

## Appendix A Experimental Details

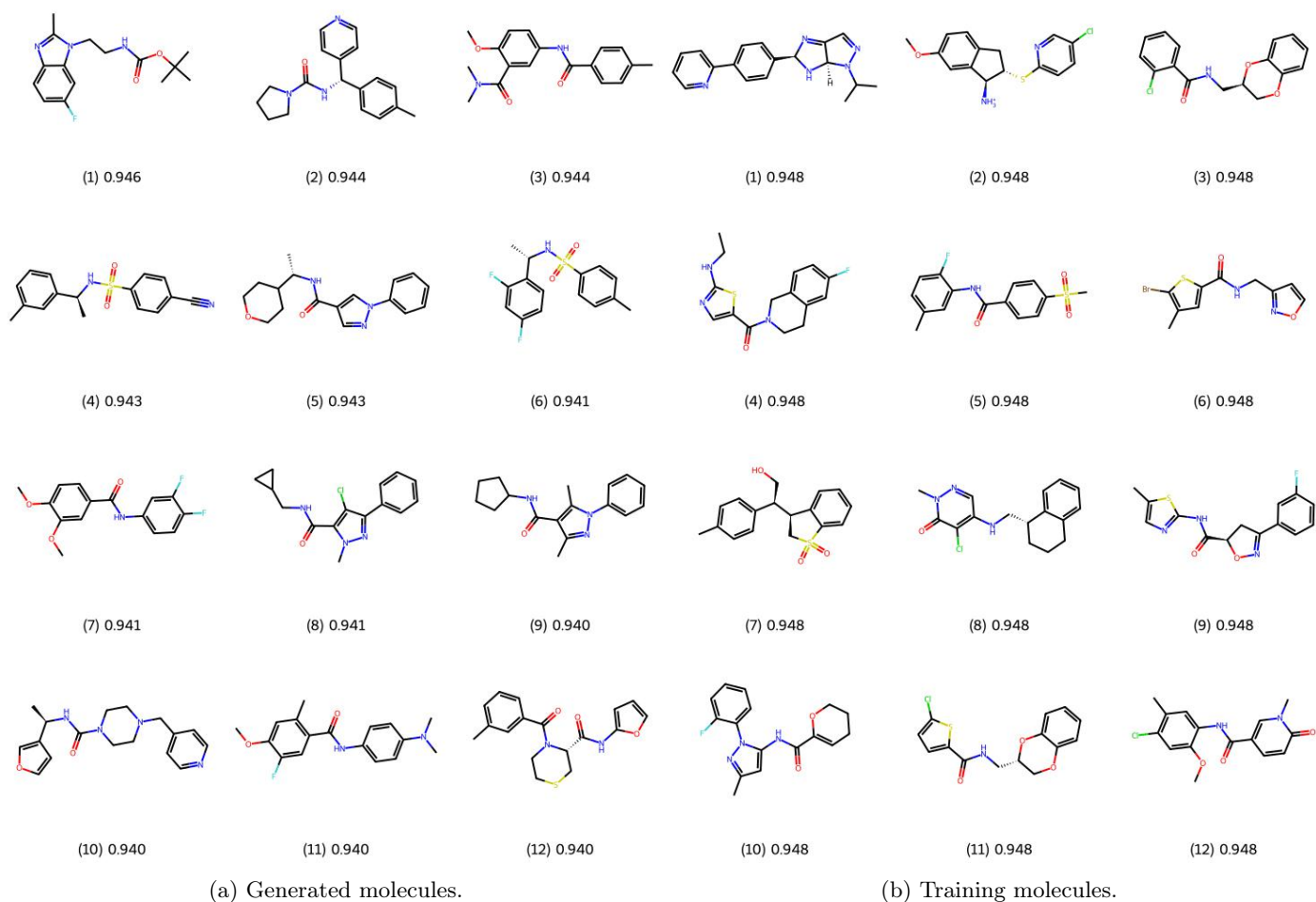
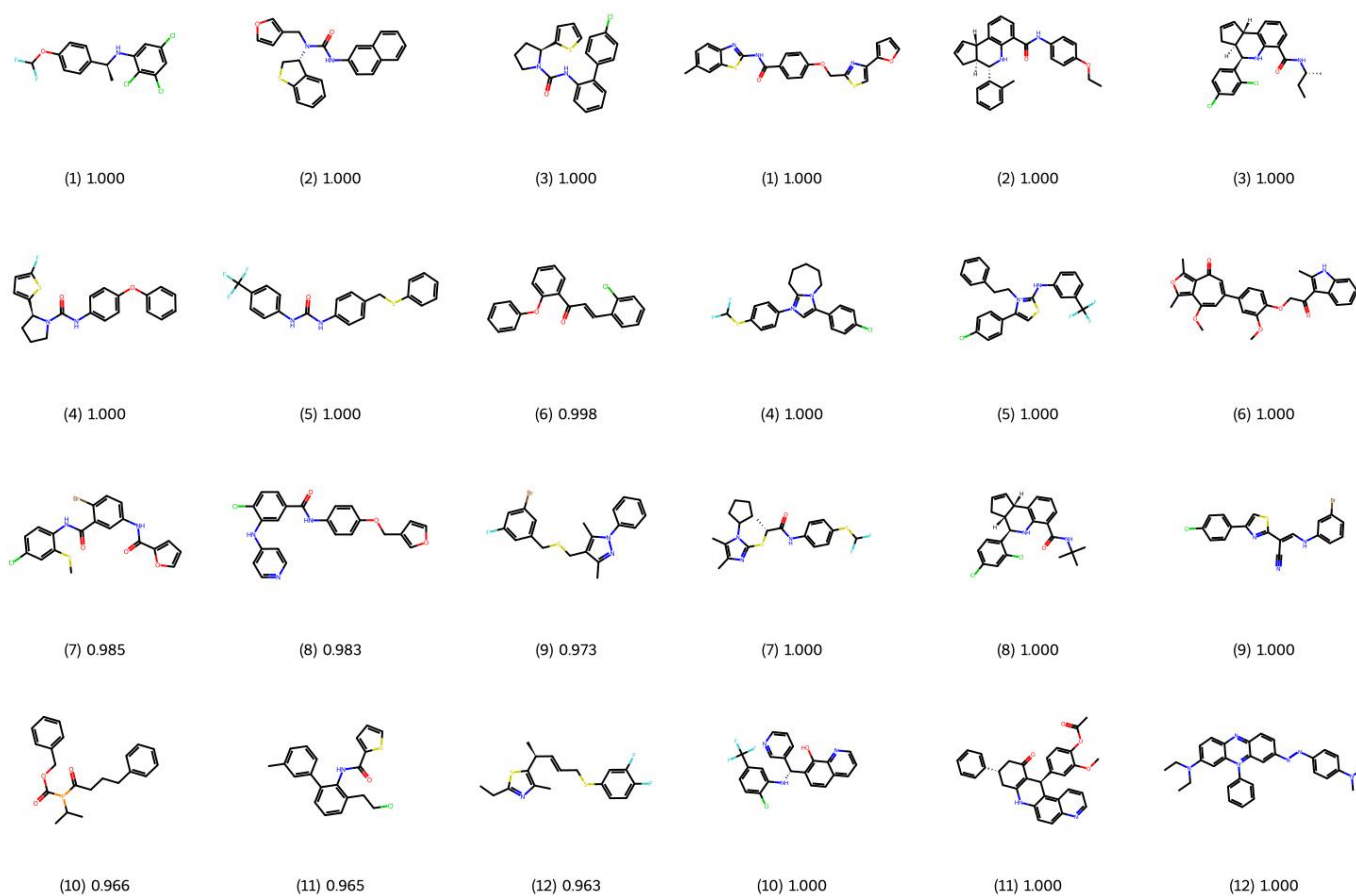


