

Table 2: Absorption, distribution, metabolism, excretion and toxicity (ADMET) properties of the benzylidene-acrylohydrazone derivatives predicted by pkCSM [33](<http://biosig.unimelb.edu.au/pkCSM/>), PREDHERG 4.2 [34] (<http://predherg.labmol.com.br/>) and DataWarrior 5.2.1 [35].

Code number	Lipinski's rule	LogP	Hepatotoxicity	BBB Permeability	Brain Permeability	CaCo2 Permeability	Intestinal Absorption	hERG I inib.	hERG II inib.	Cardiotoxicity	Mutagenic	Tumorigenic	Reproductive Effects	Irritant	Druglikeness	Molecular Mass	Rotatable bonds	Hydrogen bond acceptors (HBA)	Hydrogen bond donors (HBD)
11a	yes	5.1	yes	-0.41	-2.18	1.05	92.5	no	yes	Non-cardiotoxic	no	no	no	no	13.8	380.49	9	4	1
11b	yes	4.7	yes	-0.31	-2.18	1.45	91.5	no	yes	Non-cardiotoxic	no	no	no	no	-56.0	406.40	8	4	1
11c	yes	3.7	yes	-0.29	-2.52	1.02	95.2	no	yes	Non-cardiotoxic	no	no	low	high	16.2	368.43	9	5	1
11d	yes	5.5	yes	-0.35	-2.05	1.05	94.1	no	yes	Weak or moderate	no	no	no	no	15.9	414.51	9	4	1
12a	yes	5.2	yes	0.06	-0.72	1.45	91.7	no	yes	Non-cardiotoxic	no	no	no	no	28.0	306.41	5	2	1
12b	yes	4.9	yes	0.16	-0.83	1.45	90.7	no	yes	Non-cardiotoxic	no	no	no	no	-41.1	332.33	4	2	1
12c	yes	3.8	no	-0.10	-2.10	1.35	94.4	no	yes	Non-cardiotoxic	no	no	low	high	30.3	294.35	5	3	1
12d	yes	5.6	no	0.13	-0.58	1.09	93.3	no	yes	Non-cardiotoxic	no	no	no	no	30.8	340.43	5	2	1
13a	yes	6.7	yes	-0.03	-0.95	1.22	89.2	no	yes	Non-cardiotoxic	no	no	no	no	-29.5	388.56	6	2	1
13b	yes	6.3	yes	0.03	-0.44	1.10	87.6	no	yes	Weak or moderate	no	no	no	no	-98.8	414.47	5	2	1
13c	yes	5.3	yes	-0.07	-1.75	1.24	90.0	no	yes	Non-cardiotoxic	no	no	low	high	-26.6	376.50	6	3	1
13d	yes	7.1	yes	-0.01	-0.19	1.06	90.2	no	yes	Non-cardiotoxic	no	no	no	no	-26.9	422.57	6	2	1
16	yes	4.4	no	-0.16	-2.03	1.32	88.6	no	yes	Non-cardiotoxic	no	no	no	no	28.0	308.38	5	3	2
20a	yes	4.4	yes	-0.17	-2.08	1.07	93.6	no	yes	Non-cardiotoxic	no	no	no	no	28.0	362.43	7	4	1
20b	yes	3.5	yes	-0.37	-2.32	1.19	95.4	no	yes	Non-cardiotoxic	no	no	no	no	28.0	363.42	7	5	1
20c	yes	3.9	yes	-0.39	-2.37	1.21	94.8	no	yes	Non-cardiotoxic	no	no	no	no	28.0	363.42	7	5	1
20d	yes	3.4	yes	0.02	-0.07	1.27	91.4	no	yes	Non-cardiotoxic	no	no	no	no	40.5	351.41	7	4	2
20e	yes	3.0	yes	-1.78	-2.64	1.28	87.3	no	yes	Non-cardiotoxic	no	no	no	no	41.7	352.39	7	5	2
21a	yes	4.5	yes	0.30	-0.58	1.31	92.7	no	yes	Non-cardiotoxic	no	no	no	no	43.6	288.35	3	2	1

