Electronic Supplementary Material (ESI):

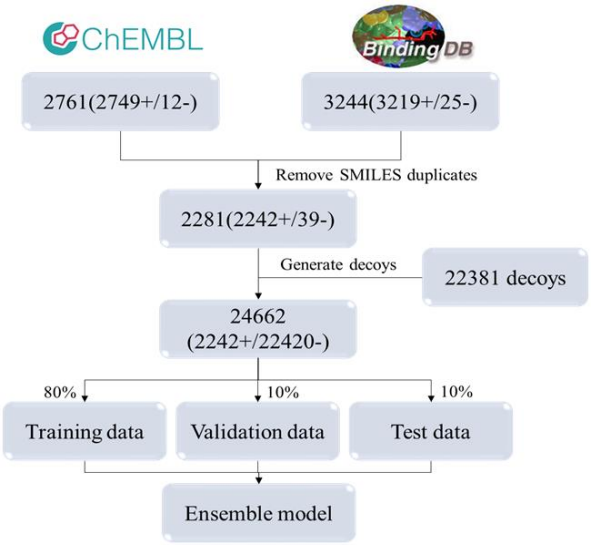

Fig. S1 Data preparation procedure for Model Bind.

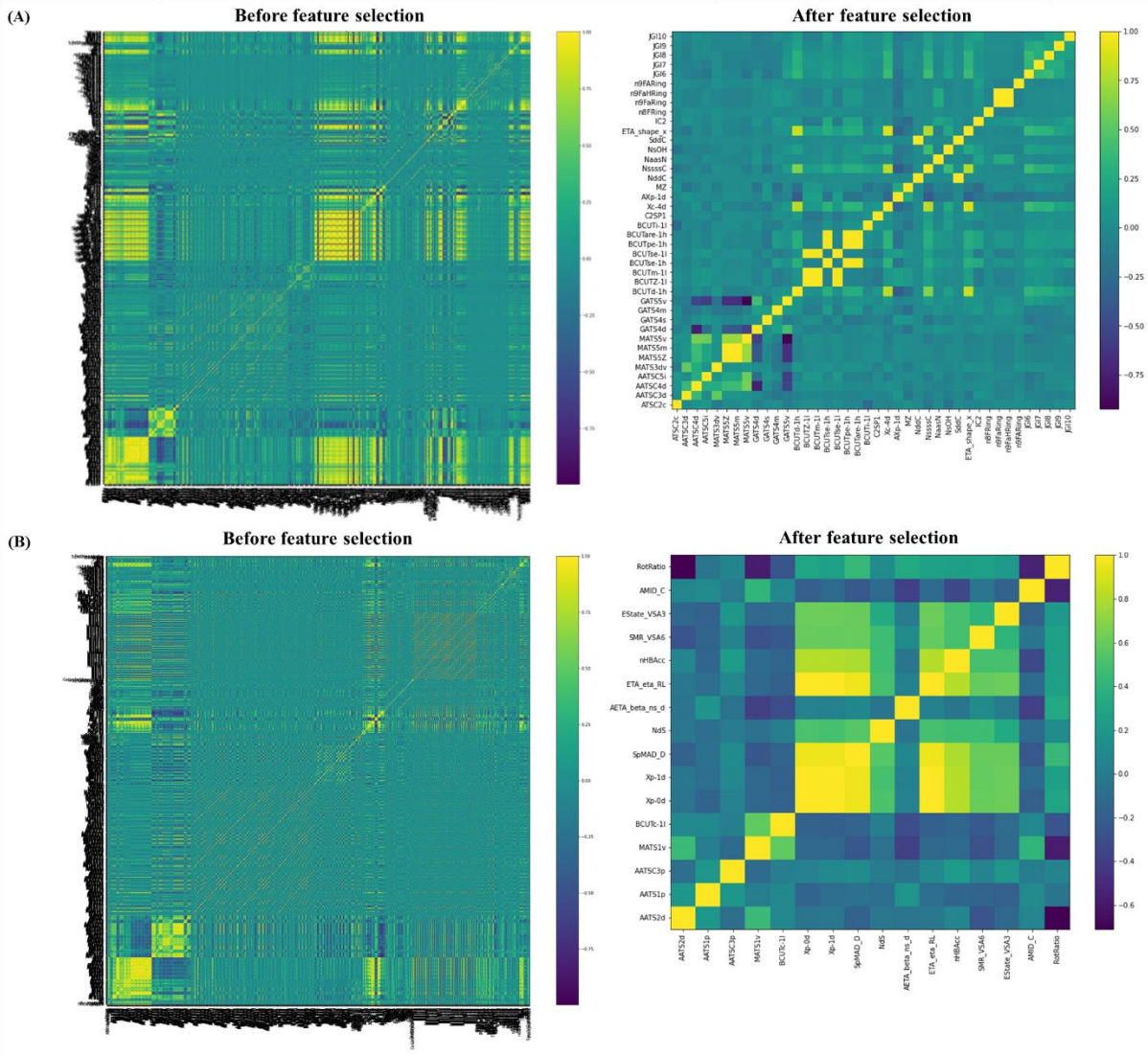

Fig. S2 Intercorrelation matrix between the molecular descriptors before and after feature selection for (A) Model Bind and (B) Model Ant.

