A Proof of Proposition 1.

First, we here denote all atom's positions in the molecules as $\boldsymbol{X}_{\mathrm{M}} \in \mathbb{R}^{N_{\mathrm{a}} \times 3}$, and in the protein as $\boldsymbol{X}_{\mathrm{M}} \in \mathbb{R}^{N_{\mathrm{aa}} \times 3}$, and linker and functional group type as $\boldsymbol{S}_{\mathrm{M}} \in \mathbb{R}^{(N_{\mathrm{aa}}+N_{\mathrm{fg}}) \times (22+M_{\mathrm{fg}}+M_{\mathrm{at}})}$. Note that one functional group may contain several atoms so that $N_{\mathrm{aa}} + N_{\mathrm{fg}} < N_{\mathrm{a}}$.

SE(3) group as a roto-translation group in $\mathbb{R}^3$, can be divided into two groups: SO(3) as the rotation group and T(3) as the translation group. For $\boldsymbol{x} \in \mathbb{R}^3$, and $g = r + v$ with $g \in \mathrm{SE}(3), r \in \mathrm{SO}(3), v \in \mathrm{T}(3)$, $T_g(\boldsymbol{x}) = T_{r+v}(\boldsymbol{x}) = T_v \circ T_r(\boldsymbol{x})$

Lemma A1. If the The equivariance and invariance of the distribution in the reverse diffusion process are listed as

$$\begin{aligned} p\left(\mathrm{T}_g(\boldsymbol{X}_{\mathrm{M}}^T), \boldsymbol{S}_{\mathrm{M}}^T | \mathrm{T}_g(\boldsymbol{X}_{\mathrm{P}}), \boldsymbol{S}_{\mathrm{P}}\right) &= p\left(\boldsymbol{X}_{\mathrm{M}}^T, \boldsymbol{S}_{\mathrm{M}}^T\right) = p\left(\boldsymbol{X}_{\mathrm{M}}^T, \boldsymbol{S}_{\mathrm{M}}^T | \boldsymbol{X}_{\mathrm{P}}, \boldsymbol{S}_{\mathrm{P}}\right) \\ p\left(\mathrm{T}_g(\boldsymbol{X}_{\mathrm{M}}^{t-1}) | \mathrm{T}_g(\boldsymbol{X}_{\mathrm{M}}^t), \boldsymbol{S}_{\mathrm{M}}^t, \mathrm{T}_g(\boldsymbol{X}_{\mathrm{P}}), \boldsymbol{S}_{\mathrm{P}}\right) &= p\left(\boldsymbol{X}_{\mathrm{M}}^{t-1} | \boldsymbol{X}_{\mathrm{M}}^t, \boldsymbol{S}_{\mathrm{M}}^t, \boldsymbol{X}_{\mathrm{P}}, \boldsymbol{S}_{\mathrm{P}}\right) \\ p\left(\boldsymbol{S}_{\mathrm{M}}^{t-1} | \mathrm{T}_g(\boldsymbol{X}_{\mathrm{M}}^t), \boldsymbol{S}_{\mathrm{M}}^t, \mathrm{T}_g(\boldsymbol{X}_{\mathrm{P}}), \boldsymbol{S}_{\mathrm{P}}\right) &= p\left(\boldsymbol{S}_{\mathrm{M}}^{t-1} | \boldsymbol{X}_{\mathrm{M}}^t, \boldsymbol{S}_{\mathrm{M}}^t, \boldsymbol{X}_{\mathrm{P}}, \boldsymbol{S}_{\mathrm{P}}\right), \end{aligned} \tag{13}$$

Then $p\left(\boldsymbol{X}_{\mathrm{M}}^T, \boldsymbol{S}_{\mathrm{M}}^T | \boldsymbol{X}_{\mathrm{P}}, \boldsymbol{S}_{\mathrm{P}}\right)$ is SE(3) invariant.