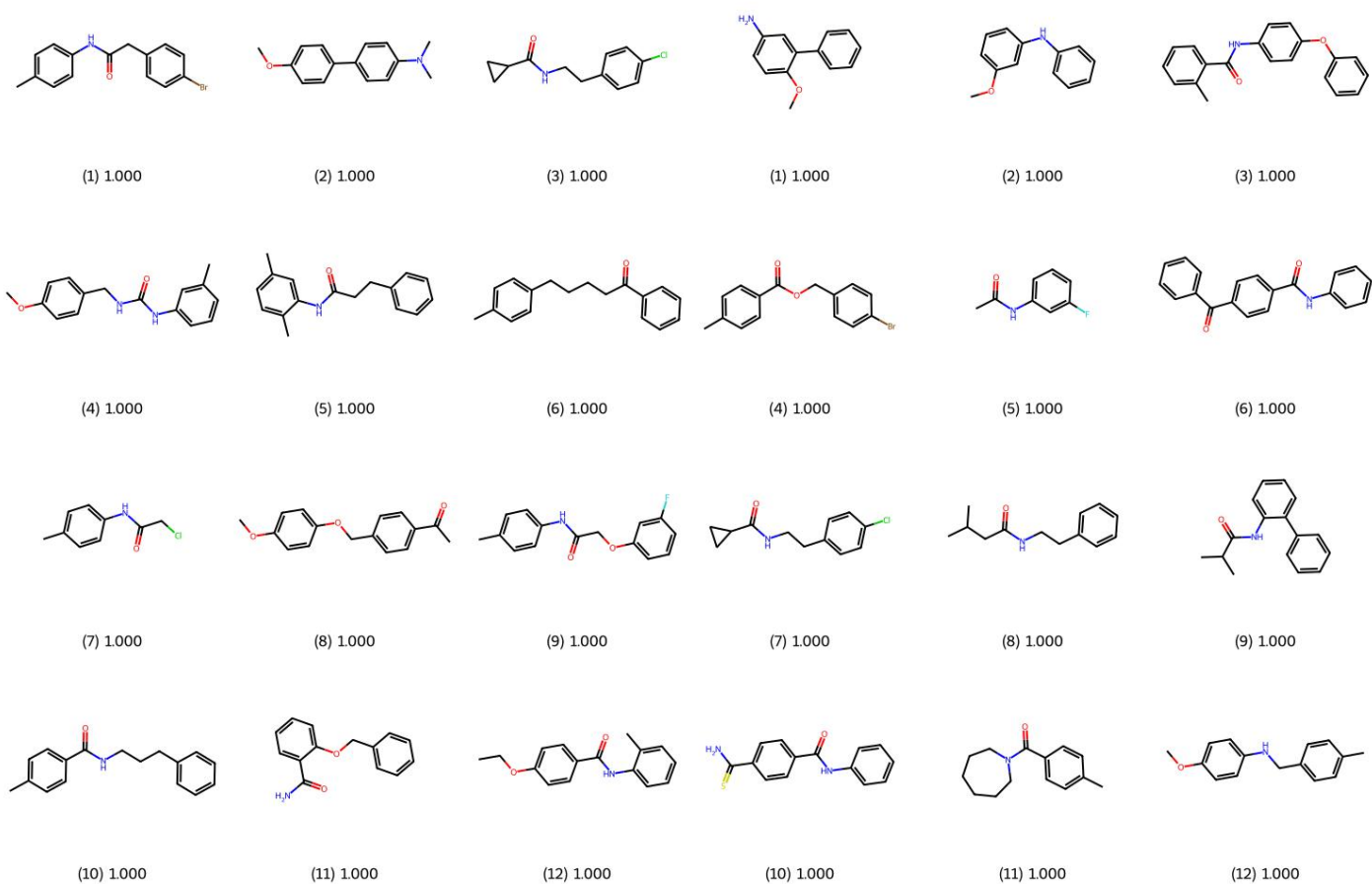
Figure A.1: Top 12 Drug-likeness (QED) molecules.



