

Table S1.

ID ChemBridge	Cluster	Kd (μ M)	Antibody Inhibition	IC50 Cell Degranulation	MW	logP	tPSA	HBD	HBA	State / FAFdrug2	Detected Problems
6752784	1	5	86.5 %	**	496.94	5.57	79.73	1	6	Accepted	-
6670340	1	16.3	81%	**	453.51	3.02	122.13	1	8	Accepted	-
6422575	single	6.2	81%	**	497.31	4.1	94.01	1	7	Rejected	Max Ring Size
6882059	1	9.4	79.5 %	**	451.53	3.35	76.27	2	7	Accepted	-
7111786	1	-	77.5 %	**	447.48	3.01	93.89	1	8	Accepted	-
6203863	1	6.1	73.5 %	**	487.50	4.71	102.37	1	8	Accepted	-
7347627	1	-	72%	**	451.53	3.35	76.27	2	7	Accepted	-
7489416	1	-	71%	**	514.38	5.27	115.31	2	6	Accepted	-
6719738	1	-	71%	**	480.48	5.04	79.73	1	6	Accepted	-
6650234	1	6.3	71%	**	480.50	5.33	125.04	1	7	Accepted	-
6652639	1	-	70.5 %	**	444.47	3.72	88.96	1	7	Accepted	-
6673225	1	-	69%	**	478.51	4.84	134.27	1	8	Accepted	-
6800873	single	4.6	67.5 %	**	467.51	4.78	76.07	1	6	Accepted	-
6879058	1	-	67.5 %	**	438.49	1.92	89.16	2	8	Accepted	-
6282824	2	5.6	67.5 %	5 μ M	458.53	4.15	111.41	1	7	Accepted	-
6750319	1	-	67%	**	448.49	4.86	125.04	1	7	Accepted	-
6474819	single	17.9	63%	**	429.57	5.63	38.53	2	4	Accepted	-
6498669	3	0.8	63%	**	467.53	2.78	127.18	3	8	Accepted	-
6651552	1	-	60%	**	467.55	4.24	67.04	2	6	Accepted	-
6453860	3	-	60%	**	454.51	5.65	76.66	2	6	Accepted	-
6853966	3	-	58%	**	469.51	2.4	131.21	3	9	Accepted	-
6866968	single	-	57.5%	**	464.61	3.82	61.78	3	6	Accepted	-
7938324	single	-	57%	**	444.52	3.49	107.5	0	6	Accepted	-
6905988	1	-	57%	**	455.49	3.08	76.27	2	7	Accepted	-
6885782	1	-	56.5%	**	532.00	3.55	94.73	2	9	Accepted	-
6663684	1	-	56.5%	**	435.53	3.78	67.04	2	6	Accepted	-
6672500	1	-	55%	**	487.95	3.22	85.5	2	8	Accepted	-
7721949	1	-	54%	**	453.55	4.07	76.27	2	7	Accepted	-
7966545	2	6.7	53.5%	**	486.52	3.33	123.27	2	8	Accepted	-
7437580	single	-	51%	**	481.56	3.0	125.46	2	8	Accepted	-
6654239	1	-	50%	**	471.49	2.7	85.5	2	8	Accepted	-
6670570	1	-	50%	**	500.58	1.8	112.8	2	9	Accepted	-
6670673	1	-	50%	**	471.49	2.7	85.5	2	8	Accepted	-
6670747	1	-	50%	**	437.50	2.99	76.27	2	7	Accepted	-
6671401	1	-	50%	**	443.46	1.99	98.64	2	9	Accepted	-
6677533	1	-	50%	**	459.53	2.61	113.74	2	8	Accepted	-
6683618	1	-	50%	**	457.92	3.25	76.27	2	7	Accepted	-
6417902	single	-	49.5%	**	478.62	4.19	66.27	1	6	Accepted	-
6437157	single	-	49.5%	**	461.89	5.48	80.75	0	6	Accepted	-
6465972	3	-	49%	**	484.56	4.17	102.55	1	8	Accepted	-
7723671	1	-	48.5%	**	485.52	3.05	85.5	2	8	Accepted	-
6648368	1	-	48.5%	**	459.91	3.74	67.04	2	6	Accepted	-
6656195	1	-	48.5%	**	453.52	3.88	67.04	2	6	Accepted	-
7778331	single	3	48%	**	475.58	1.73	105.55	3	9	Accepted	-
6994060	2	-	47.5%	**	485.98	3.15	115.85	2	8	Accepted	-
6458830	3	-	47%	**	492.65	4.56	66.27	1	6	Accepted	-