Table S1 Molecular descriptors identified via feature selection for each model.

Model	Molecular Descriptor	Description
Model Bind: GR binding prediction model	ATSC2c	averaged and centered moreau-broto autocorrelation of lag 2 weighted by gasteiger charge
	AATSC3d	averaged and centered moreau-broto autocorrelation of lag 3 weighted by sigma electrons
	AATSC4d	averaged and centered moreau-broto autocorrelation of lag 4 weighted by sigma electrons
	AATSC5i	averaged and centered moreau-broto autocorrelation of lag 5 weighted by ionization potential
	MATS3dv	moran coefficient of lag 3 weighted by valence electrons
	MATS5Z	moran coefficient of lag 5 weighted by atomic number
	MATS5m	moran coefficient of lag 5 weighted by mass
	MATS5v	moran coefficient of lag 5 weighted by vdw volume
	GATS4d	geary coefficient of lag 4 weighted by sigma electrons
	GATS4s	geary coefficient of lag 4 weighted by intrinsic state
	GATS4m	geary coefficient of lag 4 weighted by mass
	GATS5v	geary coefficient of lag 5 weighted by vdw volume
	BCUTd-1h	first highest eigenvalue of Burden matrix weighted by sigma electrons
	BCUTZ-1l	first lowest eigenvalue of Burden matrix weighted by atomic number
	BCUTm-1l	first lowest eigenvalue of Burden matrix weighted by mass
	BCUTse-1h	first highest eigenvalue of Burden matrix weighted by sanderson EN
	BCUTse-1l	first lowest eigenvalue of Burden matrix weighted by sanderson EN
	BCUTpe-1h	first highest eigenvalue of Burden matrix weighted by pauling EN
	BCUTare-1h	first heighest eigenvalue of Burden matrix weighted by allred-rocow EN
	BCUTi-1l	first lowest eigenvalue of Burden matrix weighted by ionization potential
	C2SP1	SP carbon bound to 2 other carbons
	Xc-4d	4-ordered Chi cluster weighted by sigma electrons
	AXp-1d	1-ordered averaged Chi path weighted by sigma electrons
	MZ	mean of constitutional weighted by atomic number
	NddC	number of ddC
	NssssC	number of ssssC
	NaasN	number of aasN
	NsOH	number of sOH
	SddC	sum of ddC
	ETA_shape_x	ETA shape index (type: x)
	IC2	2-ordered neighborhood information content
	n8FRing	8-membered fused ring count
	n9FaRing	9-membered aromatic fused ring count
	n9FaHRing	9-membered aromatic fused hetero ring count
	n9FARing	9-membered aromatic fused ring count
	JGI6	6-ordered mean topological charge

	JGI7	7-ordered mean topological charge
	JGI8	8-ordered mean topological charge
	JGI9	9-ordered mean topological charge
	JGI10	10-ordered mean topological charge
Model Ant: GR antagonist prediction model	AATS2d	averaged moreau-broto autocorrelation of lag 2 weighted by sigma electrons
	AATS1p	averaged moreau-broto autocorrelation of lag 1 weighted by polarizability
	AATSC3p	averaged and centered moreau-broto autocorrelation of lag 3 weighted by polarizability
	MATS1v	moran coefficient of lag 1 weighted by vdw volume
	BCUTc-1l	first lowest eigenvalue of Burden matrix weighted by gasteiger charge
	Xp-0d	0-ordered Chi path weighted by sigma electrons
	Xp-1d	1-ordered Chi path weighted by sigma electrons
	SpMAD_D	spectral mean absolute diviation from distance matrix
	NdS	number of dS
	AETA_beta_ns_d	averaged delta contribution to valence electron mobile count
	ETA_eta_RL	local ETA composite index for reference graph
	nHBAcc	number of hydrogen bond acceptor
	SMR_VSA6	MOE MR VSA Descriptor 6 (2.75 <= x < 3.05)
	EState_VSA3	EState VSA Descriptor 3 (0.29 <= x < 0.72)
	AMID_C	averaged molecular ID on C atoms
	RotRatio	rotatable bonds ratio

Table S2 Performance metrics of the four classification models to construct Model Ant.

