

# README

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## Reproduce evaluation results in Table 2.

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### 1. Installation

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Package	Version
Python	3.8
PyTorch	1.10.1
CUDA	11.3
PyTorch Geometric	2.0.4
RDKit	2022.03.5

Create the conda enviroment:

```
cd ./ipdiff
conda env create -f ipdiff.yaml
# For Vina Docking
pip install meeko==0.1.dev3 scipy pdb2pqr vina==1.2.2
python -m pip install git+https://github.com/Valdes-Tresanco-MS/AutoDockTools_py3
```

### 2. Evaluation from sampled results (.pt)

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#### a. Dataset preparation

The data used for evaluation are organized in the Google Drive folder ([https://drive.google.com/drive/folder/s/1j21cc7-97TedKh\\_El5E34yI8o5ckI7eK?usp=share\\_link](https://drive.google.com/drive/folder/s/1j21cc7-97TedKh_El5E34yI8o5ckI7eK?usp=share_link)), which is provided by TargetDiff.

```
https://drive.google.com/drive/folders/1j21cc7-97TedKh_El5E34yI8o5ckI7eK?usp=share_link
```

#### b. Evaluate the sampled molecule ligands of IPDiff

Evaluation results in Table2.

Table 2: Summary of different properties of reference molecules and molecules generated by our model and other non-diffusion (Non-Diff.) and diffusion-based (Diff.) baselines. (↑) / (↓) denotes a larger / smaller number is better. Top 2 results are highlighted with **bold text** and underlined text, respectively.

Methods		Vina Score (↓)		Vina Min (↓)		Vina Dock (↓)		High Affinity (↑)		QED (↑)		SA (↑)		Diversity (↑)	
		Avg.	Med.	Avg.	Med.	Avg.	Med.	Avg.	Med.	Avg.	Med.	Avg.	Med.	Avg.	Med.
Reference		-6.36	-6.46	-6.71	-6.49	-7.45	-7.26	-	-	0.48	0.47	0.73	0.74	-	-
Comp. with Non-Diff.	LiGAN	-	-	-	-	-6.33	-6.20	21.1%	11.1%	0.39	0.39	0.59	0.57	0.66	0.67
	GraphBP	-	-	-	-	-4.80	-4.70	14.2%	6.7%	0.43	0.45	0.49	0.48	<b>0.79</b>	<b>0.78</b>
	AR	<u>-5.75</u>	<u>-5.64</u>	-6.18	<u>-5.88</u>	-6.75	-6.62	37.9%	31.0%	0.51	0.50	<u>0.63</u>	<u>0.63</u>	0.70	0.70
	Pocket2Mol	-5.14	-4.70	<u>-6.42</u>	-5.82	<u>-7.15</u>	<u>-6.79</u>	48.4%	<u>51.0%</u>	<b>0.56</b>	<b>0.57</b>	<b>0.74</b>	<b>0.75</b>	0.69	0.71
	<b>IPDIFF</b>	<b>-6.42</b>	<b>-7.01</b>	<b>-7.45</b>	<b>-7.48</b>	<b>-8.57</b>	<b>-8.51</b>	<b>69.5%</b>	<b>75.5%</b>	<u>0.52</u>	<u>0.53</u>	0.61	0.59	<u>0.74</u>	<u>0.73</u>
Comp. with Diff.	TargetDiff	-5.47	<u>-6.30</u>	-6.64	-6.83	-7.80	-7.91	58.1%	59.1%	<u>0.48</u>	<u>0.48</u>	<u>0.58</u>	<u>0.58</u>	<u>0.72</u>	<u>0.71</u>
	DecompDiff	<u>-5.67</u>	-6.04	<u>-7.04</u>	<u>-7.09</u>	<u>-8.39</u>	<u>-8.43</u>	64.4%	<u>71.0%</u>	0.45	0.43	<b>0.61</b>	<b>0.60</b>	0.68	0.68
	<b>IPDIFF</b>	<b>-6.42</b>	<b>-7.01</b>	<b>-7.45</b>	<b>-7.48</b>	<b>-8.57</b>	<b>-8.51</b>	<b>69.5%</b>	<b>75.5%</b>	<b>0.52</b>	<b>0.53</b>	<b>0.61</b>	<u>0.59</u>	<b>0.74</b>	<b>0.73</b>

The sampled molecule ligands of IPDiff (Table 2.) are provided in the directory:

```
./sampled_results_ipdiff_official
```

## step 1. run the following command for evaluation

```
conda activate ipdiff
cd ./ipdiff
python eval.py --eval_start_index 0 --eval_end_index 99 --docking_mode vina_dock --
protein_root ./crossdocked_v1.1_rmsd1.0 --sampled_results_path
./sampled_results_ipdiff_official --eval_result_path ./eval_results_ipdiff
```

### For Vina Docking

The '**docking\_mode**' can be chosen from {'none', 'vina\_score', 'vina\_dock'}

**none**: QED, SA only;

**vina score**: QED + SA + vina score + vina min; (faster)

**vina dock**: QED + SA + vina score + vina min + vina dock. (slower)

And in our paper, we select the vina\_dock for the evaluation, the evaluation results are present in Table 2.

**! Note**: It will take some time to prepare pcdqt and pqr files when you run the evaluation code with vina\_score/vina\_dock docking mode for the first time. And we provide the evaluated results in the directory:

```
./eval_results_ipdiff_official
```

## step 2 (optional). calculate the overall evaluation results

If you evaluate the sampled results separately, you can run the following command for calculating the overall results.

```
cd ./ipdiff
python cal_overall_eval_results.py --eval_result_path ./eval_results_ipdiff --
docking_mode vina_dock
```

Or you can run the following command for calculating the overall metrics of provided evaluation results:

```
cd ./ipdiff
python cal_overall_eval_results.py --eval_result_path ./eval_results_ipdiff_official --
docking_mode vina_dock
```

## 3. Training and inference code

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We are committed to open sourcing the train/inference code upon paper acceptance.