nature machine intelligence

Article

https://doi.org/10.1038/s42256-023-00654-0

Knowledge graph-enhanced molecular contrastive learning with functional prompt

Received: 12 September 2022

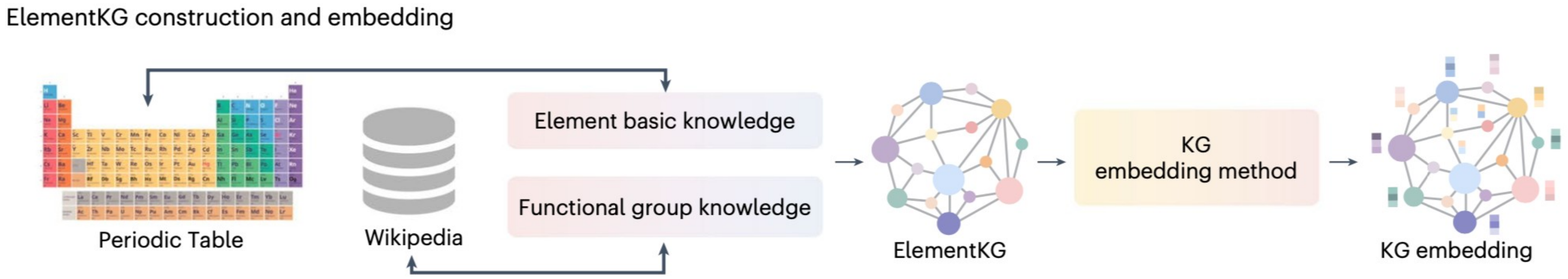
Accepted: 6 April 2023

Yin Fang [1,2,3], Qiang Zhang [1,2], Ningyu Zhang [1,4,5], Zhuo Chen [1,2], Xiang Zhuang [1,2], Xin Shao [3], Xiaohui Fan [3,6,7] & Huajun Chen [1,2,5,8]

Introduction –

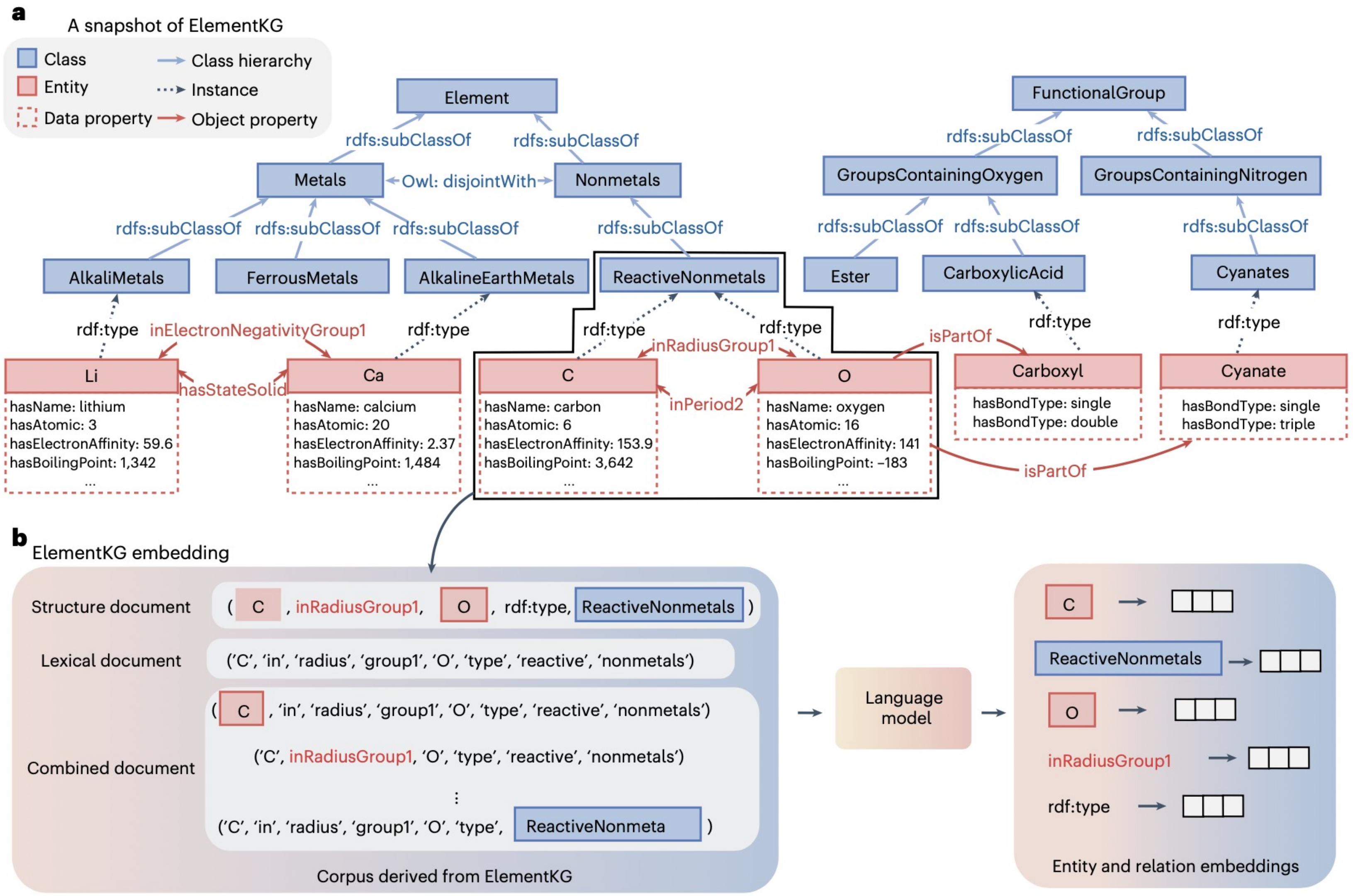
- Most current SSL methods, completely data-driven.
- Low generalizability + interpretability.
- Fundamental problems with current approaches.
- ElementKG.
- ElementKG guided Mol. graph augmentations.
- Functional prompting using ElemenetKG + strong expts.

KANO –



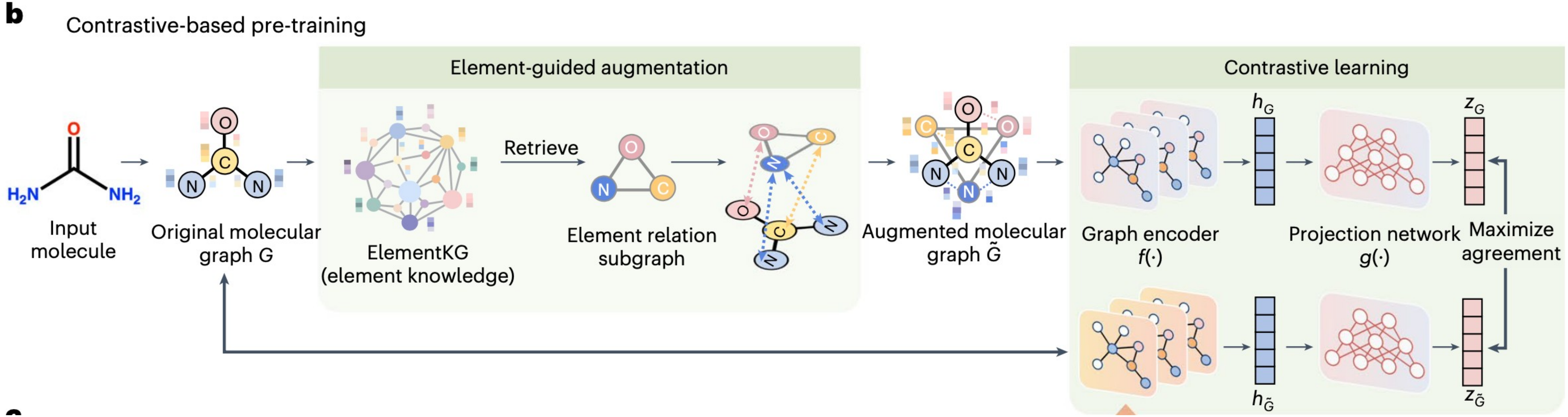
KANO –

- Use OWL2Vec to embed the KG.