(a) Generated molecules.

(b) Training molecules.

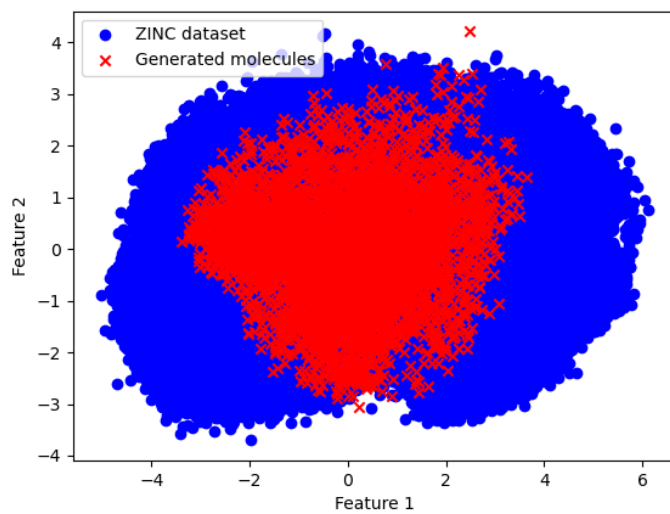
Figure A.2: Top 12 Solubility (Logp) molecules.



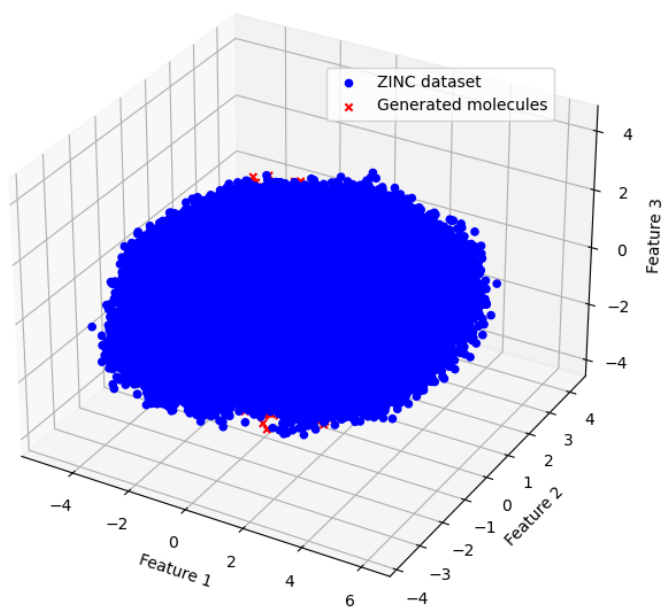
(a) Generated molecules.

(b) Training molecules.

Figure A.3: Top 12 Synthesizability molecules.



(a) Visualization of the two-dimensional scatter plot.



(b) Visualization of the three-dimensional scatter plot.

Figure A.4: Visualization of trained and generated molecules in two and three-dimensional space.