

1 Graph Attribution Benchmarks

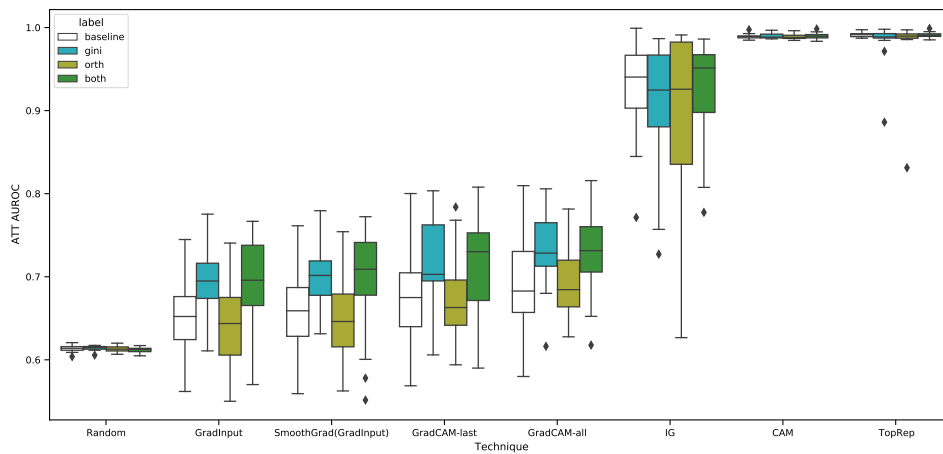


Figure 1: Benzene GCN

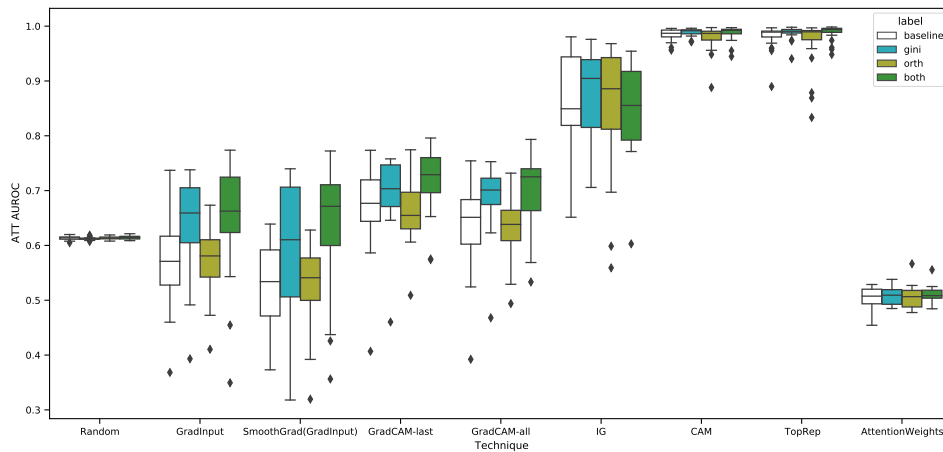


Figure 2: Benzene GAT

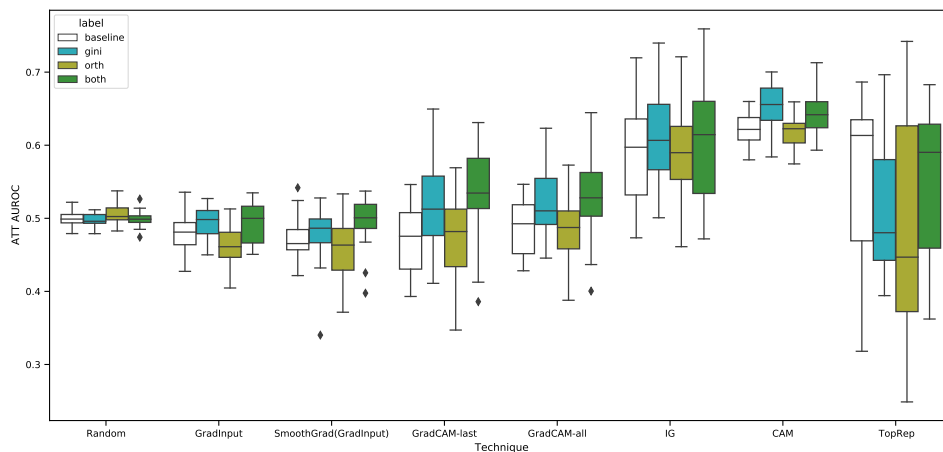


Figure 3: Amine-Ether-Benzene GCN

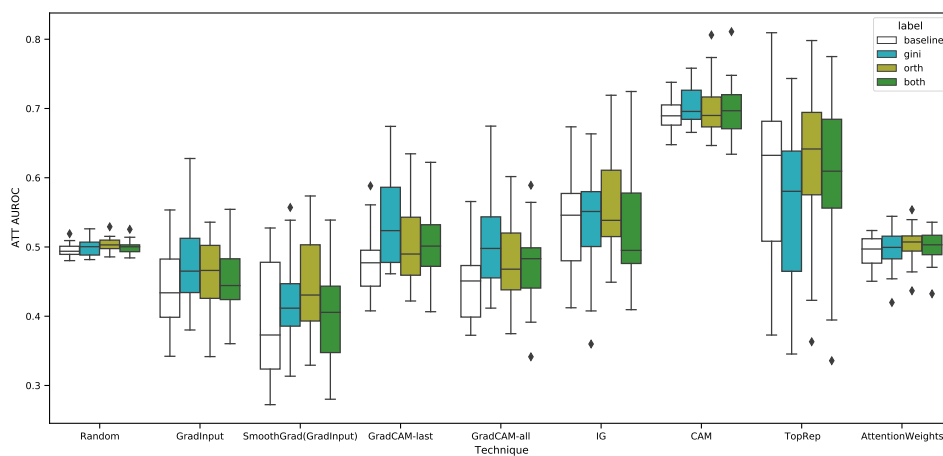


Figure 4: Amine-Ether-Benzene GAT

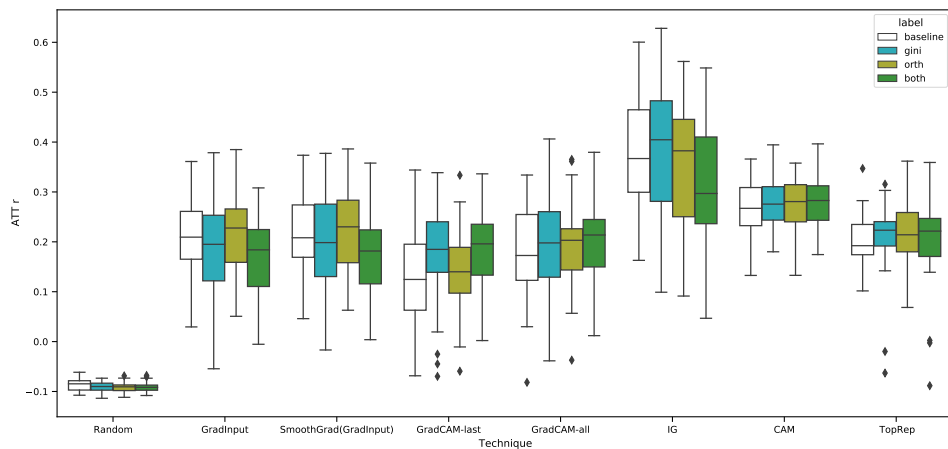


Figure 5: Crippen LogP GCN

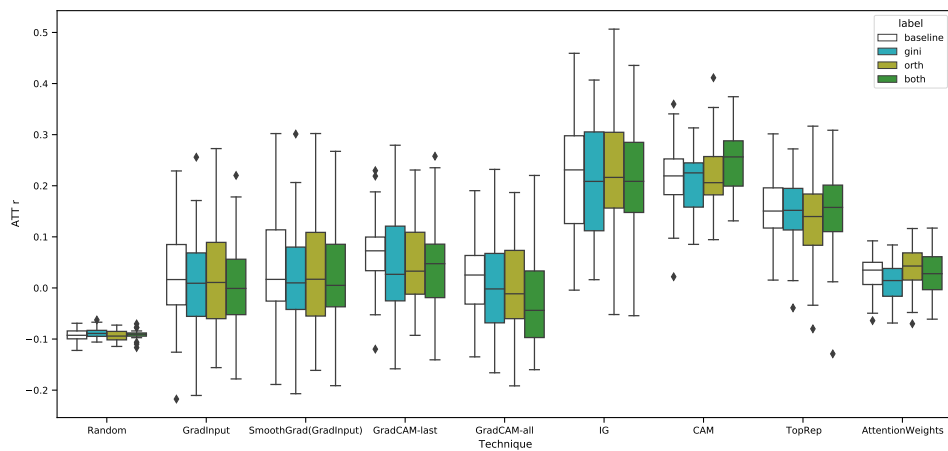


Figure 6: Crippen LogP GAT

2 Survey of medicinal chemists

SMILES strings for molecules can be found in `medchem_game_data.txt`.

Table 1: Raw count of votes per question and attribution method. Note that not all chemists voted on all questions.

Endpoint	Molecule	CAM	CAM _{BRO+Gini}	TopRep _{BRO+Gini}	Random	None
Solubility	5	1	3	5	3	0
	1	6	4	1	0	3
	7	2	1	1	7	1
	8	2	3	6	1	0
	10	2	2	5	5	0
	22	2	7	4	1	0
	13	4	3	5	2	0
	2	0	2	4	5	3
	19	5	4	4	0	0
	4	0	2	7	4	1
logD	tamoxifen	1	10	1	1	0
	chlorpromazine	1	9	2	1	1
	bifonazole	3	10	0	1	0
	tolnaftate	1	10	0	1	1
	amiodarone	1	4	3	4	2
	loratadine	7	0	6	0	1
	trifluoperazine	0	1	9	3	1
	thioridazine	0	5	7	0	2
Melting point	27	1	2	4	4	2
	36	1	4	4	4	0
	37	1	0	4	1	2
	38	1	2	5	3	2
	23	4	3	3	2	1
	32	4	3	1	1	4