

Supplementary Table 1: 139 active ingredients in Shegan mixture screened out by TCMSP database

Mol ID	Molecule Name	MW	AlogP	Hdon	Hacc	OB (%)	Caco-2	BBB	DL	FASA-	HL
MOL002322	isovitexin	432.41	-0.06	7	10	31.29	-1.24	-2.01	0.72	0.33	16.45
MOL001735	Dinatin	300.28	2.32	3	6	30.97	0.48	-0.49	0.27	0.28	16.44
MOL000449	Stigmasterol	412.77	7.64	1	1	43.83	1.44	1	0.76	0.22	5.57
MOL000351	Rhamnazin	330.31	2.01	3	7	47.14	0.53	-0.32	0.34	0.25	13.54
MOL000354	isorhamnetin	316.28	1.76	4	7	49.6	0.31	-0.54	0.31	0.32	14.34
MOL003741	anhydrobelachinal	468.74	6.34	1	4	43.57	0.81	0.05	0.78	0.3	4.83
MOL003742	ardisianone A	346.56	5.7	0	3	44.22	0.8	0.14	0.25	0.27	2.83
MOL003743	belachinal	486.76	5.58	3	5	31.24	-0.09	-0.97	0.64	0.33	5.3
MOL003744	belamcandal	528.8	5.07	3	6	30.07	0.05	-0.82	0.67	0.28	4.84
MOL003753	dihydrokaempferide	302.3	2	3	6	50.56	0.08	-0.39	0.27	0.36	14.74
MOL003754	epianhydrobelachinal	468.74	6.34	1	4	43.57	0.84	0.07	0.78	0.3	5
MOL003757	iristectorene B	685.2	12.75	2	5	32.56	0.36	-0.9	0.42	0.23	2.58
MOL003758	Iristectorigenin (9CI)	330.31	2.03	3	7	71.55	0.55	-0.16	0.34	0.23	16.32
MOL003759	Iristectorigenin A	330.31	2.03	3	7	63.36	0.54	-0.12	0.34	0.22	16.82
MOL003769	Irolone	298.26	2.1	2	6	46.87	0.57	-0.27	0.36	0.35	19.59
MOL003773	Mangiferolic acid	442.75	6.47	2	3	36.16	0.66	-0.06	0.84	0.25	5.71
MOL000006	luteolin	286.25	2.07	4	6	36.16	0.19	-0.84	0.25	0.39	15.94
MOL010921	estrone	270.4	3.77	1	2	53.56	1.01	0.83	0.32	0.3	3.5
MOL010922	Diisooctyl succinate	342.58	5.99	0	4	31.62	0.72	0.13	0.23	0.2	1.98
MOL002211	11,14-eicosadienoic acid (6Z,10E,14E,18E)- 2,6,10,15,19,23- hexamethyltetracos- 2,6,10,14,18,22-hexaene	308.56	7.3	1	2	39.99	1.22	0.76	0.2	0.23	5.6
MOL002372		410.8	11.33	0	0	33.55	2.07	1.77	0.42	0.27	3.15
MOL000359	sitosterol	414.79	8.08	1	1	36.91	1.32	0.87	0.75	0.22	5.37
MOL005030	gondoic acid	310.58	7.75	1	2	30.7	1.2	0.8	0.2	0.21	4.79
MOL000953	CLR	386.73	7.38	1	1	37.87	1.43	1.13	0.68	0.2	4.52
MOL000211	Mairin	456.78	6.52	2	3	55.38	0.73	0.22	0.78	0.26	8.87
MOL000492	(+)-catechin	290.29	1.92	5	6	54.83	-0.03	-0.73	0.24	0	0.61
MOL002311	Glycyrol	366.39	4.85	2	6	90.78	0.71	-0.2	0.67	0.28	9.85
MOL003410	Ziziphin_qt	472.78	4.39	2	4	66.95	0.49	-0.12	0.62	0.24	10
MOL004355	Spinasterol	412.77	7.64	1	1	42.98	1.44	1.04	0.76	0.21	5.32
MOL004841	Licochalcone B	286.3	2.88	3	5	76.76	0.47	-0.46	0.19	0	17.02
MOL004903	liquiritin	418.43	0.66	5	9	65.69	-1.06	-1.93	0.74	0	17.96
MOL004908	Glabridin	324.4	3.95	2	4	53.25	0.97	0.36	0.47	0	0.03
MOL005017	Phaseol	336.36	4.87	2	5	78.77	0.76	-0.06	0.58	0	9.64
MOL007207	Machiline	285.37	2.83	3	4	79.64	0.78	0.09	0.24	0.27	3.7
MOL012922	I-SPD	327.41	3.1	2	5	87.35	0.76	0.21	0.54	0.24	1.68
MOL002773	beta-carotene	536.96	12	0	0	37.18	2.25	1.52	0.58	0.33	4.36
MOL000433	FA	441.45	0.01	7	13	68.96	-1.5	-2.59	0.71	0	24.81
MOL010788	leucopelargonidin	290.29	1.36	5	6	57.97	-0.12	-0.62	0.24	0.37	1.38