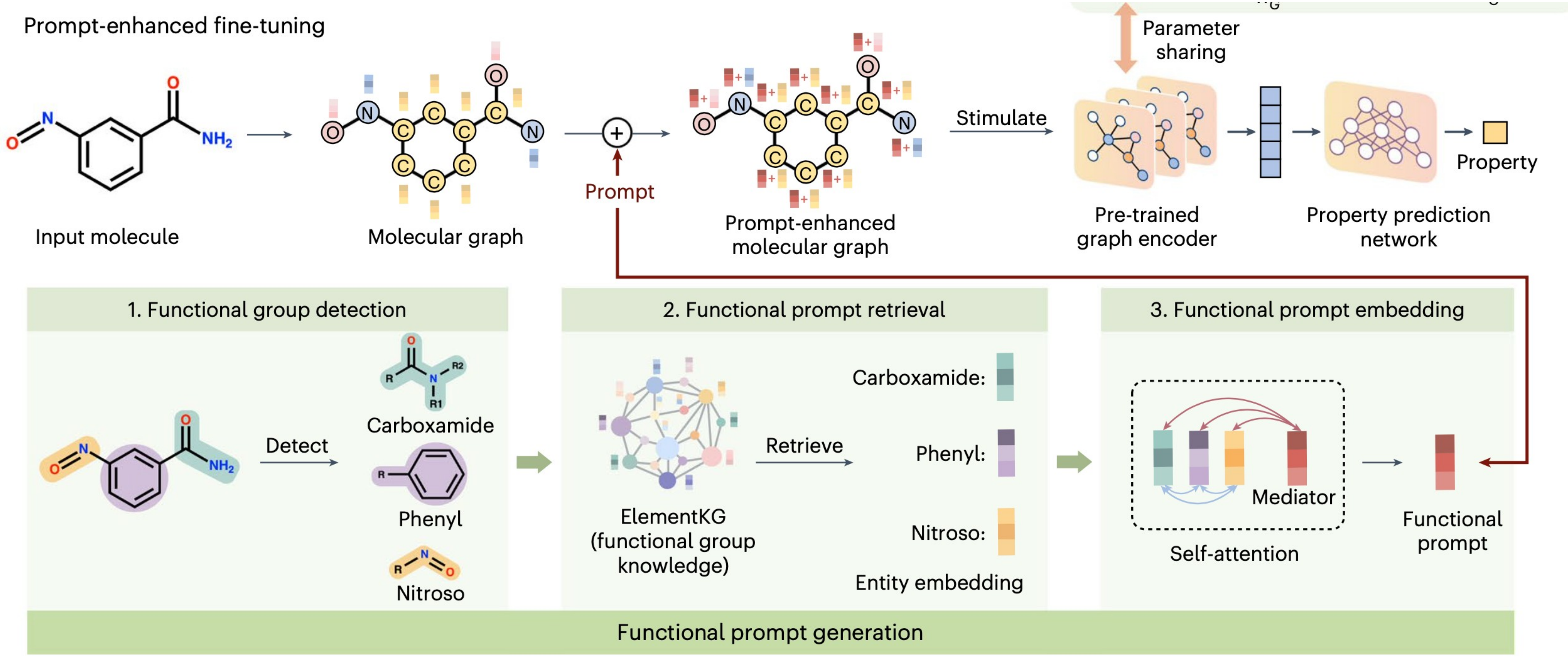
KANO –

- Contrastive Learning. (N examples to 2N)



KANO –

- Prompt based fine-tuning.



Results –

- Classification tasks.

Category	Physiology					Biophysics		
Dataset	**BBBP**	**Tox21**	**ToxCast**	**SIDER**	**ClinTox**	**BACE**	**MUV**	**HIV**
Number of molecules	**2,039**	**7,831**	**8,575**	**1,427**	**1,478**	**1,513**	**93,807**	**41,127**
Number of tasks	**1**	**12**	**617**	**27**	**2**	**1**	**17**	**1**
GCN[47]	71.8±0.9	70.9±0.3	65.0±6.1	53.6±0.3	62.5±2.8	71.6±2.0	71.6±4.0	74.0±3.0
GIN[48]	65.8±4.5	74.0±0.8	66.7±1.5	57.3±1.6	58.0±4.4	70.1±5.4	71.8±2.5	75.3±1.9
MPNN[49]	91.3±4.1	80.8±2.4	69.1±3.0	59.5±3.0	87.9±5.4	81.5±1.0	75.7±1.3	77.0±1.4
DMPNN[50]	91.9±3.0	75.9±0.7	63.7±0.2	57.0±0.7	90.6±0.6	85.2±0.6	78.6±1.4	77.1±0.5
CMPNN[26]	92.7±1.7	80.1±1.6	70.8±1.3	61.6±0.3	89.8±0.8	86.7±0.2	79.0±2.0	78.2±2.2
N-GRAM[46]	91.2±0.3	76.9±2.7	-	63.2±0.5	87.5±2.7	79.1±1.3	76.9±0.7	78.7±0.4
Hu et.al[7]	70.8±1.5	78.7±0.4	65.7±0.6	62.7±0.8	72.6±1.5	84.5±0.7	81.3±2.1	79.9±0.7
MGSSL[10]	70.5±1.1	76.4±0.4	64.1±0.7	61.8±0.8	80.7±2.1	79.7±0.8	78.7±1.5	79.5±1.1
GEM[9]	88.8±0.4	78.1±0.4	68.6±0.2	63.2±1.5	90.3±0.7	87.9±1.1	75.3±1.5	81.3±0.3
GROVER[8]	86.8±2.2	80.3±2.0	56.8±3.4	61.2±2.5	70.3±13.7	82.4±3.6	67.3±1.8	68.2±1.1
GraphMVP[51]	72.4±1.6	75.9±0.5	63.1±0.4	63.9±1.2	79.1±2.8	81.2±0.9	77.7±0.6	77.0±1.2
MolCLR[11]	73.3±1.0	74.1±5.3	65.9±2.1	61.2±3.6	89.8±2.7	82.8±0.7	78.9±2.3	77.4±0.6
$\text{MolCLR}_{\text{CMPNN}}$	72.4±0.7	78.4±2.6	69.1±1.2	59.7±3.4	88.0±4.0	85.0±2.4	74.5±2.1	77.8±5.5
KANO	**96.0±1.6**	**83.7±1.3**	**73.2±1.6**	**65.2±0.8**	**94.4±0.3**	**93.1±2.1**	**83.7±2.3**	**85.1±2.2**

*Note that the N-GRAM model on ToxCast is too time consuming to finish in time, and its results are not presented. The best-performing results are marked in bold.

Results –

- Regression tasks.

