

## Bayesian Model for the Classification of GPCR Agonists and Antagonists

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**Table S1.** Enrichment Results for Bayesian model building

Output	Category %	1%	5%	10%	25%	50%	75%	90%	95%	99%
GPCR (N = 3368)	50.03%	2%	10%	19.9%	48.8%	89.7%	99.6%	100%	100%	100%

**Table S2.** Percentile Results for Bayesian model building

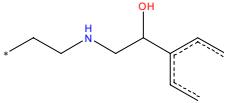
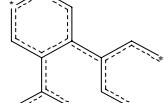
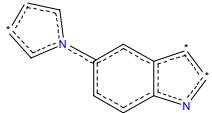
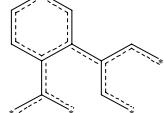
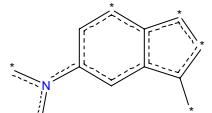
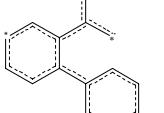
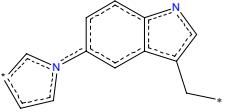
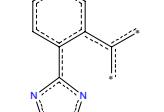
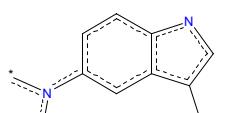
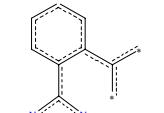
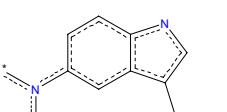
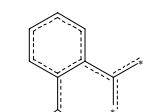
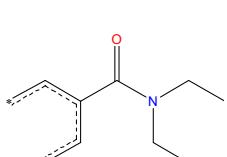
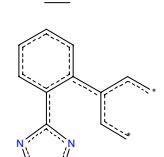
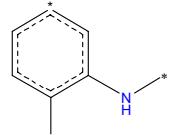
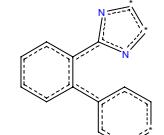
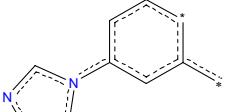
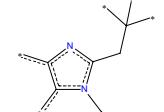
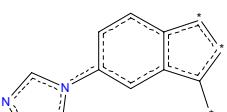
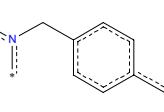
Model Name	99%	95%	90%	70%	50%	30%	10%	5%	1%
GPCR (N = 3368)	-10.472 29%/71%	-5.022 22%/78%	-2.064 18%/82%	1.206 15%/85%	1.206 10%/90%	14.442 6%/94%	17.712 5%/95%	20.671 4%/96%	26.121 2%/98%

**Table S3.** Category Statistics Results for Bayesian model building

Output	Category N	Category Mean ( $\pm$ StdDev)	Noncategory N	Noncategory Mean ( $\pm$ StdDev)
GPCR (N = 3368)	1685	7.82 ( $\pm$ 7.79)	1683	-24.26 ( $\pm$ 24.17)

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**Figure S1.** Scaffolds representing GPCR agonistic and antagonistic features from FCFP-6

GPCR agonistic features from FCFP-6			GPCR antagonistic features from FCFP-6		
ID	Feature	Bayesian score	ID	Feature	Bayesian score
G1		0.703	B1		-3.833
G2		0.703	B2		-3.823
G3		0.703	B3		-3.823
G4		0.703	B4		-3.801
G5		0.703	B5		-3.801
G6		0.703	B6		-3.790
G7		0.702	B7		-3.790
G8		0.702	B8		-3.779
G10		0.701	B9		-3.779
G12		0.701	B10		-3.597

**Figure S1.** Continued

GPCR agonistic features from FCFP-6			GPCR antagonistic features from FCFP-6		
ID	Feature	Bayesian score	ID	Feature	Bayesian score
G13		0.701	B11		-3.357
G14		0.700	B12		-3.305
G15		0.700	B13		-3.250
G16		0.699	B14		-3.212
G17		0.698	B15		-3.157
G18		0.698	B17		-3.087
G19		0.698	B18		-3.087
G20		0.696	B19		-3.064
G21		0.693	B20		-3.041
G22		0.693	B21		-3.018

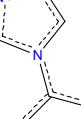
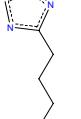
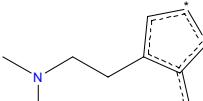
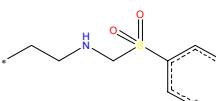
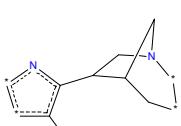
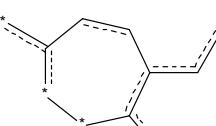
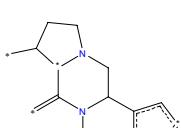
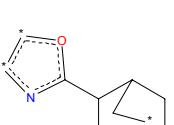
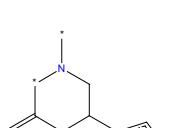
**Figure S1.** Continued

GPCR agonistic features from FCFP-6			GPCR antagonistic features from FCFP-6		
ID	Feature	Bayesian score	ID	Feature	Bayesian score
G23		0.693	B22		-2.994
G24		0.692	B23		-2.969
G25		0.692	B24		-2.969
G26		0.692	B25		-2.891
G27		0.691	B26		-2.891
G28		0.689	B27		-2.864
G29		0.689	B28		-2.864
G30		0.689	B29		-2.864
G31		0.689	B30		-2.864
G32		0.688	B31		-2.864

**Figure S1.** Continued

GPCR agonistic features from FCFP-6			GPCR antagonistic features from FCFP-6		
ID	Feature	Bayesian score	ID	Feature	Bayesian score
G33		0.688	B32		-2.864
G34		0.688	B33		-2.864
G35		0.688	B34		-2.849
G36		0.687	B35		-2.836
G37		0.687	B36		-2.836
G38		0.685	B38		-2.835
G39		0.685	B40		-2.825
G40		0.685	B42		-2.807
G41		0.684	B43		-2.807
G42		0.683	B46		-2.746

**Figure S1.** Continued

GPCR agonistic features from FCFP-6			GPCR antagonistic features from FCFP-6		
ID	Feature	Bayesian score	ID	Feature	Bayesian score
G43		0.682	B47		-2.714
G44		0.681	B48		-2.682
G46		0.680	B49		-2.682
G47		0.678			
G48		0.678			
G49		0.678			
G50		0.678			

The stars in the sketches represent ‘any atom’.