

Supplementary Table S1: Physicochemical properties of drugs used in building quantitative structure-permeability relationships for tacrine, perazine, and clobazam.

Drug Name	Molecular Weight	Log Molecular Weight	Hydrogen Bond Donors	Hydrogen Bond Acceptors	High Bond Donors + Acceptors	TPSA	Rotatable Bonds	C Bonds	N Bonds	NO Bonds	Hydroxyl Bonds	Halogen Bonds	Number of Rings	Aromatic Rings	Number of Ring (Size 5)	Number of Ring (Size 6)	Log(P)	Powder	Index of Refraction	Surface Tension	Density	Polarizability	Molar Volume	Log Molar Volume	Molar Refractivity	LogP	LogP ₁	LogP ₂	LogP ₃	LogP ₄	LogP ₅	LogP ₆	pH(pKa)
Alprazolam	246.35	2.40	2.00	3.00	5.00	45.49	8.00	9.63	0.06	0.17	0.17	0.00	1.00	1.00	0.00	1.00	1.96	607.76	1.52	36.37	1.01	29.76	367.46	2.39	70.05	0.62	2.76	0.51	0.59	0.68	0.77	0.86	13.98
Alprazolol	265.34	2.43	4.00	5.00	9.00	98.29	8.00	0.74	0.11	0.26	0.26	0.00	1.00	1.00	0.00	1.00	0.10	613.02	1.58	46.20	1.11	29.66	236.66	2.37	74.26	0.17	0.24	-0.09	-0.94	-1.05	-0.76	-0.57	13.98
Alprazololol	287.63	2.46	2.00	6.00	8.00	107.72	11.00	0.62	0.05	0.18	0.18	0.00	1.00	1.00	0.00	1.00	1.81	733.89	1.53	41.68	1.07	31.25	287.98	2.46	84.92	-0.11	0.07	0.39	0.48	0.77	0.86	0.95	13.99
Alprazolololol	310.92	2.50	2.00	7.00	9.00	117.15	12.00	0.50	0.00	0.10	0.10	0.00	1.00	1.00	0.00	1.00	2.62	820.26	1.47	36.75	1.03	31.25	310.92	2.50	98.29	-0.11	0.07	0.39	0.48	0.77	0.86	0.95	13.99
Alprazololololol	334.21	2.53	2.00	8.00	10.00	126.58	13.00	0.41	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	3.43	906.63	1.39	32.25	1.09	41.14	334.21	2.53	111.66	-0.06	0.02	0.00	0.00	0.00	0.00	0.00	13.97
Alprazolololololol	357.50	2.56	2.00	9.00	11.00	136.01	14.00	0.29	0.00	0.08	0.08	0.00	1.00	1.00	0.00	1.00	4.24	992.98	1.32	27.77	1.15	39.74	357.50	2.56	125.01	-0.17	0.02	0.00	0.00	0.00	0.00	0.00	13.96
Alprazololololololol	380.79	2.59	2.00	10.00	12.00	145.44	15.00	0.19	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	5.05	1079.33	1.25	23.27	1.21	42.33	380.79	2.59	138.36	-0.41	0.01	0.00	0.00	0.00	0.00	0.00	13.95
Alprazolololololololol	404.08	2.62	2.00	11.00	13.00	154.87	16.00	0.09	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	5.86	1165.68	1.18	18.76	1.27	44.93	404.08	2.62	151.21	-0.65	0.00	0.00	0.00	0.00	0.00	0.00	13.94
Alprazololololololololol	427.37	2.65	2.00	12.00	14.00	164.30	17.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	6.67	1252.03	1.11	14.26	1.33	47.53	427.37	2.65	164.06	-0.89	0.00	0.00	0.00	0.00	0.00	0.00	13.93
Alprazolololololololololol	450.66	2.68	2.00	13.00	15.00	173.73	18.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	7.48	1338.38	1.04	9.76	1.39	50.13	450.66	2.68	176.91	-1.13	0.00	0.00	0.00	0.00	0.00	0.00	13.92
Alprazololololololololololol	473.95	2.71	2.00	14.00	16.00	183.16	19.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	8.29	1424.73	0.97	4.26	1.45	52.73	473.95	2.71	189.76	-1.37	0.00	0.00	0.00	0.00	0.00	0.00	13.91
Alprazolololololololololololol	497.24	2.74	2.00	15.00	17.00	192.59	20.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	9.10	1511.08	0.90	-0.24	1.51	55.33	497.24	2.74	202.61	-1.61	0.00	0.00	0.00	0.00	0.00	0.00	13.90
Alprazololololololololololololol	520.53	2.77	2.00	16.00	18.00	202.02	21.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	9.91	1597.43	0.83	-4.74	1.57	57.93	520.53	2.77	215.46	-1.85	0.00	0.00	0.00	0.00	0.00	0.00	13.89
Alprazolololololololololololololol	543.82	2.80	2.00	17.00	19.00	211.45	22.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	10.72	1683.78	0.76	-9.24	1.63	60.53	543.82	2.80	228.31	-2.09	0.00	0.00	0.00	0.00	0.00	0.00	13.88
Alprazololololololololololololololol	567.11	2.83	2.00	18.00	20.00	220.88	23.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	11.53	1770.13	0.69	-13.74	1.69	63.13	567.11	2.83	241.16	-2.33	0.00	0.00	0.00	0.00	0.00	0.00	13.87
Alprazolololololololololololololololol	590.40	2.86	2.00	19.00	21.00	230.31	24.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	12.34	1856.48	0.62	-18.24	1.75	65.73	590.40	2.86	254.01	-2.57	0.00	0.00	0.00	0.00	0.00	0.00	13.86