MOL002823	Herbacetin	302.25	1.5	5	7	36.07	0.12	-0.65	0.27	0.37	14.8
MOL010489	Resivit	306.29	1.09	6	7	30.84	-0.49	-1.03	0.27	0.36	1.44
MOL000422	kaempferol	286.25	1.77	4	6	41.88	0.26	-0.55	0.24	0	14.74
MOL004798	delphinidin	303.26	1.4	6	7	40.63	-0.02	-0.81	0.28	0.35	1.16
MOL000098	quercetin	302.25	1.5	5	7	46.43	0.05	-0.77	0.28	0.38	14.4
MOL000358	beta-sitosterol	414.79	8.08	1	1	36.91	1.32	0.99	0.75	0.23	5.36
MOL001494	Mandenol	308.56	6.99	0	2	42	1.46	1.14	0.19	0.25	5.39
MOL001506	Supraene	410.8	11.33	0	0	33.55	2.08	1.73	0.42	0.27	2.72
MOL001755	24-Ethylcholest-4-en-3-one	412.77	8.18	0	1	36.08	1.46	1.22	0.76	0.25	5.49
MOL001771	poriferast-5-en-3beta-ol	414.79	8.08	1	1	36.91	1.45	1.14	0.75	0	5.07
MOL002881	Diosmetin	300.28	2.32	3	6	31.14	0.46	-0.66	0.27	0.34	16.34
MOL004328	naringenin	272.27	2.3	3	5	59.29	0.28	-0.37	0.21	0.4	16.98
MOL004576	taxifolin	304.27	1.49	5	7	57.84	-0.23	-0.8	0.27	0.39	14.41
MOL005043	campest-5-en-3beta-ol	400.76	7.63	1	1	37.58	1.32	0.94	0.71	0.23	4.43
MOL005190	eriodictyol	288.27	2.03	4	6	71.79	0.17	-0.54	0.24	0.38	15.81
MOL005573	Genkwaniin	284.28	2.59	2	5	37.13	0.63	-0.24	0.24	0.32	16.1
MOL005842	Pectolinarigenin	314.31	2.57	2	6	41.17	0.7	-0.09	0.3	0	16.56
MOL007214	(+)-Leucocyanidin	306.29	1.09	6	7	37.61	-0.45	-1	0.27	0.36	0.9
MOL011319	Trufflex OBP	334.5	6.02	0	4	43.74	0.9	0.6	0.24	0.3	4.9
MOL001689	acacetin	284.28	2.59	2	5	34.97	0.67	-0.05	0.24	0.35	17.25
MOL000173	wogonin	284.28	2.59	2	5	30.68	0.79	0.04	0.23	0.32	17.75
MOL000228	(2R)-7-hydroxy-5-methoxy-2- phenylchroman-4-one	270.3	2.82	1	4	55.23	0.87	0.26	0.2	0.34	17.02
MOL002714	baicalein	270.25	2.33	3	5	33.52	0.63	-0.05	0.21	0.36	16.25
MOL002908	5,8,2'-Trihydroxy-7- methoxyflavone	300.28	2.32	3	6	37.01	0.76	-0.07	0.27	0.28	16.17

MOL002909	5,7,2,5-tetrahydroxy-8,6-dimethoxyflavone	376.34	2.02	4	9	33.82	0.35	-0.59	0.45	0.19	15.94
MOL002910	Carthamidin	288.27	2.03	4	6	41.15	0.16	-0.42	0.24	0.36	15.81
MOL002911	2,6,2',4'-tetrahydroxy-6'-methoxychaleone	302.3	2.62	4	6	69.04	-0.07	-0.32	0.22	0.34	21.89
MOL002913	Dihydrobaicalin_qt	272.27	2.3	3	5	40.04	0.56	0.18	0.21	0.36	16.13
MOL002914	Eriodyctiol (flavanone)	288.27	2.03	4	6	41.35	0.05	-0.66	0.24	0.39	15.88
MOL002915	Salvigenin	328.34	2.82	1	6	49.07	0.86	-0.03	0.33	0.21	15.87
MOL002917	5,2',6'-Trihydroxy-7,8-dimethoxyflavone	330.31	2.3	3	7	45.05	0.48	-0.11	0.33	0.25	16.37
MOL002925	5,7,2',6'-Tetrahydroxyflavone	286.25	2.07	4	6	37.01	0.18	-0.56	0.24	0.38	18
MOL002926	dihydrooroxylin A	286.3	2.55	2	5	38.72	0.71	0.03	0.23	0.29	17.58
MOL002927	Skullcapflavone II	374.37	2.54	2	8	69.51	0.68	-0.07	0.44	0.2	16.14
MOL002928	oroxylin a	284.28	2.59	2	5	41.37	0.76	0.13	0.23	0.29	17.15
MOL002932	Panicolin	314.31	2.57	2	6	76.26	0.84	0.31	0.29	0.24	16.78
MOL002933	5,7,4'-Trihydroxy-8-methoxyflavone	300.28	2.32	3	6	36.56	0.46	-0.4	0.27	0.31	16.93
MOL002934	NEOBAICALEIN	374.37	2.54	2	8	104.34	0.74	-0.19	0.44	0.18	16.5
MOL002937	DIHYDROOROXYLIN	286.3	2.55	2	5	66.06	0.67	0.13	0.23	0.31	17.17
