



Gene	Accession	Length (bp)	GC (%)	GC3 (%)	GC4 (%)	GC5 (%)	GC6 (%)	GC7 (%)	GC8 (%)	GC9 (%)	GC10 (%)	GC11 (%)	GC12 (%)	GC13 (%)	GC14 (%)	GC15 (%)	GC16 (%)	GC17 (%)	GC18 (%)	GC19 (%)	GC20 (%)	GC21 (%)	GC22 (%)	GC23 (%)	GC24 (%)	GC25 (%)	GC26 (%)	GC27 (%)	GC28 (%)	GC29 (%)	GC30 (%)	GC31 (%)	GC32 (%)	GC33 (%)	GC34 (%)	GC35 (%)	GC36 (%)	GC37 (%)	GC38 (%)	GC39 (%)	GC40 (%)	GC41 (%)	GC42 (%)	GC43 (%)	GC44 (%)	GC45 (%)	GC46 (%)	GC47 (%)	GC48 (%)	GC49 (%)	GC50 (%)	GC51 (%)	GC52 (%)	GC53 (%)	GC54 (%)	GC55 (%)	GC56 (%)	GC57 (%)	GC58 (%)	GC59 (%)	GC60 (%)	GC61 (%)	GC62 (%)	GC63 (%)	GC64 (%)	GC65 (%)	GC66 (%)	GC67 (%)	GC68 (%)	GC69 (%)	GC70 (%)	GC71 (%)	GC72 (%)	GC73 (%)	GC74 (%)	GC75 (%)	GC76 (%)	GC77 (%)	GC78 (%)	GC79 (%)	GC80 (%)	GC81 (%)	GC82 (%)	GC83 (%)	GC84 (%)	GC85 (%)	GC86 (%)	GC87 (%)	GC88 (%)	GC89 (%)	GC90 (%)	GC91 (%)	GC92 (%)	GC93 (%)	GC94 (%)	GC95 (%)	GC96 (%)	GC97 (%)	GC98 (%)	GC99 (%)	GC100 (%)
Gene1	Accession1	Length1	GC1	GC31	GC41	GC51	GC61	GC71	GC81	GC91	GC101	GC111	GC121	GC131	GC141	GC151	GC161	GC171	GC181	GC191	GC201	GC211	GC221	GC231	GC241	GC251	GC261	GC271	GC281	GC291	GC301	GC311	GC321	GC331	GC341	GC351	GC361	GC371	GC381	GC391	GC401	GC411	GC421	GC431	GC441	GC451	GC461	GC471	GC481	GC491	GC501	GC511	GC521	GC531	GC541	GC551	GC561	GC571	GC581	GC591	GC601	GC611	GC621	GC631	GC641	GC651	GC661	GC671	GC681	GC691	GC701	GC711	GC721	GC731	GC741	GC751	GC761	GC771	GC781	GC791	GC801	GC811	GC821	GC831	GC841	GC851	GC861	GC871	GC881	GC891	GC901	GC911	GC921	GC931	GC941	GC951	GC961	GC971	GC981	GC991	GC1001

