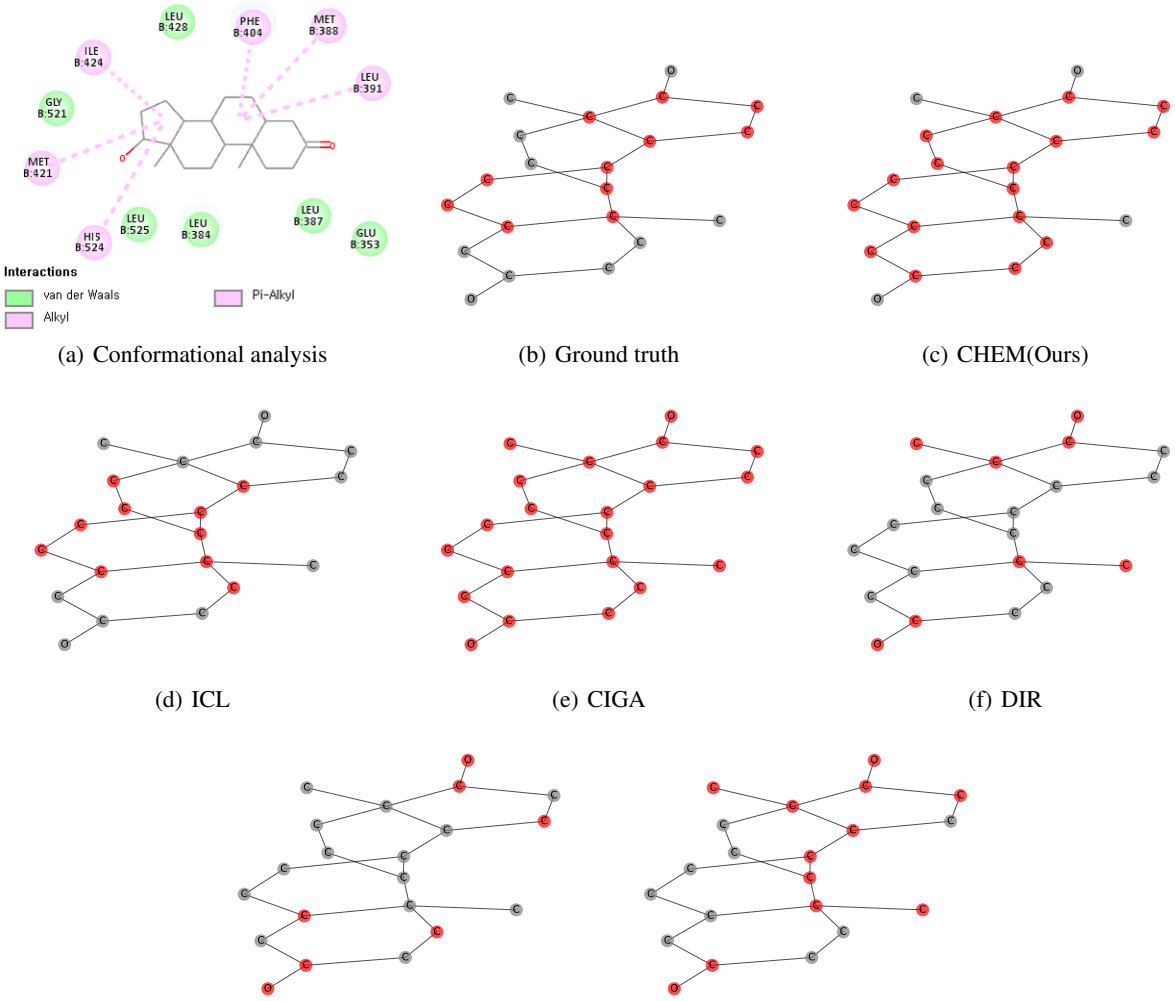
SUPPLEMENTARY MATERIAL: CHEM: CAUSALLY AND HIERARCHICALLY EXPLAINING MOLECULES

Additional Results

Table 1: Classification performance on molecular property prediction task (PRAUC).

