Supplementary Table 1. *In Vitro* Characteristics of Selected Chemicals with Docking Score Order 1–50

Lab No.*	Docking score	ChemBridge ID	MW	Relative inhibition†	Dil-LDL uptake‡	Amount of the LDLR§	Amount of PCSK9§
CBC_1	28.40	5323858	348.5	36.8%	1.55	1.72	0.97
CBC_2	27.26	5422509	419.5	49.7%	1.97	1.58	0.97
CBC_3	27.12	5423970	389.5	43.9%	1.85	1.42	0.53
CBC_4	28.18	5428460	400.5	31.7%	1.35	0.93	0.60
CBC_5	27.15	5573554	276.3	10.7%	1.08	1.03	0.29
CBC_6	27.20	5646807	393.5	17.2%	0.85	0.91	0.68
CBC_7	27.00	5679233	405.5	12.6%	1.11	0.77	0.75
CBC_8	28.45	5781565	415	37.3%	1.49	1.40	1.07
CBC_9	28.82	5834186	445.5	12.9%	0.90	0.84	0.57
CBC_10	27.78	5851930	404.5	9.9%	0.85	0.93	0.76
CBC_11	27.27	5862390	397.3	4.5%	0.94	0.81	0.49
CBC_12	28.36	5865258	430.2	-2.0%	1.08	0.74	0.68
CBC_13	28.17	6577494	455.6	41.4%	1.66	1.77	1.54
CBC_14	27.13	6578587	442.6	46.6%	2.26	1.20	1.90
CBC_15	27.10	6579857	379.5	22.9%	1.41	1.44	1.07
CBC_16	27.37	7000500	388.5	14.1%	1.01	0.26	0.01
CBC_17	28.26	7011653	327.5	45.0%	1.56	0.92	1.11
CBC_18	27.90	7017850	299.4	49.9%	1.56	0.69	0.98
CBC_19	27.50	7021996	341.5	38.3%	1.59	1.37	1.20
CBC_20	29.19	7300311	380.5	-1.6%	1.05	0.87	0.86
CBC_21	28.47	7319736	355.9	47.5%	1.36	1.09	0.72
CBC_22	27.42	7497360	449.6	11.6%	0.97	1.19	1.23
CBC_23	27.95	7596514	463.6	11.7%	0.87	1.15	0.99
CBC_24	27.52	7597336	422.6	12.9%	0.80	0.80	0.75
CBC_25	27.75	7682179	484	12.1%	1.06	1.18	0.66
CBC_26	27.48	7732594	385.4	53.4%	0.94	0.56	0.59
CBC_27	27.31	7736937	376.4	14.4%	0.95	0.88	0.86
CBC_28	28.26	7796312	416.5	-4.5%	0.90	0.79	0.98
CBC_29	27.12	7877851	416.5	3.3%	0.76	1.32	0.74
CBC_30	27.83	7883245	408.3	20.2%	0.95	1.10	1.34
CBC_31	27.05	7891362	354.4	13.0%	0.87	0.87	0.91
CBC_32	27.04	7922733	385.8	19.0%	0.81	0.64	0.20
CBC_33	28.85	7925242	341.5	52.7%	1.85	1.86	1.80
CBC_34	27.05	7925467	382.4	-2.5%	0.73	0.87	0.52
CBC_35	27.18	7926470	386.9	-12.0%	0.99	0.87	0.10
CBC_36	29.63	7926604	371.5	49.3%	1.69	1.57	1.22
CBC_37	27.06	7941561	416.6	11.3%	0.99	0.29	0.29
CBC_38	28.99	7949973	437.5	-3.2%	0.95	1.37	0.40
CBC_39	27.87	7962923	432.9	10.0%	1.05	0.81	1.01
CBC_40	29.17	7966968	383.5	39.9%	1.57	1.08	1.00
CBC_41	27.18	7968349	372.5	12.6%	1.09	0.76	0.55
CBC_42	28.00	7969162	453.5	33.6%	1.07	0.93	0.81
CBC_43	27.40	7983219	430.9	31.4%	1.49	1.04	0.80
CBC_44	27.58	7984456	405.9	18.2%	1.46	1.43	1.15
CBC_45	28.76	7990813	440.5	-6.5%	1.08	0.83	0.98
CBC_46	27.70	7998682	384.4	30.9%	1.15	0.92	0.76
CBC_47	27.38	9024196	384.5	22.9%	1.31	0.99	0.68
CBC_48	27.11	9025824	346.5	25.0%	1.09	1.08	0.67
CBC_49	27.63	9070071	371.5	30.5%	1.39	1.43	1.64
CBC_50	27.47	9148410	415.5	38.7%	1.39	1.17	1.15

MW, molecular weight; LDL, low density lipoprotein; LDLR, LDL receptor; PCSK9, proprotein convertase subtilisin/kexin type 9.
*Lab No. is arbitrarily denoted according to the order of the ChemBridge ID number, †Relative inhibition represents the difference in percentile between the intensity of PCSK9-LDLR in the presence of the chemical and that in the presence of the vehicle (DMSO), which was set as 100%, ‡Dil-LDL uptake denotes the factor of the mean fluorescence intensity in HepG2 cells treated with each chemical compared to that in cells treated with the vehicle, §The amount of LDLR or PCSK9 denotes the factor of the signal for LDLR or PCSK9, respectively, from immunoblot data analyzed by ImageJ.