Supplementary Table 2. *In Vitro* Characteristics of Selected Chemicals with Docking Score Order 51–100

Lab No.*	Docking score	ChemBridge ID	MW	Relative inhibition†	Dil-LDL uptake‡	LDLR§	PCSK9§
CBC_51	26.99	7127155	468.5	-2.6%	0.95	0.74	0.85
CBC_52	26.99	7010655	295.4	15.4%	1.80	1.41	0.60
CBC_53	26.98	6707210	409.6	28.4%	1.74	1.16	0.75
CBC_54	26.98	7980928	391.9	2.6%	1.74	1.09	0.87
CBC_55	26.97	7059604	448.4	-5.3%	1.03	0.51	0.67
CBC_56	26.95	9006787	370.4	26.1%	1.02	1.40	0.50
CBC_57	26.94	6991769	318.5	12.5%	2.18	1.10	0.46
CBC_58	26.89	7116267	469.6	-27.9%	1.49	1.43	0.23
CBC_59	26.86	6587027	339.8	-5.8%	1.18	0.53	0.00
CBC_60	26.85	5537034	332.4	4.6%	0.94	0.61	0.16
CBC_61	26.84	6578162	459.6	14.9%	1.03	1.26	0.74
CBC_62	26.81	9011745	356.4	4.7%	1.02	0.70	0.15
CBC_63	26.81	7913488	402.5	-11.1%	0.90	0.45	0.57
CBC_64	26.79	6447900	400.5	-0.6%	2.04	1.27	0.72
CBC_65	26.79	7261073	353.5	-1.8%	1.17	0.98	0.26
CBC_66	26.78	7943026	493.4	10.2%	1.93	0.83	0.60
CBC_67	26.75	5252938	378.4	-10.6%	1.08	0.44	0.79
CBC_68	26.74	5426872	389.5	10.0%	0.52	0.65	0.41
CBC_69	26.74	7970741	345.5	5.8%	1.22	1.18	0.88
CBC_70	26.73	9025813	348.4	9.8%	2.06	1.23	0.59
CBC_71	26.69	7547620	361.4	-8.5%	1.01	0.68	0.41
CBC_72	26.69	5723280	330.4	25.8%	1.21	1.06	1.28
CBC_73	26.68	5425499	345.5	18.9%	1.93	1.76	1.26
CBC_74	26.67	7968546	341.5	19.6%	1.94	1.48	1.49
CBC_75	26.67	5665101	459.5	-1.5%	1.23	0.52	0.75
CBC_76	26.66	7873145	381.5	7.0%	1.10	0.70	0.33
CBC_77	26.66	9036091	337.4	16.0%	1.18	0.82	1.06
CBC_78	26.64	7543524	368.4	-2.7%	1.44	0.77	0.23
CBC_79	26.62	5427177	398.5	52.3%	1.76	0.98	0.62
CBC_80	26.62	7924529	299.4	6.9%	1.49	1.36	1.18
CBC_81	26.62	7232922	431.5	-10.0%	1.35	1.20	0.15
CBC_82	26.61	6759201	397.6	12.1%	1.32	1.65	1.45
CBC_83	26.61	9014232	327.8	22.5%	2.08	0.97	0.61
CBC_84	26.59	7997500	377.5	11.9%	1.34	1.62	1.80
CBC_85	26.59	7924880	329.5	18.6%	1.44	1.31	1.22
CBC_86	26.58	9038237	348.4	8.4%	1.54	1.22	0.89
CBC_87	26.55	7966644	385.5	11.2%	1.80	1.60	1.37
CBC_88	26.48	7595292	373.9	3.3%	1.09	0.65	0.08
CBC_89	26.48	7968661	475.5	3.2%	1.26	1.21	0.39
CBC_90	26.47	7839314	389.4	6.2%	0.76	1.47	0.95
CBC_91	26.44	7889540	366.4	2.5%	1.12	2.08	0.76
CBC_92	26.43	9030034	422.4	1.1%	1.46	1.44	0.59
CBC_93	26.41	6484579	375.5	2.3%	1.18	1.26	0.78
CBC_94	26.39	7280568	366.5	-5.6%	1.11	1.03	0.91
CBC_95	26.35	7934110	416.5	-12.5%	0.91	1.19	0.64
CBC_96	26.34	6659178	403.4	-11.3%	1.01	0.59	0.86
CBC_97	26.33	9019728	371.5	-0.2%	1.44	0.97	1.01
CBC_98	26.32	7633305	397.4	6.0%	1.05	0.97	0.05
CBC_99	26.31	7791626	434.6	11.5%	0.91	0.74	0.84
CBC_100	26.24	7933432	444.5	-3.0%	0.85	0.62	0.68

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.