MOL000525	Norwogonin	270.25	2.33	3	5	39.4	0.6	-0.17	0.21	0.39	16.93
MOL000552	5,2'-Dihydroxy-6,7,8-trimethoxyflavone	344.34	2.55	2	7	31.71	0.93	0	0.35	0.22	16.47
MOL000073	ent-Epicatechin	290.29	1.92	5	6	48.96	0.02	-0.64	0.24	0.34	0.63
MOL001458	coptisine	320.34	3.25	0	4	30.67	1.21	0.32	0.86	0.26	9.33
MOL001490	bis[(2S)-2-ethylhexyl] benzene-1,2-dicarboxylate	390.62	7.57	0	4	43.59	0.98	0.68	0.35	0.28	3.02
MOL002879	Diop	390.62	7.44	0	4	43.59	0.79	0.26	0.39	0.28	3.6
MOL008206	Moslosooflavone	298.31	2.84	1	5	44.09	1.01	0.54	0.25	0.26	17.02
MOL010415	11,13-Eicosadienoic acid, methyl ester	322.59	7.55	0	2	39.28	1.46	1.24	0.23	0.21	5.44
MOL012245	5,7,4'-trihydroxy-6-methoxyflavanone	302.3	2.28	3	6	36.63	0.43	-0.32	0.27	0.28	16.12
MOL012246	5,7,4'-trihydroxy-8-methoxyflavanone	302.3	2.28	3	6	74.24	0.37	-0.43	0.26	0.31	16.85
MOL012266	rivularin	344.34	2.55	2	7	37.94	0.65	-0.13	0.37	0.21	16.25
MOL013076	(8S,9R)-9-hydroxy-8-(2-hydroxypropan-2-yl)-8,9-dihydrofuro[2,3-h]chromen-2-one	262.28	1.2	2	5	37.3	0.1	-0.19	0.2	0.35	3
MOL013077	Decursin	328.39	3.96	0	5	39.27	0.77	0.25	0.38	0.29	-1.77
MOL013078	praeruptorin E	428.52	4.88	0	7	51.22	0.37	-0.05	0.66	0.35	5.37
MOL013079	dl-praeruptorin a	386.43	3.5	0	7	46.46	0.52	0.09	0.53	0.31	4.5
MOL013081	Decussine	301.42	3.43	0	2	39.83	1.74	1.12	0.65	0.2	9.29
MOL013083	Skimmin (8Cl)	324.31	-0.27	4	8	38.35	-1.02	-1.57	0.32	0.3	3.57
MOL013087	Peucedanocoumarin II	386.43	3.5	0	7	63.48	0.25	-0.26	0.53	0.38	3.17
MOL013093	rubicauloside	602.65	-1.5	7	15	58.36	-1.94	-2.52	0.71	0.24	1.28
MOL013094	8-[(2R)-2,3-dihydroxy-3-methylbutyl]-5,7-dimethoxy-coumarin	308.36	1.66	2	6	48.57	-0.03	-0.5	0.21	0.24	2.05
MOL013095	Sporidesmin	474	1.35	2	9	58.31	-0.08	-0.54	0.76	0.38	15.31
MOL013098	[(9R)-8,8-dimethyl-2-oxo-9,10-dihydropyrano[6,5-h]chromen-9-yl] (Z)-2-methylbut-2-enoate	328.39	3.96	0	5	87.48	0.61	0.3	0.37	0.36	1.98
MOL013100	(2S)-2-(1-hydroxy-1-methyl-ethyl)-9-[(2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6-methylol-tetrahydropyran-2-yl]oxy-2,3-dihydrofuro[3,2-g]chromen-7-one	424.44	-0.14	5	10	45.33	-1.31	-1.65	0.73	0.27	5.23
MOL013101	rutarin_qt	262.28	1.76	2	5	70.1	0.2	-0.28	0.2	0.32	3.11
MOL013103	532-16-1	366.54	7	0	3	46.57	1.43	0.85	0.44	0.31	3.69
MOL001941	Ammidin	270.3	3.65	0	4	34.55	1.13	0.92	0.22	0.28	-1.35
MOL001942	isoimperatorin	270.3	3.65	0	4	45.46	0.97	0.66	0.23	0.27	-1.44
MOL002644	Phellopterin	300.33	3.64	0	5	40.19	0.98	0.48	0.28	0.24	-1.64
MOL004653	(+)-Anomalin	426.5	5.05	0	7	46.06	0.46	0	0.66	0.36	1.03
MOL004792	nodakenin	408.44	0.28	4	9	57.12	-0.79	-1.42	0.69	0.27	7.16
MOL005100	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)chroman-4-one	302.3	2.28	3	6	47.74	0.28	-0.3	0.27	0.31	16.51
MOL007154	tanshinone iia	294.37	4.66	0	3	49.89	1.05	0.7	0.4	0.31	23.56
MOL009361	13,15-Dideoxyaconitine	613.82	0.34	1	10	34.67	0.2	-0.31	0.25	0.2	20.74