Gene	Accession	Length (bp)	GC (%)	GC3 (%)	GC4 (%)	GC5 (%)	GC6 (%)	GC7 (%)	GC8 (%)	GC9 (%)	GC10 (%)	GC11 (%)	GC12 (%)	GC13 (%)	GC14 (%)	GC15 (%)	GC16 (%)	GC17 (%)	GC18 (%)	GC19 (%)	GC20 (%)	GC21 (%)	GC22 (%)	GC23 (%)	GC24 (%)	GC25 (%)	GC26 (%)	GC27 (%)	GC28 (%)	GC29 (%)	GC30 (%)	GC31 (%)	GC32 (%)	GC33 (%)	GC34 (%)	GC35 (%)	GC36 (%)	GC37 (%)	GC38 (%)	GC39 (%)	GC40 (%)	GC41 (%)	GC42 (%)	GC43 (%)	GC44 (%)	GC45 (%)	GC46 (%)	GC47 (%)	GC48 (%)	GC49 (%)	GC50 (%)	GC51 (%)	GC52 (%)	GC53 (%)	GC54 (%)	GC55 (%)	GC56 (%)	GC57 (%)	GC58 (%)	GC59 (%)	GC60 (%)	GC61 (%)	GC62 (%)	GC63 (%)	GC64 (%)	GC65 (%)	GC66 (%)	GC67 (%)	GC68 (%)	GC69 (%)	GC70 (%)	GC71 (%)	GC72 (%)	GC73 (%)	GC74 (%)	GC75 (%)	GC76 (%)	GC77 (%)	GC78 (%)	GC79 (%)	GC80 (%)	GC81 (%)	GC82 (%)	GC83 (%)	GC84 (%)	GC85 (%)	GC86 (%)	GC87 (%)	GC88 (%)	GC89 (%)	GC90 (%)	GC91 (%)	GC92 (%)	GC93 (%)	GC94 (%)	GC95 (%)	GC96 (%)	GC97 (%)	GC98 (%)	GC99 (%)	GC100 (%)
Gene2	Accession2	Length2	GC2	GC32	GC42	GC52	GC62	GC72	GC82	GC92	GC102	GC112	GC122	GC132	GC142	GC152	GC162	GC172	GC182	GC192	GC202	GC212	GC222	GC232	GC242	GC252	GC262	GC272	GC282	GC292	GC302	GC312	GC322	GC332	GC342	GC352	GC362	GC372	GC382	GC392	GC402	GC412	GC422	GC432	GC442	GC452	GC462	GC472	GC482	GC492	GC502	GC512	GC522	GC532	GC542	GC552	GC562	GC572	GC582	GC592	GC602	GC612	GC622	GC632	GC642	GC652	GC662	GC672	GC682	GC692	GC702	GC712	GC722	GC732	GC742	GC752	GC762	GC772	GC782	GC792	GC802	GC812	GC822	GC832	GC842	GC852	GC862	GC872	GC882	GC892	GC902	GC912	GC922	GC932	GC942	GC952	GC962	GC972	GC982	GC992	GC1002

Gene	Accession	Length (bp)	GC (%)	GC3 (%)	GC4 (%)	GC5 (%)	GC6 (%)	GC7 (%)	GC8 (%)	GC9 (%)	GC10 (%)	GC11 (%)	GC12 (%)	GC13 (%)	GC14 (%)	GC15 (%)	GC16 (%)	GC17 (%)	GC18 (%)	GC19 (%)	GC20 (%)	GC21 (%)	GC22 (%)	GC23 (%)	GC24 (%)	GC25 (%)	GC26 (%)	GC27 (%)	GC28 (%)	GC29 (%)	GC30 (%)	GC31 (%)	GC32 (%)	GC33 (%)	GC34 (%)	GC35 (%)	GC36 (%)	GC37 (%)	GC38 (%)	GC39 (%)	GC40 (%)	GC41 (%)	GC42 (%)	GC43 (%)	GC44 (%)	GC45 (%)	GC46 (%)	GC47 (%)	GC48 (%)	GC49 (%)	GC50 (%)	GC51 (%)	GC52 (%)	GC53 (%)	GC54 (%)	GC55 (%)	GC56 (%)	GC57 (%)	GC58 (%)	GC59 (%)	GC60 (%)	GC61 (%)	GC62 (%)	GC63 (%)	GC64 (%)	GC65 (%)	GC66 (%)	GC67 (%)	GC68 (%)	GC69 (%)	GC70 (%)	GC71 (%)	GC72 (%)	GC73 (%)	GC74 (%)	GC75 (%)	GC76 (%)	GC77 (%)	GC78 (%)	GC79 (%)	GC80 (%)	GC81 (%)	GC82 (%)	GC83 (%)	GC84 (%)	GC85 (%)	GC86 (%)	GC87 (%)	GC88 (%)	GC89 (%)	GC90 (%)	GC91 (%)	GC92 (%)	GC93 (%)	GC94 (%)	GC95 (%)	GC96 (%)	GC97 (%)	GC98 (%)	GC99 (%)	GC100 (%)
Gene3	Accession3	Length3	GC3	GC33	GC43	GC53	GC63	GC73	GC83	GC93	GC103	GC113	GC123	GC133	GC143	GC153	GC163	GC173	GC183	GC193	GC203	GC213	GC223	GC233	GC243	GC253	GC263	GC273	GC283	GC293	GC303	GC313	GC323	GC333	GC343	GC353	GC363	GC373	GC383	GC393	GC403	GC413	GC423	GC433	GC443	GC453	GC463	GC473	GC483	GC493	GC503	GC513	GC523	GC533	GC543	GC553	GC563	GC573	GC583	GC593	GC603	GC613	GC623	GC633	GC643	GC653	GC663	GC673	GC683	GC693	GC703	GC713	GC723	GC733	GC743	GC753	GC763	GC773	GC783	GC793	GC803	GC813	GC823	GC833	GC843	GC853	GC863	GC873	GC883	GC893	GC903	GC913	GC923	GC933	GC943	GC953	GC963	GC973	GC983	GC993	GC1003



The image displays a vertical column of 11 small, illegible table thumbnails. Each thumbnail appears to be a table with multiple columns and rows, but the text is too small to read. The thumbnails are arranged in a single vertical line, separated by small gaps.