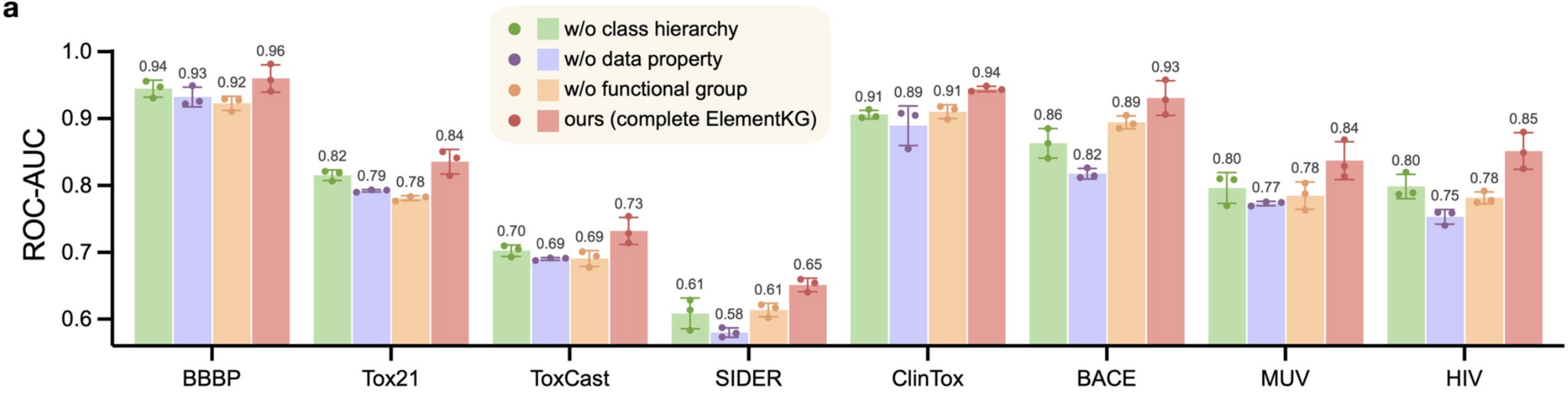
Category	Physical chemistry			Quantum mechanics		
Dataset	**ESOL**	**FreeSolv**	**Lipophilicity**	**QM7**	**QM8**	**QM9**
Number of molecules	**1,128**	**642**	**4,200**	**7,160**	**21,786**	**133,885**
Number of tasks	**1**	**1**	**1**	**1**	**12**	**3**
GCN[47]	1.431±0.050	2.870±0.135	0.712±0.049	122.9±2.2	0.0366±0.000	0.00835±0.00001
GIN[48]	1.452±0.020	2.765±0.180	0.850±0.071	124.8±0.7	0.0371±0.001	0.00824±0.00004
MPNN[49]	1.167±0.430	1.621±0.952	0.672±0.051	111.4±0.9	0.0148±0.001	0.00522±0.00003
DMPNN[50]	1.050±0.008	1.673±0.082	0.683±0.016	103.5±8.6	0.0156±0.001	0.00514±0.00001
CMPNN[26]	0.798±0.112	1.570±0.442	0.614±0.029	75.1±3.1	0.0153±0.002	0.00405±0.00002
N-GRAM[46]	1.100±0.030	2.510±0.191	0.880±0.121	125.6±1.5	0.0320±0.003	0.00964±0.00031
Hu et.al[7]	1.100±0.006	2.764±0.002	0.739±0.003	113.2±0.6	0.0215±0.001	0.00922±0.00004
GEM[9]	0.813±0.028	1.748±0.114	0.674±0.022	60.0±2.7	0.0163±0.001	0.00562±0.00007
GROVER[8]	1.423±0.288	2.947±0.615	0.823±0.010	91.3±1.9	0.0182±0.001	0.00719±0.00208
MolCLR[11]	1.113±0.023	2.301±0.247	0.789±0.009	90.9±1.7	0.0185±0.013	0.00480±0.00003
$MolCLR_{CMPNN}$	0.911±0.082	2.021±0.133	0.875±0.003	89.8±6.3	0.0179±0.001	0.00475±0.00001
KANO	**0.670±0.019**	**1.142±0.258**	**0.566±0.007**	**56.4±2.8**	**0.0123±0.000**	**0.00320±0.00001**

*The best-performing results are marked in bold.

Results –

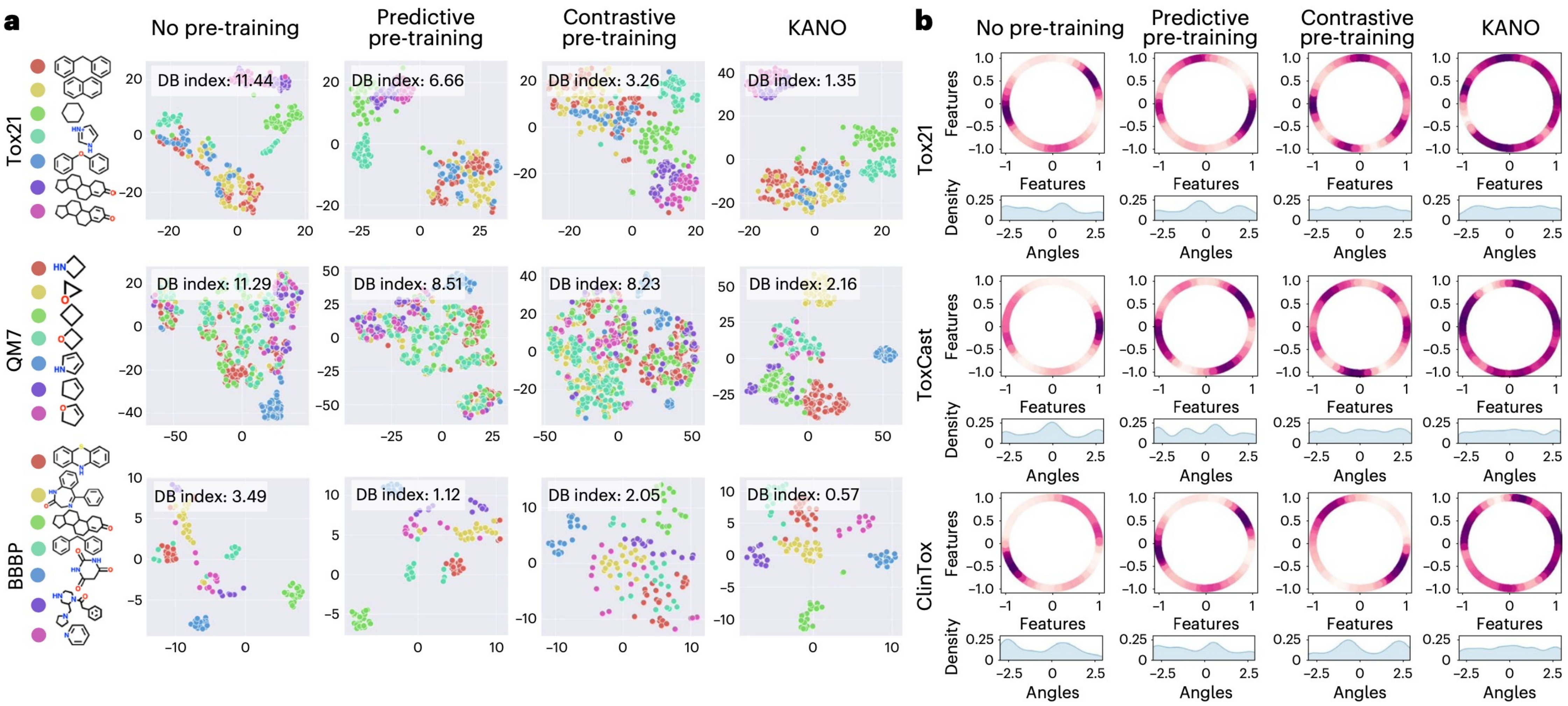
- Robust Representations.