Proof. Since $\mathbf{T}_{\boldsymbol{g}}(\mathcal{M}) = \{\boldsymbol{S}, \mathrm{T}_g(\boldsymbol{X}_{\mathrm{M}})\}$, we can write the joint generative process as

$$\begin{aligned} & p\left(\mathrm{T}_g(\boldsymbol{X}_{\mathrm{M}}), \boldsymbol{S}_{\mathrm{M}} | \mathrm{T}_g(\boldsymbol{X}_{\mathrm{P}}), \boldsymbol{S}_{\mathrm{P}}\right) \\ =& \int p\left(\mathrm{T}_g(\boldsymbol{X}_{\mathrm{M}}^T), \boldsymbol{S}_{\mathrm{M}}^T | \mathrm{T}_g(\boldsymbol{X}_{\mathrm{P}}), \boldsymbol{S}_{\mathrm{P}}\right) \prod_{t=0}^{T-1} p\left(\mathrm{T}_g(\boldsymbol{X}_{\mathrm{M}}^{t-1}), \boldsymbol{S}_{\mathrm{M}}^{t-1} | \mathrm{T}_g(\boldsymbol{X}_{\mathrm{M}}^t), \boldsymbol{S}_{\mathrm{M}}^t, \mathrm{T}_g(\boldsymbol{X}_{\mathrm{P}}), \boldsymbol{S}_{\mathrm{P}}\right) d\mathcal{M}^{0:T-1} \\ =& \int p\left(\boldsymbol{X}_{\mathrm{M}}^T, \boldsymbol{S}_{\mathrm{M}}^T | \boldsymbol{X}_{\mathrm{P}}, \boldsymbol{S}_{\mathrm{P}}\right) \prod_{t=0}^{T-1} p\left(\mathrm{T}_g(\boldsymbol{X}_{\mathrm{M}}^{t-1}), \boldsymbol{S}_{\mathrm{M}}^{t-1} | \mathrm{T}_g(\boldsymbol{X}_{\mathrm{M}}^t), \boldsymbol{S}_{\mathrm{M}}^t, \mathrm{T}_g(\boldsymbol{X}_{\mathrm{P}}), \boldsymbol{S}_{\mathrm{P}}\right) d\mathcal{M}^{0:T-1} \\ =& \int p\left(\boldsymbol{X}_{\mathrm{M}}^T, \boldsymbol{S}_{\mathrm{M}}^T | \boldsymbol{X}_{\mathrm{P}}, \boldsymbol{S}_{\mathrm{P}}\right) \prod_{t=0}^{T-1} p\left(\mathrm{T}_g(\boldsymbol{X}_{\mathrm{M}}^{t-1}) | \mathrm{T}_g(\mathcal{M}^t, \mathcal{P})\right) p\left(\boldsymbol{S}_{\mathrm{M}}^{t-1} | \mathrm{T}_g(\mathcal{M}^t, \mathcal{P})\right) d\mathcal{M}^{0:T-1} \\ =& \int p\left(\boldsymbol{X}_{\mathrm{M}}^T, \boldsymbol{S}_{\mathrm{M}}^T | \boldsymbol{X}_{\mathrm{P}}, \boldsymbol{S}_{\mathrm{P}}\right) \prod_{t=0}^{T-1} p\left(\boldsymbol{X}_{\mathrm{M}}^{t-1} | \mathcal{M}^t, \mathcal{P}\right) p\left(\boldsymbol{S}_{\mathrm{M}}^{t-1} | \mathcal{M}^t, \mathcal{P}\right) d\mathcal{M}^{0:T-1} \\ =& \int p\left(\boldsymbol{X}_{\mathrm{M}}^T, \boldsymbol{S}_{\mathrm{M}}^T | \boldsymbol{X}_{\mathrm{P}}, \boldsymbol{S}_{\mathrm{P}}\right) \prod_{t=0}^{T-1} p\left(\boldsymbol{X}_{\mathrm{M}}^{t-1}, \boldsymbol{S}_{\mathrm{M}}^{t-1} | \boldsymbol{X}_{\mathrm{M}}^t, \boldsymbol{S}_{\mathrm{M}}^t, \boldsymbol{X}_{\mathrm{P}}, \boldsymbol{S}_{\mathrm{P}}\right) d\mathcal{M}^{0:T-1} \\ =& p\left(\boldsymbol{X}_{\mathrm{M}}, \boldsymbol{S}_{\mathrm{M}} | \boldsymbol{X}_{\mathrm{P}}, \boldsymbol{S}_{\mathrm{P}}\right) \end{aligned} \tag{14}$$

