Appendix for: Active Causal Machine Learning for Molecular Property Prediction

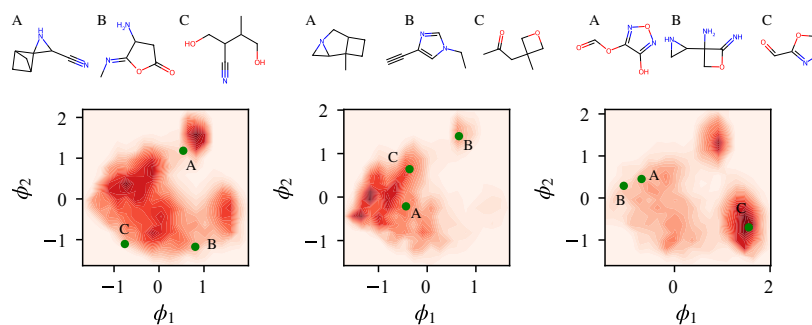**Anonymous Author(s)**
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1 Appendix

Figure A1: Density plot of the molecules' projected onto the principle components of extended connectivity fingerprint (ECFPs) for each of the data subsets, along with three representative molecules from each data subset.
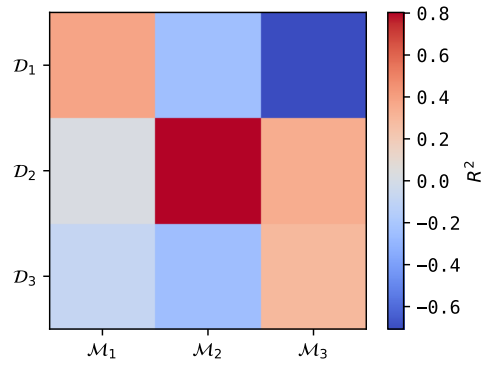
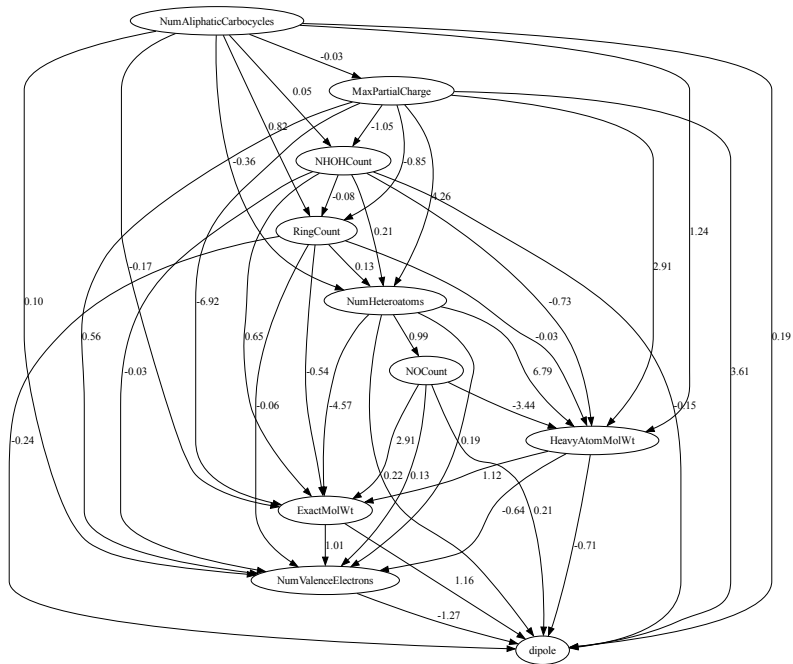Figure A2: Models trained on different data subsets do not generalize well.
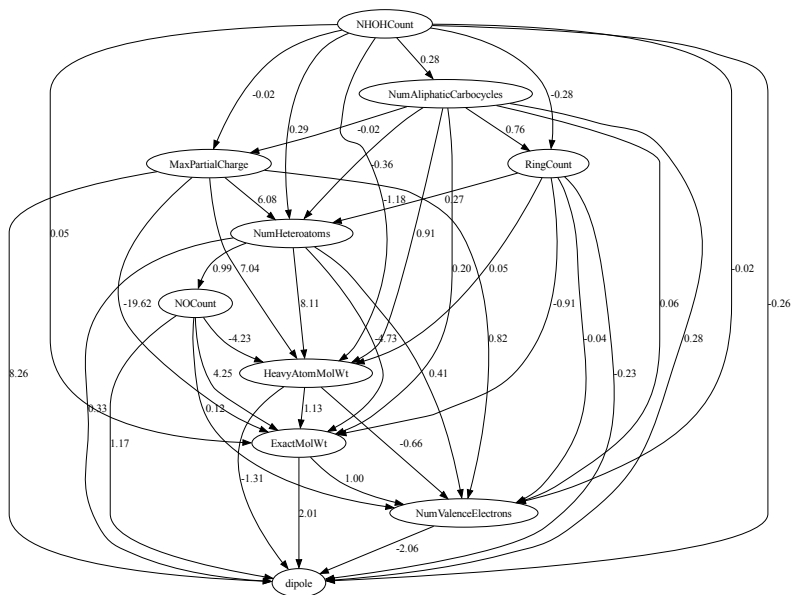
Figure A3: Causal maps associated with $\mathcal{D}_1$.