a



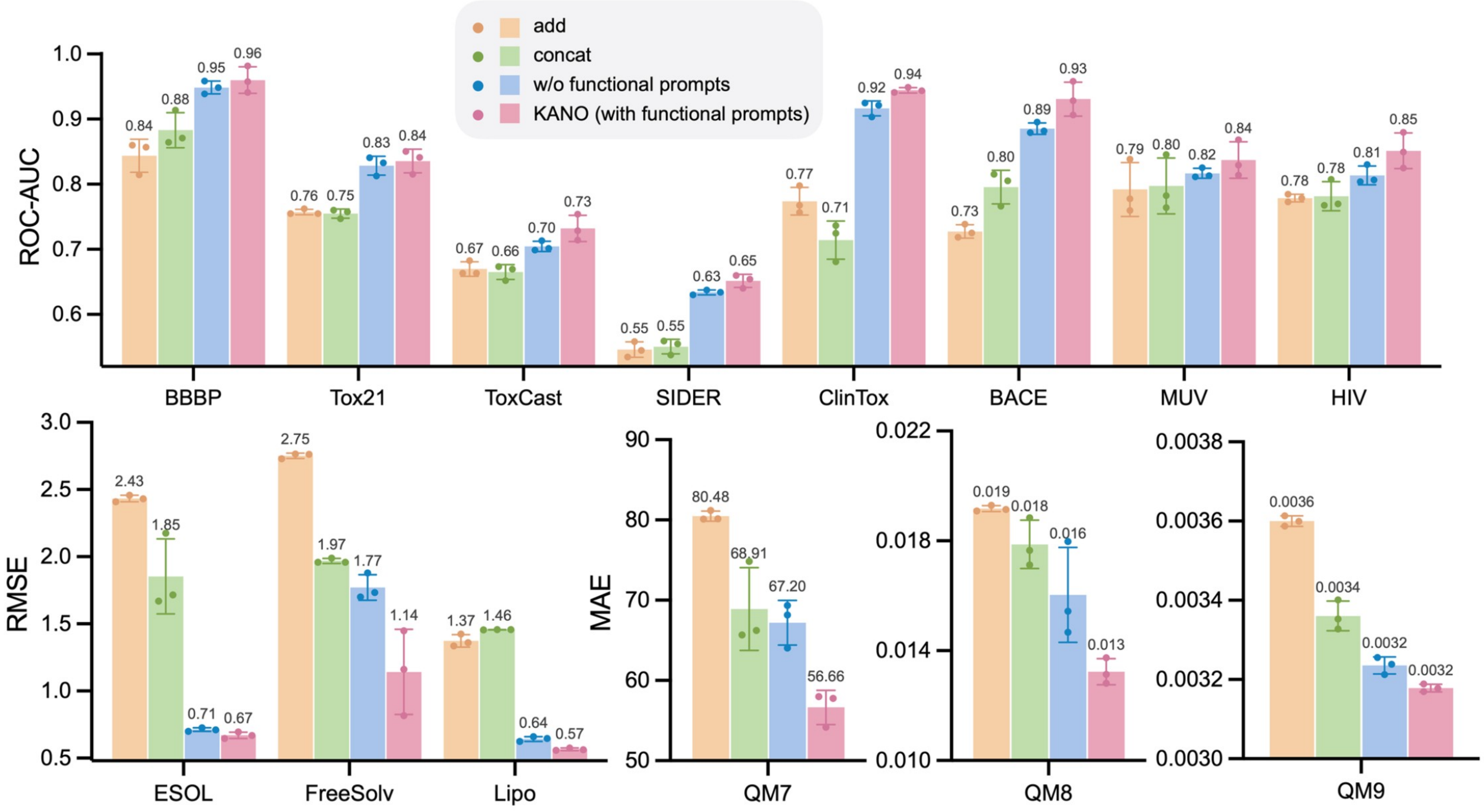
Results –

- Alignment and uniformity.



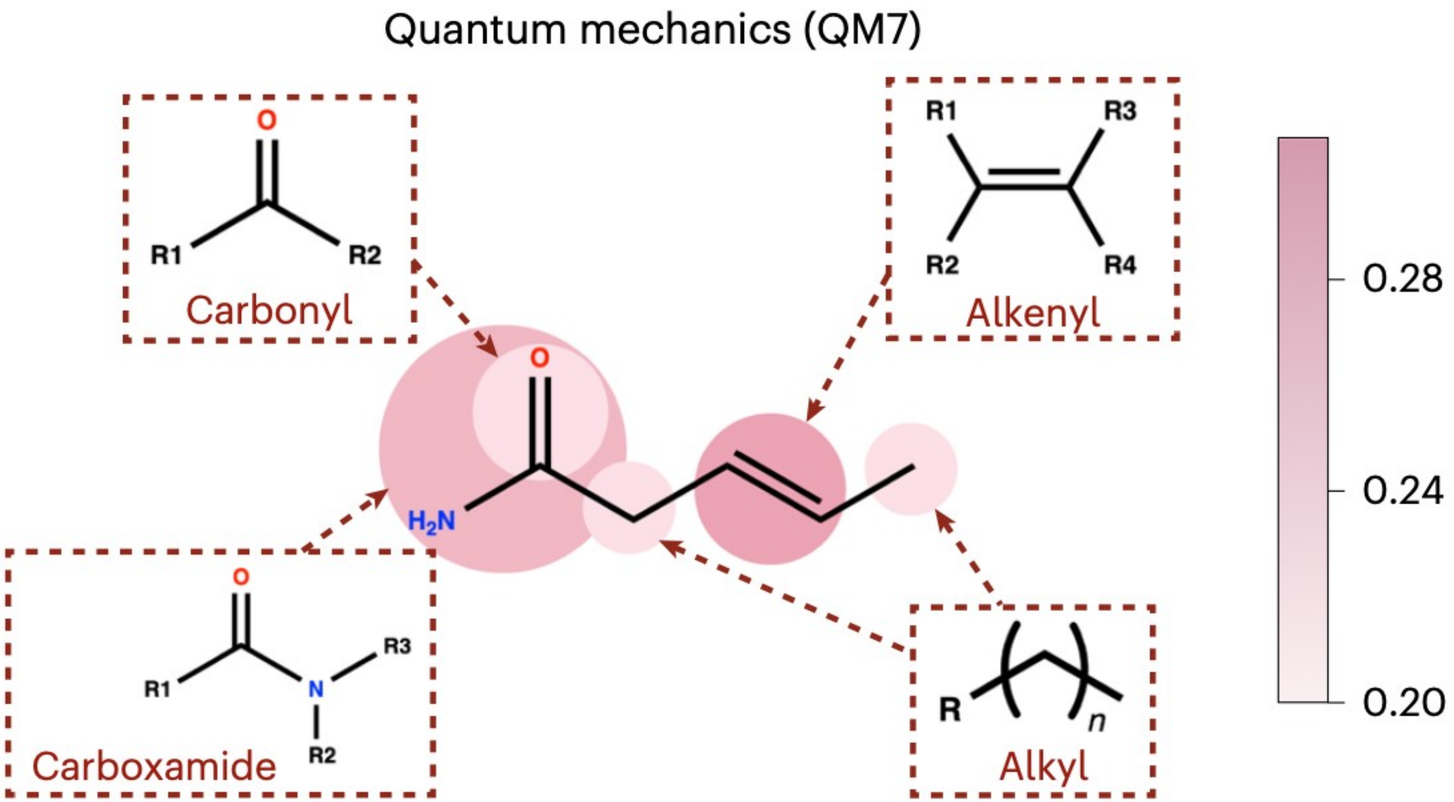
Results –

- Importance of functional prompts.