Alprazololololololololololololololololol	613.69	2.89	2.00	20.00	22.00	239.74	25.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	13.15	1942.83	0.55	-22.74	1.81	68.33	613.69	2.89	266.86	-2.81	0.00	0.00	0.00	0.00	0.00	0.00	13.85
Alprazolololololololololololololololololol	636.98	2.92	2.00	21.00	23.00	249.17	26.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	13.96	2029.18	0.48	-27.24	1.87	70.93	636.98	2.92	279.71	-3.05	0.00	0.00	0.00	0.00	0.00	0.00	13.84
Alprazololololololololololololololololololol	660.27	2.95	2.00	22.00	24.00	258.60	27.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	14.77	2115.53	0.41	-31.74	1.93	73.53	660.27	2.95	292.56	-3.29	0.00	0.00	0.00	0.00	0.00	0.00	13.83
Alprazol	683.56	2.98	2.00	23.00	25.00	268.03	28.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	15.58	2201.88	0.34	-36.24	1.99	76.13	683.56	2.98	305.41	-3.53	0.00	0.00	0.00	0.00	0.00	0.00	13.82
Alprazol	706.85	3.01	2.00	24.00	26.00	277.46	29.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	16.39	2288.23	0.27	-40.74	2.05	78.73	706.85	3.01	318.26	-3.77	0.00	0.00	0.00	0.00	0.00	0.00	13.81
Alprazol	730.14	3.04	2.00	25.00	27.00	286.89	30.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	17.20	2374.58	0.20	-45.24	2.11	81.33	730.14	3.04	331.11	-4.01	0.00	0.00	0.00	0.00	0.00	0.00	13.80
Alprazol	753.43	3.07	2.00	26.00	28.00	296.32	31.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	18.01	2460.93	0.13	-49.74	2.17	83.93	753.43	3.07	343.96	-4.25	0.00	0.00	0.00	0.00	0.00	0.00	13.79
Alprazol	776.72	3.10	2.00	27.00	29.00	305.75	32.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	18.82	2547.28	0.06	-54.24	2.23	86.53	776.72	3.10	356.81	-4.49	0.00	0.00	0.00	0.00	0.00	0.00	13.78
Alprazol	800.01	3.13	2.00	28.00	30.00	315.18	33.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	19.63	2633.63	0.00	-58.74	2.29	89.13	800.01	3.13	369.66	-4.73	0.00	0.00	0.00	0.00	0.00	0.00	13.77
Alprazol	823.30	3.16	2.00	29.00	31.00	324.61	34.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	20.44	2720.00	0.00	-63.24	2.35	91.73	823.30	3.16	382.51	-4.97	0.00	0.00	0.00	0.00	0.00	0.00	13.76
Alprazol	846.59	3.19	2.00	30.00	32.00	334.04	35.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	21.25	2806.35	0.00	-67.74	2.41	94.33	846.59	3.19	395.36	-5.21	0.00	0.00	0.00	0.00	0.00	0.00	13.75
Alprazol	869.88	3.22	2.00	31.00	33.00	343.47	36.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	22.06	2892.70	0.00	-72.24	2.47	96.93	869.88	3.22	408.21	-5.45	0.00	0.00	0.00	0.00	0.00	0.00	13.74
Alprazol	893.17	3.25	2.00	32.00	34.00	352.90	37.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	22.87	2979.05	0.00	-76.74	2.53	99.53	893.17	3.25	421.06	-5.69	0.00	0.00	0.00	0.00	0.00	0.00	13.73
Alprazol	916.46	3.28	2.00	33.00	35.00	362.33	38.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	23.68	3065.40	0.00	-80.74	2.59	102.13	916.46	3.28	433.91	-5.93	0.00	0.00	0.00	0.00	0.00	0.00	13.72
Alprazol	939.75	3.31	2.00	34.00	36.00	371.76	39.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	24.49	3151.75	0.00	-84.74	2.65	104.73	939.75	3.31	446.76	-6.17	0.00	0.00	0.00	0.00	0.00	0.00	13.71
Alprazol	963.04	3.34	2.00	35.00	37.00	381.19	40.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	25.30	3238.10	0.00	-88.74	2.71	107.33	963.04	3.34	459.61	-6.41	0.00	0.00	0.00	0.00	0.00	0.00	13.70
Alprazol	986.33	3.37	2.00	36.00	38.00	390.62	41.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	26.11	3324.45	0.00	-92.74	2.77	109.93	986.33	3.37	472.46	-6.65	0.00	0.00	0.00	0.00	0.00	0.00	13.69
Alprazol	1009.62	3.40	2.00	37.00	39.00	400.05	42.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00	26.92	3410.80	0.00	-96.74	2.83	112.53	1009.62	3.40	485.31	-6.89	0.00	0.00	0.00	0.00	0.00	0.00	13.68
Alprazol	1032.91	3.43	2.00	38.00	40.00	409.48	43.00	0.00	0.00	0.09	0.09	0.00	1.00	1.00	0.00	1.00																	