21b	yes	3.6	yes	0.13	-1.89	1.39	94.5	no	yes	Non-cardiotoxic	no	no	no	no	43.6	289.34	3	3	1
21c	yes	4.0	yes	0.46	-1.94	1.40	93.95	no	yes	Non-cardiotoxic	no	no	no	no	43.6	289.34	3	3	1
21d	yes	3.5	yes	0.26	-1.89	1.32	91.3	no	yes	Non-cardiotoxic	no	no	no	no	55.2	277.33	3	2	2
21e	yes	3.1	yes	-0.62	-2.22	1.29	87.2	no	yes	Non-cardiotoxic	no	no	no	no	56.7	278.32	3	3	2
22a	yes	3.7	yes	-0.06	-1.91	1.29	91.6	no	yes	Non-cardiotoxic	no	no	no	no	44.2	290.32	3	3	2
22b	yes	2.8	no	-0.06	-2.15	1.05	93.4	no	yes	Non-cardiotoxic	no	no	no	no	44.2	291.31	3	4	2
22c	yes	3.2	no	-0.08	-2.21	1.12	92.9	no	yes	Non-cardiotoxic	no	no	no	no	44.2	291.31	3	4	2
22d	yes	2.7	no	-0.55	-2.16	1.20	90.2	no	yes	Non-cardiotoxic	no	no	no	no	55.7	279.30	3	3	3
22e	yes	2.3	yes	-0.79	-2.49	1.10	86.1	no	yes	Non-cardiotoxic	no	no	no	no	57.3	280.29	3	4	3
23a	yes	5.9	yes	0.17	-0.18	1.08	89.6	no	yes	Non-cardiotoxic	no	no	no	no	-15.4	370.50	4	2	1
23b	yes	5.1	yes	-0.01	-1.50	1.11	91.4	no	yes	Non-cardiotoxic	no	no	no	no	-15.4	371.48	4	3	1
23c	yes	5.5	yes	0.32	-1.55	1.13	90.8	no	yes	Weak or moderate	no	no	no	no	-15.4	371.48	4	3	1
23d	yes	4.9	yes	0.13	-1.50	1.21	88.1	no	yes	Weak or moderate	no	no	no	no	-0.2	359.47	4	2	2
23e	yes	4.6	yes	-0.60	-1.82	1.22	84.1	yes	yes	Weak or moderate	no	no	no	no	-0.2	360.46	4	3	2
27	yes	4.7	no	-0.23	-2.29	1.15	92.7	no	yes	Non-cardiotoxic	no	no	no	no	-50.6	410.51	9	5	1
28	yes	4.8	no	0.01	-1.88	1.10	92.6	no	yes	Non-cardiotoxic	no	no	no	no	-36.5	336.44	5	3	1
29	yes	4.0	no	0.07	-2.14	1.05	91.5	no	yes	Non-cardiotoxic	no	no	no	no	-36.5	338.41	5	4	2
35	yes	5.1	yes	0.07	-2.04	0.65	89.1	no	yes	Weak or moderate	no	no	no	no	-0.9	409.53	8	4	2
36	yes	5.2	yes	-0.01	-1.62	1.22	89.0	no	yes	Non-cardiotoxic	no	no	no	no	0.5	355.45	4	2	2
37	yes	4.4	yes	-0.57	-1.88	0.85	87.9	no	yes	Non-cardiotoxic	no	no	no	no	0.5	337.42	4	3	3
38	yes	6.6	yes	-0.15	-1.23	1.19	85.8	no	yes	Weak or moderate	no	no	no	no	-5.2	417.60	5	2	2
41	yes	4.3	no	0.07	-2.38	1.12	90.8	no	yes	Strong or extreme	high	no	high	no	12.5	371.51	9	4	2
42	yes	4.4	yes	0.28	-0.84	1.54	90.7	no	yes	Strong or extreme	high	no	high	no	27.6	297.43	5	2	2
43	yes	3.6	no	0.03	-2.22	1.30	89.6	no	yes	Strong or extreme	high	no	high	no	27.7	299.40	5	3	3
44	yes	5.9	yes	0.13	-0.39	1.02	87.6	no	yes	Strong or extreme	high	no	high	no	-25.8	379.57	6	2	2
