

Supplementary Table 1: Calculated physicochemical descriptors and pharmaceutically relevant properties

molecule	dipole	SASA	FOSA	FISA	PISA	WPSA	volume	dip ² /V	glob	QPpoIrz	QPlogPC16	QPlogP oct	Rot or
3h	12.1	520.	27.1	101.	264.	127.	903.9	0.162	0.8				
	1	36	7	59	45	15	6	1	69	29.98	9.37	15.85	4
3i	12.0	523.	26.6	94.9	253.	148.	923.7	0.157	0.8				
	5	63	5	0	87	22	3	2	76	30.67	10.14	16.10	4
3j	11.9	535.	25.8	93.7	249.	166.	947.8	0.151	0.8				
	8	62	7	3	81	21	6	4	71	31.60	10.91	16.42	4
3o	7.14	534.	66.9	79.3	290.	98.0	955.3	0.053	0.8				
	7.19	543.	66.2	74.9	279.	121.	978.9	0.052	0.8	31.64	9.80	14.73	5
3p	06	7	3	98	88	0	8	78	32.49	10.58	15.11	5	
	3.91	599.	63.9	89.4	350.	95.4	1041.	0.014	0.8				
4a-S	45	2	5	60	9	68	7	29	37.60	11.69	16.51	2	
	4.84	590.	53.8	90.2	345.	100.	1033.	0.022	0.8				
4a-R	10	8	0	94	07	43	7	38	37.22	11.63	16.54	2	
	4.33	608.	60.6	91.2	326.	130.	1057.	0.017	0.8				
4b-S	79	4	5	56	34	80	7	25	38.01	11.45	16.83	2	
	3.99	603.	54.1	96.6	326.	125.	1054.	0.015	0.8				
4b-R	16	9	5	90	41	56	1	31	37.89	11.45	16.77	2	
	2.30	607.	63.9	89.4	311.	142.	1057.	0.005	0.8				
4c-S	42	3	6	81	22	98	0	27	37.88	11.27	16.64	2	
	2.86	599.	53.9	90.3	308.	146.	1050.	0.007	0.8				
4c-R	28	9	8	12	79	21	8	34	37.53	11.22	16.60	2	
	2.49	606.	63.8	88.9	311.	142.	1057.	0.005	0.8				
4d-S	34	6	3	30	25	62	8	28	37.86	11.26	16.65	2	
	3.44	599.	54.0	90.2	308.	146.	1049.	0.011	0.8				
4d-R	21	2	2	16	81	99	3	34	37.53	11.21	16.65	2	
	4.28	619.	58.6	90.2	321.	149.	1082.	0.017	0.8				
4e-S	69	9	8	30	42	15	0	23	38.94	12.26	17.22	2	
	3.93	614.	51.3	96.6	320.	145.	1078.	0.014	0.8				
4e-R	18	4	6	23	93	14	4	28	38.77	12.24	17.16	2	
	2.38	622.	63.9	89.2	301.	166.	1085.	0.005	0.8				
4f-S	01	5	9	88	89	58	2	21	38.89	12.27	17.09	2	
	2.99	613.	54.4	90.3	297.	171.	1077.	0.008	0.8				
4f-R	85	4	3	61	47	84	3	28	38.54	12.21	17.06	2	
	2.50	621.	63.8	88.9	301.	166.	1085.	0.005	0.8				
4g-S	36	6	3	63	94	66	7	22	38.89	12.26	17.10	2	
	3.46	614.	54.0	90.1	298.	171.	1078.	0.011	0.8				
4g-R	25	5	9	51	51	04	1	28	38.56	12.22	17.10	2	
	5.15	608.	61.2	86.1	306.	154.	1064.	0.024	0.8				
4h-S	00	4	5	22	39	22	9	29	38.08	11.17	17.03	2	
	5.15	607.	61.2	86.1	306.	154.	1064.	0.024	0.8				
4h-R	99	4	5	22	38	21	9	29	38.08	11.17	17.03	2	
	7.21	606.	57.8	87.7	295.	165.	1079.	0.048	0.8				
4i-S	66	5	8	22	82	44	2	39	38.58	11.80	17.61	2	
	7.21	606.	57.8	87.7	295.	165.	1079.	0.048	0.8				
4i-R	65	5	8	21	81	44	2	39	38.58	11.80	17.61	2	
	6.96	619.	56.4	85.5	291.	186.	1104.	0.043	0.8				
4j-S	63	4	1	22	47	72	9	34	39.55	12.50	17.97	2	
	6.98	619.	56.4	85.5	291.	186.	1104.	0.044	0.8				
4j-R	63	4	8	18	43	74	1	34	39.55	12.50	17.97	2	
	6.95	545.	105.	102.	258.	79.6	1022.	0.047	0.8				
4k-S	80	20	95	00	6	39	3	99	35.30	11.07	16.18	3	
	2.92	612.	90.5	90.6	335.	95.7	1093.	0.007	0.8				
4k-R	72	7	2	81	1	14	8	38	38.87	12.11	16.86	3	
	6.80	546.	101.	103.	230.	111.	1041.	0.044	0.9				
4l-S	59	28	19	55	56	70	3	09	35.81	11.32	16.48	3	
	3.23	640.	85.5	94.7	310.	149.	1135.	0.009	0.8				
4l-R	76	7	9	90	50	62	2	22	40.34	12.73	17.59	3	
	5.31	559.	104.	102.	232.	120.	1058.	0.026	0.8	36.48	11.48	16.48	3

		09	28	42	18	20	02	7	98				
4m-R	5.30	559.	104.	102.	232.	120.	1058.	0.026	0.8				
		21	29	40	45	07	16	5	98	36.49	11.49	16.48	3
4n-S	5.12	555.	105.	103.	216.	130.	1053.	0.024	0.9				
		42	15	63	34	30	44	9	01	36.14	11.43	16.38	3
4n-R	3.00	640.	94.2	94.7	285.	165.	1139.	0.007	0.8				
		42	8	7	59	78	47	9	24	40.25	12.70	17.59	3
4o-S	8.17	548.	102.	100.	218.	126.	1039.	0.064	0.9				
		96	81	48	74	93	30	2	04	35.60	10.62	16.70	3
4o-R	8.17	548.	102.	100.	218.	126.	1039.	0.064	0.9				
		95	81	48	74	93	29	3	04	35.60	10.62	16.70	3
4p-S	8.12	551.	101.	98.6	211.	140.	1057.	0.062	0.9				
		69	63	5	28	14	90	3	10	36.27	11.19	16.98	3
4p-R	8.12	551.	101.	98.6	211.	140.	1057.	0.062	0.9				
		76	62	3	37	13	98	3	10	36.28	11.19	16.98	3