MOL009380	bisdehydrostemoninine	385.5	4.09	0	5	38.51	0.51	-0.21	0.73	0.29	2.41
MOL009436	stemotinine	335.44	1.94	0	6	38.69	0.26	-0.05	0.46	0.27	1.84
MOL009423	sessilistemonamine A	391.56	2.86	1	6	40.28	-0.12	-0.44	0.73	0.29	2.31

MOL009424	sessilistemonamine B	391.56	2.86	1	6	40.64	0.29	-0.29	0.73	0.28	3.15
MOL009409	oxystemoninine	407.56	2.43	1	7	42.79	-0.03	-0.51	0.77	0.28	2.69
MOL009419	sessilifoliamide H	421.54	1.31	1	8	43.68	-0.15	-0.57	0.68	0.3	6.36
MOL009394	stemonamine	317.42	2.12	0	5	45.19	0.56	0.48	0.35	0.28	5.97
MOL009411	protostemotinine	415.53	2.74	0	7	45.99	0.03	-0.19	0.75	0.32	3.86
MOL009382	bisdehydrostemoninine B	387.52	4.16	1	5	46.05	0.33	-0.45	0.64	0.26	1.96
MOL009377	bisdehydroneotuberostemonine	371.52	4.37	0	4	51.14	0.68	0.15	0.74	0.27	9.3
MOL009387	didehydrotuberostemonine	371.52	4.37	0	4	51.91	0.7	0.19	0.74	0.27	8.12
MOL009386	3,3'-bis-(3,4-dihydro-4-hydroxy-6-methoxy)-2H-1-benzopyran	358.42	1.82	2	6	52.11	0.14	-0.55	0.54	0.26	3.76
MOL009363	tuberostemonine C	375.56	3.6	0	5	55.34	0.68	0.45	0.74	0.27	11.17
MOL001558	sesamin	354.38	2.24	0	6	56.55	0.75	-0.08	0.83	0.31	13.44
MOL005384	suchilactone	368.41	3.73	0	6	57.52	0.82	0.28	0.56	0.28	9.03
MOL005360	malkangunin	432.56	1.84	2	7	57.71	0.22	-0.17	0.63	0.3	4.09
MOL009422	sessilifoline B	277.45	2.8	0	3	58.81	1.23	1.28	0.29	0.23	9.95
MOL009374	7-methoxy-3-methyl-2,5-dihydroxy-9,10-dihydrophenanthrene	256.32	3.88	2	3	59	1.12	0.49	0.21	0.3	-0.42
MOL009381	bisdehydrostemoninine A	401.5	3.59	1	6	62.64	0.06	-0.49	0.68	0.28	15.49
MOL009414	sessilifoliamide C	291.43	2.78	0	4	65.87	0.72	0.47	0.2	0.29	4.99
MOL009434	stemoninoamide	305.41	1.8	0	5	66.7	0.42	0	0.33	0.28	2.98
MOL009430	stemonamide	329.43	0.95	0	5	67.46	0.24	-0.08	0.38	0.29	5.51
MOL009388	dihydrostemoninine	391.56	3.01	0	6	68.01	0.44	-0.08	0.72	0.26	3.14
MOL000392	formononetin	268.28	2.58	1	4	69.67	0.78	0.02	0.21	0	17.04
MOL009379	2-oxostenine	291.43	2.04	0	4	72.94	0.68	0.4	0.34	0.27	8.15
MOL009433	stemoninine B	387.52	3.74	0	5	74.77	0.53	-0.17	0.73	0.25	2.32
MOL009431	stemonine	389.54	3.36	0	6	81.75	0.51	-0.07	0.72	0.3	3.33
MOL009441	(3S,3'R,4'R,9S,9aS)-4'-hydroxy-3'-methyl-3-[(2S,4S)-4-methyl-5-oxoxolan-2-yl]spiro[1,2,3,5,6,7,8,9a-octahydropyrrolo[1,2-a]azepine-9,5'-oxolane]-2'-one	337.46	1.95	1	6	85.52	-0.02	-0.53	0.38	0.29	2.88
MOL002897	epiberberine	336.39	3.45	0	4	43.09	1.17	0.4	0.78	0.19	6.1

ID, molecular name, and various parameters corresponding to each active ingredients. These parameters include molecular weight (MW), AlogP for representing the partition coefficient between octanol and water, Hdon and Hacc for number of possible hydrogen-bond donors and acceptors, respectively, oral bioavailability (OB), Caco-2 permeability to represent the intestinal epithelial permeability, blood-brain barrier (BBB), drug-likeness (DL), Fractional water accessible surface area of all atoms with negative partial charge (FASA-), and drug half-life (HL).