Results –

- Example of attention mechanism. (they have reported several others)



Multi-Grained Multimodal Interaction Network for Entity Linking

Pengfei Luo
School of Computer Science and Technology, University of Science and Technology of China & State Key Laboratory of Cognitive Intelligence
Hefei, Anhui, China
pfluo@mail.ustc.edu.cn

Tong Xu*
School of Computer Science and Technology, University of Science and Technology of China & State Key Laboratory of Cognitive Intelligence
Hefei, Anhui, China
tongxu@ustc.edu.cn

Shiwei Wu
School of Data Science, University of Science and Technology of China & State Key Laboratory of Cognitive Intelligence
Hefei, Anhui, China
dwustc@mail.ustc.edu.cn

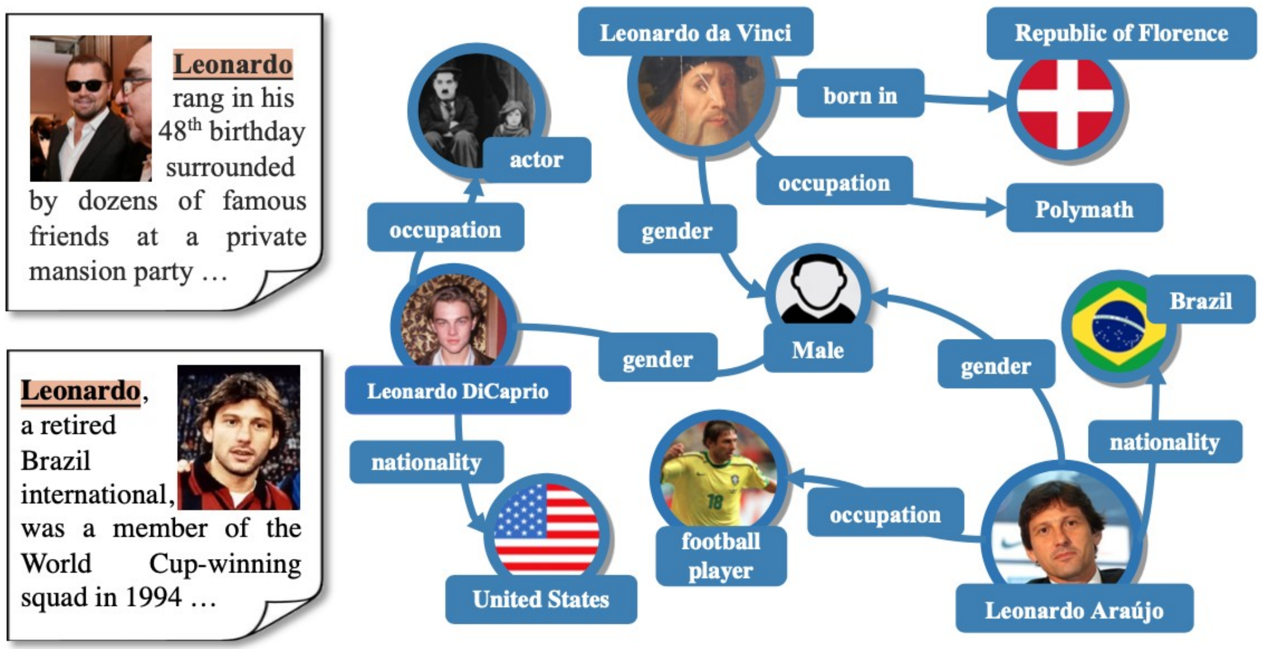
Chen Zhu
Career Science Lab, BOSS Zhipin & School of Management, University of Science and Technology of China
Beijing, China
zc3930155@gmail.com

Linli Xu
School of Computer Science and Technology, University of Science and Technology of China & State Key Laboratory of Cognitive Intelligence
Hefei, Anhui, China
linlixu@ustc.edu.cn

Enhong Chen*
School of Computer Science and Technology, University of Science and Technology of China & State Key Laboratory of Cognitive Intelligence
Hefei, Anhui, China
cheneh@ustc.edu.cn

Introduction –

- Entity disambiguation (linking) in a MMKG.



- MEL is a tough task.

Introduction –

- **M**ulti-Gra**I**ned **M**ultimodal **I**ntera**C**tion network (MIMIC)
- SOTA results + strong ablation studies.

Related Work –

- Text-based entity linking local/global.
- Multimodal entity linking.

Problem Formulation –

- Entity – $\mathbf{E}_i = (\mathbf{e}_{n_i}, \mathbf{e}_{v_i}, \mathbf{e}_{d_i}, \mathbf{e}_{a_i})$ Mention – $\mathbf{M}_j = (\mathbf{m}_{w_j}, \mathbf{m}_{s_j}, \mathbf{m}_{v_j})$

Problem Formulation –

- Goal – $\theta^* = \max_{\theta} \sum_{(\mathbf{M}_j, \mathbf{E}_i) \in \mathcal{D}} \log p_\theta \left(\mathbf{E}_i | \mathbf{M}_j, \mathcal{E} \right)$

Methodology –

- For encoding images of both Entities and Messages, ViT.
  Global feature = embedding of [CLS] token; and
  Local feature = full hidden state.

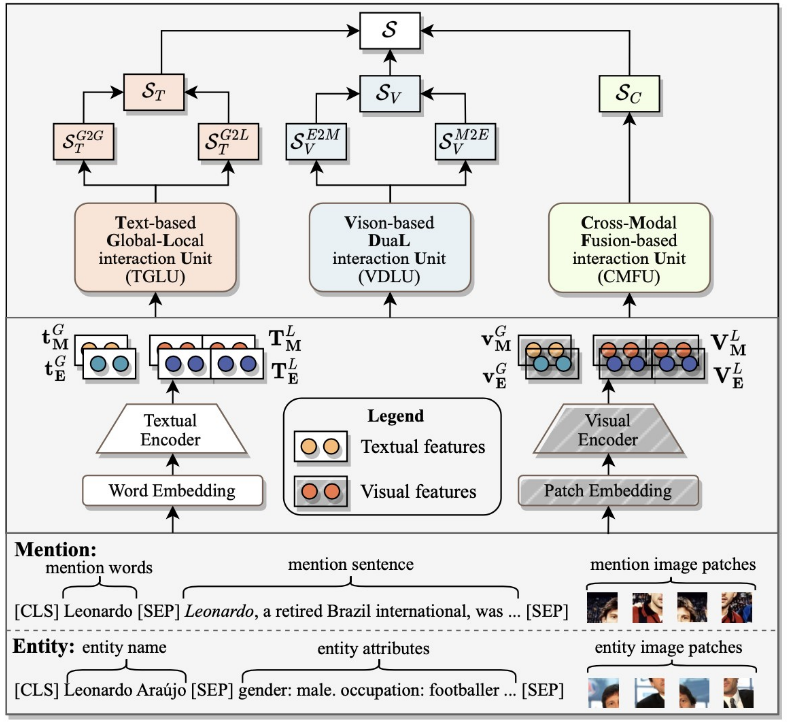
$$\mathbf{V}_{\mathbf{E}_i} = \left[\mathbf{v}^0_{[\mathrm{CLS}]}; \mathbf{v}^1_{\mathbf{E}_i}; \ldots; \mathbf{v}^n_{\mathbf{E}_i} \right] \in \mathbb{R}^{(n+1) \times d_v}$$

