

Supporting Information

Imidazolopiperazines: Lead optimization of the second generation antimalarial agents

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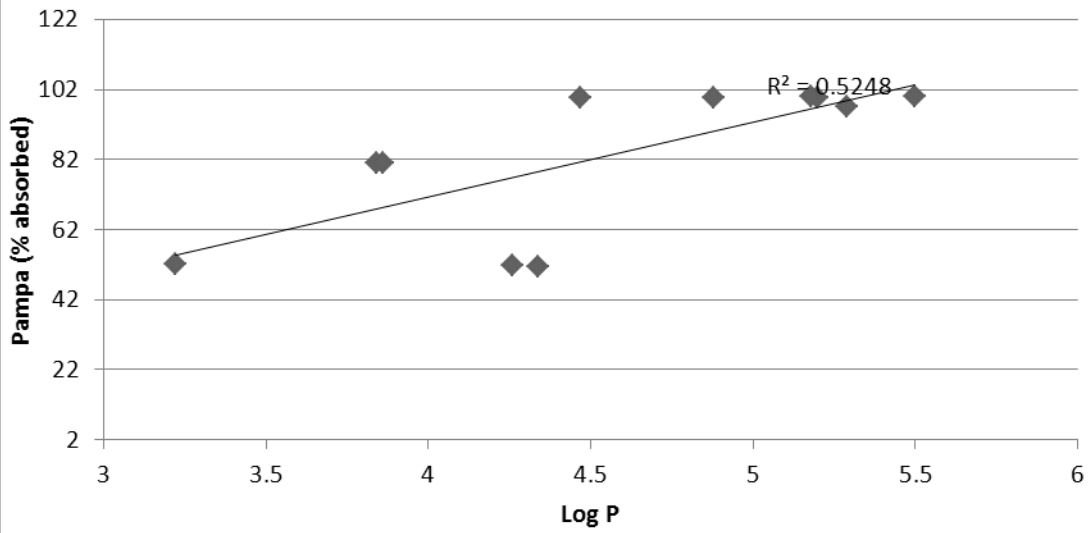
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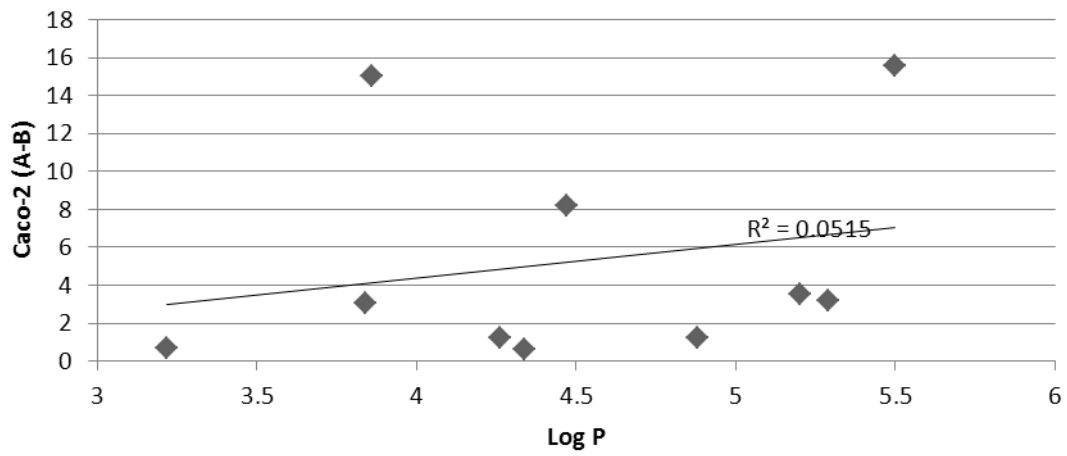
Supporting Information:Supporting information Table 1. *In vitro* ADME of selected analogs

Entry	Log P (calculated)	Polar surface area (PSA)	PAMPA (% Absorbed)	Caco-2 A-B (cm/sec $\times 10^6$)	Caco-2 B-A (cm/se $c \times 10^6$)	Ratio Caco-2 A-B/B- A
15	3.22	76.18	52	0.70	2.55	0.27
22	4.26	76.18	51.8	1.26	2.99	0.42
24	4.34	76.18	51.5	0.61	1.3	0.47
27	3.84	76.18	81	3.05	8.38	0.36
28	4.88	76.18	99.5	1.2	0.97	1.24
29	5.2	76.18	99.5	3.5	2.37	1.48
31	4.47	41.88	99.5	8.2	2.36	3.47
32	3.86	58.95	80.9	15	14.37	1.04
33	4.89	58.95	n.t	n.t	n.t	
34	5.29	58.95	97.1	3.22	3.35	0.96
35	5.5	41.88	99.9	15.56	6.96	2.24
36	5.18	41.88	99.9	n.t	n.t	

