Dataset Units	Solubility log Mol/L	Drug efficacy EC_{50} in nM	Photovoltaic efficiency percent	Toxicity (binary)
Predict mean	4.29 ± 0.40	1.47 ± 0.07	6.40 ± 0.09	-
	3.79	1.38	6.29	0.41
Circular FPs + linear layer	1.71 ± 0.13	1.13 ± 0.03	2.63 ± 0.09	-
	1.57	1.11	2.52	0.25
Circular FPs + neural net	1.40 ± 0.13	1.36 ± 0.10	2.00 ± 0.09	-
	1.13	1.26	1.97	0.26
Neural FPs + linear layer	0.77 ± 0.11	1.15 ± 0.02	2.58 ± 0.18	-
	0.58	1.08	2.10	0.25
Neural FPs + neural net	0.52 ± 0.07	1.16 ± 0.03	1.43 ± 0.09	-
	0.41	1.07	1.25	0.24