

Supplementary data

	MW (Da)	cLogP	TPSA (Å <sup>2</sup> )	#rings	#HBD	#HBA	#RB
<b>Minimum</b>	144.1	-0.34	52.6	0.00	0.00	2.00	2.00
<b>10% Percentile</b>	226.7	0.37	63.0	1.00	1.00	3.60	2.60
<b>25% Percentile</b>	441.6	1.62	81.0	2.50	2.00	6.50	4.50
<b>Median</b>	615.5	4.13	150.0	3.00	3.00	10.0	7.00
<b>Mean</b>	621.8	4.15	143.7	4.04	2.68	9.48	7.76
<b>75% Percentile</b>	831.0	6.41	198.5	5.50	3.00	13.5	11.5
<b>90% Percentile</b>	931.8	7.65	222.2	8.40	4.40	14.4	14.0
<b>Maximum</b>	1030	10.3	242.0	9.00	6.00	16.0	15.0

**Supplementary Table 1.** Mean, median and percentile values for physicochemical properties of approved PPI Modulators

	<b>MW (Da)</b>	<b>cLogP</b>	<b>TPSA (Å<sup>2</sup>)</b>	<b>#rings</b>	<b>#HBD</b>	<b>#HBA</b>	<b>#RB</b>
<b>Minimum</b>	26.04	-16.57	0	0.00	0.00	0.00	0.00
<b>10% Percentile</b>	167.2	-2.448	21.26	0.00	0.00	2.00	1.00
<b>25% Percentile</b>	247.7	-0.151	41.62	1.00	1.00	2.00	2.00
<b>Median</b>	335.5	2.062	72.83	3.00	2.00	4.00	5.00
<b>Mean</b>	384.7	1.623	91.90	2.65	2.24	4.91	6.03
<b>75% Percentile</b>	444.5	3.671	109.7	4.00	3.00	6.00	8.00
<b>90% Percentile</b>	609.7	4.969	167.9	5.00	4.00	9.00	12.0
<b>Maximum</b>	2002	18.23	805.5	18.00	25.0	48.0	58.0

**Supplementary Table 2.** Mean, median and percentile values for physicochemical properties of non-PPI approved drugs.

	<b>MW (Da)</b>	<b>cLogP</b>	<b>TPSA (Å<sup>2</sup>)</b>	<b>#rings</b>	<b>#HBD</b>	<b>#HBA</b>	<b>#RB</b>
<b>Minimum</b>	283.4	1.16	49.4	1.00	0.00	3.00	2.00
<b>10% Percentile</b>	332.1	1.59	66.2	3.00	0.10	3.10	3.10
<b>25% Percentile</b>	444.6	2.75	90.2	4.00	1.00	5.00	5.00
<b>Median</b>	558.6	3.57	104.0	5.00	2.00	7.00	7.00
<b>Mean</b>	544.7	4.27	108.9	4.47	2.17	6.80	7.33
<b>75% Percentile</b>	624.5	4.69	128.3	5.00	3.00	8.00	9.00
<b>90% Percentile</b>	724.7	8.69	157.8	6.00	3.90	10.0	14.5
<b>Maximum</b>	974.6	12.39	195.0	7.00	8.00	14.0	17.0

**Supplementary Table 3.** Mean, median and percentile values for physicochemical properties of PPI modulators in clinical trials