Methodology –

- For textual encoding of both Entities and Messages, BERT.

$$\mathbf{I}_{\mathbf{E}_i} = [\mathrm{CLS}]\mathbf{e}_{n_i}[\mathrm{SEP}]\mathbf{e}_{a_i}[\mathrm{SEP}]$$
$$\mathbf{I}_{\mathbf{M}_j} = [\mathrm{CLS}]\mathbf{m}_{w_j}[\mathrm{SEP}]\mathbf{m}_{s_j}[\mathrm{SEP}]$$

And similarly, [CLS] token = “Global” textual feature and full embedding is the “local” textual feature.



Methodology –

- Overall equations using **Text-based Global-Local interaction Unit** (TGLU), **Vision-based DuaL interaction Unit** (VDLU) and **Cross-Modal Fusion- based interaction Unit** (CMFU).

$$\mathcal{S}_T = \mathcal{U}_T\left(\mathbf{M}, \mathbf{E}\right) = (\mathcal{S}_T^{G2G} + \mathcal{S}_T^{G2L})/2,$$

$$\mathcal{S}_V = \mathcal{U}_V\left(\mathbf{M}, \mathbf{E}\right) = (\mathcal{S}_V^{E2M} + \mathcal{S}_V^{M2E})/2,$$

$$\mathcal{S}_C = \mathcal{U}_C\left(\mathbf{M}, \mathbf{E}\right),$$

$$\mathcal{S} = \mathcal{U}\left(\mathbf{M}, \mathbf{E}\right) = (\mathcal{S}_V + \mathcal{S}_T + \mathcal{S}_C)/3,$$

Methodology –

- TGLU –

$$\mathcal{S}_T^{G2G} = \mathbf{t}_{\mathbf{E}}^G \cdot \mathbf{t}_{\mathbf{M}}^G$$

$$Q, K, V = \mathbf{T}_{\mathbf{E}}^L \boldsymbol{W}_{tq}, \mathbf{T}_{\mathbf{M}}^L \boldsymbol{W}_{tk}, \mathbf{T}_{\mathbf{M}}^L \boldsymbol{W}_{tv},$$

$$H_t = \mathrm{softmax}(\frac{QK^T}{\sqrt{d_T}})V,$$

$$h_t = \mathrm{LayerNorm}\left(\mathrm{MeanPooling}\left(H_t\right)\right),$$

$$\mathbf{S}_T^{G2L} = \mathrm{FC}\left(\mathbf{t}_{\mathbf{E}}^G\right) \cdot h_t,$$

Methodology –

- VDLU –

$$\mathcal{S}_V^{E2M} = \mathrm{DUAL}_{E2M}\left(\mathbf{v}_{\mathbf{E}}^{G}, \mathbf{v}_{\mathbf{M}}^{G}, \mathbf{V}_{\mathbf{M}}^{L}\right),$$
$$\mathcal{S}_V^{M2E} = \mathrm{DUAL}_{M2E}\left(\mathbf{v}_{\mathbf{M}}^{G}, \mathbf{v}_{\mathbf{E}}^{G}, \mathbf{V}_{\mathbf{E}}^{L}\right),$$

$\mathrm{DUAL}_{A2B}(v_A, v_B, V_B)$ is as follows –

$$\bar{h}_p = \mathrm{MeanPooling}\left(\mathbf{V}_{\mathbf{B}}^{L}\right),$$
$$h_{vc} = \mathrm{FC}\left(\mathrm{LayerNorm}\left(\bar{h}_p + \mathbf{v}_{\mathbf{A}}^{G}\right)\right),$$
$$h_{vg} = \mathrm{Tanh}\left(\mathrm{FC}\left(h_{vc}\right)\right),$$
$$h_v = \mathrm{LayerNorm}\left(h_{vg} * h_{vc} + \mathbf{v}_{\mathbf{B}}^{G}\right),$$
$$\mathcal{S}_V^{A2B} = h_v \cdot \mathbf{v}_{\mathbf{A}}^{G}$$

Methodology –

- CMFU –

$$h_{et}, h_{mt} = \mathrm{FC}_{c1}\left(\mathbf{t}_{\mathbf{E}}^{G}\right), \mathrm{FC}_{c1}\left(\mathbf{t}_{\mathbf{M}}^{G}\right),$$

$$H_{ev}, H_{mv} = \mathrm{FC}_{c2}\left(\mathbf{V}_{\mathbf{E}}^{L}\right), \mathrm{FC}_{c2}\left(\mathbf{V}_{\mathbf{M}}^{L}\right),$$

$$\alpha_i = \frac{\exp\left(h_{et} \cdot H_{ev}^{i}\right)}{\sum_{i}^{n+1} \exp\left(h_{et} \cdot H_{ev}^{i}\right)},$$

$$h_{ec} = \sum_{i}^{n+1} \alpha_i * H_{ev}^{i}, i \in [1, 2, \ldots, (n+1)]$$

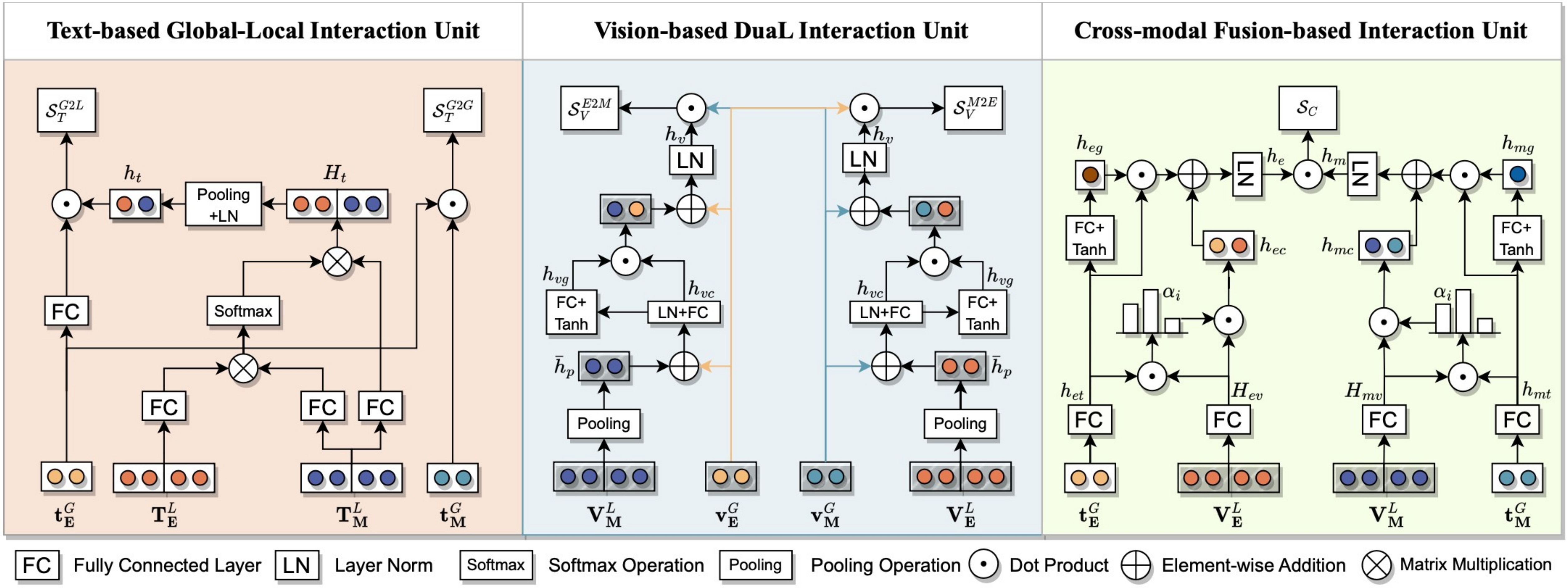
$$h_{eg} = \mathrm{Tanh}\left(\mathrm{FC}_{c3}\left(h_{et}\right)\right),$$