Model	MUTAG	BBBP	BACE	ClinTox	Tox21	SIDER	SynM-0.5	SynM-0.7	SynM-0.9
GCN	$96.07_{\pm 7.25}$	$68.28_{\pm 2.67}$	$77.00_{\pm 2.22}$	$\underline{68.26}_{\pm 3.89}$	$\underline{35.50}_{\pm 1.10}$	$\mathbf{64.28}_{\pm 0.50}$	$77.44_{\pm 5.28}$	$76.81_{\pm 4.84}$	$74.72_{\pm 8.64}$
GIN	$\underline{97.32}_{\pm 3.21}$	$66.64_{\pm 3.07}$	$78.32_{\pm 1.56}$	$67.05_{\pm 3.46}$	$35.11_{\pm 1.30}$	$63.52_{\pm 0.51}$	$\underline{84.44}_{\pm 9.35}$	$79.85_{\pm 8.34}$	$72.39_{\pm 8.82}$
GAT	$96.71_{\pm 4.84}$	$67.23_{\pm 3.58}$	$78.27_{\pm 2.01}$	$68.11_{\pm 3.73}$	$35.39_{\pm 1.18}$	$\underline{63.92}_{\pm 0.63}$	$53.14_{\pm 13.29}$	$55.85_{\pm 19.33}$	$49.52_{\pm 10.26}$
ICL	$94.86_{\pm 7.80}$	$64.04_{\pm 3.95}$	$76.76_{\pm 3.05}$	$70.51_{\pm 4.20}$	$34.67_{\pm 1.29}$	$62.91_{\pm 0.55}$	$75.66_{\pm 9.97}$	$78.19_{\pm 9.18}$	$65.96_{\pm 13.29}$
CIGA	$94.34_{\pm 6.27}$	$68.38_{\pm 4.51}$	$73.59_{\pm 5.88}$	$64.26_{\pm 4.61}$	$37.44_{\pm 1.67}$	$60.76_{\pm 0.63}$	$60.33_{\pm 12.65}$	$63.75_{\pm 14.31}$	$60.73_{\pm 10.70}$
DIR	$94.51_{\pm 4.65}$	$68.43_{\pm 3.03}$	$73.34_{\pm 2.19}$	$64.99_{\pm 4.48}$	$30.44_{\pm 1.83}$	$61.99_{\pm 0.68}$	$72.99_{\pm 11.44}$	$63.42_{\pm 14.10}$	$50.52_{\pm 9.53}$
DisC	$95.19_{\pm 5.83}$	$\underline{69.53}_{\pm 1.71}$	$\underline{78.39}_{\pm 3.68}$	$65.11_{\pm 3.42}$	$34.61_{\pm 1.11}$	$60.79_{\pm 0.55}$	$75.39_{\pm 6.67}$	$79.94_{\pm 9.78}$	$65.61_{\pm 13.40}$
CAL	$97.07_{\pm 2.25}$	$68.92_{\pm 2.18}$	$76.95_{\pm 3.67}$	$68.20_{\pm 1.91}$	$\mathbf{38.04}_{\pm 1.23}$	$63.38_{\pm 0.60}$	$82.12_{\pm 2.60}$	$\underline{82.63}_{\pm 4.75}$	$\mathbf{82.06}_{\pm 4.17}$
CHEM(Ours)	$\mathbf{97.70}_{\pm 1.90}$	$\mathbf{71.16}_{\pm 4.85}$	$\mathbf{80.14}_{\pm 2.27}$	$\mathbf{69.41}_{\pm 2.23}$	$34.35_{\pm 1.47}$	$63.13_{\pm 0.63}$	$\mathbf{87.37}_{\pm 5.42}$	$\mathbf{83.50}_{\pm 5.39}$	$\underline{80.65}_{\pm 7.79}$

