# UniMatch: Universal matching from Atom to Task for Few-shot Drug Discovery

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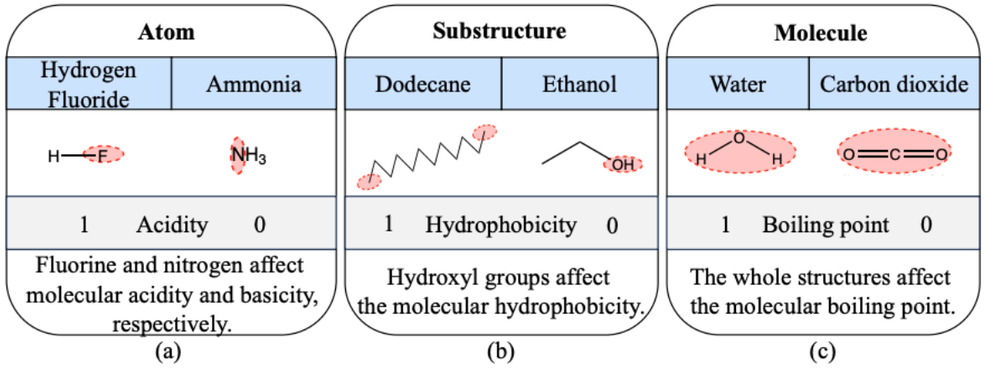
## Motivation

- Different levels of structural information contribute to distinct molecular properties.
- Matching Learning is useful in few-shot learning task.




## Contribution

- We introduce a universal matching approach that spans from the atoms level to the task level for few-shot drug discovery.
- We propose an explicit hierarchical molecular matching mechanism that integrates information from atoms to higher-level structures.

## Universal Matching: Bridging Data & Task:

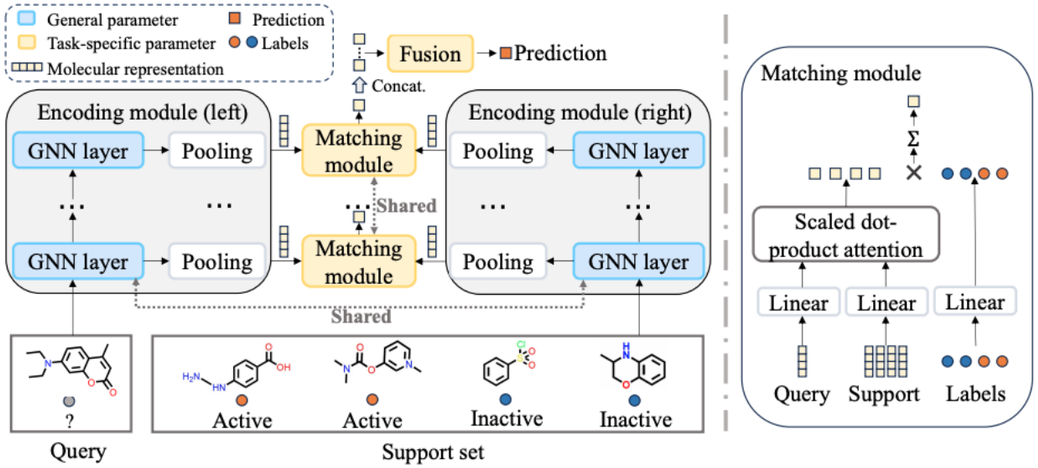
### Hierarchical molecular matching & Meta-learning

#### Model

- Encoding Module.
- Matching Module.
- Fusion.

#### Training and Inference

- Inner Loop.
- Outer Loop.




## Benchmark Results and Downstream Applications

- State-of-the-Art MPP Prediction on MoleculeNet and FS-Mol Benchmark.
- Validated in cross-domain experiment on Meta-MolNet Benchmark.

| Method | Tox21 (12) ↑ | SIDER (27) ↑ | MUV (17) ↑ | ToxCast (617) ↑ |
|---|---|---|---|---|
| CHEF (Adler et al., 2020) | 61.97 ± 0.65 | 57.34 ± 0.82 | 53.17 ± 4.21 | 56.52 ± 1.24 |
| MixHop (Abu-El-Haija et al., 2019) | 78.14 ± 0.33 | 72.01 ± 0.87 | 78.04 ± 3.01 | 77.19 ± 0.93 |
| Siamese (Koch et al., 2015) | 80.40 ± 0.35 | 71.10 ± 4.32 | 59.59 ± 5.13 | - |
| ProtoNet (Snell et al., 2017) | 74.98 ± 0.32 | 64.54 ± 0.89 | 65.88 ± 4.11 | 63.70 ± 1.26 |
| MAML (Finn et al., 2017) | 80.21 ± 0.24 | 70.43 ± 0.76 | 63.90 ± 2.28 | 66.79 ± 0.85 |
| TPN (Liu et al., 2018) | 76.05 ± 0.24 | 67.84 ± 0.95 | 65.22 ± 5.82 | 62.74 ± 1.45 |
| EGNN (Kim et al., 2019) | 81.21 ± 0.16 | 72.87 ± 0.73 | 65.20 ± 2.08 | 63.65 ± 1.57 |
| IterRefLSTM (Altae-Tran et al., 2017) | 81.10 ± 0.17 | 69.63 ± 0.31 | 45.56 ± 5.12 | - |
| PAR (Wang et al., 2021) | 82.06 ± 0.12 | **74.68 ± 0.31** | 66.48 ± 2.12 | 69.72 ± 1.63 |
| ADKF-IFT (Chen et al., 2023) | 82.43 ± 0.60 | 67.72 ± 1.21 | **98.18 ± 3.05** | 72.07 ± 0.81 |
| MHNFs (Schimunek et al., 2023) | 80.23 ± 0.84 | 65.89 ± 1.17 | 73.81 ± 2.53 | 74.91 ± 0.73 |
| **UniMatch (Ours)** | **82.62 ± 0.43** | 68.13 ± 1.54 | 79.40 ± 3.14 | **77.74 ± 0.75** |
| Pre-GNN (Hu et al., 2020) | 82.14 ± 0.08 | 73.96 ± 0.08 | 67.14 ± 1.58 | 73.68 ± 0.74 |
| GNN-MAML (Guo et al., 2021) | 82.97 ± 0.10 | 75.43 ± 0.21 | 68.99 ± 1.84 | - |
| Pre-PAR (Wang et al., 2021) | 84.93 ± 0.11 | 78.08 ± 0.16 | 69.96 ± 1.37 | 75.12 ± 0.84 |
| Pre-ADKF-IFT (Chen et al., 2023) | 86.06 ± 0.35 | 70.95 ± 0.60 | **95.74 ± 0.37** | 76.22 ± 0.13 |
| **Pre-UniMatch (Ours)** | **86.35 ± 0.13** | **80.34 ± 0.45** | 86.35 ± 0.76 | **81.63 ± 0.73** |