$$h_e = \mathrm{LayerNorm}\left(h_{eg} * h_{et} + h_{ec}\right)$$

$$\mathcal{S}_C = h_e \cdot h_m$$

Methodology –

- Full diagram.



Methodology –

- Unit consistent loss function.

$$\mathcal{L}_O = -\log \frac{\exp\left(\mathcal{U}(\mathbf{M}, \mathbf{E})\right)}{\sum_i \exp\left(\mathcal{U}(\mathbf{M}, \mathbf{E}_i')\right)},$$

$$\mathcal{L}_X = -\log \frac{\exp\left(\mathcal{U}_X(\mathbf{M}, \mathbf{E})\right)}{\sum_i \exp\left(\mathcal{U}_X(\mathbf{M}, \mathbf{E}_i')\right)}, X \in \{T, V, C\},$$

$$\mathcal{L} = \mathcal{L}_O + \underbrace{\mathcal{L}_T + \mathcal{L}_V + \mathcal{L}_C}_{\text{unit-consistent loss function}}.$$

Experiments –

- Questions –

- **RQ1.** How does the proposed MIMIC perform compared with various baselines?
- **RQ2.** How do the generalization abilities of MIMIC and other baselines perform in low-resource scenarios?
- **RQ3.** How do the three proposed interaction units and unit-consistent objective function affect performance?
- **RQ4.** How does the model performance change with the parameters?

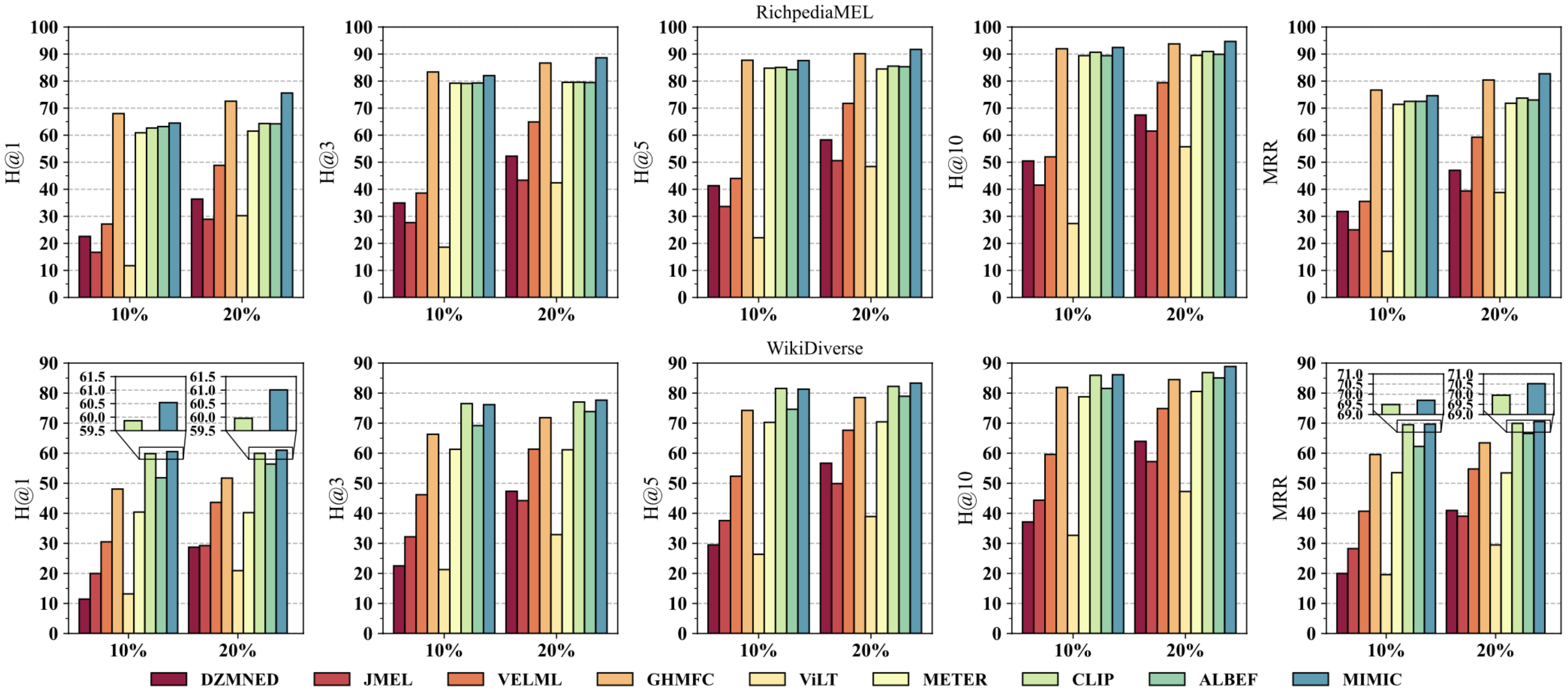
Experiments –

- RQ1 (vs Baselines) –

Model	WikiMEL					RichpediaMEL					WikiDiverse				
	H@1↑	H@3↑	H@5↑	MRR↑	MR↓	H@1↑	H@3↑	H@5↑	MRR↑	MR↓	H@1↑	H@3↑	H@5↑	MRR↑	MR↓
BLINK [38]	74.66	86.63	90.57	81.72	51.48	58.47	81.51	88.09	71.39	178.57	57.14	78.04	85.32	69.15	332.03
BERT [9]	74.82	86.79	90.47	81.78	51.23	59.55	81.12	87.16	71.67	278.08	55.77	75.73	83.11	67.38	373.96
RoBERTa [23]	73.75	85.85	89.80	80.86	31.02	61.34	81.56	87.15	72.80	218.16	59.46	78.54	85.08	70.52	405.22
DZMNED [26]	78.82	90.02	92.62	84.97	152.58	68.16	82.94	87.33	76.63	313.85	56.90	75.34	81.41	67.59	563.26
JMEL [1]	64.65	79.99	84.34	73.39	285.14	48.82	66.77	73.99	60.06	470.90	37.38	54.23	61.00	48.19	996.63
VELML [43]	76.62	88.75	91.96	83.42	102.72	67.71	84.57	89.17	77.19	332.85	54.56	74.43	81.15	66.13	463.25
GHMFC [35]	76.55	88.40	92.01	83.36	54.75	72.92	86.85	90.60	80.76	214.64	60.27	79.40	84.74	70.99	628.87
CLIP [29]	83.23	92.10	94.51	88.23	17.60	67.78	85.22	90.04	77.57	107.16	61.21	79.63	85.18	71.69	313.35
ViLT [18]	72.64	84.51	87.86	79.46	220.76	45.85	62.96	69.80	56.63	675.93	34.39	51.07	57.83	45.22	2421.49
ALBEF [21]	78.64	88.93	91.75	84.56	47.95	65.17	82.84	88.28	75.29	122.30	60.59	75.59	81.30	69.93	291.17
METER [11]	72.46	84.41	88.17	79.49	111.90	63.96	82.24	87.08	74.15	376.42	53.14	70.93	77.59	63.71	944.48
MIMIC	**87.98***	**95.07***	**96.37***	**91.82***	**11.02**	**81.02***	**91.77***	**94.38***	**86.95***	**55.11***	**63.51***	**81.04**	**86.43***	**73.44***	**227.08**