Then, let's consider a single atom's position. We here denote each atom's $\boldsymbol{x}_{\mathrm{M}}^t$ as

$$\boldsymbol{x}_{\mathrm{M}}^t = \boldsymbol{x}_{\mathrm{C}}^t + \boldsymbol{x}_{\mathrm{R}}^t \boldsymbol{O}_c^t \tag{15}$$

where $\boldsymbol{x}_{\mathrm{C}}^t$ is the defined center atom's position in the functional group, $\boldsymbol{x}_{\mathrm{R}}^t$ is the relative position of the atom in the local coordinate system centering at $\boldsymbol{x}_{\mathrm{C}}^t$, $\boldsymbol{O}_{\mathrm{C}}^t$ is the rotation matrices of the local coordinate system with respect to the global system. Moreover, because the functional group is regarded as rigid bodies, $\boldsymbol{x}_{\mathrm{R}}^t = \boldsymbol{x}_{\mathrm{R}}$ is constant. To be specific, if $\boldsymbol{x}_{\mathrm{M}}^t$ refers to linker's position, $\boldsymbol{O}_{\mathrm{C}}^t = \mathbf{0}$.

Proposition A2. If each atom's relative positions in the local coordinate systems are fixed, and $p(\boldsymbol{x}_{\mathrm{C}}^{t-1} | \mathcal{M}^t, \mathcal{P})$ is SE(3)-equivariant and $p(\boldsymbol{O}_{\mathrm{C}}^{t-1} | \mathcal{M}^t, \mathcal{P})$ is SO(3)-equivariant and T(3)-invariant, such that $p\left(\mathrm{T}_g(\boldsymbol{x}_{\mathrm{C}}^{t-1}) | \mathrm{T}_g(\mathcal{M}^t, \mathcal{P})\right) = p\left(\boldsymbol{x}_{\mathrm{C}}^{t-1} | \mathcal{M}^t, \mathcal{P}\right)$ and $p\left(\mathrm{T}_r(\boldsymbol{O}_{\mathrm{C}}^{t-1}) | \mathrm{T}_g(\mathcal{M}^t, \mathcal{P})\right) = p\left(\boldsymbol{O}_{\mathrm{C}}^{t-1} | \mathcal{M}^t, \mathcal{P}\right)$, where $r \in \mathrm{SO}(3), v \in \mathrm{T}(3), r + v = g \in \mathrm{SE}(3)$, then $p(\boldsymbol{x}_{\mathrm{M}}^{t-1} | \mathcal{M}^t, \mathcal{P})$ is SO(3)-equivariant.

Proof. According to the convolution formula in probability theory, if $w = u + v$, then

$$p(w) = \int p(u, w-u) du = \int p(w-v, v) dv \tag{16}$$

By using the Eq. (16), we can write every single atom's position density function as

$$\begin{aligned}
&p\left(\boldsymbol{x}_{\mathrm{M}}^{t-1}|\mathcal{M}^t,\mathcal{P}\right)\\
=&p\left(\boldsymbol{x}_{\mathrm{C}}^{t-1}+\boldsymbol{x}_{\mathrm{R}}\boldsymbol{O}_{\mathrm{C}}^{t-1}|\mathcal{M}^t,\mathcal{P}\right)\\
=&\int p\left(\boldsymbol{x}_{\mathrm{C}}^{t-1},\boldsymbol{x}_{\mathrm{M}}^{t-1}-\boldsymbol{x}_{\mathrm{C}}^{t-1}|\mathcal{M}^t,\mathcal{P}\right)d\boldsymbol{x}_{\mathrm{C}}^{t-1}\\
=&\int p\left(\boldsymbol{x}_{\mathrm{C}}^{t-1}|\mathcal{M}^t,\mathcal{P}\right)p\left(\boldsymbol{x}_{\mathrm{M}}^{t-1}-\boldsymbol{x}_{\mathrm{C}}^{t-1}|\mathcal{M}^t,\mathcal{P}\right)d\boldsymbol{x}_{\mathrm{C}}^{t-1}
\end{aligned} \tag{17}$$

Since

$$p\left(\mathrm{T}_g(\boldsymbol{x}_{\mathrm{C}}^{t-1})|\mathrm{T}_g(\mathcal{M}^t,\mathcal{P})\right)=p\left(\boldsymbol{x}_{\mathrm{C}}^{t-1}|\mathcal{M}^t,\mathcal{P}\right), \tag{18}$$

and

$$p\left(\mathrm{T}_r(\boldsymbol{O}_{\mathrm{C}}^{t-1})|\mathrm{T}_g(\mathcal{M}^t,\mathcal{P})\right)=p\left(\boldsymbol{O}_{\mathrm{C}}^{t-1}|\mathcal{M}^t,\mathcal{P}\right). \tag{19}$$

