

Table S1 Compound Constitution of Formula. In this table, the constitution information of formula is presented. Each record of compound information contains herb name and compound CASRN.

TCM herb	CAS	TCM herb	CAS	TCM herb	CAS
Gan-cao	103000-77-7	Yin-hua	520-32-1	Lian-qiao	1616-93-9
Gan-cao	104-46-1	Yin-hua	520-32-1	Lian-qiao	522-12-3
Gan-cao	104691-86-3	Yin-hua	5373-11-5	Lian-qiao	21637-25-2
Gan-cao	105038-43-5	Yin-hua	578-74-5	Lian-qiao	482-36-0
Gan-cao	1157-39-7	Yin-hua	60077-47-6	Lian-qiao	55954-61-5
Gan-cao	117038-82-1	Yin-hua	6151-25-3	Lian-qiao	548-04-9
Gan-cao	117-39-5	Yin-hua	639-99-6	Lian-qiao	11079-53-1
Gan-cao	118524-14-4	Yin-hua	639-99-6	Lian-qiao	54328-09-5
Gan-cao	118525-49-8	Yin-hua	6753-98-6	Lian-qiao	548-03-8
Gan-cao	120-46-7	Yin-hua	7212-44-4	Lian-qiao	4852-22-6
Gan-cao	121687-83-0	Yin-hua	74518-57-3	Lian-qiao	491-60-1
Gan-cao	121709-66-8	Yin-hua	77-53-2	Lian-qiao	491-70-3
Gan-cao	123914-44-3	Yin-hua	8007-87-2	Lian-qiao	520-18-3
Gan-cao	124596-86-7	Yin-hua	301-00-8	Lian-qiao	529-44-2
Gan-cao	124596-87-8	Yin-hua	1191-41-9	Lian-qiao	1617-53-4
Gan-cao	124596-88-9	Yin-hua	112-63-0	Lian-qiao	89-83-8
Gan-cao	124596-89-0	Yin-hua	544-35-4	Lian-qiao	6753-98-6
Gan-cao	125310-04-5	Yin-hua	17306-46-6	Lian-qiao	97-53-0
Gan-cao	126716-36-7	Yin-hua	76-49-3	Lian-qiao	2955-23-9
Gan-cao	129145-50-2	Yin-hua	472-70-8	Lian-qiao	79-92-5
Gan-cao	129145-51-3	Yin-hua	144-68-3	Lian-qiao	3387-41-5
Gan-cao	129145-52-4	Yin-hua	489-86-1	Lian-qiao	13466-78-9
Gan-cao	129145-53-5	Yin-hua	8047-15-2	Lian-qiao	487-36-5
Gan-cao	129145-54-6	Yin-hua	21368-68-3	Lian-qiao	99-86-5
Gan-cao	129280-33-7	Yin-hua	74563-64-7	Lian-qiao	10385-78-1
Gan-cao	129314-37-0	Yin-hua	628-97-7	Lian-qiao	76-22-2
Gan-cao	129314-37-0	Yin-hua	565-00-4	Lian-qiao	543-39-5
Gan-cao	129-66-8	Yin-hua	120-72-9	Lian-qiao	515-00-4
Gan-cao	131-11-3	Yin-hua	91-22-5	Lian-qiao	123-35-3
Gan-cao	134958-52-4	Yin-hua	89-83-8	Lian-qiao	23202-85-9
Gan-cao	134958-53-5	Yin-hua	83-46-5	Lian-qiao	98-55-5
Gan-cao	134958-54-6	Yin-hua	83-48-7	Lian-qiao	15297-99-1
Gan-cao	134958-55-7	Yin-hua	905-99-7	Lian-qiao	5392-40-5
Gan-cao	134958-56-8	Yin-hua	327-97-9	Lian-qiao	6617-34-1
Gan-cao	134958-57-9	Yin-hua	14534-61-3	Lian-qiao	138-86-3
Gan-cao	136-60-7	Yin-hua	2450-53-5	Lian-qiao	13877-91-3
Gan-cao	139163-15-8	Yin-hua	57378-72-0	Lian-qiao	18530-03-5
Gan-cao	143986-30-5	Yin-hua	331-39-5	Lian-qiao	7299-42-5
Gan-cao	143986-30-5	Yin-hua	77-95-2	Lian-qiao	81525-13-5
Gan-cao	144506-14-9	Yin-hua	22255-40-9	Lian-qiao	60976-49-0
Gan-cao	144506-15-0	Yin-hua	59472-23-0	Lian-qiao	78-70-6
Gan-cao	150853-98-8	Yin-hua	499-75-2	Lian-qiao	24189-95-5
Gan-cao	150853-99-9	Yin-hua	98-55-5	Lian-qiao	17884-88-7
Gan-cao	153-18-4	Yin-hua	69671-15-4	Lian-qiao	27978-14-9
Gan-cao	17038-80-9	Yin-hua	17699-14-8	Lian-qiao	498-45-3
Gan-cao	19725-44-1	Yin-hua	80-56-8	Bo-he	480-44-4
Gan-cao	220860-37-7	Yin-hua	51317-08-9	Bo-he	520-36-5
Gan-cao	23013-84-5	Yin-hua	120-51-4	Bo-he	626-93-7
Gan-cao	27762-99-8	Yin-hua	55290-63-6	Bo-he	491-71-4

Gan-cao	2859-88-3	Yin-hua	475-20-7	Bo-he	41365-32-6
Gan-cao	30508-27-1	Yin-hua	78-70-6	Bo-he	520-34-3
Gan-cao	32383-76-9	Yin-hua	1365-19-1	Bo-he	2798-20-1
Gan-cao	34221-41-5	Yin-hua	334-48-5	Bo-he	29202-00-4
Gan-cao	3809-79-5	Yin-hua	51419-48-8	Bo-he	437-64-9
Gan-cao	41983-91-9	Yin-hua	474-58-8	Bo-he	1447-88-7
Gan-cao	4382-17-6	Zhi-mu	83-46-5	Bo-he	18085-97-7
Gan-cao	46763-58-8	Zhi-mu	82597-74-8	Bo-he	10176-71-3
Gan-cao	480-10-4	Zhi-mu	113558-15-9	Bo-he	71-41-0
Gan-cao	481-34-5	Zhi-mu	123-41-1	Bo-he	23494-48-6
Gan-cao	485-72-3	Zhi-mu	4773-96-0	Bo-he	22384-63-0
Gan-cao	486-62-4	Zhi-mu	1401-55-4	Bo-he	2623-23-6
Gan-cao	486-62-4	Zhi-mu	512-04-9	Bo-he	19103-54-9
Gan-cao	51847-92-8	Zhi-mu	64809-67-2	Bo-he	23130-22-5
Gan-cao	51938-32-0	Zhi-mu	59-67-6	Bo-he	76844-67-2
Gan-cao	520-18-3	Zhi-mu	98-92-0	Bo-he	589-98-0
Gan-cao	551-15-5	Zhi-mu	24699-16-9	Bo-he	16545-23-6
Gan-cao	552-59-0	Zhi-mu	139051-27-7	Bo-he	5208-59-3
Gan-cao	562-49-2	Zhi-mu	136656-07-0	Bo-he	470-82-6
Gan-cao	565-59-3	Zhi-mu	82597-74-8	Bo-he	89-83-8
Gan-cao	578-86-9	Zhi-mu	79-83-4	Bo-he	494-90-6
Gan-cao	584-94-1	Zhi-mu	64809-67-2	Bo-he	93-58-3
Gan-cao	58749-22-7	Zhi-mu	41059-79-4	Bo-he	15932-80-6
Gan-cao	58749-23-8	Zhi-mu	142759-74-8	Bo-he	481-74-3
Gan-cao	589-43-5	Zhi-mu	138831-68-2	Bo-he	518-82-1
Gan-cao	590-35-2	Zhi-mu	28591-01-7	Bo-he	521-61-9
Gan-cao	59870-65-4	Zhi-mu	17676-24-3	Bo-he	5524-05-0
Gan-cao	59870-68-7	Zhi-mu	136565-73-6	Bo-he	13877-91-3
Gan-cao	60008-02-8	Zhi-mu	22910-60-7	Bo-he	87-44-5
Gan-cao	60008-03-9	Zhi-mu	477-17-8	Bo-he	97-42-7
Gan-cao	604-80-8	Zhi-mu	13878-92-7	Bo-he	3387-41-5
Gan-cao	604-80-8	Zhi-mu	4184-34-3	Bo-he	18794-84-8
Gan-cao	61153-77-3	Zhi-mu	13849-08-6	Bo-he	565-00-4
Gan-cao	617-78-7	Zhi-mu	122021-74-3	Bo-he	10385-78-1
Gan-cao	64742-82-1	Zhi-mu	5187-84-8	Bo-he	481-72-1
Gan-cao	66056-18-6	Zhi-mu	54-11-5	Bo-he	6753-98-6
Gan-cao	66056-30-2	Zhi-mu	50802-21-6	Bo-he	80225-53-2
Gan-cao	66067-26-3	Zhi-mu	107259-46-1	Bo-he	138-86-3
Gan-cao	73513-42-5	Huang-qin	480-40-0	Bo-he	508-02-1
Gan-cao	74148-41-7	Huang-qin	480-40-0	Bo-he	546-79-2
Gan-cao	81202-36-0	Huang-qin	480-44-4	Bo-he	3338-55-4
Gan-cao	82209-75-4	Huang-qin	51059-44-0	Bo-he	8000-41-7
Gan-cao	822-50-4	Huang-qin	632-85-9	Bo-he	29066-34-0
Gan-cao	87746-47-2	Huang-qin	479-54-9	Bo-he	112-17-4
Gan-cao	89-78-1	Huang-qin	21967-41-9	Bo-he	80-26-2
Gan-cao	92-61-5	Huang-qin	491-67-8	Bo-he	491-07-6
Gan-cao	94805-82-0	Huang-qin	41060-16-6	Bo-he	123-35-3
Gan-cao	94805-83-1	Huang-qin	55084-08-7	Bo-he	2216-51-5
Gan-cao	961-29-5	Huang-qin	480-11-5	Bo-he	1168-42-9
Gan-cao	96-14-0	Huang-qin	491-70-3	Zhe-bei-mu	59803-98-4
Gan-cao	96-37-7	Huang-qin	520-36-5	Zhe-bei-mu	80-78-4
Gan-cao	128564-83-2	Huang-qin	1090-65-9	Zhe-bei-mu	23496-41-5
Ma-huang	1334-76-5	Huang-qin	61276-17-3	Zhe-bei-mu	18059-10-4
Ma-huang	111-14-8	Huang-qin	41365-32-6	Zhe-bei-mu	83-46-5