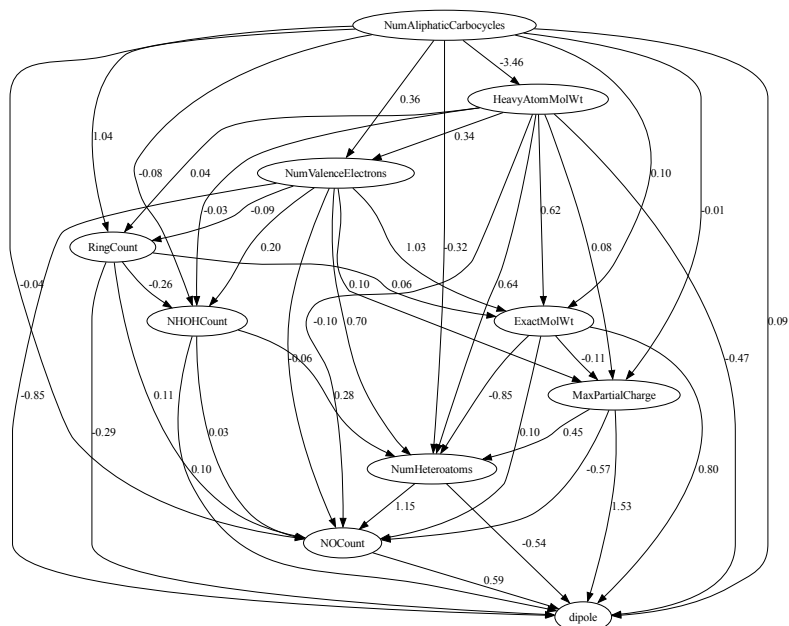Figure A4: Causal maps associated with $\mathcal{D}_2$.

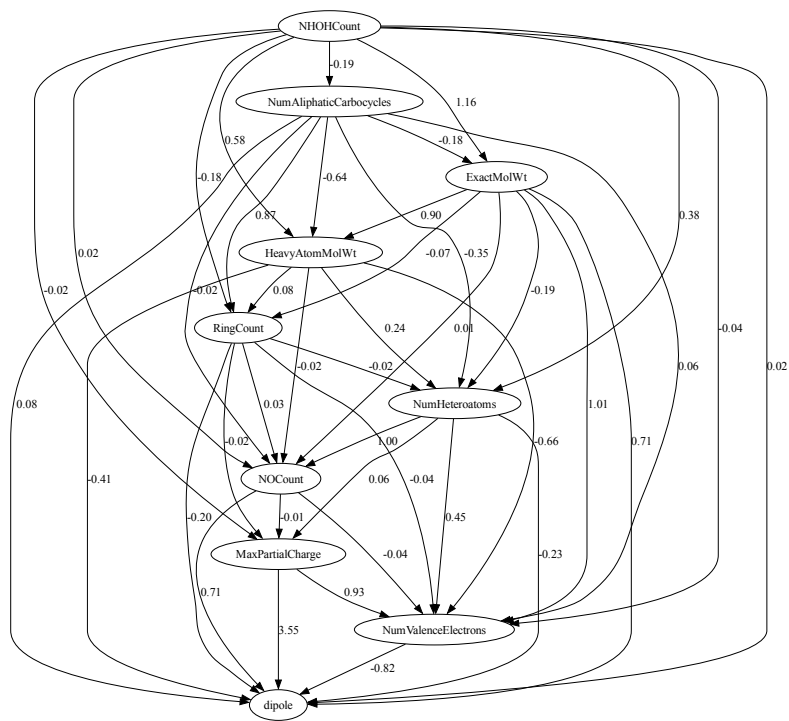Figure A5: Causal maps associated with $\mathcal{D}_3$.

Figure A6: Causal maps associated with $\mathcal{D}_\rho$.