We can obtain that

$$\begin{aligned}
&p\left(\mathrm{T}_r(\boldsymbol{x}_{\mathrm{M}}^{t-1}-\boldsymbol{x}_{\mathrm{C}}^{t-1})|\mathrm{T}_g(\mathcal{M}^t,\mathcal{P})\right)\\
=&p\left(\mathrm{T}_r(\boldsymbol{x}_{\mathrm{R}}\boldsymbol{O}_{\mathrm{C}}^{t-1})|\mathrm{T}_g(\mathcal{M}^t,\mathcal{P})\right)\\
=&\frac{1}{\boldsymbol{x}_{\mathrm{R}}}p\left(\mathrm{T}_r(\boldsymbol{O}_{\mathrm{C}}^{t-1})|\mathrm{T}_g(\mathcal{M}^t,\mathcal{P})\right)\\
=&\frac{1}{\boldsymbol{x}_{\mathrm{R}}}p\left(\boldsymbol{O}_{\mathrm{C}}^{t-1}|\mathcal{M}^t,\mathcal{P}\right)\\
=&p\left(\boldsymbol{x}_{\mathrm{R}}\boldsymbol{O}_{\mathrm{C}}^{t-1}|\mathcal{M}^t,\mathcal{P}\right)\\
=&p\left(\boldsymbol{x}_{\mathrm{M}}^{t-1}-\boldsymbol{x}_{\mathrm{C}}^{t-1}|\mathcal{M}^t,\mathcal{P}\right)
\end{aligned} \tag{20}$$

Therefore, according to Eq. (18), (20), and (17)

$$\begin{aligned}
&p\left(\mathrm{T}_g(\boldsymbol{x}_{\mathrm{M}}^{t-1})|\mathrm{T}_g(\mathcal{M}^t,\mathcal{P})\right)\\
=&\int p\left(\mathrm{T}_g\boldsymbol{x}_{\mathrm{C}}^{t-1})|\mathrm{T}_g(\mathcal{M}^t,\mathcal{P})\right)p\left(\mathrm{T}_{r+v}(\boldsymbol{x}_{\mathrm{M}}^{t-1}-\boldsymbol{x}_{\mathrm{C}}^{t-1})|\mathrm{T}_g(\mathcal{M}^t,\mathcal{P})\right)d\boldsymbol{x}_{\mathrm{C}}^{t-1}\\
=&\int p\left(\mathrm{T}_g\boldsymbol{x}_{\mathrm{C}}^{t-1})|\mathrm{T}_g(\mathcal{M}^t,\mathcal{P})\right)p\left(\mathrm{T}_r(\boldsymbol{x}_{\mathrm{M}}^{t-1}-\boldsymbol{x}_{\mathrm{C}}^{t-1})|\mathrm{T}_g(\mathcal{M}^t,\mathcal{P})\right)d\boldsymbol{x}_{\mathrm{C}}^{t-1}\\
=&\int p\left(\boldsymbol{x}_{\mathrm{C}}^{t-1}|\mathcal{M}^t,\mathcal{P}\right)p\left(\boldsymbol{x}_{\mathrm{M}}^{t-1}-\boldsymbol{x}_{\mathrm{C}}^{t-1}|\mathcal{M}^t,\mathcal{P}\right)d\boldsymbol{x}_{\mathrm{C}}^{t-1}\\
=&p\left(\boldsymbol{x}_{\mathrm{M}}^{t-1}|\mathcal{M}^t,\mathcal{P}\right)
\end{aligned} \tag{21}$$

Proof of Proposition 1. The sufficiency of SE(3)-invariance of $p(\boldsymbol{s}^{t-1}|\mathcal{M}^t,\mathcal{P})$ and $p(\boldsymbol{s}^T)$ is given in **Lemma A.1**, and the sufficiency of SE(3)-equivariance of $p(\boldsymbol{x}^{t-1}|\mathcal{M}^t,\mathcal{P})$, and SO(3)-equivariance and T(3)-invariance of $p(\boldsymbol{O}^{t-1}|\mathcal{M}^t,\mathcal{P})$ is given in **Proposition A.2**. Besides, it is easy to obtain that if $p(\boldsymbol{O}^T)$ and $p(\boldsymbol{x}^T)$ is SE(3)-invariant distribution, then $p(\boldsymbol{x}_{\mathrm{M}}^T)$ will be invariant.

