

Supplementary Information

2D Chemical Drawings Correlate to Bioactivities: MIA-QSAR Modelling of Antimalarial Activities of 2,5-Diaminobenzophenone Derivatives

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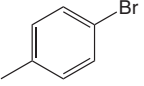
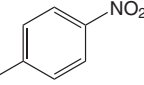
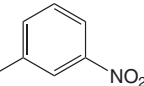
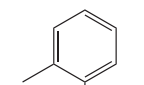
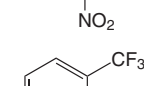
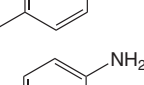
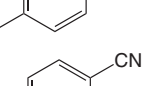
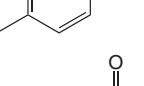
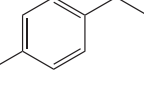
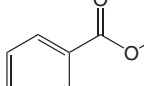
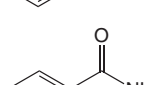
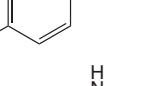
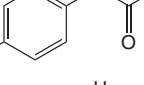
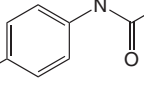
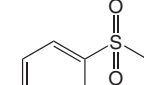
Table S1. Structures of data set, and experimental, predicted and cross-validated (LOO) pIC₅₀ for the series of 2,5-diaminobenzophenone derivatives

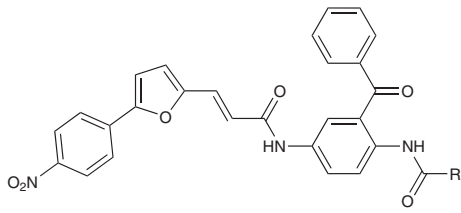
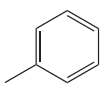
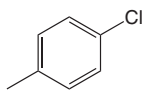
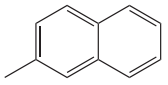
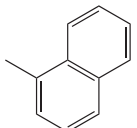
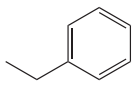
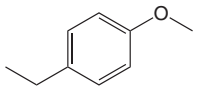
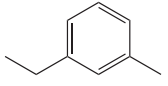
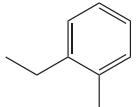
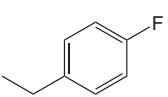
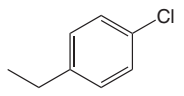
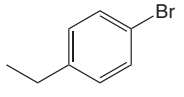
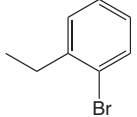
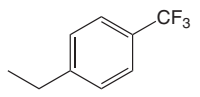
Compound	Structure	pIC _{50(Exp)}	pIC _{50(Pred)}	pIC _{50(LOO CV)}
1		5.57	5.58	5.65
Compound		pIC _{50(Exp)}	pIC _{50(Pred)}	pIC _{50(LOO CV)}
	R			
2 ^[a]	-H	5.24	5.60	-
3	-NO ₂	5.19	5.36	5.69
4	-CHO	4.4	4.67	5.41
5	-COOCH ₃	6.00	5.64	5.22
6	-CF ₃	5.24	5.41	5.68
7	-Cl	5.26	5.52	5.73
8	-Br	5.49	5.16	5.08
9 ^[a]	-NH ₂	5.26	5.14	-
10	-CH=C(CN) ₂	4.37	4.40	5.46
11	-CH ₃	5.85	5.19	4.90
12	-O-CH ₃	5.89	5.96	5.95
13	-CH ₂ -CH ₃	5.92	5.77	5.70
14	-CH(CH ₃) ₂	5.92	5.82	5.69
15	-C(CH ₃) ₃	5.52	5.74	5.91
16	-O-CH ₂ -CH ₃	6.07	5.94	5.77
17	-O-(CH ₂) ₃ -CH ₃	5.96	5.85	5.64
18	-O-(CH ₂) ₂ -CH ₃	6.47	6.53	6.34