Supplementary Table 2: Active Ingredients-related targets in SGM

Mol ID	Molecule Name	Target Symbol	Target Name
MOL000211	Mairin	PGR	Progesterone receptor
MOL002311	Glycyrol	NOS2	Nitric oxide synthase, inducible
MOL002311	Glycyrol	ESR1	Estrogen receptor
MOL002311	Glycyrol	PPARG	Peroxisome proliferator activated receptor gamma
MOL002311	Glycyrol	PTGS2	Prostaglandin G/H synthase 2
MOL002311	Glycyrol	VEGFR2	Vascular endothelial growth factor receptor 2
MOL002311	Glycyrol	MAPK14	Mitogen-activated protein kinase 14
MOL002311	Glycyrol	GSK3B	Glycogen synthase kinase-3 beta
MOL002311	Glycyrol	CHEK1	Serine/threonine-protein kinase Chk1
MOL002311	Glycyrol	PIM1	Proto-oncogene serine/threonine-protein kinase Pim-1
MOL002311	Glycyrol	CCNA2	Cyclin-A2
MOL004903	liquiritin	F10	Coagulation factor Xa
MOL004903	liquiritin	F7	Coagulation factor VII
MOL004903	liquiritin	CALM1	Calmodulin
MOL004903	liquiritin	PTGS2	Prostaglandin G/H synthase 2
MOL004903	liquiritin	VEGFR2	Vascular endothelial growth factor receptor 2
MOL004903	liquiritin	SOD1	Superoxide dismutase [Cu-Zn]
MOL004908	Glabridin	NOS2	Nitric oxide synthase, inducible
MOL004908	Glabridin	CHRM1	Muscarinic acetylcholine receptor M1
MOL004908	Glabridin	ESR1	Estrogen receptor
MOL004908	Glabridin	AR	Androgen receptor
MOL004908	Glabridin	SCN5A	Sodium channel protein type 5 subunit alpha
MOL004908	Glabridin	PPARG	Peroxisome proliferator activated receptor gamma
MOL004908	Glabridin	PTGS2	Prostaglandin G/H synthase 2
MOL004908	Glabridin	RXRA	Retinoic acid receptor RXR-alpha
MOL004908	Glabridin	ACHE	Acetylcholinesterase
MOL004908	Glabridin	ADRA1B	Alpha-1B adrenergic receptor
MOL004908	Glabridin	ADRB2	Beta-2 adrenergic receptor
MOL004908	Glabridin	ESR2	Estrogen receptor beta
MOL004908	Glabridin	MAPK14	Mitogen-activated protein kinase 14
MOL004908	Glabridin	GSK3B	Glycogen synthase kinase-3 beta
MOL004908	Glabridin	CDK2	Cell division protein kinase 2
MOL004908	Glabridin	CHEK1	Serine/threonine-protein kinase Chk1
MOL004908	Glabridin	PRKACA	mRNA of PKA Catalytic Subunit C-alpha
MOL004908	Glabridin	RXRB	Retinoic acid receptor RXR-beta
MOL004908	Glabridin	IGHG1	Ig gamma-1 chain C region
MOL004908	Glabridin	PRSS1	Trypsin-1
MOL004908	Glabridin	PIM1	Proto-oncogene serine/threonine-protein kinase Pim-1
MOL004908	Glabridin	CCNA2	Cyclin-A2
MOL004908	Glabridin	NCOA2	Nuclear receptor coactivator 2
MOL004908	Glabridin	NCOA1	Nuclear receptor coactivator 1
MOL004908	Glabridin	CALM1	Calmodulin
MOL005017	Phaseol	ESR1	Estrogen receptor
MOL005017	Phaseol	AR	Androgen receptor
MOL005017	Phaseol	PPARG	Peroxisome proliferator activated receptor gamma
MOL005017	Phaseol	PTGS2	Prostaglandin G/H synthase 2
MOL005017	Phaseol	VEGFR2	Vascular endothelial growth factor receptor 2
MOL005017	Phaseol	MAPK14	Mitogen-activated protein kinase 14
MOL005017	Phaseol	GSK3B	Glycogen synthase kinase-3 beta
MOL005017	Phaseol	HSP90	Heat shock protein HSP 90
MOL005017	Phaseol	CDK2	Cell division protein kinase 2
MOL005017	Phaseol	CHEK1	Serine/threonine-protein kinase Chk1
MOL005017	Phaseol	PRKACA	mRNA of PKA Catalytic Subunit C-alpha
MOL005017	Phaseol	PIM1	Proto-oncogene serine/threonine-protein kinase Pim-1
MOL005017	Phaseol	CCNA2	Cyclin-A2
MOL012922	I-SPD	PTGS1	Prostaglandin G/H synthase 1
MOL012922	I-SPD	DRD1	Dopamine D1 receptor
MOL012922	I-SPD	CHRM3	Muscarinic acetylcholine receptor M3
MOL012922	I-SPD	KCNH2	Potassium voltage-gated channel subfamily H member 2
MOL012922	I-SPD	CHRM1	Muscarinic acetylcholine receptor M1
MOL012922	I-SPD	DRD5	D(1B) dopamine receptor
MOL012922	I-SPD	SCN5A	Sodium channel protein type 5 subunit alpha
MOL012922	I-SPD	F10	Coagulation factor Xa
MOL012922	I-SPD	CHRM5	Muscarinic acetylcholine receptor M5
MOL012922	I-SPD	PTGS2	Prostaglandin G/H synthase 2