Experiments –

- RQ2 (Low resource setting, x% training data) –



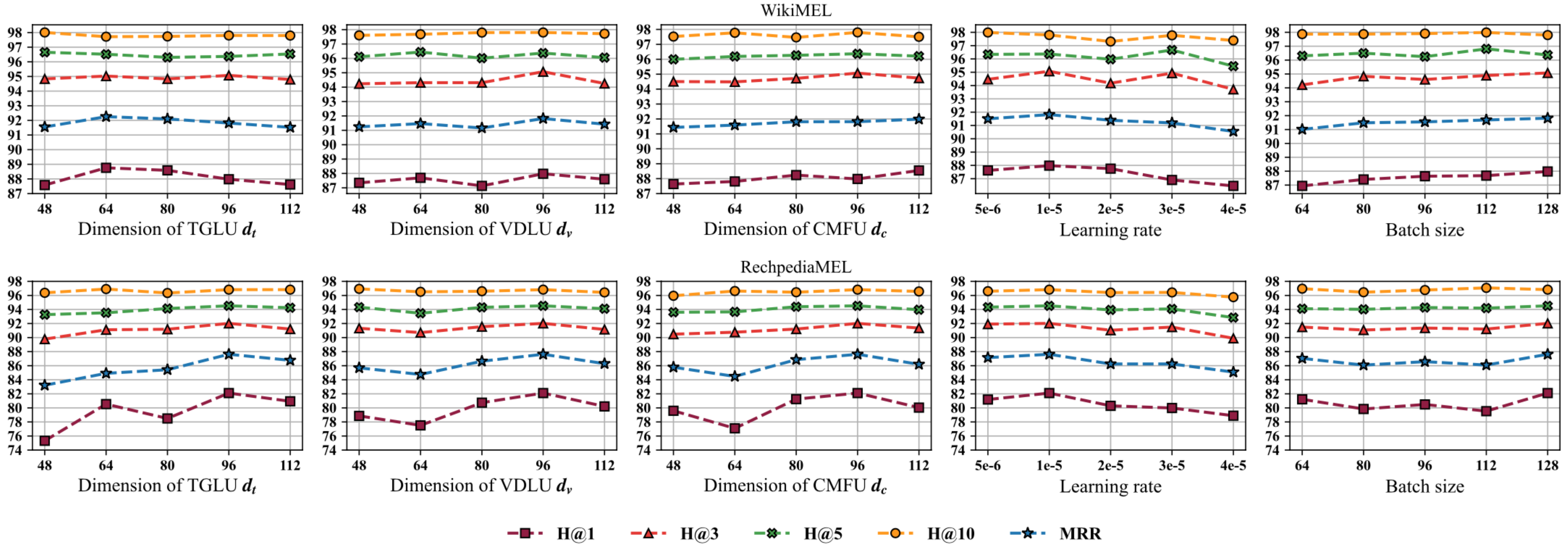
Experiments –

- RQ3 (Ablation Study) –

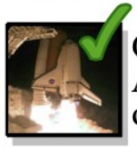
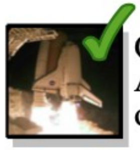
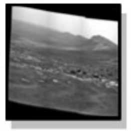
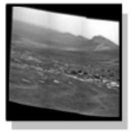
Model	WikiMEL						RichpediaMEL					
	H@1↑	H@3↑	H@5↑	H@10↑	H@20↑	MRR↑	H@1↑	H@3↑	H@5↑	H@10↑	H@20↑	MRR↑
MIMIC	**87.98**	**95.07**	**96.37**	97.80	98.73	**91.82**	**81.02**	**91.77**	**94.38**	**96.69**	**98.04**	**86.95**
w/o $\mathcal{L}_T$	86.13	93.69	95.74	97.66	98.57	90.42	72.82	89.05	93.12	96.15	97.61	81.61
w/o $\mathcal{L}_V$	86.71	94.43	96.25	**98.01**	**98.80**	90.94	78.72	90.23	93.66	96.04	97.61	85.15
w/o $\mathcal{L}_C$	86.67	94.04	95.69	97.21	98.18	90.74	79.65	89.89	92.56	94.92	96.94	85.38
w/o TGLU + $\mathcal{L}_T$	85.03	92.36	94.35	95.94	97.27	89.18	74.48	85.37	88.71	92.00	94.02	80.74
w/o VDLU + $\mathcal{L}_V$	83.46	93.33	95.47	97.23	98.18	88.74	74.12	89.47	92.81	95.82	97.61	82.37
w/o CMFU + $\mathcal{L}_C$	84.60	92.90	94.82	96.42	97.35	89.14	76.98	88.29	91.30	94.22	96.15	83.39

Experiments –

- RQ4 (Parameter Sensitivity) –



Example –

Mention	Ground Truth Entity		MIMIC		GHMFC		CLIP
 Official photo of *Endeavour's* final crew, taken in January 2010.	 Q182508 **Endeavour** American Space Shuttle orbiter	Top1	 Q182508 | Endeavour | American Space Shuttle orbiter	Top1	 Q96206891 | Endeavour | Crew Dragon space capsule manufactured by SpaceX	Top1	Q2151914 | Endeavour | british television series
		Top2	 Q96206891 | Endeavour | Crew Dragon space capsule manufactured by SpaceX	Top2	 Q182508 | Endeavour | American Space Shuttle orbiter	Top2	 Q182508 | Endeavour | American Space Shuttle orbiter
		Top3	 Q96206891 | Endeavour | village in Saskatchewan, Canada	Top3	 Q508018 | Endeavour | ship	Top3	 Q96206891 | Endeavour | village in Saskatchewan, Canada
 *Bush* with Iraqi Prime Minister Nouri al-Maliki in 2006.	 Q207 **George W. Bush** president of the United States from 2001 to 2009	Top1	 Q207 | George W. Bush | president of the United States from 2001 to 2009	Top1	 Q247949 | Bush | British rock band	Top1	 Q247949 | Bush | British rock band
		Top2	 Q247949 | Bush | British rock band	Top2	 Q2743830 | Bush family | American family prominent in the fields of politics, sports and business	Top2	Q2743830 | George Bush | racing driver
		Top3	 Q96206891 | presidency of George W. Bush | 43rd presidential administration and cabinet of the USA (2001-2009)	Top3	 Q5537488 | George Bush | American biblical scholar and pastor (1796–1859)	Top3	 Q5537488 | George Bush | American biblical scholar and pastor (1796–1859)