Ma-huang	106-73-0	Huang-qin	464-71-1	Zhe-bei-mu	139893-27-9
Ma-huang	334-48-5	Huang-qin	122622-16-6	Zhe-bei-mu	16836-31-0
Ma-huang	621-82-9	Huang-qin	38232-08-5	Zhe-bei-mu	14696-33-4
Ma-huang	89-81-6	Huang-qin	83529-62-8	Niu-bang-zi	19549-87-2
Ma-huang	117-39-5	Huang-qin	67884-12-2	Niu-bang-zi	2363-88-4
Ma-huang	142-62-1	Huang-qin	520-12-7	Niu-bang-zi	80466-34-8
Ma-huang	108-39-4	Huang-qin	102-61-4	Niu-bang-zi	123-73-9
Ma-huang	122-00-9	Xing-ren	2724-57-4	Niu-bang-zi	505-57-7
Ma-huang	552-79-4	Xing-ren	50-28-2	Niu-bang-zi	137-32-6
Ma-huang	51018-28-1	Xing-ren	2363-88-4	Niu-bang-zi	96-17-3
Ma-huang	64-18-6	Xing-ren	2463-63-0	Niu-bang-zi	3777-69-3
Ma-huang	502-61-4	Xing-ren	2305-21-7	Niu-bang-zi	86632-03-3
Ma-huang	536-60-7	Xing-ren	505-57-7	Niu-bang-zi	105-57-7
Ma-huang	84-74-2	Xing-ren	3913-71-1	Niu-bang-zi	14534-61-3
Ma-huang	84-66-2	Xing-ren	10067-06-8	Niu-bang-zi	2450-53-5
Ma-huang	84-69-5	Xing-ren	2305-21-7	Niu-bang-zi	327-97-9
Ma-huang	64-67-5	Xing-ren	327-97-9	Niu-bang-zi	928-96-1
Ma-huang	153-18-4	Xing-ren	562-74-3	Niu-bang-zi	123-51-3
Ma-huang	19078-35-4	Xing-ren	123-76-2	Niu-bang-zi	590-86-3
Ma-huang	16251-46-0	Xing-ren	327-97-9	Niu-bang-zi	589-34-4
Ma-huang	299-42-3	Xing-ren	4233-57-2	Niu-bang-zi	32451-88-0
Ma-huang	105-87-3	Xing-ren	98-55-5	Niu-bang-zi	19870-46-3
Ma-huang	3033-23-6	Xing-ren	83-46-5	Niu-bang-zi	17608-52-5
Ma-huang	91-20-3	Xing-ren	9-77-6	Niu-bang-zi	93451-44-6
Ma-huang	624-15-7	Xing-ren	706-14-9	Niu-bang-zi	4461-48-7
Ma-huang	520-36-5	Xing-ren	695-06-7	Niu-bang-zi	89-80-5
Ma-huang	14838-15-4	Xing-ren	532-28-5	Niu-bang-zi	4411-89-6
Ma-huang	14838-15-4	Xing-ren	53-16-7	Niu-bang-zi	515-13-9
Ma-huang	124-19-6	Xing-ren	57-88-5	Niu-bang-zi	17066-67-0
Ma-huang	112-05-0	Xing-ren	83-48-7	Niu-bang-zi	71-43-2
Ma-huang	110-27-0	Xing-ren	128-37-0	Niu-bang-zi	108-95-2
Ma-huang	593-50-0	Xing-ren	505-57-7	Niu-bang-zi	1182-34-9
Ma-huang	520-18-3	Xing-ren	78-70-6	Niu-bang-zi	100-44-7
Ma-huang	27234-05-5	Xing-ren	122-32-7	Niu-bang-zi	629-97-0
Ma-huang	593-45-3	Xing-ren	28880-24-2	Niu-bang-zi	638-67-5
Ma-huang	57-11-4	Xing-ren	2091-39-6	Niu-bang-zi	646-31-1
Ma-huang	143-07-7	Xing-ren	506-30-9	Niu-bang-zi	112-95-8
Ma-huang	111-82-0	Xing-ren	5561-99-9	Niu-bang-zi	629-94-7
Ma-huang	629-92-5	Xing-ren	6917-35-7	Niu-bang-zi	111-71-7
Ma-huang	628-97-7	Xing-ren	111-02-4	Niu-bang-zi	142-82-5
Ma-huang	112-39-0	Xing-ren	29883-15-6	Niu-bang-zi	83-46-5
Ma-huang	629-78-7	Xing-ren	1921-70-6	Niu-bang-zi	112-31-2
Ma-huang	629-59-4	Xing-ren	84-74-2	Niu-bang-zi	89-80-5
Ma-huang	544-63-8	Xing-ren	84-69-5	Niu-bang-zi	1241-87-8
Ma-huang	1002-84-2	Xing-ren	327-97-9	Niu-bang-zi	108-38-3
Ma-huang	6753-98-6	Xing-ren	624-15-7	Niu-bang-zi	111-02-4
Ma-huang	527-95-7	Xing-ren	5561-99-9	Niu-bang-zi	98-01-1
Ma-huang	16721-38-3	Xing-ren	74-90-8	Niu-bang-zi	629-76-5
Ma-huang	19894-97-4	Xing-ren	544-63-8	Niu-bang-zi	20362-31-6
Ma-huang	562-74-3	Xing-ren	112-85-6	Niu-bang-zi	77770-78-7
Ma-huang	90-82-4	Xing-ren	373-49-9	Niu-bang-zi	124-19-6
Ma-huang	480-17-1	Xing-ren	506-12-7	Niu-bang-zi	629-92-5
Ma-huang	121-34-6	Xing-ren	544-63-8	Niu-bang-zi	68917-75-9
Ma-huang	3387-41-5	Xing-ren	327-97-9	Niu-bang-zi	616-25-1

Ma-huang	499-75-2	Xing-ren	463-40-1	Niu-bang-zi	301-00-8
Ma-huang	106-22-9	Xing-ren	2197-37-7	Niu-bang-zi	2197-37-7
Ma-huang	6379-73-3	Xing-ren	68605-14-1	Niu-bang-zi	112-63-0
Ma-huang	520-32-1	Xing-ren	99-18-3	Niu-bang-zi	95-92-1
Ma-huang	68526-83-0	Xing-ren	67701-08-0	Niu-bang-zi	100-41-4
Ma-huang	124-07-2	Xing-ren	57-11-4	Niu-bang-zi	78-83-1
Ma-huang	111-11-5	Xing-ren	27234-05-5	Qing-hao	76-49-3
Ma-huang	6415-59-4	Xing-ren	112-80-1	Qing-hao	125-12-2
Ma-huang	463-40-1	Xing-ren	112-62-9	Qing-hao	115-95-7
Ma-huang	2197-37-7	Xing-ren	143-07-7	Qing-hao	80-26-2
Ma-huang	1365-19-1	Xing-ren	630-02-4	Qing-hao	25154-56-7
Ma-huang	99-18-3	Xing-ren	629-97-0	Qing-hao	138-86-3
Ma-huang	928-96-1	Xing-ren	630-03-5	Qing-hao	486-21-5
Ma-huang	64-17-5	Xing-ren	630-01-3	Qing-hao	855-96-9
Ma-huang	64-19-7	Xing-ren	593-49-7	Qing-hao	569-80-2
Ma-huang	76-49-3	Xing-ren	638-67-5	Qing-hao	87-44-5
Ma-huang	79-20-9	Xing-ren	646-31-1	Qing-hao	6753-98-6
Ma-huang	115-95-7	Xing-ren	112-95-8	Qing-hao	508-32-7
Ma-huang	74-84-0	Xing-ren	629-99-2	Qing-hao	519-96-0
Ma-huang	79-31-2	Xing-ren	629-94-7	Qing-hao	117-39-5
Ma-huang	95910-36-4	Xing-ren	544-85-4	Qing-hao	7787-20-4
Ma-huang	25465-65-0	Xing-ren	630-05-7	Qing-hao	520-18-3
Ma-huang	489-84-9	Xing-ren	14167-59-0	Qing-hao	120-08-1
Ma-huang	99-50-3	Xing-ren	638-68-6	Qing-hao	559-74-0
Ma-huang	76-22-2	Xing-ren	630-07-9	Qing-hao	5085-72-3
Ma-huang	150-86-7	Xing-ren	630-04-6	Qing-hao	491-70-3
Ma-huang	138-86-3	Xing-ren	593-45-3	Qing-hao	69-72-7
Ma-huang	2111-75-3	Xing-ren	629-92-5	Qing-hao	123-35-3
Ma-huang	557-61-9	Xing-ren	629-73-2	Qing-hao	10385-78-1
Ma-huang	630-03-5	Xing-ren	629-78-7	Qing-hao	34334-69-5
Ma-huang	25154-56-7	Xing-ren	629-50-5	Qing-hao	63968-64-9
Ma-huang	638-67-5	Xing-ren	629-59-4	Qing-hao	56121-42-7
Ma-huang	646-31-1	Xing-ren	629-62-9	Qing-hao	92-61-5
Ma-huang	18733-57-8	Xing-ren	150-86-7	Qing-hao	5188-73-8
Ma-huang	506-30-9	Xing-ren	502-69-2	Qing-hao	124-76-5
Ma-huang	629-94-7	Xing-ren	638-36-8	Qing-hao	76-50-6
Ma-huang	4602-84-0	Xing-ren	373-49-9	Qing-hao	546-49-6
Ma-huang	2463-53-8	Xing-ren	2091-29-4	Qing-hao	78-70-6
Ma-huang	106-28-5	Lian-qiao	7770-78-7	Qing-hao	83-48-7
Ma-huang	6874-10-8	Lian-qiao	29388-59-8	Qing-hao	5779-62-4
Ma-huang	87-44-5	Lian-qiao	480-10-4	Qing-hao	82442-48-6
Ma-huang	78-70-6	Lian-qiao	20362-31-6	Qing-hao	145941-07-7
Ma-huang	13270-61-6	Lian-qiao	331-39-5	Qing-hao	101020-89-7
Ma-huang	21391-98-0	Lian-qiao	75775-36-9	Qing-hao	546-49-6
Yin-hua	60047-17-8	Lian-qiao	40661-45-8	Qing-hao	80286-58-4
Yin-hua	106-22-9	Lian-qiao	25488-59-9	Qing-hao	99-85-4
Yin-hua	624-15-7	Lian-qiao	6883-44-9	Qing-hao	562-74-3
Yin-hua	624-15-7	Lian-qiao	24404-50-0	Qing-hao	98-55-5
Yin-hua	1139-30-6	Lian-qiao	149-32-6	Qing-hao	138-87-4
Yin-hua	117-39-5	Lian-qiao	487-39-8	Qing-hao	586-81-2
Yin-hua	118627-52-4	Lian-qiao	43043-09-0	Qing-hao	3917-48-4
Yin-hua	122739-11-1	Lian-qiao	21637-25-2	Qing-hao	502-61-4
Yin-hua	136849-88-2	Lian-qiao	580-72-3	Qing-hao	3856-25-5
Yin-hua	140360-29-8	Lian-qiao	508-02-1	Qing-hao	40939-72-8