MOL012922	I-SPD	CA2	Carbonic anhydrase II
MOL012922	I-SPD	ADRA2C	Alpha-2C adrenergic receptor

MOL012922	I-SPD	CHRM4	Muscarinic acetylcholine receptor M4
MOL012922	I-SPD	RXRA	Retinoic acid receptor RXR-alpha
MOL012922	I-SPD	OPRD1	Delta-type opioid receptor
MOL012922	I-SPD	HTR2A	5-hydroxytryptamine 2A receptor
MOL012922	I-SPD	ADRA1A	Alpha-1A adrenergic receptor
MOL012922	I-SPD	HTR2C	5-hydroxytryptamine 2C receptor
MOL012922	I-SPD	CHRM2	Muscarinic acetylcholine receptor M2
MOL012922	I-SPD	ADRA2B	Alpha-2B adrenergic receptor
MOL012922	I-SPD	ADRA1B	Alpha-1B adrenergic receptor
MOL012922	I-SPD	DRD3	D(3) dopamine receptor
MOL012922	I-SPD	SLC6A3	Sodium-dependent dopamine transporter
MOL012922	I-SPD	ADRB2	Beta-2 adrenergic receptor
MOL012922	I-SPD	ADRA1D	Alpha-1D adrenergic receptor
MOL012922	I-SPD	SLC6A4	Sodium-dependent serotonin transporter
MOL012922	I-SPD	OPRM1	Mu-type opioid receptor
MOL012922	I-SPD	HSP90	Heat shock protein HSP 90
MOL012922	I-SPD	PRKACA	mRNA of PKA Catalytic Subunit C-alpha
MOL012922	I-SPD	CALM1	Calmodulin
MOL000433	FA	CDK2	Cell division protein kinase 2
MOL000433	FA	GSK3B	Glycogen synthase kinase-3 beta
MOL013078	praeruptorin E	KCNH2	Potassium voltage-gated channel subfamily H member 2
MOL013078	praeruptorin E	F10	Coagulation factor Xa
MOL013078	praeruptorin E	PTGS2	Prostaglandin G/H synthase 2
MOL013078	praeruptorin E	CA2	Carbonic anhydrase II
MOL013078	praeruptorin E	TOP2	DNA topoisomerase II
MOL013078	praeruptorin E	HSP90	Heat shock protein HSP 90
MOL013078	praeruptorin E	PRSS1	Trypsin-1
MOL013078	praeruptorin E	CALM1	Calmodulin
MOL013078	praeruptorin E	NCOA1	Nuclear receptor coactivator 1
MOL013087	Peucedanocoumarin II	KCNH2	Potassium voltage-gated channel subfamily H member 2
MOL013087	Peucedanocoumarin II	F10	Coagulation factor Xa
MOL013087	Peucedanocoumarin II	PTGS2	Prostaglandin G/H synthase 2
MOL013087	Peucedanocoumarin II	PTPN1	mRNA of Protein-tyrosine phosphatase, non-receptor type 1
MOL013087	Peucedanocoumarin II	TOP2	DNA topoisomerase II
MOL013087	Peucedanocoumarin II	DPP4	Dipeptidyl peptidase IV
MOL013087	Peucedanocoumarin II	HSP90	Heat shock protein HSP 90
MOL013087	Peucedanocoumarin II	NCOA1	Nuclear receptor coactivator 1
MOL013087	Peucedanocoumarin II	KCNMA1	Calcium-activated potassium channel subunit alpha 1
MOL004792	nodakenin	ESR1	Estrogen receptor
MOL004792	nodakenin	PTGS2	Prostaglandin G/H synthase 2
MOL004792	nodakenin	PIM1	Proto-oncogene serine/threonine-protein kinase Pim-1
MOL004792	nodakenin	ACHE	Acetylcholinesterase
MOL001558	sesamin	F10	Coagulation factor Xa
MOL001558	sesamin	PTGS2	Prostaglandin G/H synthase 2
MOL001558	sesamin	SCN5A	Sodium channel protein type 5 subunit alpha
MOL001558	sesamin	CCND1	G1/S-specific cyclin-D1
MOL001558	sesamin	IL10	Interleukin-10
MOL001558	sesamin	FASN	Fatty acid synthase
MOL001558	sesamin	ACACA	Acetyl-CoA carboxylase 1
MOL001558	sesamin	H6PD	Glucose-6-phosphate 1-dehydrogenase
MOL001558	sesamin	NOS3	Nitric oxide synthase, endothelial
MOL001558	sesamin	ECE1	Endothelin-converting enzyme 1
MOL001558	sesamin	ACADM	Medium-chain specific acyl-CoA dehydrogenase, mitochondrial
MOL001558	sesamin	CYP2B6	Cytochrome P450 2B6
MOL001558	sesamin	UGT1A1	UDP-glucuronosyltransferase 1-1
MOL001558	sesamin	SREBF1	Sterol regulatory element-binding protein 1
MOL001558	sesamin	NOX3	NADPH oxidase 3
MOL001558	sesamin	NOX1	NADPH oxidase 1
MOL001558	sesamin	ACOX1	Peroxisomal acyl-coenzyme A oxidase 1
MOL001558	sesamin	ACLY	ATP-citrate synthase
MOL001558	sesamin	EHHADH	Peroxisomal bifunctional enzyme
MOL001558	sesamin	AUH	Methylglutaconyl-CoA hydratase, mitochondrial
MOL001558	sesamin	HADHB	Trifunctional enzyme subunit beta, mitochondrial
MOL001558	sesamin	DECR1	2,4-dienoyl-CoA reductase, mitochondrial
MOL001558	sesamin	EC11	3,2-trans-enoyl-CoA isomerase, mitochondrial