A grid of approximately 10 rows and 10 columns. The central column is shaded grey. The text within the cells is extremely small and illegible.A grid of approximately 10 rows and 10 columns. The central column is shaded grey. The text within the cells is extremely small and illegible.A grid of approximately 10 rows and 10 columns. The central column is shaded grey. The text within the cells is extremely small and illegible.







Supplementary Table S7 ADMET data of the 18 selected compounds in VGP													
	MOE ID	MOE00018	MOE00042	MOE00098	MOE00154	MOE00178	MOE00238	MOE00412	MOE00443	MOE00499	MOE00518	Unit	
Physicochemical Properties	Compound name	Isotretinoin	Isotretinoin	Isotretinoin	Isotretinoin	Isotretinoin	Isotretinoin	Isotretinoin	Isotretinoin	Isotretinoin	Isotretinoin		
	Pubchem ID	111214	7338	35631	111134	71734	111147	37663	111720	25674	7137		
	SMILES	CC1=C(C)C(=O)C(C)C(C)C1=O	CC1=C(C)C(=O)C(C)C(C)C1=O	CC1=C(C)C(=O)C(C)C(C)C1=O	CC1=C(C)C(=O)C(C)C(C)C1=O	CC1=C(C)C(=O)C(C)C(C)C1=O	CC1=C(C)C(=O)C(C)C(C)C1=O	CC1=C(C)C(=O)C(C)C(C)C1=O	CC1=C(C)C(=O)C(C)C(C)C1=O	CC1=C(C)C(=O)C(C)C(C)C1=O	CC1=C(C)C(=O)C(C)C(C)C1=O	CC1=C(C)C(=O)C(C)C(C)C1=O	
	mw	300.34	301.31	301.31	316.38	444.39	414.37	386.37	397.34	411.37	314.34		
	LogP (Distribution Coefficient)	2.81	2.86	1.98	2.81	6.21	6.23	2.82	2.84	2.80	2.21		
	LogP (Stability)	-1.63	-2.38	-3.34	-1.63	-6.71	-6.71	-3.27	-3.23	-6.62	-4.18	Source (log mol/L)	
Absorption	TPSA	100.11	81.8	171.36	126.36	26.21	26.21	111.11	80.91	26.21	15.36		
	100-150	16.47	77.01	86.41	89.6	16.91	16.91	41.84	49.19	41.83	16.51		
	Biorelevant Area	6.91	6.91	6.91	6.91	6.91	6.91	6.91	6.91	6.91	6.91		
	Case 2	-5.126	-6.181	-6.181	-5.227	-4.726	-4.726	-3.674	-4.489	-4.774	-4.811	Source (log Part in 10 ⁷ mol/L)	
	30s Permeability	-6.1	-7.47	-7.68	-6.9	-2.2	-2.2	-6.7	-6.68	-2.14	-6.56	Source (log Part)	
	Permeability	-	-	-	-	-	-	-	-	-	-	Category (1-5)	
Distribution	PPH (Percent Protein Bound)	88.8%	88.7%	88.8%	88.71%	77.56%	77.76%	88.87%	71.86%	81.87%	87.88%		
	VD (Volume Distribution)	-0.44	-0.218	-1.36	-0.912	0.134	0.134	-0.977	1.267	0.89	0.241		
	SA absorption	High	High	High	High	Low	Low	High	High	Low	High		
Metabolism	CYP1A2 substrate	+++	-	-	-	-	-	-	-	-	-	Category (1-5)	
	CYP2A2 substrate	-	-	-	-	-	-	-	-	-	-	Category (1-5)	
	CYP1A4 substrate	-	-	-	-	-	-	-	-	-	-	Category (1-5)	
	CYP1A4 inhibitor	-	-	-	-	-	-	-	-	-	-	Category (1-5)	
	CYP2C9 substrate	-	-	-	-	-	-	-	-	-	-	Category (1-5)	
	CYP2C9 inhibitor	-	-	-	-	-	-	-	-	-	-	Category (1-5)	
	CYP2C19 substrate	-	-	-	-	-	-	-	-	-	-	Category (1-5)	
	CYP2C19 inhibitor	-	-	-	-	-	-	-	-	-	-	Category (1-5)	
	CYP2D6 substrate	-	-	-	-	-	-	-	-	-	-	Category (1-5)	
Toxicity	T.1/2 (Half Life Time)	1.097 h	1.646 h	8.2 h	6.658 h	1.865 h	1.865 h	6.679 h	1.811 h	1.928 h	1.997 h	h	
	CL (Clearance Rate)	4.977	2.689	2.641	1.911	1.135	1.135	1.981	2.142	6.974	1.871	ml/min/kg	
	MBC (MBC) (Breasts)	-	-	-	-	-	-	-	-	-	-	Category (1-5)	
Exposure	HIT (Human Hepatotoxicity)	-	-	-	-	-	-	-	-	-	-	Category (1-5)	
	AMR (Acute Myelotoxicity)	++	-	-	-	-	-	-	-	-	-	Category (1-5)	
	Melan (New melanocytes)	-	-	-	-	-	-	-	-	-	-	Category (1-5)	
	LD50 (LD50) (rat body weight)	614.608	145.791	498.794	684.92	273.171	273.171	645.211	562.996	211.546	555.658	mg/kg	
	DLI (Drug Induced Liver Injury)	+++	-	-	-	-	-	-	-	-	-	Category (1-5)	
Exposure	TOXNET (Maximum Recommended Daily Dose)	-	-	-	-	-	-	-	-	-	-	Category (1-5)	