Yin-hua	14215-86-2	Lian-qiao	487-41-2	Qing-hao	483-76-1
Yin-hua	153-18-4	Lian-qiao	487-36-5	Qing-hao	603-61-2
Yin-hua	15486-34-7	Lian-qiao	117-39-5	Qing-hao	99-48-9
Yin-hua	18103-41-8	Lian-qiao	29388-59-8	Qing-hao	91-64-5
Yin-hua	18524-94-2	Lian-qiao	57-11-4	Qing-hao	470-82-6
Yin-hua	20549-47-7	Lian-qiao	110-15-6	Qing-hao	14787-34-9
Yin-hua	22255-40-9	Lian-qiao	77-52-1	Qing-hao	5208-49-1
Yin-hua	2415-24-9	Lian-qiao	121-34-6	Qing-hao	80-56-8
Yin-hua	25406-64-8	Lian-qiao	80-56-8	Qing-hao	18172-67-3
Yin-hua	29548-30-9	Lian-qiao	83-46-5	Qing-hao	479-90-3
Yin-hua	327-97-9	Lian-qiao	127-91-3	Qing-hao	515-13-9
Yin-hua	33289-85-9	Lian-qiao	4481-62-3	Qing-hao	29873-99-2
Yin-hua	27013-91-8	Lian-qiao	156-38-7	Qing-hao	569-92-6
Yin-hua	37839-63-7	Lian-qiao	78-70-6	Qing-hao	90-19-7
Yin-hua	3856-25-5	Lian-qiao	51059-44-0	Qing-hao	6601-62-3
Yin-hua	471271-55-3	Lian-qiao	474-58-8	Qing-hao	76-22-2
Yin-hua	482-35-9	Lian-qiao	487-39-8	Qing-hao	79-92-5
Yin-hua	482-36-0	Lian-qiao	61276-17-3	Qing-hao	63968-64-9
Yin-hua	489-39-4	Lian-qiao	153-18-4	Shi-gao	7778-18-9
Yin-hua	489-86-1	Lian-qiao	23202-85-9		
Yin-hua	491-70-3	Lian-qiao	10338-51-9		

Table S2 Compound Information. In this table, information of all the distinct compounds is presented. Each record introduces one compound. Information contains compound CASRN, compound name, compound frequency and a tick on whether this compound has Associated Genes in CTD Database. Compound frequency refers to the number of times the compound occurs in the constitution information of formula. “G” in the last column tells that the compound has Associated Genes.

CAS	compound name	frequency	Associated Genes	CAS	compound name	frequency	Associated Genes
327-97-9	lvyuansuan beta-	7	G	134958-57-9	Vgancaonin V	1	
83-46-5	Sitosterol	6		593-49-7	N-HEPTACOSANE	1	
78-70-6	linalool	6	G	124596-87-8	gancaonin C	1	
117-39-5	quercetin	5	G	81525-13-5	ForsythosideB	1	
6753-98-6	caryophyllene	5		81202-36-0	choerospondin	1	
138-86-3	limonene	4	G	76844-67-2	thymonin	1	
153-18-4	rutin	4	G	18794-84-8	beta-Farnesene	1	
520-18-3	kaempferol	4	G	77-95-2	Quinic acid	1	G
491-70-3	luteolin	4	G	481-34-5	α-cadinol	1	
98-55-5	α-terpineol	4		66056-18-6	glycyrin	1	
624-15-7	geraniol	4	G	77-52-1	uraolic acid	1	G
89-83-8	Thymol	3	G	6883-44-9	EGENINE	1	
87-44-5	trans-caryophyllene	3		19103-54-9	salvigenin	1	
520-36-5	apigenin	3	G	112-31-2	Decaldehyde	1	G
544-63-8	Myristic acid	3	G	144506-15-0	licochalcone D	1	
520-32-1	tricin	3		111-11-5	octanoic acid methyl ester	1	
629-92-5	N-NONADECANE	3		89-78-1	Racementhol	1	
57-11-4	octadecanoic acid	3	G	905-99-7	4-caffeoylquinic acid	1	
10385-78-1	Borneol	3	G	17608-52-5	4-caffeoylquinic acid	1	
646-31-1	tetracosane	3		544-85-4	DOTRIACONTANE	1	
629-94-7	N-HENEICOSANE	3		111-14-8	heptanoic acid	1	G
2197-37-7	linoleic acid	3	G	512-04-9	Spirost-5-en-3-ol, (3beta, 25S)-Ethyl	1	G
638-67-5	tricosane	3		544-35-4	linoleate	1	

Table S2

3387-41-5	sabinene	3		552-59-0	prunetin	1	G
83-48-7	stigmasterol	3	G	124596-88-9	gancaonin D	1	
76-49-3	bornyl acetate	3		100-41-4	Ethylbenzene	1	G
562-74-3	4-terpineol	3		17038-80-9	licopyranocoumarin	1	
76-22-2	camphor	3	G	19894-97-4	Myrtenol	1	G
505-57-7	2-hexenal	3	G	25406-64-8	morroneiside	1	
123-35-3	myrcene	3		41060-16-6	Skullcapflavone I	1	
80-56-8	alpha-Pinene	3	G	16836-31-0	kauran-16 α , 17-diol	1	
13877-91-3	beta-trans-Ocimene	2		10338-51-9	Rhodioloside	1	
480-44-4	acacetin	2	G	515-00-4	2-Pinen-10-ol	1	
2305-21-7	2-hexenol	2		78-83-1	Isobutyl alcohol	1	G
565-00-4	Camphene	2		13849-08-6	Marmesin	1	
480-40-0	Chrysin	2	G	58749-23-8	Licochalcone B	1	
79-92-5	camphene	2		569-92-6	rhamnocitrin	1	
1365-19-1	linalool oxide	2		1921-70-6	pristane	1	G
41365-32-6	cirsilineol	2		6617-34-1	(+)-Car-3-ene-2, 5-dione	1	
89-80-5	Menthone	2	G	80286-58-4	artemisinic acid	1	
121-34-6	vanillic acid	2	G	118627-52-4	epi-vogeloside	1	
470-82-6	cineole	2	G	552-79-4	methylephedrine	1	
546-49-6	isoartemisiaketone	2		90-82-4	pseudoephedrine	1	
3856-25-5	α -copaene	2		40661-45-8	cornoside	1	
604-80-8	narcissin	2		112-17-4	Acetic acid, decyl ester	1	
499-75-2	carvacrol	2	G	2091-39-6	Eicosadienoic acid	1	
25154-56-7	nonacosanol	2		150853-99-9	uralene	1	
143986-30-5	uralenneoside	2		543-39-5	myrcenol	1	G
150-86-7	Phytol	2	G	2724-57-4	12-Methyl-tridecanoicacid	1	
629-59-4	tetradecane	2		28880-24-2	di-iso-octyl succinate	1	
14534-61-3	3, 4-Dicaffeoylquinicacid	2		71-43-2	Benzene	1	G

Table S2

506-30-9	Eicosanoic acid	2		4233-57-2	6-Oxo-octanoic acid	1	
129314-37-0	Licorisoflavan A	2		479-90-3	artemetin	1	
2363-88-4	Decadienal	2	G	481-72-1	Aloe emodin	1	G
27234-05-5	octadecanoic acid methyl ester	2		90-19-7	rhamnetin	1	G
112-95-8	N-EICOSANE	2		55954-61-5	pseudo-hypericin	1	G
82597-74-8	Sarsasapogenin	2	G	15297-99-1	norlapachol	1	
928-96-1	Leaf alcohol	2	G	27762-99-8	Agancaonin A	1	
639-99-6	Elemol	2		629-99-2	N-PENTACOSANE	1	
629-97-0	N-DOCOSANE	2		480-11-5	Aoroxylin, oroxylin A	1	G
20362-31-6	ARCTIIN	2	G	125310-04-5	glycyroside	1	
480-10-4	astragalin	2	G	626-93-7	2-Hexanol	1	
334-48-5	Decanoic acid	2	G	695-06-7	γ -hexanolactone	1	
23202-85-9	matairesinonide	2		69-72-7	salicylic acid	1	G
14838-15-4	norephedrine	2	G	101020-89-7	artemisitenene	1	
331-39-5	Caffeic acid	2	G	64-18-6	formic acid	1	G
486-62-4	ononin	2		41983-91-9	glabranin	1	
29388-59-8	SECOISOLARICIRESINOL	2	G	536-60-7	Cumic alcohol	1	
301-00-8	Methyl linolenate	2		59803-98-4	Brimonidine	1	G
61276-17-3	acetoside	2	G	472-70-8	Cryptoxanthin	1	G
143-07-7	dodecanoic acid	2	G	120-72-9	Indole	1	G
5561-99-9	Eicosenoic acid	2		27013-91-8	α -hederin	1	G
84-69-5	Diisobutyl phthalate	2	G	111-71-7	N-Heptanal	1	G
22255-40-9	loganic acid	2		123-41-1	Sincaline	1	
92-61-5	scopoletin	2	G	28591-01-7	F-gitonin	1	
80-26-2	4-terpinyl acetate	2		124-07-2	octanoic acid	1	G
482-36-0	hyperoside	2	G	64-17-5	ethanol	1	G
502-61-4	farnesene	2		629-62-9	N-PENTADECANE	1	
373-49-9	hexadecenoic acid	2		23494-48-6	nodifloretin	1	
111-02-4	squalene	2	G	38232-08-5	gaylussacin	1	
63968-64-9	qinghaosuIII	2	G	67701-08-0	Isooleic acid	1	

Table S2

112-63-0	methylinoleate	2		74518-57-3	xylostosidine	1	
106-22-9	Citronellol	2		855-96-9	eupatorin	1	G
515-13-9	β -elemene	2	G	519-96-0	patuletin	1	
84-74-2	Dibutyl phthalate	2	G	137-32-6	2-Methyl-1-butanol	1	
629-78-7	N-HEPTADECANE	2		475-20-7	Longifolene	1	
115-95-7	acetic acid linalool ester	2		5208-59-3	beta-Bourbonene	1	
628-97-7	Palmiticacid, ethylester	2		24699-16-9	Isomangiferin	1	
487-36-5	(+)-Pinoresinol	2		491-71-4	chrysoeriol	1	G
64809-67-2	Neomangiferin	2		75775-36-9	cedrusin	1	
124-19-6	Nonanal 3,5-Dicaffeoylquinic acid	2	G	100-44-7	Benzyl chloride	1	
2450-53-5		2		43043-09-0	forsythide	1	
99-18-3	Prunasin	2		580-72-3	MATAIRESINOL	1	
51059-44-0	Oroxindin	2		94805-82-0	Glycycoumarin	1	
593-45-3	Octadecane	2		98-92-0	Niacinamide	1	G
508-02-1	Oleanolic acid (+)-pinoresinolmonomethyl ether	2	G	144506-14-9	licochalcone C	1	
487-39-8		2		487-41-2	PHILLYRIN	1	
474-58-8	alexandrin	2		494-90-6	Menthofuran	1	G
463-40-1	Linolenic acid	2	G	138-87-4	β -terpineol	1	
21637-25-2	ISOQUERCETIN	2		506-12-7	Heptadecanoic acid	1	
630-03-5	nonacosane	2		3033-23-6	roseoxide	1	
2798-20-1	gardenin B	1		961-29-5	isoliquiritigenin	1	G
89-81-6	Piperitone	1		13270-61-6	delphinidin	1	G
131-11-3	dimethyl phthalate	1	G	41059-79-4	TimosaponinA-III	1	
61153-77-3	Licoflavone A	1		7778-18-9	Calcium sulfate	1	
3913-71-1	2-Decenal	1	G	108-95-2	Phenol	1	G
106-28-5	Farnesol	1		136849-88-2	macranthoidin B	1	
127-91-3	beta-Pinene	1	G	25465-65-0	isopinocampheol	1	
18530-03-5	Campherenol	1		122-00-9	methylacetophenone	1	