	RF	XGB	SVM	DL
MCC	0.646 (0.050)	0.646 (0.045)	0.650 (0.046)	0.653 (0.061)
Accuracy	0.809 (0.026)	0.797 (0.032)	0.814 (0.026)	0.803 (0.042)
Precision	0.928 (0.034)	0.976 (0.014)	0.918 (0.027)	0.963 (0.022)
Recall	0.697 (0.038)	0.0634 (0.073)	0.722 (0.039)	0.664 (0.077)
AUC	0.818 (0.026)	0.808 (0.032)	0.823 (0.022)	0.817 (0.035)

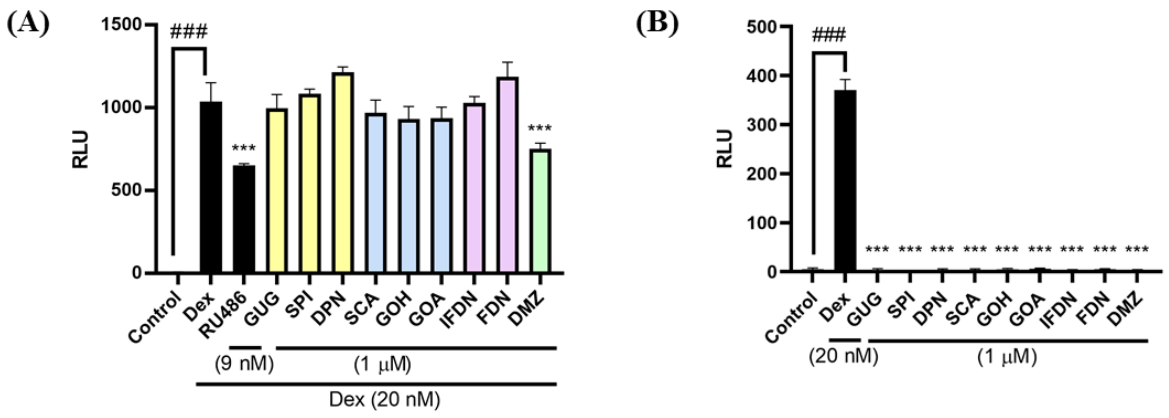

Fig. S3 (A) Inhibition of Dex (20 nM)-induced luciferase activity by the predicted phytochemicals (1 μM) and RLU measurements. (B) RLU induced by the predicted phytochemicals at a concentration of 1 μM without treatment with Dex. The data are represented as mean ± standard deviation (n=3). ###, significantly different from control by ($p < 0.001$). Significantly different from Dex by *** ($p < 0.001$).

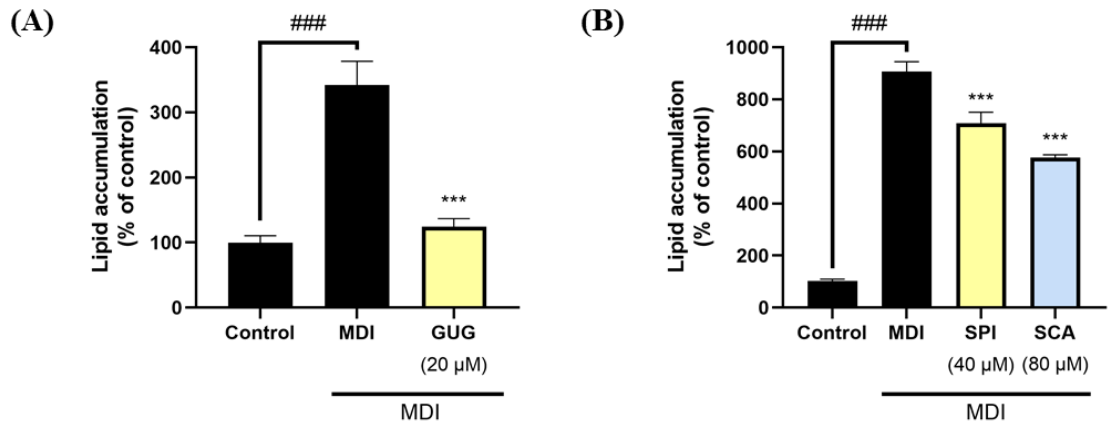

Fig. S4. Effects of the phytochemicals on intracellular lipid accumulations in 3T3-L1 mature adipocytes. The 3T3-L1 preadipocytes were treated with phytochemicals for 6 days of differentiation. The data are represented as mean ± standard deviation (n=3). ###, significantly different from control by ($p < 0.001$). Significantly different from MDI-treated group by *** ($p < 0.001$).