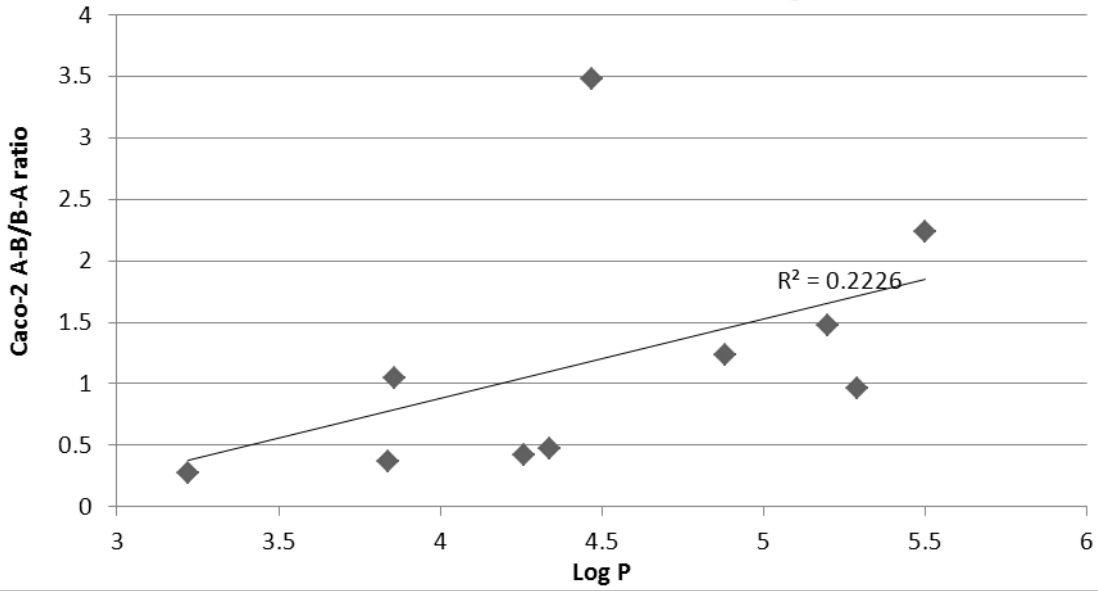
Pampa (%absorbed) vs. Log P



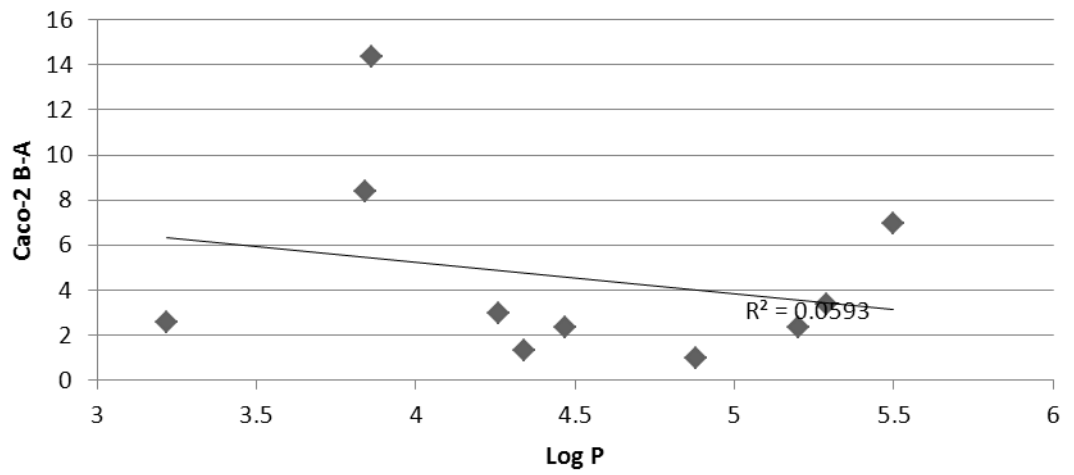
Caco-2 (A-B) vs. log P



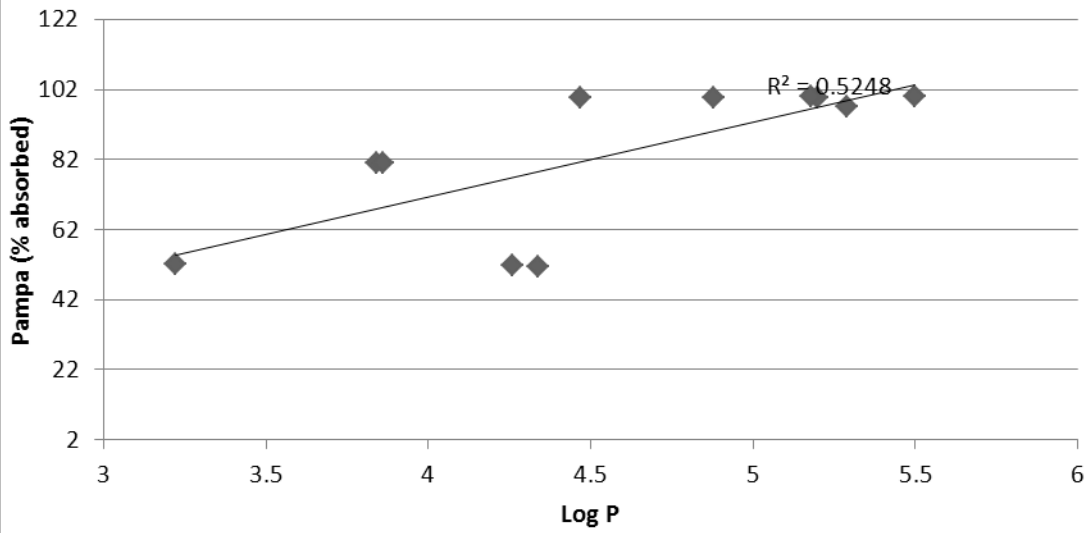
Caco-2 A-B/B-A ratio vs Log P