Table S2

124596-89-0	gancaonin E	1		480-17-1	leucocyanidin	1	
74-84-0	ethane	1	G	520-34-3	diosmetin	1	G
5187-84-8	Neoglucobrassicin	1	G	64-19-7	acetic acid	1	G
95-92-1	Diethyl oxalate	1		18059-10-4	Imperialine	1	
76-50-6	bornyl isovalerate	1		630-05-7	N-TRITRIACONTANE	1	
5392-40-5	geranial	1	G	56121-42-7	aurantiamideacetate	1	
30508-27-1	licoricidin	1		19870-46-3	1,3-dicaffeoylquinic acid	1	
126716-36-7	Gancaonin I	1		68605-14-1	methyl linoleate	1	
54-11-5	Nicotine	1	G	55290-63-6	Atractylodin	1	
483-76-1	δ -cadinol/ δ -cadinene	1		84-66-2	diethyl phthalate	1	G
64742-82-1	Hexane	1		129145-54-6	Pgancaonin P	1	
124596-86-7	gancaonin B	1		589-34-4	Hexane, 3-methyl-	1	
144-68-3	Zeaxanthin	1	G	629-50-5	n-Tridecane	1	
498-45-3	Scopine	1		67884-12-2	martynoside	1	
1616-93-9	β -amyrin acetate	1		59472-23-0	secologanoside	1	
68917-75-9	Wintergreen Oil	1		74563-64-7	Phytantriol	1	
60008-02-8	glabrone	1		120-51-4	benzylbenzoate	1	
120-08-1	aesculetindimethyl ether	1	G	479-54-9	Carthamidin	1	
110-15-6	SUCCINIC acid	1	G	82442-48-6	arteannuin A	1	
97-53-0	eugenol	1	G	19078-35-4	patchoulane	1	
104-46-1	Benzene, 1-methoxy-4-1-propenyl	1	G	94805-83-1	isolicoflavonol	1	
5373-11-5	luteolin-7-O- β -D-glucoside	1	G	16251-46-0	ephedroxane	1	
3777-69-3	Furan, 2-pentyl-	1		142759-74-8	pseudoprototimosaponinA-III	1	
23130-22-5	sorbifolin	1		66056-30-2	licoisoflavone B	1	
120-46-7	dibenzoylmethane	1	G	477-17-8	Hippeastrine	1	
74148-41-7	3-Hydroxyglabrol	1		80466-34-8	2,4-Hexadienal	1	G

Table S2

	7-methoxy-2-methylisoflavone					G
19725-44-1		1		18524-94-2	loganin	1
13466-78-9	3-carene	1		24189-95-5	Matatabiether 2,3-dimethylpentane	1
121709-66-8	apioglycyrrhizin	1		565-59-3		1
77770-78-7	Arctigenin 7,4'-Dimethoxyisoflavone	1		29202-00-4	gardenin D	1
1157-39-7	Emodinanthrone	1		129280-33-7	semilicoisoflavone B	1
491-60-1		1		118524-14-4	licocoumarone	1
77-53-2	Cedrol	1		16721-38-3	cis-piperitol	1
5188-73-8	axillarin	1		123914-44-3	Glyuranolide	1
40939-72-8	γ -cadinene	1		149-32-6	ERYTHRITOL	1
5779-62-4	β -sitosterol	1	G	82209-75-4	liconeolignan	1
518-82-1	Emodin	1	G	4481-62-3	Lup-20(29)-en-28-oic acid, 3-oxo-	1
134958-53-5	Rgancaonin R	1		629-76-5	1-Pentadecanol	1
2463-53-8	2-Nonenal	1	G	118525-49-8	licorice-saponin C2	1
17066-67-0	beta-Selinene	1		142-62-1	hexanoic acid	1
586-81-2	γ -terpineol	1		104691-86-3	lupiwighteone	1
27978-14-9	Safynol	1		53-16-7	estrone	1
66067-26-3	liscoisoflavone	1		97-42-7	Carvyl acetate	1
58749-22-7	liscochalcone A	1	G	617-78-7	3-ethylpentane	1
18085-97-7	jaceosidin	1		589-98-0	3-Octanol	1
630-02-4	n-Octacosane	1		29883-15-6	amygdalin 1,5-dicaffeoylquinic acid	1
2415-24-9	Catalpol	1		1182-34-9	quercetin-3-O-beta-D-glucoside	1
138831-68-2	smilageninoside	1		482-35-9		1
603-61-2	tamarixetin	1		638-68-6	N-TRIACONTANE 5,6,7,4'-tetramethoxyflavone	1
71-41-0	3-Pentanol	1	G	1168-42-9		1

Table S2

578-74-5	cosmosiin	1		93451-44-6	4-p-coumaroylquinic acid	1	
95910-36-4	isoleucene	1		485-72-3	formononetin	1	G
14215-86-2	sweroside	1		19549-87-2	1-Heptene, 2, 4-dimethyl-	1	
150853-98-8	uralenol-3-methylether	1		8007-87-2	Oils, cubeb	1	
481-74-3	Chrysophanic acid	1		590-86-3	Isovaleraldehyde	1	
145941-07-7	artemisinin B Methyl	1		106-73-0	heptanoic acid methyl ester	1	
93-58-3	benzoate	1		111-82-0	Methyl dodecanoate	1	
99-50-3	protocatechuic acid	1	G	486-21-5	6, 8-dimethoxy-7-hydroxycoumarin	1	
1002-84-2	Pentadecanoic acid	1		529-44-2	Myricetin	1	G
24404-50-0	epipinoresinol	1		34221-41-5	echinatin	1	
112-39-0	Methyl palmitate	1		123-73-9	(E)-Crotonaldehyde	1	
21391-98-0	Phellandral	1		10067-06-8	2-Hydroxy-hexadecanoic acid	1	
6379-73-3	carvacrol methyl ether	1		508-32-7	tricyclene	1	
87746-47-2	uralenin	1		156-38-7	4-Hydroxyphenylacetic acid	1	G
632-85-9	Wogonin	1	G	4773-96-0	mangiferin	1	G
548-03-8	protohypericin	1		638-36-8	phytane	1	
15486-34-7	7, 3', 4'-trimethyl-luteolin	1		105-87-3	geranyl acetate	1	
299-42-3	ephedrine	1	G	706-14-9	γ -Decanolactone	1	G
139893-27-9	peimisine	1		2216-51-5	Levomenthol	1	
121687-83-0	Araboglycyrrhizin	1		37839-63-7	germacrene-D	1	
551-15-5	liquiritin	1		99-48-9	carveol	1	G
122622-16-6	galericulin	1		105-57-7	Acetal	1	

Table S2

593-50-0	n- triacontanol	1		74-90-8	hydrogen cyanide	1	G
6151-25-3	Quercetin dihydrate	1		17884-88-7	Myricadiol	1	
79-83-4	Pantothenic Acid	1	G	4382-17-6	quercetin- 3',3'- dimethylether	1	
32451-88-0	4,5- dicaffeoylqui nic acid	1		17306-46-6	rhoifolin	1	
621-82-9	cinnamic acid 2,4-	1	G	18733-57-8	trichloroeicos yl-Silane	1	
589-43-5	dimethylhexan e	1		128-37-0	Butylated hydroxytoluene	1	G
79-20-9	Methyl acetate	1		139163-15-8	uralenol 1-	1	
68526-83-0	octanol	1	G	1241-87-8	caffeoylquinic acid	1	
51847-92-8	licoricone	1		110-27-0	isopropyl myristate	1	
18172-67-3	β -pinene	1		102-61-4	pinosylvin	1	G
54328-09-5	protopseudohy pericin	1		14696-33-4	kaur-15-en-17- ol	1	
57-88-5	cholesterol	1	G	112-05-0	nonanoic acid	1	G
437-64-9	genkwanin	1	G	136656-07-0	Timosaponin b- II	1	
50-28-2	17 β - estradiol	1	G	559-74-0	friedelin	1	G
112-80-1	oleic acid delta-	1	G	532-28-5	Mandelonitrile	1	
7299-42-5	Terpineol	1		108-39-4	m-Cresol	1	G
69671-15-4	α -Muurolene	1		22910-60-7	Ginkgolic acid	1	
136-60-7	butyl benzoate	1		117038-82-1	isoglycycoumar in	1	
124-76-5	isoborneol	1		112-85-6	Behenic acid	1	
17699-14-8	alpha- cubebene	1		569-80-2	penduletin	1	
91-22-5	quinoline	1	G	4184-34-3	Mangiferolic acid	1	
112-62-9	methyl oleate	1		1139-30-6	(-)-beta- Caryophyllene	1	
98-01-1	Furfural	1		7212-44-4	epoxide	1	
4602-84-0	Nerolidol	1	G	1447-88-7	hispidulin	1	
21368-68-3	farnesol	1		4852-22-6	Procyanidin	1	G
23013-84-5	Camphor	1		18103-41-8	corymbosin	1	
	neoglycyrol	1					

Table S2

129145-50-2	gancaonin L	1		220860-37-7	Kanzonol Z	1	
139051-27-7	Anemarsaponin B	1		502-69-2	Phytone	1	
134958-54-6	Sgancaonin S	1		16545-23-6		1	
50802-21-6	Tingenone	1		125-12-2	isobornyl acetate	1	
129145-53-5	Ogancaonin O	1		6917-35-7	inositol	1	G
79-31-2	isobutyric acid	1		83529-62-8	leucosceptoside	1	
562-49-2	3, 3-dimethylpentane	1		59-67-6	Niacin	1	G
590-35-2	2, 2-dimethylpentane	1		13878-92-7	Isomangiferolic acid	1	
105038-43-5	uralsaponinB	1		91-64-5	coumarin	1	G
578-86-9	liquiritogenin	1		51419-48-8	hydnocarpin	1	
7787-20-4	fenchone	1		2859-88-3	7-hydroxy-2-methylisoflavone	1	
34334-69-5	cirsiliol	1	G	1401-55-4	Tannic acid	1	
108-38-3	3-Xylene	1	G	14167-59-0	N-TETRATRIACONTANE	1	
80225-53-2	Rosmarinic acid	1		60077-47-6	vogeloside	1	
464-71-1	clerodin	1		521-61-9	Physcione	1	
489-84-9	guaiazulene	1		96-37-7	methylcyclopentane	1	
5085-72-3	3 β -friedelanol	1		17676-24-3	hinokiresinol	1	
8000-41-7	Terpineol	1		629-73-2	N-HEXADECANE	1	
520-12-7	pectolinarigenin	1		1334-76-5	methyl furoate	1	
630-01-3	N-HEXACOSANE	1		60976-49-0	Geraniin	1	G
123-76-2	4-Oxo-pentanoicacid	1		3917-48-4	α -thujene	1	
11079-53-1	hyperforin	1	G	5524-05-0	d-Dihydrocarvone (E)-aldosecologanin	1	
103000-77-7	uralsaponinA	1		471271-55-3		1	
96-17-3	Butanal, 2-methyl-	1		6601-62-3	cirsimaritin	1	
29873-99-2	γ -elemene	1		29066-34-0	Menthyl acetate	1	