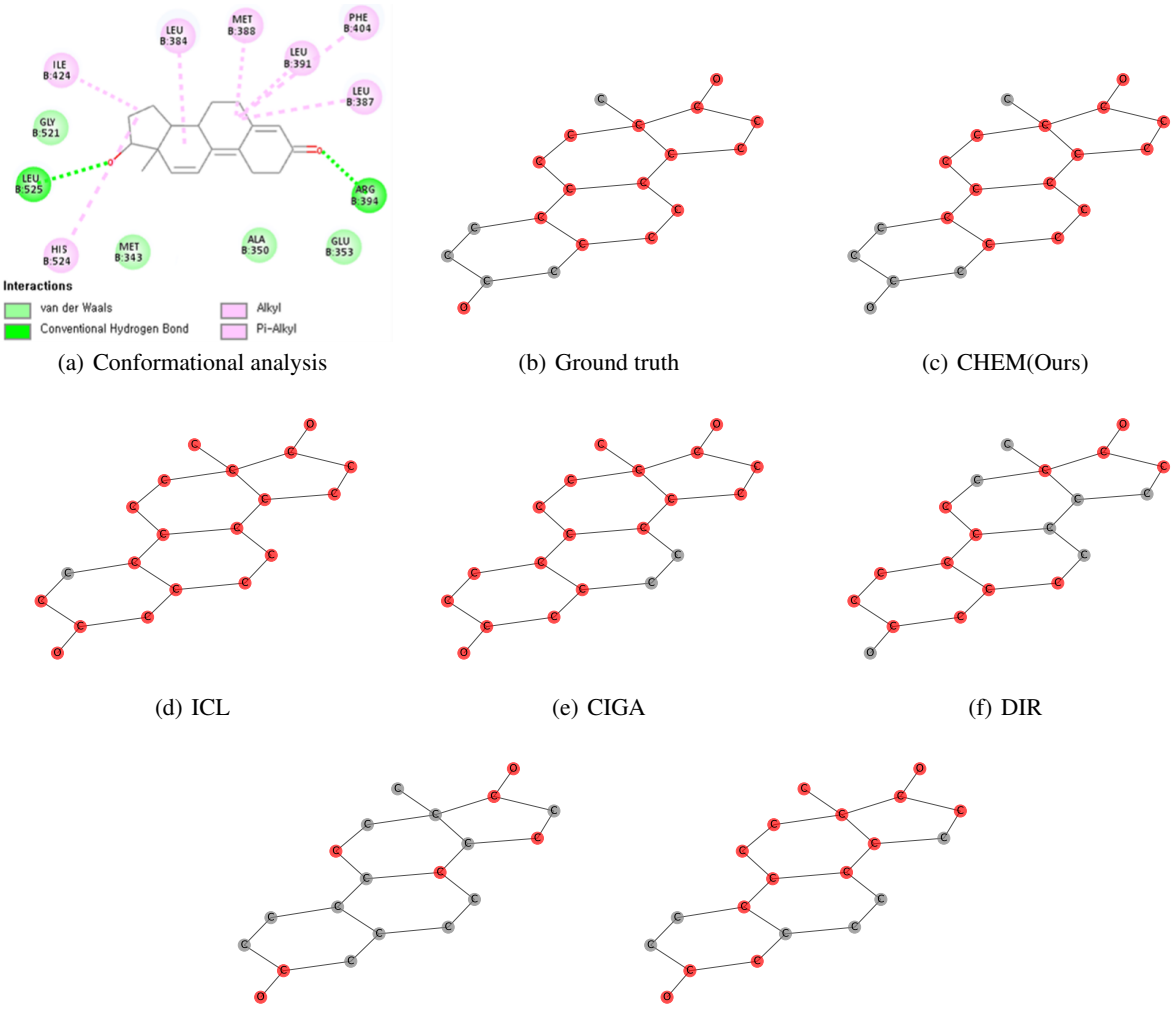


(a) Conformational analysis (b) Ground truth (c) CHEM(Ours)

(d) ICL (e) CIGA (f) DIR

(g) DisC (h) CAL

Figure 1: Result of causal subgraph analysis in NCGC00258540-01.



(a) Conformational analysis (b) Ground truth (c) CHEM(Ours)

(d) ICL (e) CIGA (f) DIR

(g) DisC (h) CAL

Figure 2: Result of causal subgraph analysis in NCGC00258093-01.