

1 Overview of GOOD Results

covariate	GOOD-HIV↑				GOOD-PCBA↑				GOOD-ZINC↓				GOOD-CMNIST↑			
	scaffold		size		scaffold		size		scaffold		size		color			
	ID _{ID}	OOD _{OOD}	ID _{ID}	OOD _{OOD}	ID _{ID}	OOD _{OOD}	ID _{ID}	OOD _{OOD}	ID _{ID}	OOD _{OOD}	ID _{ID}	OOD _{OOD}	ID _{ID}	OOD _{OOD}		
ERM	82.79	69.58	83.72	59.94	33.45	16.89	34.31	17.86	0.1224	0.1995	0.1199	0.2427	77.96	28.60	graph	
IRM	81.35	67.97	81.33	59.00	33.56	16.90	34.28	18.05	0.1213	0.2025	0.1222	0.2403	77.92	27.83		
VREx	82.11	70.77	83.47	58.53	33.88	16.98	34.09	17.79	0.1211	0.2094	0.1234	0.2384	77.98	28.48		
GroupDRO	82.60	70.64	83.79	58.98	33.81	16.98	33.95	17.59	0.1168	0.1934	0.1180	0.2423	77.98	29.07		
DANN	81.18	70.63	83.90	58.68	33.63	16.90	34.17	17.86	0.1186	0.2004	0.1188	0.2439	78.00	29.14		
Deep Coral	82.53	68.61	84.70	60.11	33.47	16.93	34.49	17.94	0.1185	0.2036	0.1134	0.2505	78.64	29.05		
Mixup	82.29	68.88	83.16	59.03	30.22	16.59	30.63	17.06	0.1279	0.2240	0.1255	0.2748	77.40	26.47	graph	
DIR	82.54	67.47	80.46	57.11	32.55	14.98	32.89	16.61	0.3799	0.6493	0.1541	0.5482	31.09	20.60		
CIGAv1	79.03	69.40	82.20	61.81	-	-	-	-	-	-	-	-	74.46	32.22		
CIGAv2	79.17	69.40	82.40	59.55	-	-	-	-	-	-	-	-	71.56	32.11		
covariate	GOOD-Motif↑				GOOD-SST2↑				concept	GOOD-Motif↑				GOOD-SST2↑		
	base		size		length		base			size		length				
	ID _{ID}	OOD _{OOD}	ID _{ID}	OOD _{OOD}	ID _{ID}	OOD _{OOD}	ID _{ID}	OOD _{OOD}		ID _{ID}	OOD _{OOD}	ID _{ID}	OOD _{OOD}	ID _{ID}	OOD _{OOD}	
ERM	92.60	68.66	92.28	51.74	89.82	81.30	ERM	92.02	81.44	91.73	70.75	94.43	72.43	graph		
IRM	92.60	70.65	92.18	51.41	89.41	79.91		92.00	80.71	91.68	69.77	94.10	77.47			
VREx	92.60	71.47	92.25	52.67	89.51	80.64		VREx	92.05	81.56	91.67	70.24	94.26		73.16	
GroupDRO	92.61	68.24	92.29	51.95	89.59	81.35		GroupDRO	92.01	81.43	91.67	69.98	94.41		71.86	
DANN	92.60	65.47	92.23	51.46	89.60	79.71		DANN	92.02	81.33	91.81	70.72	94.02		76.03	
Deep Coral	92.61	68.88	92.22	50.97	89.68	79.81		Deep Coral	92.01	81.37	91.68	70.49	94.25		72.34	
Mixup	92.68	70.08	92.02	51.48	89.78	80.88	Mixup	91.89	77.63	91.45	67.81	94.12	73.34	graph		
DIR	87.73	61.50	84.53	50.41	84.30	77.65	DIR	91.60	72.14	73.10	56.28	93.71	68.76			
CIGAv1	90.78	66.43	89.25	49.14	84.02	80.44	CIGAv1	90.39	72.50	85.26	58.63	88.78	71.18			
CIGAv2	91.01	67.15	92.08	54.42	84.92	80.46	CIGAv2	90.12	77.48	90.14	70.65	92.20	70.33			
concept	GOOD-HIV↑				GOOD-PCBA↑					GOOD-ZINC↓				GOOD-CMNIST↑		
	scaffold		size		scaffold		size			scaffold		size		color		
	ID _{ID}	OOD _{OOD}	ID _{ID}	OOD _{OOD}	ID _{ID}	OOD _{OOD}	ID _{ID}	OOD _{OOD}		ID _{ID}	OOD _{OOD}	ID _{ID}	OOD _{OOD}	ID _{ID}	OOD _{OOD}	
ERM	84.22	72.33	88.05	63.26	25.95	21.63	32.54	15.36	ERM	0.1222	0.1306	0.1315	0.1403	90.00	42.87	graph
IRM	82.89	72.59	88.62	59.90	25.89	21.22	32.99	16.07		0.1225	0.1314	0.1278	0.1368	90.02	42.80	
VREx	83.84	72.60	88.28	60.23	26.62	22.02	32.49	15.59		0.1186	0.1270	0.1309	0.1419	89.99	43.31	
GroupDRO	83.40	73.64	88.28	61.37	26.32	21.83	33.03	15.99		0.1207	0.1281	0.1251	0.1369	90.02	43.32	
DANN	83.87	71.92	87.28	65.27	26.07	21.64	32.74	15.78		0.1172	0.1256	0.1253	0.1339	89.94	43.11	
Deep Coral	84.65	72.97	87.88	62.28	26.38	21.95	32.67	16.20		0.1187	0.1279	0.1287	0.1370	89.94	43.16	
Mixup	82.36	72.03	87.64	64.87	23.73	19.78	30.23	13.36	ERM	0.1353	0.1475	0.1423	0.1522	89.95	40.96	graph
DIR	83.28	69.05	79.19	72.61	25.85	22.20	30.53	16.86		0.3501	0.3865	0.2348	0.2871	86.76	22.69	
CIGAv1	81.62	70.79	78.74	72.80	-	-	-	-		-	-	-	-	88.82	35.48	
CIGAv2	81.76	71.65	76.34	73.62	-	-	-	-		-	-	-	-	89.87	41.73	

Table 1: ID_{ID} and OOD_{OOD} performances of 10 baselines on 11 datasets.