51	yes	4.2	yes	-0.02	-1.97	1.22	89.6	no	yes	Non-cardiotoxic	no	no	no	no	-19.4	368.48	6	3	2
52	yes	5.0	yes	0.21	-0.96	1.59	89.2	no	yes	Non-cardiotoxic	no	no	no	no	-2.1	322.45	4	1	2

53	yes	4.5	yes	0.17	-0.97	1.59	89.4	no	yes	Non-cardiotoxic	no	no	no	no	-2.1	308.43	4	1	2
54	yes	2.6	no	-0.14	-2.29	1.35	91.8	no	yes	Non-cardiotoxic	no	no	no	no	11.4	312.37	6	3	2
55	yes	3.4	yes	0.31	-1.22	1.60	89.8	no	yes	Non-cardiotoxic	no	no	no	no	10.2	266.34	4	1	2
58	yes	5.3	yes	0.20	-0.87	1.46	88.1	no	yes	Non-cardiotoxic	no	no	no	no	-29.5	308.43	3	1	2
59	yes	4.5	yes	-0.07	-1.65	1.38	87.5	no	yes	Non-cardiotoxic	no	no	no	no	-29.0	310.40	3		2
60	yes	3.7	no	0.35	-0.99	1.33	88.8	no	no	Non-cardiotoxic	no	no	no	no	0.1	252.32	3	1	2
61	yes	2.9	no	-0.01	-1.96	1.30	87.9	no	yes	Non-cardiotoxic	no	no	no	no	0.2	254.29	3	2	3
69	yes	4.5	no	0.05	-2.20	0.74	90.8	no	yes	Weak or moderate	no	no	no	no	-4.0	410.51	7	4	2
70	yes	4.7	yes	0.19	-1.78	1.51	91.2	no	yes	Weak or moderate	no	no	no	no	-26.1	336.44	3	2	2
71	yes	5.5	yes	0.10	-1.87	1.00	93.1	no	yes	Weak or moderate	no	no	no	no	-42.3	392.50	7	5	0
72	yes	5.6	yes	0.47	-1.00	1.72	93.8	no	yes	Non-cardiotoxic	no	no	no	no	-28.5	318.42	3	3	0
77	yes	5.3	yes	-0.04	-2.02	1.04	95.8	no	yes	Strong or extreme	no	no	no	no	-54.8	394.52	8	5	0
78	yes	5.4	yes	0.38	-1.07	1.68	95.1	no	yes	Strong or extreme	no	no	no	no	-41.0	320.44	4	3	0
79	yes	3.8	yes	-0.18	-2.30	1.09	96.2	no	yes	Strong or extreme	no	no	no	no	-2.4	338.41	8	5	0
80	yes	3.9	no	0.54	-1.31	1.81	95.7	no	yes	Strong or extreme	no	no	no	no	-1.0	264.33	4	3	0
82	yes	4.6	yes	0.00	-1.85	1.39	93.3	no	yes	Weak or moderate	no	no	no	no	-40.4	322.41	4	4	1
88	yes	4.9	yes	0.10	-1.95	1.02	94.4	no	yes	Weak or moderate	no	no	no	no	-44.3	380.49	7	5	0
89	yes	5.0	yes	0.47	-1.06	1.75	95.2	no	yes	Non-cardiotoxic	no	no	no	no	-30.5	306.41	3	3	0
93	yes	4.6	no	0.26	-1.31	1.90	97.6	no	no	Strong or extreme	no	no	no	no	-2.1	263.34	4	3	0
98	yes	5.6	no	0.05	-1.61	0.27	79.5	no	yes	Non-cardiotoxic	low	no	high	no	-26.6	333.44	3	2	2
99	yes	5.1	no	0.01	-1.68	-2.97	13.4	no	yes	Non-cardiotoxic	no	no	high	no	-26.6	319.41	45,123	3	2
100	yes	5.5	no	0.03	-1.73	0.25	79.7	no	yes	Weak or moderate	low	no	high	no	-24.0	335.45	4	2	2
101	yes	5.0	no	-0.02	-1.79	1.33	80.8	no	yes	Weak or moderate	no	no	high	no	-24.0	321.42	4	2	2