

## ANEXO 3

Tabla con valores de los 13 descriptores elegidos para los 39 ligandos del modelo predictivo.

ID	a_aro	a_nS	chi1 C	PEOE_PC-	E_sol	KierFlex	a_acc
L01	17	1	6.618592	-2.01059	-20.7374	5.347043	4
L02	23	2	9.568082	-2.32483	-29.7582	7.309276	5
L03	17	1	9.02684	-3.05445	-89.1657	7.328529	5
L04	34	2	18.05368	-5.80804	-520.43	16.3486	10
L05	23	1	7.765986	-1.73702	-63.4501	3.982799	2
L06	12	1	6.541242	-1.12108	-571.426	5.017261	1
L07	12	1	6.618592	-2.05996	-6.48871	4.487842	4
L08	17	1	6.041242	-1.89026	-7.33234	4.305722	3
L09	18	1	10.26599	-2.25324	-8.2916	6.581814	2
L10	17	1	6.618592	-2.1282	-28.1122	5.135141	4
L11	17	1	7.357738	-1.85092	27.58533	4.223736	3
L12	17	1	8.195942	-2.26562	12.78072	6.348061	4
L13	17	1	7.265986	-1.62515	1.197815	3.795592	2
L14	12	1	8.191072	-1.88215	-20.1374	4.147818	4
L17	23	2	9.159833	-2.1971	-38.3979	5.851624	4
L18	17	1	6.618592	-2.18784	-17.9388	4.43495	4
L19	23	2	9.659833	-2.58502	-33.6112	6.809387	5
L20	12	2	10.15983	-1.87242	-55.6341	7.879178	4
L21	18	2	11.65983	-2.10565	-39.4093	9.147623	4
L22	22	2	7.357738	-1.5037	-41.6583	4.619968	1
L23	22	1	7.357738	-1.74769	-63.2251	3.873049	1
L24	17	1	8.765986	-1.65006	-30.5268	4.907259	1
L25	23	1	7.765986	-1.73702	-100.347	3.982799	2
L26	23	1	9.840901	-1.47365	-38.6907	3.845117	1
L27	22	2	7.857738	-1.3767	-143.265	4.702222	1
L28	26	2	9.415816	-1.84613	-75.201	4.32409	1
L29	23	1	7.765986	-1.73318	-62.6535	3.982799	2
L30	23	1	10.25159	-1.76037	-37.877	5.130753	1
L31	27	1	10.74915	-1.81947	5.21E-06	4.135734	1
L32	22	2	7.357738	-1.71859	-65.5285	4.249537	1
L34	17	1	7.357738	-1.78878	-99.8406	4.443115	2
L35	23	1	7.857738	-1.75962	-62.7649	3.982799	2
L37	12	1	7.248348	-2.04934	-15.1403	4.945916	2
L38	18	2	11.65983	-2.39153	-18.8899	7.71333	4
L39	12	1	7.656597	-2.2798	-13.4074	5.550423	3
L40	12	2	6.618592	-1.97643	-15.139	5.565877	2
L41	18	1	10.97309	-2.33036	-11.9565	7.096067	2
L42	12	1	7.156597	-2.34827	-45.8091	5.395108	3
L43	12	1	5.94949	-1.85311	-90.8807	5.020299	3

ID	a_hyd	SlogP_VSA1	std_dim2	polararea	surfarea	pka
L01	16	58.73969	2.540972	111.1	636	6.04
L02	23	58.73969	2.841022	169.9	816.9	6.04
L03	21	50.33725	2.601988	205.2	826.6	6.39
L04	42	100.6745	2.502639	215.7	818	6.04
L05	18	51.58181	2.369205	212.6	800.1	6.04
L06	16	0.693079	2.37833	154.8	602.7	6.75
L07	15	46.58822	2.484637	140.4	617.9	8.14
L08	15	35.47015	2.447579	137.3	592.6	6.71
L09	25	37.92059	2.965257	89.3	773.2	6.48
L10	17	61.864	2.782596	98.7	676.2	7.91
L11	17	35.47015	2.450183	140.5	603.9	7.95
L12	21	56.60522	2.77552	84.4	716.1	7.04
L13	17	53.4809	2.384925	71	651.4	6.5
L14	18	43.50489	2.193003	91.4	697.1	6.04
L17	21	82.82553	2.481751	165.2	767.3	6.04
L18	15	58.73969	2.542818	166.5	640.6	6.04
L19	22	82.82553	2.790282	204.3	786.1	6.04
L20	25	40.05507	2.675888	173.8	824.7	6.04
L21	27	40.05507	2.981313	211.9	868.5	7
L22	18	34.79628	2.438119	137.7	655.4	6.04
L23	16	34.79628	2.254042	123.3	652.4	6.39
L24	19	34.79628	2.378252	99.4	704.5	6.39
L25	18	51.58181	2.139882	123.7	675.6	6.04
L26	21	34.79628	2.367306	109.1	691	6.39
L27	19	16.78553	2.536071	152.8	697.5	6.62
L28	22	34.79628	2.310737	133.1	729.1	6.39
L29	18	51.58181	2.304328	124.2	674.7	6.008
L30	22	34.79628	2.307339	100.1	760.4	6.9
L31	23	34.79628	2.217432	99	741.2	6.85
L32	18	16.78553	2.439555	144.7	660	6.008
L34	17	34.79628	2.103166	116.1	674.3	6.85
L35	17	51.58181	2.383653	119.6	679.5	6.22
L37	18	19.90984	2.556301	128	644.4	6.67
L38	28	46.30369	2.875037	156.6	856.2	7.59
L39	19	43.17938	2.880834	101.2	698.9	6.04
L40	18	43.17938	2.686104	127.2	673.5	6.04
L41	26	37.92059	2.371787	76.4	757.5	6.4
L42	18	43.17938	2.365946	98	661.2	6.71
L43	17	19.90984	2.417862	137.1	328.9	6.74