MW: molecular weight; TPSA: Top polar surface area; ClogP: ClogP; BBB: blood-brain barrier

Supplementary Table S8 Details of targets and components for molecular docking							
Target	PDB ID	Center coordinates	Docking grid box size	Compounds Mol ID	PubChem ID	Compounds Name	Compound type
VEGFA	1bj1	24.8,-25,-6.1	49.3,46.5,67.9	MOL005530	5318214	hydroxygenkwanin	flavonoids
IL6	1alu	0.5,-19.8,9.7	54.2,58, 49	MOL009042	23205	helenalin	sesquiterpene lactone
TP53	5ole	98.2, 79.9,-30.4	49,55.6,57	MOL000098	5280343	quercetin	flavonoids
TNF	1tnf	20,51.9,41	71.3,73.3,70.7	MOL000354	5281654	isorhamnetin	flavonoids
ALB	1ao6	31.2,30.9,22	83.3,71.6,89.6	MOL000358	222284	beta-sitosterol	phytosterols
IL1B	1i1b	38.9,-10.7,22.2	49.2,55,54.9	MOL000359	12303645	sitosterol	phytosterols
				MOL000422	5280863	kaempferol	tetrahydroxyflavone
				MOL000443	5317205	erythraline	alkaloid
				MOL000449	5280794	stigmasterol	sterol
				MOL001558	72307	sesamin	lignan

Supplementary Table S9 Details of each ligand-protein interaction molecular docking results			
Interacting group	Amino acid residue	Distance	Interaction type
TNF- Stigmasterol	Glu-116	2.9	Conventional Hydrogen Bond
	Lys-98		Carbon Hydrogen Bond
	Arg-103		Alkyl
ALB- Sesamin	Try-161,Phe-134		Carbon Hydrogen Bond
	Leu-115		Pi-sigma
	Tyr-138		Pi-Pi T-shaped
	Ala-126,Lys-137		Alky,Pi-Alkyl
IL1B- Sesamin	Glu-64	2.8	Conventional Hydrogen Bond
	Ser-43	2.4	Conventional Hydrogen Bond
	Ser-5	2.3	Conventional Hydrogen Bond
	Leu-6		Carbon Hydrogen Bond
	Ser-153,Asn-7,Pro-87,Asn-66,Tyr-90,Tyr-68,Pro-91		Van der Waals
TP53- Hydroxygenkwanin	His-115	3.1	Conventional Hydrogen Bond
	Phe-113	3.0,3.4	Conventional Hydrogen Bond
	Asp-268	3.1,3.4	Conventional Hydrogen Bond
	Ser-269	3.1,3.2	Conventional Hydrogen Bond
	Trp-146,Gly-112		Pi-sigma
	Tyr-126		Pi-Donor Hydrogen Bond
IL6- Stigmasterol	Met-117	3.6	Conventional Hydrogen Bond
	Tyr-31		Pi-sigma
	Arg-30,Lys-27,Val-121		Alky,Pi-Alkyl
VEGFA- Stigmasterol	Tyr-21		Pi-sigma
	Met-18,Phe-17,Tyr-25		Alky,Pi-Alkyl