Table S2

15932-80-6	R-Pulegone	1	G	522-12-3	quercitrin	1	G
113558-15-9	Baohuoside I	1		21967-41-9	baicalin	1	G
8047-15-2	Saponins	1		57378-72-0	4, 5-Dicaffeoylquinic acid	1	
107259-46-1	Xuelianlactone	1		99-85-4	β -terpinene	1	
2111-75-3	perillaldehyde	1	G	59870-68-7	glabridin	1	G
5208-49-1	4-carene	1		99-86-5	alpha-Terpinene	1	
60008-03-9	glabrene	1		1090-65-9	Alpinetin	1	
7770-78-7	ARCTIGENIN	1	G	23496-41-5	Verticine	1	
527-95-7	herbacetin	1		557-61-9	octacosanol	1	
122021-74-3	Monomethyl lithospermate	1	G	22384-63-0	pedalitin	1	
142-82-5	Heptane	1		616-25-1	1-Penten-3-ol	1	
32383-76-9	medicarpin	1		2463-63-0	2-Heptenal	1	G
73513-42-5	hexanes	1		86632-03-3	3, 4, 5-tricaffeoylquinic acid	1	
64-67-5	Diethylsulfate	1	G	3809-79-5	liquoric acid	1	
122739-11-1	fulvotomentoside A	1		6415-59-4	Sedanolid	1	
134958-52-4	Qgancaonin Q	1		123-51-3	Isoamyl alcohol	1	G
630-04-6	N-HENTRIACONTANE	1		584-94-1	2, 3-dimethylhexane	1	
122-32-7	triolein	1	G	129145-52-4	Ngancaonin N	1	
91-20-3	Naphthalene	1	G	6874-10-8	trans-ocimene	1	
140360-29-8	macranthoidin A	1		2955-23-9	olivil	1	
491-67-8	baicalein	1	G	134958-55-7	Tgancaonin T	1	
10176-71-3	ladanein	1		51938-32-0	schaftoside	1	
46763-58-8	glypallichalcone1	1		134958-56-8	Ugancaonin U	1	
2091-29-4	Palmitoleic acid	1	G	25488-59-9	DI methyl MATAIRESINOL	1	
4461-48-7	4-Methylpent-2-ene	1		1191-41-9	ethyl linolenate	1	
96-14-0	3-methylpentane	1		136565-73-6	Timosaponin E	1	
33289-85-9	dipsacoside	1		491-07-6	Isomenthone	1	
630-07-9	N-PENTATRIACONTANE	1		1617-53-4	Amentoflavone	1	G

Table S2

2623-23-6	1-Menthyl acetate	1		59870-65-4	glabrol methylpseudoep	1	
548-04-9	Hypericin	1	G	51018-28-1	hedrine Skullcapflavon	1	
129145-51-3	Gancaonin M	1		55084-08-7	e II	1	
80-78-4	Solanidine	1					
51317-08-9	2-Naphthalenemethanol, decahydro-alpha, alpha, 4a, 8-tetramethyl-					1	
489-39-4	(1AR-(1aalpha, 4aalpha, 7alpha, 7abeta, 7balph)))-decahydro-1, 1, 7-					1	
20549-47-7	Cyclohexanol, 2-methyl-5-(1-methylethenyl)-, (1R-					1	G
29548-30-9	2, 6, 10-Dodecatrien-1-ol, 3, 7, 11-trimethyl-, acetate					1	
4411-89-6	Benzeneacetaldehyde, alpha-ethylidene-					1	
60047-17-8	2-Furanmethanol, 5-ethenyltetrahydro-alpha, alpha, 5-trimethyl-					1	
128564-83-2	4H-Pyran-4-one, 2, 3-dihydro-3, 5-dihydroxy-6-methy					1	
546-79-2	2-Methyl-5-(1-methylethyl)bicyclo(3. 1. 0)hexan-2-ol					1	
9-77-6	4-(2, 6, 6-Trimethyl-1-cyclohexenyl)-3-buten-2-one					1	
489-86-1	trimethyl-4-methylene-1H-cycloprop(e)azulene					2	
129-66-8	METHYL12-METHYLTETRADECANOATE					1	
822-50-4	1, 2-TRANS-DIMETHYLCYCLOPENTANE					1	
14787-34-9	5-hydroxy-3, 6, 7, 4'-tetramethoxyflavone					1	
3338-55-4	1, 3, 6-Octatriene, 3, 7-dimethyl-, (3Z)-					1	

Table S2

Table S3 The 153 compounds. In this table, the 153 compounds that have Associated Genes information are presented. These compounds are used to predict active drug components and gene targets.

CAS	compound name	CAS	compound name
327-97-9	lvyuansuan	1921-70-6	pristane
78-70-6	linalool	543-39-5	myrcenol
117-39-5	quercetin	71-43-2	Benzene
138-86-3	limonene	481-72-1	Aloe emodin
153-18-4	rutin	90-19-7	rhamnetin
520-18-3	kaempferol	55954-61-5	pseudo-hypericin
491-70-3	luteolin	480-11-5	Aoroxylin, oroxylin A
624-15-7	Nerol	69-72-7	salicylic acid
89-83-8	Thymol	64-18-6	formic acid
520-36-5	apigenin	59803-98-4	Brimonidine
544-63-8	Myristic acid	472-70-8	Cryptoxanthin
57-11-4	octadecanoicacid	120-72-9	Indole
10385-78-1	Borneol	27013-91-8	α -hederin
2197-37-7	linoleic acid	111-71-7	N-Heptanal
83-48-7	stigmasterol	124-07-2	octanoicacid
76-22-2	camphor	64-17-5	ethanol
505-57-7	2-hexenal	855-96-9	eupatorin
80-56-8	alpha-Pinene	491-71-4	chrysoeriol
480-44-4	acacetin	98-92-0	Niacinamide
480-40-0	Chrysin	494-90-6	Menthofuran
89-80-5	Menthone	961-29-5	isoliquiritigenin
121-34-6	vanillic acid	13270-61-6	delphinidin
470-82-6	cineole	108-95-2	Phenol
499-75-2	carvacrol	520-34-3	diosmetin
150-86-7	Phytol	64-19-7	acetic acid
2363-88-4	2, 4-Decadienal	84-66-2	diethyl phthalate
82597-74-8	Sarsasapogenin	80466-34-8	2, 4-Hexadienal
928-96-1	Leaf alcohol	18524-94-2	loganin
20362-31-6	ARCTIIN	53-16-7	estrone
480-10-4	astragalin	97-42-7	Carvyl acetate
334-48-5	Decanoic acid	485-72-3	formononetin
14838-15-4	norephedrine	529-44-2	Myricetin
331-39-5	Caffeic acid	156-38-7	4-Hydroxyphenylacetic acid
29388-59-8	SECOISOLARICIRESinOL	4773-96-0	mangiferin
61276-17-3	acetoside	706-14-9	γ -Decanolactone
143-07-7	dodecanoic acid	99-48-9	carveol
84-69-5	Diisobutyl phthalate	74-90-8	hydrogen cyanide
92-61-5	scopoletin	128-37-0	Butylated hydroxytoluene
482-36-0	hyperoside	102-61-4	pinosylvlin
111-02-4	squalene	112-05-0	nonanoic acid
63968-64-9	qinghaosuIII	559-74-0	friedelin
515-13-9	β -elemene	108-39-4	m-Cresol
84-74-2	Dibutyl phthalate	4852-22-6	Procyanidin
124-19-6	Nonanal	6917-35-7	inositol
508-02-1	Oleanolic acid	59-67-6	Niacin
463-40-1	Linolenic acid	91-64-5	coumarin
131-11-3	dimethyl phthalate	60976-49-0	Geraniin
3913-71-1	2-Decenal	522-12-3	quercitrin
127-91-3	beta-Pinene	21967-41-9	baicalin
74-84-0	ethane	59870-68-7	glabridin
5187-84-8	Neoglucobrassicin	2463-63-0	2-Heptenal
5392-40-5	geranial	123-51-3	Isoamyl alcohol
54-11-5	nicotine	299-42-3	ephedrine
144-68-3	Zeaxanthin	79-83-4	Pantothenic Acid

Table S3

120-08-1	aesculetindimethyl ether	621-82-9	cinnamic acid
110-15-6	SUCCINIC acid	68526-83-0	octanol
97-53-0	eugenol	57-88-5	cholesterol
104-46-1	Benzene, 1-methoxy-4-1-propenyl	437-64-9	genkwanin
5373-11-5	luteolin-7-O- β -D-glucoside	50-28-2	17 β -estradiol
120-46-7	dibenzoylmethane	112-80-1	oleic acid
5779-62-4	β -sitosterol	91-22-5	quinoline
518-82-1	Emodin	4602-84-0	farnesol
2463-53-8	2-Nonenal	34334-69-5	cirsiliol
58749-22-7	licochalcone A	108-38-3	3-Xylene
71-41-0	3-Pentanol	11079-53-1	hyperforin
99-50-3	protocatechuic acid	15932-80-6	R-Pulegone
632-85-9	Wogonin	2111-75-3	perillaldehyde
77-95-2	Quinic acid	7770-78-7	ARCTIGENIN
77-52-1	uraolic acid	122021-74-3	Monomethyl lithospermate
112-31-2	Decaldehyde	64-67-5	Diethylsulfate
111-14-8	heptanoic acid	122-32-7	triolein
512-04-9	Spirost-5-en-3-ol, (3 β , 25S)-	91-20-3	Naphthalene
552-59-0	prunetin	491-67-8	baicalein
100-41-4	Ethylbenzene	2091-29-4	Palmitoleic acid
19894-97-4	Myrtenol	548-04-9	Hypericin
78-83-1	Isobutyl alcohol	1617-53-4	Amentoflavone
20549-47-7	Cyclohexanol, 2-methyl-5-(1-methylethenyl)-,		(1R-(1 α , 2 β , 5 α))-

Table S4 Pathway Information. In this table, KEGG pathway information of the 152 selected genes is presented with KEGG Pathway entries.