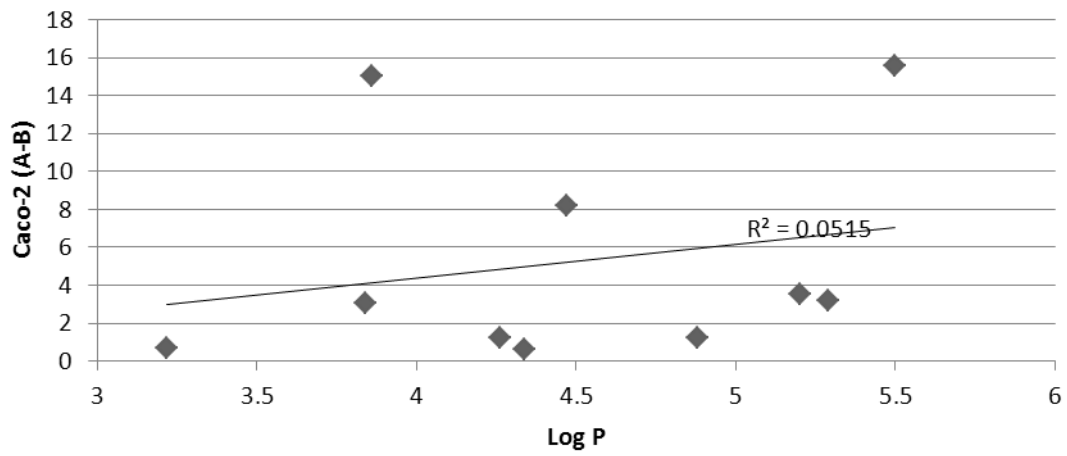
Caco-2 (B-A) vs. Log P



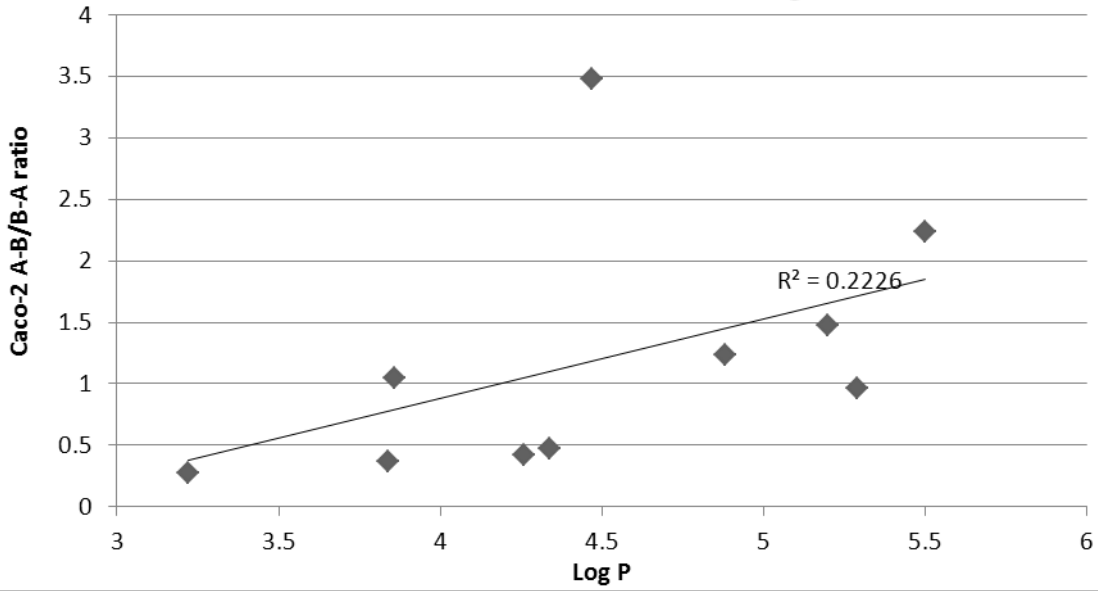
Pampa (%absorbed) vs. Log P



Caco-2 (A-B) vs. log P



Caco-2 A-B/B-A ratio vs Log P



Caco-2 (B-A) vs. Log P