B Method Details

Amino acid context encoding. Several geometric or type features are embedded to encode amino acids. For the geometric features including torsion angles/dihedrals, and pairwise distances, they are all roto-translational invariant, since the geometric features are all scalars obtained from relative coordinates. Besides, the local coordinates of atoms in a single amino acid are also invariant because it is always fixed in the local frame established by C_α, C and N. For the type features including amino acid types, sequential relationships, and pair of amino acid types, the translational and rotational operation is unrelated to them. Thus, the encoded amino acid contexts are roto-translational invariant, leading to the invariance of all the follow-up embeddings.

Equivariant neural network for linkers. For the roto-translational equivariance of positions for single atoms, since $\boldsymbol{O}_j^t=\boldsymbol{I}$, Eq. 12 will be written as $G\left(\mathcal{M}^t,\mathcal{P}\right)[j]=\mathrm{MLP}_G(\boldsymbol{h}_j')$, unable to satisfy

the equivariance. In this way, we revised it for single atoms by using the EGNN[33] stacked in the final layer for updating the positions, which reads

$$G\left(\mathcal{M}^t, \mathcal{P}\right)[j] = \boldsymbol{x}_j + \frac{1}{C_j} \sum_{i \in \mathcal{I}_{\mathrm{at}} \cup \mathcal{I}_{\mathrm{fg}}} (\boldsymbol{x}_j - \boldsymbol{x}_i) \boldsymbol{h}'_i, \tag{22}$$

where we choose $C_j = \|\boldsymbol{x}_j\|_2 + 1$.

C Data Preprocessing

Local frame establishment. In 3D Euclidian space, for a rigid body including more than mass points that are not co-linear, a local frame can be established. We first choose a center node (center point) A as the origin, and a second node B, leading to $\vec{AB}$ as the direction of x-axis. Then, a third node C is selected. By Schmidt orthogonalization of $\vec{AC}$ with respect to $\vec{AB}$, the direction of y-axis can be computed. And finally, the direction of z-axis is obtained by the cross-product of the unit vectors in the x direction and y direction. By this means, the local frame is established by the three nodes, and the other nodes' local coordinates can be determined in the local frame. Because the local frame requires at least three points to establish, the functional groups including only 2 atoms are divided into two linkers.

Functional group datasets. We give detailed information on the included functional groups, including 2D graph, 3D structure, time of occurrence in the CrossDocked2020, and the center node (node A), node B, and node C of the functional group in Table. 8.

Note that in beneze, the symmetric structures lead the frame nodes to be any three consecutive points on the hexagon. Besides, for the functional groups of 'NS(=O)=O' and 'O=CNO', two stable conformations exist, so we in practice regard them as four different types.

D Experiment Details

Platform. We use a single NVIDIA A100(81920MiB) GPU for a trial. The codes are implemented in Python 3.9 mainly with Pytorch 1.12, and run on Ubuntu Linux.

Model Details. In the diffusion of orientation and position, we employ a cosine variance schedule for $\bar{\alpha}_t$, which reads

$$\bar{\alpha}_t = \cos^2\left(\frac{\pi}{2}(\frac{t}{T} + s)/(1+s)\right) / \cos^2\left(\frac{\pi}{2} s/(1+s)\right), \tag{23}$$

where $s = 0.01$. In the diffusion of atom type, β_t is set as $\beta_t = \frac{t}{T}$. For the denoiser, the layer number is set as 6, and the embedding size is set as 256. The model is trained with Adam optimizer in 5000 epochs.

Functional group and Atom type analysis. We give a detailed analysis of functional groups and atom types, in Table. 5, 6 and 7.

Table 5: Frequency of the top ten functional groups that occur most frequently in Crossdocked2020.

Functional Group	Ref.	Pocket2Mol	TargetDiff	DiffSBDD	D3FG(Joint)	D3FG(Stage)
c1ccccc1	0.392	0.491	0.277	0.007	0.372	0.409
NC=O	0.147	0.075	0.142	0.201	0.082	0.107
O=CO	0.119	0.169	0.303	0.579	0.154	0.085
c1ccncc1	0.045	0.072	0.049	0.018	0.027	0.052
c1ncc2nc[nH]c2n1	0.034	0.001	0.000	0.000	0.001	0.020
NS(=O)=O	0.030	0.000	0.000	0.008	0.001	0.001
O=P(O)(O)O	0.022	0.003	0.193	0.000	0.007	0.010
OCO	0.019	0.024	0.091	0.016	0.045	0.050
c1cncnc1	0.017	0.008	0.138	0.000	0.002	0.009
c1cn[nH]c1	0.016	0.011	0.001	0.000	0.003	0.004
JSD	-	0.248	0.301	0.553	0.223	0.201

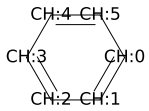
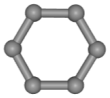
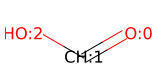
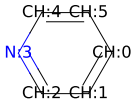
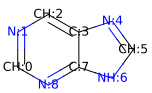
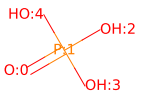
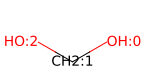
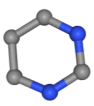
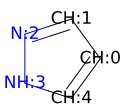
Table 6: Ratio of the atoms.

