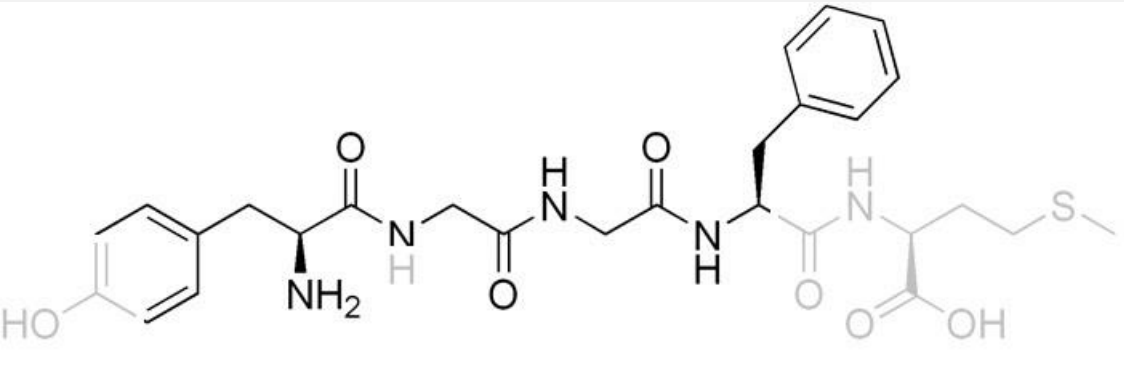
NÁVRH MODELU

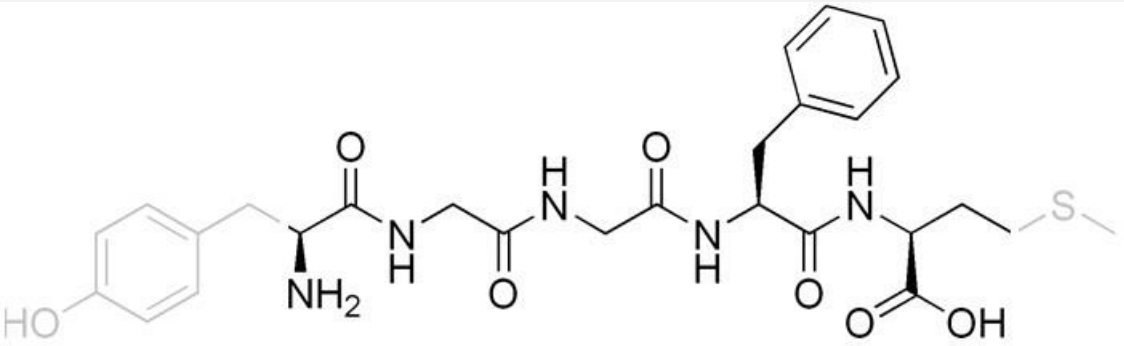


GRAFOVÉ VÝSEKY

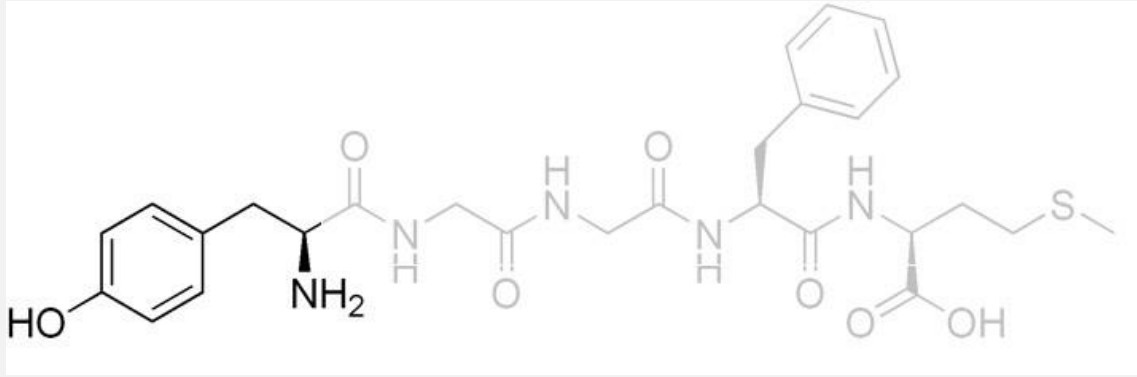


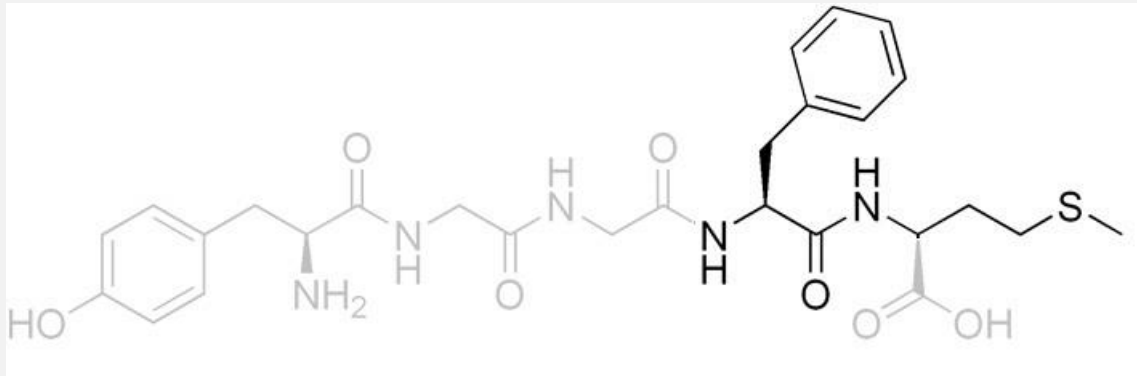
Globálne

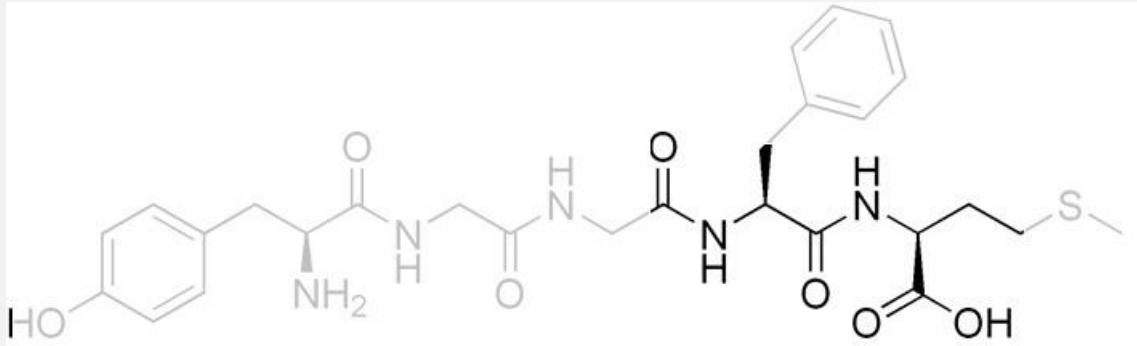




Lokálne







AKTUÁLNY STAV

- Prehľad v metódach klasifikácie a predikcie vlastností molekúl
- Prehľad v samo-kontrolovaných metódach využitých v oblasti počítačového videnia
  - DINO - metóda samo-kontrolovaného učenia
- Návrh vlastného riešenia
  - Dáta na predtréning
  - Návrh a implementácia architektúry
  - Navrh a implementácia dátových transformácií
  - Vyše 20 hyperparametrov

ĎALŠIE KROKY

- Finalizácia implementácie
  - Oprava chýb
- Identifikácia doležitých hyperparametrov
- Tréning modelu
  - Prehľadávanie priestoru hyperparametrov
  - Nájdenie optimálneho modelu
- Porovnanie výsledkov

ĎAKUJEM ZA POZORNOSŤ

ZDROJE A UŽITOČNÉ ODKAZY

- https://arxiv.org/pdf/1703.00564.pdf
- https://arxiv.org/abs/2104.14294
- https://arxiv.org/pdf/1706.03762.pdf
- https://arxiv.org/pdf/2103.03404.pdf
- https://towardsdatascience.com/on-dino-self-distillation-with-no-labels-c29e9365e382
- https://www.youtube.com/watch?v=h3ij3F3cPIk&ab_channel=YannicKilcher
- https://towardsdatascience.com/transformers-an-exciting-revolution-from-text-to-videos-dc70a15e617b
- https://www.youtube.com/watch?v=iDulhoQ2pro&t=10s&ab_channel=YannicKilcher