MOL005384	suchilactone	KCNH2	Potassium voltage-gated channel subfamily H member 2
MOL005384	suchilactone	SCN5A	Sodium channel protein type 5 subunit alpha
MOL005384	suchilactone	F10	Coagulation factor Xa
MOL005384	suchilactone	PTGS2	Prostaglandin G/H synthase 2
MOL005384	suchilactone	F7	Coagulation factor VII

MOL005384	suchilactone	PTPN1	mRNA of Protein-tyrosine phosphatase, non-receptor type 1
MOL005384	suchilactone	ADRB2	Beta-2 adrenergic receptor
MOL005384	suchilactone	HSP90	Heat shock protein HSP 90
MOL005384	suchilactone	NCOA1	Nuclear receptor coactivator 1
MOL005384	suchilactone	KCNMA1	Calcium-activated potassium channel subunit alpha 1
MOL005384	suchilactone	CALM1	Calmodulin
MOL005384	suchilactone	PTGS1	Prostaglandin G/H synthase 1
MOL005384	suchilactone	RXRA	Retinoic acid receptor RXR-alpha
MOL005384	suchilactone	PDE3A	CGMP-inhibited 3',5'-cyclic phosphodiesterase A
MOL005384	suchilactone	ADRA1D	Alpha-1D adrenergic receptor
MOL005384	suchilactone	PRKACA	mRNA of PKA Catalytic Subunit C-alpha
MOL009363	tuberostemonine C	AR	Androgen receptor
MOL009363	tuberostemonine C	CHRM2	Muscarinic acetylcholine receptor M2
MOL009363	tuberostemonine C	NR3C2	Mineralocorticoid receptor
MOL009363	tuberostemonine C	OPRM1	Mu-type opioid receptor
MOL009377	bisdehydroneotuberostemonine	NOS2	Nitric oxide synthase, inducible
MOL009377	bisdehydroneotuberostemonine	DRD1	Dopamine D1 receptor
MOL009377	bisdehydroneotuberostemonine	CHRM3	Muscarinic acetylcholine receptor M3
MOL009377	bisdehydroneotuberostemonine	CHRM1	Muscarinic acetylcholine receptor M1
MOL009377	bisdehydroneotuberostemonine	AR	Androgen receptor
MOL009377	bisdehydroneotuberostemonine	CHRM5	Muscarinic acetylcholine receptor M5
MOL009377	bisdehydroneotuberostemonine	PTGS2	Prostaglandin G/H synthase 2
MOL009377	bisdehydroneotuberostemonine	CHRM4	Muscarinic acetylcholine receptor M4
MOL009377	bisdehydroneotuberostemonine	ADRA1A	Alpha-1A adrenergic receptor
MOL009377	bisdehydroneotuberostemonine	CHRM2	Muscarinic acetylcholine receptor M2
MOL009377	bisdehydroneotuberostemonine	ADRA1B	Alpha-1B adrenergic receptor
MOL009377	bisdehydroneotuberostemonine	ADRB2	Beta-2 adrenergic receptor
MOL009377	bisdehydroneotuberostemonine	DRD2	D(2) dopamine receptor
MOL009377	bisdehydroneotuberostemonine	OPRM1	Mu-type opioid receptor
MOL009377	bisdehydroneotuberostemonine	CHRNA7	Neuronal acetylcholine receptor protein, alpha-7 chain
MOL009381	bisdehydrostemoninine A	AR	Androgen receptor
MOL009381	bisdehydrostemoninine A	PTGS2	Prostaglandin G/H synthase 2
MOL009386	3,3'-bis-(3,4-dihydro-4-hydroxy-6-methoxy)-2H-1-benzopyran	KCNH2	Potassium voltage-gated channel subfamily H member 2
MOL009386	3,3'-bis-(3,4-dihydro-4-hydroxy-6-methoxy)-2H-1-benzopyran	ESR1	Estrogen receptor
MOL009386	3,3'-bis-(3,4-dihydro-4-hydroxy-6-methoxy)-2H-1-benzopyran	PTGS2	Prostaglandin G/H synthase 2
MOL009386	3,3'-bis-(3,4-dihydro-4-hydroxy-6-methoxy)-2H-1-benzopyran	ADRB2	Beta-2 adrenergic receptor
MOL009386	3,3'-bis-(3,4-dihydro-4-hydroxy-6-methoxy)-2H-1-benzopyran	HSP90	Heat shock protein HSP 90
MOL009386	3,3'-bis-(3,4-dihydro-4-hydroxy-6-methoxy)-2H-1-benzopyran	PIM1	Proto-oncogene serine/threonine-protein kinase Pim-1
MOL009386	3,3'-bis-(3,4-dihydro-4-hydroxy-6-methoxy)-2H-1-benzopyran	CCNA2	Cyclin-A2
MOL009386	3,3'-bis-(3,4-dihydro-4-hydroxy-6-methoxy)-2H-1-benzopyran	CALM1	Calmodulin
MOL009387	didehydrotuberostemonine	CHRM3	Muscarinic acetylcholine receptor M3
MOL009387	didehydrotuberostemonine	CHRM1	Muscarinic acetylcholine receptor M1
MOL009387	didehydrotuberostemonine	AR	Androgen receptor
MOL009387	didehydrotuberostemonine	SCN5A	Sodium channel protein type 5 subunit alpha
MOL009387	didehydrotuberostemonine	CHRM5	Muscarinic acetylcholine receptor M5