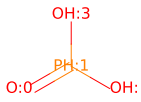
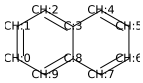
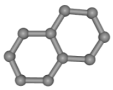
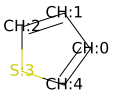
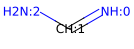
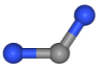
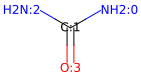
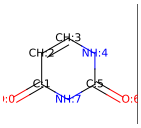
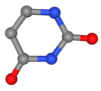
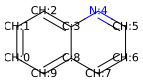
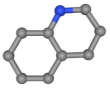
Atom	Ref.	Pocket2Mol	TargetDiff	DiffSBDD	D3FG(Joint)	D3FG(Stage)
C	15.866	14.956	17.744	13.526	17.766	15.999
N	2.765	1.956	2.192	2.236	2.157	1.943
O	4.006	2.538	4.389	3.071	3.732	3.353
F	0.309	0.084	0.239	0.160	0.193	0.170
P	0.263	0.024	0.119	0.034	0.969	0.088
S	0.266	0.038	0.104	0.149	0.169	0.153
Cl	0.152	0.016	0.064	0.006	0.145	0.122
MAE	-	0.573	0.471	0.627	0.528	0.294

Table 7: Frequency of the atoms.

Atom	Ref.	Pocket2Mol	TargetDiff	DiffSBDD	D3FG(Joint)	D3FG(Stage)
C	0.672	0.762	0.714	0.702	0.741	0.733
N	0.117	0.100	0.088	0.116	0.124	0.089
O	0.170	0.129	0.176	0.159	0.175	0.154
F	0.013	0.004	0.009	0.008	0.009	0.008
P	0.011	0.001	0.005	0.002	0.002	0.004
S	0.011	0.002	0.004	0.007	0.001	0.007
Cl	0.006	0.001	0.002	0.003	0.001	0.006
JSD	-	0.098	0.059	0.054	0.075	0.056

Table 8: The included functional groups in D3FG. 'T' is the occurrence times of the functional group in the datasets (100,000 ligands).

Smiles	2D graph	3D structures	A	B	C	T
c1ccccc1			1	0	2	131148
NC=O			1	0	2	49023
O=CO			1	0	2	39863
c1ccncc1			3	2	4	15115
c1ncc2nc[nH]c2n1			7	3	6	11369
NS(=O)=O			1	0	2	10121
O=P(O)(O)O			1	0	2	7451
OCO			1	0	2	6405
c1cncnc1			3	2	4	5965
c1cn[nH]c1			2	3	1	5404

Smiles	2D graph	3D structures	A	B	C	T
O=P(O)O			0	1	center(2,3)	5271
c1ccc2ccccc2c1			3	2	4	4742
c1ccsc1			3	2	4	4334
N=CN			1	0	2	4315
NC(N)=O			2	1	3	4167
O=c1cc[nH]c(=O)[nH]1			7	1	5	4145
c1ccc2ncccc2c1			3	2	4	3519
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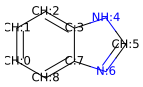
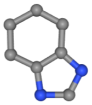
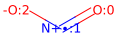
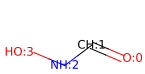
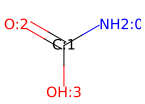
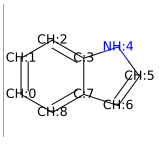
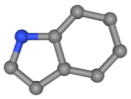
c1ccc2[nH]cnc2c1			5	4	6	3462
c1c[nH]cn1			3	2	4	2964
O=[N+][O-]			1	0	2	2702

Smiles	2D graph	3D structures	A	B	C	T
O=CNO			1	0	2	2477
NC(=O)O			1	0	2	2438
O=S=O			1	0	2	2375
c1ccc2[nH]ccc2c1			3	4	2	2301