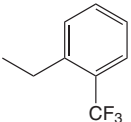
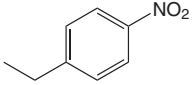
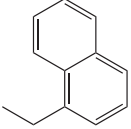
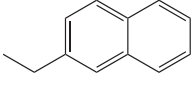
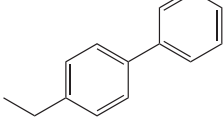
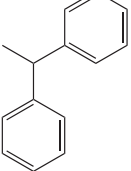
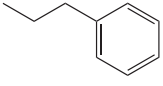
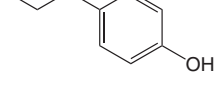
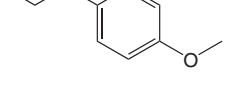
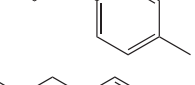
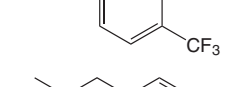
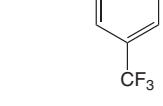
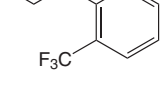
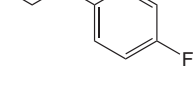
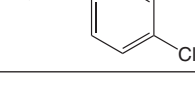
*e-mail: matheus@dqi.ufla.br

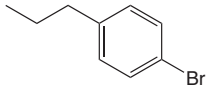
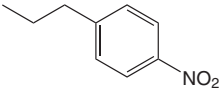
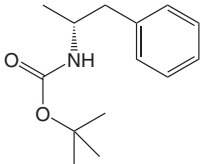
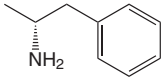
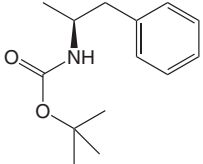
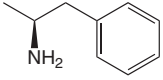
Compound	Structure	$pIC_{50(Exp)}$	$pIC_{50(Pred)}$	$pIC_{50(LOO CV)}$
	R			
19		5.05	4.92	4.90
20 ^[a]		5.47	5.50	-
21		5.6	6.10	6.18
22 ^[a]		5.89	6.56	-
23		5.62	5.86	6.06
24		6.46	6.31	6.00
25		6.51	6.36	6.08
26		6.00	5.72	5.87
27		6.92	6.79	6.29
28		4.62	4.76	5.41
29		4.64	4.57	5.55

Compound	Structure	$pIC_{50(Exp)}$	$pIC_{50(Pred)}$	$pIC_{50(LOO CV)}$
	R			
30 ^[a]		6.38	6.52	-
31		6.00	6.13	6.74
32		6.70	6.65	6.65
33		6.92	6.89	6.85
34		7.06	6.96	6.88
35		7.07	6.98	6.88
36 ^[a]		6.52	6.83	-
37		6.89	6.91	6.89
38		6.52	6.41	6.51
39		6.12	6.19	6.72
40		6.68	6.77	6.83
41 ^[a]		7.08	6.83	-
42		6.49	6.48	6.60
43		6.84	6.78	6.59

44		6.9	6.83	6.72
45		7.12	6.77	6.53
46 ^[a]		6.23	6.55	-
47		6.17	6.29	6.45
48		7.11	6.91	6.61
49		6.59	6.87	7.00
50		6.66	6.79	6.73
51		7.17	6.79	6.56
52		6.77	6.81	6.91
53		6.25	6.60	6.97
54		6.55	6.63	6.54
55 ^[a]		6.25	6.48	-
56		7.43	7.07	6.77
57		7.22	7.17	6.88
58		6.7	6.89	7.10

Structures				
Compound		pIC _{50(Exp)}	pIC _{50(Pred)}	pIC _{50 (LOO CV)}
	R			
59		5.52	5.61	5.75
60 ^[a]		5.6	5.58	-
61		5.6	5.45	5.69
62		6.11	6.19	6.20
63		6.57	6.79	6.71
64 ^[a]		6.49	6.95	-
65		6.82	6.82	6.59
66		6.19	6.10	6.12
67		6.64	7.06	7.05
68 ^[a]		7.19	7.14	-
69		7.15	7.25	7.07
70 ^[a]		6.00	6.61	-
71		7.33	7.15	6.84

72		6.00	6.35	6.61
73		5.85	6.24	7.01
74		6.60	6.55	6.38
75		6.68	6.76	6.58
76		6.00	5.65	5.57
77		5.26	5.17	6.30
78		6.51	6.40	6.38
79		5.48	5.71	6.21
80 ^[a]		5.89	6.33	-
81		6.36	6.27	6.18
82 ^[a]		7.21	6.89	-
83		6.2	6.17	6.16
84		5.96	6.05	6.38
85		6.36	6.32	6.26
86 ^[a]		6.89	6.38	-

87		6.77	6.46	6.31
88 ^[a]		5.85	5.83	-
89		6.05	6.10	6.33
90 ^[a]		5.92	6.29	-
91		6.38	6.14	6.03
92		6.24	6.33	6.53

^[a] Prediction set compounds.