MOL009387	didehydrotuberostemonine	PTGS2	Prostaglandin G/H synthase 2
MOL009387	didehydrotuberostemonine	CHRM4	Muscarinic acetylcholine receptor M4
MOL009387	didehydrotuberostemonine	CHRM2	Muscarinic acetylcholine receptor M2
MOL009387	didehydrotuberostemonine	ADRA1B	Alpha-1B adrenergic receptor
MOL009387	didehydrotuberostemonine	OPRM1	Mu-type opioid receptor
MOL009387	didehydrotuberostemonine	DPP4	Dipeptidyl peptidase IV
MOL009388	dihydrostemoninine	AR	Androgen receptor
MOL009431	stemonine	AR	Androgen receptor
MOL009433	stemoninine B	NOS2	Nitric oxide synthase, inducible
MOL009433	stemoninine B	CHRM3	Muscarinic acetylcholine receptor M3
MOL009433	stemoninine B	CHRM1	Muscarinic acetylcholine receptor M1
MOL009433	stemoninine B	AR	Androgen receptor
MOL009433	stemoninine B	PTGS2	Prostaglandin G/H synthase 2
MOL009433	stemoninine B	CHRM2	Muscarinic acetylcholine receptor M2
MOL009433	stemoninine B	ADRA1B	Alpha-1B adrenergic receptor

Supplementary Table 3: A total of 63 potential targets of SGM in the treatment of asthma

UniProt ID	Target Symbol	Details
P06401	PGR	Progesterone receptor
P35228	NOS2	Nitric oxide synthase, inducible
P03372	ESR1	Estrogen receptor
P37231	PPARG	Peroxisome proliferator activated receptor gamma
P35354	PTGS2	Prostaglandin G/H synthase 2
Q16539	MAPK14	Mitogen-activated protein kinase 14
P49841	GSK3B	Glycogen synthase kinase-3 beta
O14757	CHEK1	Serine/threonine-protein kinase Chk1
P11309	PIM1	Proto-oncogene serine/threonine-protein kinase Pim-1
P20248	CCNA2	Cyclin-A2
P00742	F10	Coagulation factor Xa
P08709	F7	Coagulation factor VII
P0DP23	CALM1	Calmodulin
P00441	SOD1	Superoxide dismutase [Cu-Zn]
P11229	CHRM1	Muscarinic acetylcholine receptor M1
P10275	AR	Androgen receptor
Q14524	SCN5A	Sodium channel protein type 5 subunit alpha
P22303	ACHE	Acetylcholinesterase
P35368	ADRA1B	Alpha-1B adrenergic receptor
P07550	ADRB2	Beta-2 adrenergic receptor
Q92731	ESR2	Estrogen receptor beta
P24941	CDK2	Cell division protein kinase 2
P28702	RXRB	Retinoic acid receptor RXR-beta
P01857	IGHG1	Ig gamma-1 chain C region
P07477	PRSS1	Trypsin-1
Q15596	NCOA2	Nuclear receptor coactivator 2
Q15788	NCOA1	Nuclear receptor coactivator 1
P07900	HSP90	Heat shock protein HSP 90
P23219	PTGS1	Prostaglandin G/H synthase 1
P21728	DRD1	Dopamine D1 receptor
P20309	CHRM3	Muscarinic acetylcholine receptor M3
P21918	DRD5	D(1B) dopamine receptor
P08912	CHRM5	Muscarinic acetylcholine receptor M5
P00918	CA2	Carbonic anhydrase II
P18825	ADRA2C	Alpha-2C adrenergic receptor
P08173	CHRM4	Muscarinic acetylcholine receptor M4
P41143	OPRD1	Delta-type opioid receptor
P28223	HTR2A	5-hydroxytryptamine 2A receptor
P35348	ADRA1A	Alpha-1A adrenergic receptor
P28335	HTR2C	5-hydroxytryptamine 2C receptor
P08172	CHRM2	Muscarinic acetylcholine receptor M2
P18089	ADRA2B	Alpha-2B adrenergic receptor
P35462	DRD3	D(3) dopamine receptor
Q01959	SLC6A3	Sodium-dependent dopamine transporter
P25100	ADRA1D	Alpha-1D adrenergic receptor
P31645	SLC6A4	Sodium-dependent serotonin transporter
P35372	OPRM1	Mu-type opioid receptor
P11388	TOP2	DNA topoisomerase II
P18031	PTPN1	mRNA of Protein-tyrosine phosphatase, non-receptor type 1
P27487	DPP4	Dipeptidyl peptidase IV
Q12791	KCNMA1	Calcium-activated potassium channel subunit alpha 1
P24385	CCND1	G1/S-specific cyclin-D1
P22301	IL10	Interleukin-10
P29474	NOS3	Nitric oxide synthase, endothelial
P42892	ECE1	Endothelin-converting enzyme 1
P22309	UGT1A1	UDP-glucuronosyltransferase 1-1
Q9HBY0	NOX3	NADPH oxidase 3
Q9Y5S8	NOX1	NADPH oxidase 1
P55084	HADHB	Trifunctional enzyme subunit beta, mitochondrial
Q14432	PDE3A	CGMP-inhibited 3',5'-cyclic phosphodiesterase A
P08235	NR3C2	Mineralocorticoid receptor
P14416	DRD2	D(2) dopamine receptor
P36544	CHRNA7	Neuronal acetylcholine receptor protein, alpha-7 chain