Entrez Gene ID	Pathways
7124	hsa04010; hsa04060; hsa04210; hsa04350; hsa04380; hsa04612; hsa04620; hsa04621; hsa04622; hsa04640; hsa04650; hsa04660; hsa04664; hsa04920; hsa04930; hsa04940; hsa05010; hsa05014; hsa05133; hsa05134; hsa05140; hsa05142; hsa05143; hsa05144; hsa05145; hsa05146; hsa05152; hsa05160; hsa05164; hsa05166; hsa05168; hsa05310; hsa05322; hsa05323; hsa05330; hsa05332; hsa05410; hsa05414;
1543	hsa00140; hsa00380; hsa00830; hsa00980; hsa01100;
836	hsa04010; hsa04115; hsa04210; hsa04650; hsa04726; hsa05010; hsa05012; hsa05014; hsa05016; hsa05120; hsa05133; hsa05134; hsa05145; hsa05146; hsa05152; hsa05168; hsa05200; hsa05210; hsa05416;
5970	hsa04010; hsa04062; hsa04210; hsa04380; hsa04620; hsa04621; hsa04622; hsa04623; hsa04660; hsa04662; hsa04722; hsa04920; hsa05030; hsa05120; hsa05131; hsa05132; hsa05133; hsa05134; hsa05140; hsa05142; hsa05145; hsa05146; hsa05152; hsa05160; hsa05162; hsa05164; hsa05166; hsa05168; hsa05169; hsa05200; hsa05202; hsa05212; hsa05215; hsa05220; hsa05221; hsa05222;
4843	hsa00330; hsa01100; hsa04020; hsa04146; hsa05132; hsa05133; hsa05140; hsa05142; hsa05145; hsa05146; hsa05152; hsa05200; hsa05222;
5743	hsa00590; hsa01100; hsa04370; hsa04723; hsa04726; hsa05140; hsa05200; hsa05222;
3569	hsa04060; hsa04620; hsa04621; hsa04623; hsa04630; hsa04640; hsa04672; hsa05020; hsa05132; hsa05133; hsa05134; hsa05142; hsa05143; hsa05144; hsa05146; hsa05152; hsa05162; hsa05164; hsa05166; hsa05168; hsa05200; hsa05202; hsa05232; hsa05332; hsa05410;
596	hsa04141; hsa04210; hsa04510; hsa04722; hsa04725; hsa05014; hsa05145; hsa05152; hsa05169; hsa05200; hsa05210; hsa05215; hsa05222;
847	hsa00380; hsa00630; hsa01100; hsa04146; hsa05014;
5594	hsa04010; hsa04012; hsa04062; hsa04114; hsa04150; hsa04270; hsa04320; hsa04350; hsa04360; hsa04370; hsa04380; hsa04510; hsa04520; hsa04540; hsa04620; hsa04621; hsa04650; hsa04660; hsa04662; hsa04664; hsa04666; hsa04720; hsa04722; hsa04723; hsa04724; hsa04725; hsa04726; hsa04730; hsa04810; hsa04910; hsa04912; hsa04914; hsa04916; hsa04930; hsa04960; hsa05010; hsa05020; hsa05034; hsa05131; hsa05132; hsa05133; hsa05140; hsa05142; hsa05145; hsa05152; hsa05160; hsa05164; hsa05200; hsa05210; hsa05211; hsa05212; hsa05213; hsa05214; hsa05215; hsa05216; hsa05218; hsa05219; hsa05220; hsa05221; hsa05223;
4792	hsa04062; hsa04210; hsa04380; hsa04620; hsa04621; hsa04622; hsa04623; hsa04660; hsa04662; hsa04722; hsa04920; hsa05120; hsa05131; hsa05134; hsa05140; hsa05142; hsa05145; hsa05160; hsa05162; hsa05164; hsa05166; hsa05168; hsa05169; hsa05200; hsa05215; hsa05220; hsa05222;
3553	hsa04010; hsa04060; hsa04210; hsa04380; hsa04620; hsa04621; hsa04623; hsa04640; hsa04940; hsa05010; hsa05020; hsa05132; hsa05133; hsa05134; hsa05140; hsa05142; hsa05143; hsa05144; hsa05146; hsa05152; hsa05162; hsa05164; hsa05168; hsa05323; hsa05332;

5595	hsa04010;hsa04012;hsa04062;hsa04114;hsa04150;hsa04270;hsa04320;hsa04350;hsa04360;hsa04370;hsa04380;hsa04510;hsa04520;hsa04540;hsa04620;hsa04621;hsa04650;hsa04660;hsa04662;hsa04664;hsa04666;hsa04720;hsa04722;hsa04723;hsa04724;hsa04725;hsa04726;hsa04730;hsa04810;hsa04910;hsa04912;hsa04914;hsa04916;hsa04930;hsa04960;hsa05010;hsa05020;hsa05034;hsa05131;hsa05132;hsa05133;hsa05140;hsa05142;hsa05145;hsa05152;hsa05160;hsa05164;hsa05200;hsa05210;hsa05211;hsa05212;hsa05213;hsa05214;hsa05215;hsa05216;hsa05218;hsa05219;hsa05220;hsa05221;hsa05223;
1545	hsa00140;hsa00380;hsa00980;
581	hsa04115;hsa04141;hsa04210;hsa04722;hsa05014;hsa05016;hsa05020;hsa05152;hsa05166;hsa05200;hsa05210;
3162	hsa00860;hsa04978;
1544	hsa00232;hsa00380;hsa00591;hsa00830;hsa00980;hsa00982;hsa01100;
142	hsa03410;
207	hsa04010;hsa04012;hsa04062;hsa04150;hsa04210;hsa04370;hsa04380;hsa04510;hsa04530;hsa04620;hsa04630;hsa04660;hsa04662;hsa04664;hsa04666;hsa04722;hsa04725;hsa04728;hsa04910;hsa04914;hsa04920;hsa04973;hsa05142;hsa05145;hsa05152;hsa05160;hsa05162;hsa05164;hsa05166;hsa05169;hsa05200;hsa05210;hsa05211;hsa05212;hsa05213;hsa05214;hsa05215;hsa05218;hsa05220;hsa05221;hsa05222;hsa05223;
3725	hsa04010;hsa04012;hsa04310;hsa04380;hsa04510;hsa04620;hsa04660;hsa04662;hsa04722;hsa04912;hsa05030;hsa05031;hsa05120;hsa05132;hsa05133;hsa05140;hsa05142;hsa05164;hsa05166;hsa05168;hsa05169;hsa05200;hsa05210;hsa05211;hsa05323;
3576	hsa04060;hsa04062;hsa04620;hsa04621;hsa04622;hsa05120;hsa05131;hsa05132;hsa05133;hsa05134;hsa05142;hsa05144;hsa05146;hsa05160;hsa05164;hsa05200;hsa05202;hsa05219;hsa05323;
1026	hsa04012;hsa04110;hsa04115;hsa05160;hsa05166;hsa05169;hsa05200;hsa05202;hsa05214;hsa05215;hsa05218;hsa05219;hsa05220;
2099	hsa04961;
1571	hsa00590;hsa00591;hsa00980;hsa00982;hsa01100;
4790	hsa04010;hsa04062;hsa04210;hsa04380;hsa04620;hsa04621;hsa04622;hsa04623;hsa04660;hsa04662;hsa04722;hsa04920;hsa05030;hsa05120;hsa05131;hsa05132;hsa05133;hsa05134;hsa05140;hsa05142;hsa05145;hsa05146;hsa05152;hsa05160;hsa05162;hsa05164;hsa05166;hsa05168;hsa05169;hsa05200;hsa05202;hsa05212;hsa05215;hsa05220;hsa05221;hsa05222;
5468	hsa03320;hsa04380;hsa05016;hsa05200;hsa05202;hsa05216;
7157	hsa04010;hsa04110;hsa04115;hsa04210;hsa04310;hsa04722;hsa05014;hsa05016;hsa05160;hsa05162;hsa05166;hsa05168;hsa05169;hsa05200;hsa05202;hsa05210;hsa05212;hsa05213;hsa05214;hsa05215;hsa05216;hsa05217;hsa05218;hsa05219;hsa05220;hsa05222;hsa05223;
2353	hsa04010;hsa04380;hsa04620;hsa04660;hsa04662;hsa04725;hsa04728;hsa05031;hsa05132;hsa05133;hsa05140;hsa05142;hsa05166;hsa05168;hsa05200;hsa05210;hsa05323;

Table S4

842	hsa04115;hsa04210;hsa04370;hsa05010;hsa05012;hsa05014;hsa05016;hsa05134;hsa05145;hsa05152;hsa05164;hsa05200;hsa05210;hsa05212;hsa05213;hsa05215;hsa05222;hsa05223;hsa05416;
6347	hsa04060;hsa04062;hsa04621;hsa05142;hsa05144;hsa05164;hsa05168;hsa05323;
1576	hsa00140;hsa00591;hsa00830;hsa00980;hsa00982;hsa00983;hsa01100;hsa04976;
54577	hsa00040;hsa00053;hsa00140;hsa00500;hsa00514;hsa00830;hsa00860;hsa00980;hsa00982;hsa00983;hsa01100;
5465	hsa03320;hsa04920;hsa05160;
54575	hsa00040;hsa00053;hsa00140;hsa00500;hsa00514;hsa00830;hsa00860;hsa00980;hsa00982;hsa00983;hsa01100;
54576	hsa00040;hsa00053;hsa00140;hsa00500;hsa00514;hsa00830;hsa00860;hsa00980;hsa00982;hsa00983;hsa01100;
4846	hsa00330;hsa01100;hsa04020;hsa04370;
54205	hsa04115;hsa04210;hsa05010;hsa05012;hsa05014;hsa05016;hsa05134;hsa05145;hsa05152;hsa05164;hsa05168;hsa05200;hsa05210;hsa05222;hsa05416;
3383	hsa04514;hsa04650;hsa04670;hsa05143;hsa05144;hsa05150;hsa05164;hsa05166;hsa05169;hsa05323;hsa05416;
2950	hsa00480;hsa00980;hsa00982;hsa05200;hsa05215;
2729	hsa00480;hsa01100;
2194	hsa00061;hsa01100;hsa04910;
54659	hsa00040;hsa00053;hsa00140;hsa00500;hsa00514;hsa00830;hsa00860;hsa00980;hsa00982;hsa00983;hsa01100;
2936	hsa00480;
4609	hsa04010;hsa04012;hsa04110;hsa04310;hsa04350;hsa04630;hsa05166;hsa05169;hsa05200;hsa05202;hsa05210;hsa05213;hsa05216;hsa05219;hsa05220;hsa05221;hsa05222;
231	hsa00040;hsa00051;hsa00052;hsa00561;hsa00620;hsa01100;
5599	hsa04010;hsa04012;hsa04141;hsa04310;hsa04380;hsa04510;hsa04620;hsa04621;hsa04622;hsa04664;hsa04722;hsa04723;hsa04728;hsa04910;hsa04912;hsa04914;hsa04920;hsa04930;hsa05120;hsa05131;hsa05132;hsa05133;hsa05142;hsa05145;hsa05152;hsa05160;hsa05164;hsa05166;hsa05168;hsa05169;hsa05200;hsa05210;hsa05212;
7422	hsa04060;hsa04150;hsa04370;hsa04510;hsa05200;hsa05211;hsa05212;hsa05219;hsa05323;
54600	hsa00040;hsa00053;hsa00140;hsa00500;hsa00514;hsa00830;hsa00860;hsa00980;hsa00982;hsa00983;hsa01100;
54658	hsa00040;hsa00053;hsa00140;hsa00500;hsa00514;hsa00830;hsa00860;hsa00980;hsa00982;hsa00983;hsa01100;
3458	hsa03050;hsa04060;hsa04140;hsa04350;hsa04380;hsa04612;hsa04630;hsa04650;hsa04660;hsa04940;hsa05132;hsa05140;hsa05142;hsa05143;hsa05144;hsa05145;hsa05146;hsa05152;hsa05162;hsa05164;hsa05168;hsa05169;hsa05222;hsa05323;hsa05330;hsa05332;
6647	hsa04146;hsa05014;hsa05016;hsa05020;
4318	hsa04670;hsa05200;hsa05202;hsa05219;
5925	hsa04110;hsa05166;hsa05169;hsa05200;hsa05212;hsa05214;hsa05215;hsa05218;hsa05219;hsa05220;hsa05222;hsa05223;
1906	hsa04916;
3552	hsa04010;hsa04060;hsa04210;hsa04380;hsa04640;hsa04940;hsa05020;hsa05132;hsa05133;hsa05140;hsa05152;hsa05162;hsa05164;hsa05323;hsa05332;