7524107	2	5.5	46.5%	**	445.48	5.2	104.4	2	7	Accepted	-
6661524	1	-	46.5%	**	541.46	3.79	103.57	2	8	Accepted	-
7739436	1	-	46%	**	438.49	2.86	89.16	2	8	Accepted	-
6881804	1	-	46%	**	445.48	2.74	98.64	2	9	Accepted	-
6907921	1	-	45.5%	**	427.47	2.42	89.41	2	8	Accepted	-
7495334	2	1.6	43%	10 μ M	450.46	2.69	145.65	1	9	Accepted	-
7509862	4	-	42.5	10 μ M	515.58	4.37	131.3	2	8	Intermediate	Flagged Group Nitrile
7325385	1	-	42%	**	495.58	3.68	85.5	2	8	Accepted	-
6669449	4	-	42%	**	424.40	4.39	127.16	3	8	Intermediate	Flagged Group Nitrile
7348779	single	-	40%	**	438.55	4.58	59.08	0	6	Accepted	-
7501888	2	8.2	40%	4 μ M	539.04	5.27	112.8	1	8	Accepted	-
6946138	4	-	40%	**	415.41	5.47	85.64	0	6	Accepted	-
7722851	5	21.8	39.5%	4 μ M	523.00	3.59	128.09	1	8	Accepted	-
7517583	single	-	38.5%	**	476.47	2.22	102.45	0	9	Accepted	-
6634701	single	-	38.5%	10 μ M	470.54	4.23	102.74	0	7	Rejected	-
7726450	1	-	37.5%	**	458.46	2.74	110.69	1	9	Accepted	-
6662088	1	-	37%	**	515.60	1.09	125.69	2	10	Accepted	-
7752193	2	8	35%	10 μ M	451.54	3.1	115.85	2	8	Intermediate	Flagged Group Alkene
7238569	single	-	32%	**	478.56	3.54	132.82	4	8	Accepted	-
7724000	1	-	30%	**	469.48	2.92	85.5	2	8	Accepted	-
7443270	2	-	30%	10 μ M	451.49	3.26	120.89	1	8	Accepted	-
7245019	single	-	30%	**	428.47	4.99	76.05	1	6	Accepted	-
6909597	1	-	29%	**	457.92	3.25	76.27	2	7	Accepted	-
7661882	2	-	28%	**	443.49	4.01	74.86	1	7	Accepted	-
7667791	single	-	28%	**	434.48	3.5	82.21	2	7	Accepted	-
6891745	1	-	27.5%	**	467.53	2.95	85.5	2	8	Accepted	-
7783660	2	4.8	27%	10 μ M	507.60	3.74	132.92	2	9	Intermediate	Flagged Group Alkene
7653478	single	-	27%	**	451.54	3.12	91.36	2	9	Accepted	-
7723330	5	-	26%	**	501.48	2.88	114.48	1	10	Accepted	-
7199725	2	-	25%	**	440.55	4.62	49.61	2	5	Accepted	-
6987235	single	-	25%	**	476.00	5.28	50.77	0	4	Rejected	Max Ring Size
7140931	single	-	24.5%	**	472.59	3.47	92.37	0	7	Accepted	-
7787455	3	-	20%	**	454.49	3.36	110.39	1	8	Accepted	-
7660465	single	3.2	20%	15 μ M	536.87	4.33	106.62	2	7	Accepted	-
7661751	1	-	19%	**	466.50	1.66	98.39	2	9	Accepted	-
7722914	5	15.6	19%	15 μ M	513.62	2.29	116.79	2	9	Accepted	-
7745040	1	-	18%	**	542.39	4.05	89.41	2	8	Accepted	-
7735385	1	-	17%	**	464.53	3.79	93.07	2	8	Accepted	-
7756003	single	-	11%	10 μ M	484.61	4.5	104.57	0	7	Accepted	-