Table S4

7412	hsa04514;hsa04670;hsa05143;hsa05144;hsa05166;
5243	hsa02010;hsa04976;
595	hsa04110;hsa04115;hsa04310;hsa04510;hsa04630;hsa05162;hsa05166;hsa05200;hsa05210;hsa05212;hsa05213;hsa05214;hsa05215;hsa05216;hsa05218;hsa05219;hsa05220;hsa05221;hsa05222;hsa05223;hsa05416;
7040	hsa04010;hsa04060;hsa04110;hsa04144;hsa04350;hsa04380;hsa04672;hsa05140;hsa05142;hsa05144;hsa05145;hsa05146;hsa05152;hsa05166;hsa05200;hsa05210;hsa05211;hsa05212;hsa05220;hsa05323;hsa05410;hsa05414;
1958	hsa05020;hsa05166;
3565	hsa04060;hsa04630;hsa04640;hsa04660;hsa04664;hsa04672;hsa05140;hsa05162;hsa05310;hsa05320;hsa05330;
841	hsa04115;hsa04210;hsa04620;hsa04621;hsa04622;hsa05010;hsa05016;hsa05134;hsa05142;hsa05145;hsa05152;hsa05168;hsa05200;hsa05416;
2876	hsa00480;hsa00590;hsa05014;hsa05016;
4363	hsa02010;hsa04977;
891	hsa04110;hsa04114;hsa04115;hsa04914;
331	hsa04120;hsa04210;hsa04510;hsa04621;hsa05145;hsa05166;hsa05200;hsa05222;
6720	hsa04910;
1277	hsa04510;hsa04512;hsa04974;hsa05146;
2539	hsa00030;hsa00480;hsa01100;
598	hsa04210;hsa04630;hsa05014;hsa05145;hsa05166;hsa05200;hsa05202;hsa05212;hsa05220;hsa05222;
6352	hsa04060;hsa04062;hsa04620;hsa04621;hsa04623;hsa05020;hsa05120;hsa05142;hsa05164;hsa05168;hsa05323;
1956	hsa04010;hsa04012;hsa04020;hsa04060;hsa04144;hsa04320;hsa04510;hsa04520;hsa04540;hsa04810;hsa04912;hsa05120;hsa05160;hsa05200;hsa05212;hsa05213;hsa05214;hsa05215;hsa05218;hsa05219;hsa05223;
6648	hsa04146;hsa05016;
983	hsa04110;hsa04114;hsa04115;hsa04540;hsa04914;hsa05168;hsa05169;
1244	hsa02010;hsa04976;
183	hsa04614;
1437	hsa04060;hsa04630;hsa04640;hsa04650;hsa04660;hsa04664;hsa05132;hsa05146;hsa05166;hsa05202;hsa05323;
5443	hsa04916;hsa04920;
367	hsa04114;hsa05200;hsa05215;
9370	hsa03320;hsa04920;hsa04930;
5111	hsa03030;hsa03410;hsa03420;hsa03430;hsa04110;hsa05166;
2308	hsa04910;hsa05200;hsa05202;hsa05215;
6817	hsa00920;
5054	hsa04115;hsa04610;hsa05142;
2554	hsa04080;hsa04723;hsa04727;hsa05032;hsa05033;
4780	hsa04141;
3952	hsa04060;hsa04080;hsa04630;hsa04920;
335	hsa03320;hsa04975;hsa04977;hsa05143;
1559	hsa00590;hsa00591;hsa00830;hsa00980;hsa00982;hsa01100;hsa04726;
9429	hsa02010;hsa04976;
3309	hsa03060;hsa04141;hsa04612;hsa05020;
355	hsa04010;hsa04060;hsa04115;hsa04210;hsa04650;hsa04940;hsa05010;hsa05142;hsa05143;hsa05162;hsa05164;hsa05168;hsa05200;hsa05320;hsa05330;hsa05332;

Table S4

351	hsa04726;hsa05010;
3091	hsa04150;hsa05200;hsa05211;
3156	hsa00900;hsa01100;hsa04976;
387	hsa04062;hsa04144;hsa04270;hsa04310;hsa04350;hsa04360;hsa04510;hsa04520;hsa04530;hsa04660;hsa04670;hsa04722;hsa04810;hsa04972;hsa05100;hsa05130;hsa05133;hsa05152;hsa05200;hsa05210;
3586	hsa04060;hsa04630;hsa04660;hsa04672;hsa05133;hsa05140;hsa05142;hsa05143;hsa05144;hsa05145;hsa05146;hsa05150;hsa05152;hsa05169;hsa05310;hsa05320;hsa05322;hsa05330;
5444	hsa01100;
1027	hsa04012;hsa04110;hsa05162;hsa05169;hsa05200;hsa05202;hsa05215;hsa05220;hsa05222;
2938	hsa00480;hsa00980;hsa00982;
7296	hsa00240;hsa00450;
338	hsa04975;hsa04977;
332	hsa05200;hsa05210;
1649	hsa04010;hsa04141;hsa05202;
572	hsa04012;hsa04210;hsa04370;hsa04510;hsa04722;hsa04910;hsa05010;hsa05014;hsa05145;hsa05152;hsa05160;hsa05200;hsa05210;hsa05212;hsa05213;hsa05215;hsa05218;hsa05220;hsa05221;hsa05223;
1950	hsa04010;hsa04012;hsa04060;hsa04144;hsa04510;hsa04540;hsa04810;hsa05160;hsa05200;hsa05212;hsa05213;hsa05214;hsa05215;hsa05218;hsa05219;hsa05223;
1031	hsa04110;hsa05166;hsa05202;
2940	hsa00480;hsa00980;hsa00982;
4313	hsa04670;hsa04912;hsa05200;hsa05219;
8644	hsa00140;hsa00590;hsa00980;
7037	hsa04144;hsa04145;hsa04640;
2730	hsa00480;hsa01100;
1557	hsa00590;hsa00591;hsa00830;hsa00980;hsa00982;hsa01100;hsa04726;
19	hsa02010;hsa04975;
217	hsa00010;hsa00040;hsa00053;hsa00071;hsa00280;hsa00310;hsa00330;hsa00340;hsa00380;hsa00410;hsa00561;hsa00620;hsa00640;hsa01100;
31	hsa00061;hsa00620;hsa00640;hsa01100;hsa04910;
47	hsa00020;hsa01100;
4502	hsa04978;
3558	hsa04060;hsa04630;hsa04660;hsa04672;hsa04940;hsa05142;hsa05162;hsa05166;hsa05320;hsa05330;hsa05332;
7184	hsa04141;hsa04621;hsa05200;hsa05215;
4199	hsa00620;hsa01100;hsa03320;
834	hsa04621;hsa04623;hsa05014;hsa05132;hsa05133;hsa05134;hsa05164;
330	hsa04120;hsa04210;hsa04510;hsa04621;hsa05145;hsa05166;hsa05200;hsa05202;hsa05222;
1548	hsa00232;hsa00830;hsa00980;hsa00982;hsa00983;hsa01100;
4353	hsa04145;hsa05202;
7364	hsa00040;hsa00053;hsa00140;hsa00500;hsa00514;hsa00830;hsa00860;hsa00980;hsa00982;hsa00983;hsa01100;
2944	hsa00480;hsa00980;hsa00982;
5971	hsa04010;hsa04380;hsa05166;hsa05169;
10891	hsa04910;hsa04920;hsa05016;
6783	hsa00140;hsa00920;

Table S4

4616	hsa04010;hsa04110;hsa04115;
5580	hsa04062;hsa04270;hsa04530;hsa04664;hsa04666;hsa04722;hsa04912;hsa04930;
3949	hsa04144;hsa04976;hsa05145;hsa05160;
1080	hsa02010;hsa04971;hsa04972;hsa04976;hsa05110;
3630	hsa04114;hsa04140;hsa04150;hsa04810;hsa04910;hsa04914;hsa04930;hsa04940;hsa04950;hsa04960;hsa05215;
948	hsa03320;hsa04145;hsa04512;hsa04640;hsa04920;hsa04975;hsa05144;
949	hsa04145;hsa04975;hsa04976;hsa04977;hsa05160;
7132	hsa04010;hsa04060;hsa04210;hsa04380;hsa04920;hsa05010;hsa05014;hsa05142;hsa05145;hsa05152;hsa05160;hsa05164;hsa05166;hsa05168;
1432	hsa04010;hsa04370;hsa04380;hsa04620;hsa04621;hsa04622;hsa04660;hsa04664;hsa04670;hsa04722;hsa04723;hsa04728;hsa04912;hsa04914;hsa05014;hsa05120;hsa05131;hsa05132;hsa05133;hsa05140;hsa05142;hsa05145;hsa05152;hsa05160;hsa05164;hsa05169;
329	hsa04120;hsa04210;hsa04510;hsa04621;hsa05145;hsa05166;hsa05200;hsa05222;
43	hsa00564;hsa04725;
2203	hsa00010;hsa00030;hsa00051;hsa01100;hsa04910;
54578	hsa00040;hsa00053;hsa00140;hsa00500;hsa00514;hsa00830;hsa00860;hsa00980;hsa00982;hsa00983;hsa01100;
59	hsa04270;
7039	hsa04012;hsa05200;hsa05211;hsa05212;hsa05214;hsa05215;hsa05223;
3315	hsa04010;hsa04370;hsa05146;hsa05169;
4953	hsa00330;hsa00480;hsa01100;
3292	hsa00140;hsa01100;
1499	hsa04310;hsa04510;hsa04520;hsa04530;hsa04670;hsa04916;hsa05100;hsa05130;hsa05166;hsa05200;hsa05210;hsa05213;hsa05215;hsa05216;hsa05217;hsa05412;
1869	hsa04110;hsa05166;hsa05200;hsa05212;hsa05214;hsa05215;hsa05218;hsa05219;hsa05220;hsa05222;hsa05223;
1509	hsa04142;hsa05152;
2932	hsa04012;hsa04062;hsa04110;hsa04310;hsa04340;hsa04360;hsa04510;hsa04660;hsa04662;hsa04722;hsa04728;hsa04910;hsa04916;hsa05010;hsa05160;hsa05162;hsa05164;hsa05166;hsa05169;hsa05200;hsa05210;hsa05213;hsa05215;hsa05217;

Table S5 Pathway Pattern Detail. In this table, the Pathway Pattern before filtering is presented. The Pathway Pattern consists of 1-item association rules, 2-item association rules and 3-item association rules. Each rule is introduced with KEGG pathway entry, pathway description and frequency.

1-item rules

KEGG Pathway	Pathway Description	frequency
hsa05200	Pathways in cancer	49
hsa01100	Metabolic pathways	33
hsa05166	HTLV-I infection	32
hsa05215	Prostate cancer	25
hsa05152	Tuberculosis	25
hsa05145	Toxoplasmosis	25
hsa05142	Chagas disease (American trypanosomiasis)	25
hsa05164	Influenza A MAPK	24
hsa04010	signaling pathway Metabolism of	24
hsa00980	xenobiotics by cytochrome P450	21
hsa04210	Apoptosis Epstein-Barr	21
hsa05169	virus infection	20
hsa05160	Hepatitis C	20
hsa05210	Colorectal cancer	20
hsa04060	Cytokine-cytokine receptor interaction	19
hsa05168	Herpes simplex infection	19
hsa05222	Small cell lung cancer	19

hsa04621	NOD-like receptor signaling pathway	19
hsa04380	Osteoclast differentiat ion	18
hsa00982	Drug metabolism - cytochrome P450	18
hsa04510	Focal adhesion	18
hsa05212	Pancreatic cancer	18
hsa05133	Pertussis T cell	18
hsa04660	receptor signaling pathway	17
hsa05140	Leishmaniasi s	17
hsa05202	Transcriptio nal misregulatio n in cancer	17
hsa04620	Toll-like receptor signaling pathway	16
hsa05132	Salmonella infection	16
hsa05220	Chronic myeloid leukemia	16
hsa04722	Neurotrophin signaling pathway	16
hsa05162	Measles	15
hsa05014	Amyotrophic lateral sclerosis (ALS)	15
hsa00830	Retinol metabolism	14
hsa04110	Cell cycle	14
hsa05219	Bladder cancer	14
hsa00140	Steroid hormone biosynthesis	14

hsa05323	Rheumatoid arthritis	14
hsa05146	Amoebiasis	14

2-item rules

KEGG Pathway 1	Pathway Description	KEGG Pathway 2	Pathway Description	frequency
hsa05145	Toxoplasmosis	hsa05152	Tuberculosis	19
hsa00980	Metabolism of xenobiotics by cytochrome P450	hsa00982	Drug metabolism - cytochrome P450	18
hsa05142	Chagas disease (American trypanosomiasis)	hsa05164	Influenza A	18
hsa05142	Chagas disease (American trypanosomiasis)	hsa05152	Tuberculosis	16
hsa04210	Apoptosis	hsa05145	Toxoplasmosis	16
hsa04620	Toll-like receptor signaling pathway	hsa05142	Chagas disease (American trypanosomiasis)	16
hsa05142	Chagas disease (American trypanosomiasis)	hsa05145	Toxoplasmosis	15
hsa04010	MAPK signaling pathway	hsa04380	Osteoclast differentiation	15
hsa05152	Tuberculosis	hsa05164	Influenza A	15
hsa05142	Chagas disease (American trypanosomiasis)	hsa05168	Herpes simplex infection	15
hsa04380	Osteoclast differentiation	hsa05142	Chagas disease (American trypanosomiasis)	15

hsa05164	Influenza A	hsa05168	Herpes simplex infection	14
hsa04010	MAPK signaling pathway	hsa05142	Chagas disease (American trypanosomiasis)	14
hsa04621	NOD-like receptor signaling pathway	hsa05164	Influenza A	14
hsa04620	Toll-like receptor signaling pathway	hsa05164	Influenza A	14
hsa04210	Apoptosis	hsa05152	Tuberculosis	14
hsa05212	Pancreatic cancer	hsa05215	Prostate cancer	14
hsa04621	NOD-like receptor signaling pathway	hsa05142	Chagas disease (American trypanosomiasis)	14
hsa05132	Salmonella infection	hsa05133	Pertussis	14
hsa00830	Retinol metabolism	hsa00980	Metabolism of xenobiotics by cytochrome P450	14
hsa05140	Leishmaniasis	hsa05142	Chagas disease (American trypanosomiasis)	14
hsa05133	Pertussis	hsa05142	Chagas disease (American trypanosomiasis)	14
hsa04380	Osteoclast differentiation	hsa05164	Influenza A	14
hsa05133	Pertussis	hsa05152	Tuberculosis	14

3-item rules

KEGG Pathway 1	Pathway Description	KEGG Pathway 2	Pathway Description	KEGG Pathway 3	Pathway Description	frequency
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hsa05142	Chagas disease (American trypanosomia sis)	hsa05145	Toxoplasmosis	hsa05152	Tuberculosis	14
hsa04620	Toll-like receptor signaling pathway	hsa05142	Chagas disease (American trypanosomias is)	hsa05164	Influenza A	14

Table S6 Gene Score Detail. In this table, all the gene scores are presented. Genes are ranked according to their scores.

gene	score	gene	score	gene	score
3553	0. 907407	5925	0. 037037	5580	0
5970	0. 907407	4616	0. 037037	10891	0
4790	0. 907407	217	0. 018519	6647	0
7124	0. 865079	54600	0. 018519	2554	0
5599	0. 846561	1509	0. 018519	9370	0
3569	0. 822751	5743	0. 018519	5465	0
5595	0. 780423	1499	0. 018519	5468	0
5594	0. 780423	1544	0. 018519	1958	0
1432	0. 780423	1548	0. 018519	6720	0
3725	0. 727513	1557	0. 018519	3949	0
207	0. 685185	1559	0. 018519	3309	0
4792	0. 666667	598	0. 018519	7039	0
3576	0. 648148	7364	0. 018519	2308	0
6352	0. 62963	3952	0. 018519	6783	0
3458	0. 304233	54659	0. 018519	367	0
7132	0. 296296	54658	0. 018519	2936	0
2353	0. 267196	3156	0. 018519	5243	0
3552	0. 261905	1543	0. 018519	59	0
841	0. 230159	847	0. 018519	3091	0
6347	0. 230159	31	0. 018519	1244	0
355	0. 224868	1649	0. 018519	338	0
4843	0. 187831	4953	0. 018519	335	0
3586	0. 18254	2194	0. 018519	332	0
7040	0. 15873	2730	0. 018519	1906	0
54205	0. 145503	3292	0. 018519	3162	0
836	0. 140212	2203	0. 018519	2938	0
834	0. 121693	1031	0. 018519	1080	0
7157	0. 111111	1869	0. 018519	7412	0
2932	0. 111111	5111	0. 018519	183	0
842	0. 103175	5054	0. 018519	7296	0
596	0. 097884	231	0. 018519	3630	0
387	0. 097884	4199	0. 018519	2950	0
572	0. 079365	47	0. 018519	19	0
3558	0. 074074	54577	0. 018519	4353	0
1437	0. 074074	4846	0. 018519	4363	0
581	0. 060847	891	0. 018519	7037	0
1956	0. 055556	2729	0. 018519	6817	0
329	0. 055556	1277	0. 018519	2944	0
3565	0. 055556	54578	0. 018519	2940	0
595	0. 055556	5444	0. 018519	9429	0
3383	0. 055556	54575	0. 018519	4313	0
331	0. 055556	54576	0. 018519	142	0
330	0. 055556	2539	0. 018519	2876	0
983	0. 055556	1571	0. 018519	4318	0
4609	0. 055556	7184	0. 018519	4502	0
1027	0. 055556	1576	0. 018519	8644	0
7422	0. 055556	43	0	948	0
1950	0. 055556	2099	0	949	0
3315	0. 037037	4780	0	5443	0
5971	0. 037037	1545	0	351	0
1026	0. 037037	6648	0		

Table S7 Compound Efficacy Index Detail. In this table, all the Compound Efficacy Indexes are presented. Compounds are ranked according to their Efficacy Index. Additionally, eHiTS Score of each compound is also presented in the last column.

Compound	Efficacy Score	eHiTS Score	Compound	Efficacy Score	eHiTS Score
480-11-5	0.635196992	-5.465	334-48-5	0.251716528	-3.72
480-10-4	0.586752766	-7.065	64-67-5	0.251716528	-3.47
520-36-5	0.569648189	-5.405	480-44-4	0.250572176	-5.26
153-18-4	0.568893751	-8.77	470-82-6	0.250572176	-3.965
20362-31-6	0.552149747	-6.01	3913-71-1	0.250572176	-3.6
5373-11-5	0.552149747	-7.165	472-70-8	0.250572176	-8.73
491-70-3	0.551756186	-5.585	80466-34-8	0.250572176	-2.825
4773-96-0	0.529132977	-5.905	522-12-3	0.250572176	-7.215
58749-22-7	0.528036619	-6.435	34334-69-5	0.250572176	-6.055
60976-49-0	0.526728789	-7.68	143-07-7	0.250351479	-4.205
15932-80-6	0.526728789	-4.31	463-40-1	0.24976062	-5.335
520-18-3	0.519763872	-5.73	327-97-9	0.242709473	-4.765
117-39-5	0.517647083	-5.23	53-16-7	0.229482606	-5.6
559-74-0	0.506048717	-4.315	97-42-7	0.229482606	-4.73
54-11-5	0.505550797	-4.015	331-39-5	0.224104325	-3.73
59870-68-7	0.504495668	-5.85	1921-70-6	0.221233565	-6.145
92-61-5	0.504005231	-4.17	1617-53-4	0.206375674	-4.92
515-13-9	0.501880007	-5.46	491-71-4	0.201144352	-5.58
112-31-2	0.501144352	-3.715	84-74-2	0.199926086	-5.11
706-14-9	0.501144352	-3.855	138-86-3	0.194237561	-3.875
61276-17-3	0.500572176	-6.645	57-11-4	0.187522793	
124-19-6	0.500572176	-3.44	112-05-0	0.180684976	-3.61
111-02-4	0.500572176	-7.83	21967-41-9	0.172486513	-7.225
552-59-0	0.500572176	-5.535	19894-97-4	0.169691025	-3.655
55954-61-5	0.500572176	-5.365	2111-75-3	0.169691025	-3.76
111-71-7	0.500572176	-3.135	91-20-3	0.168426863	-3.665
494-90-6	0.500572176	-4.175	2363-88-4	0.167238843	-3.69
2463-63-0	0.500572176	-3.055	74-84-0	0.167238843	
437-64-9	0.500572176	-5.715	2091-29-4	0.167238843	-5.515
122021-74-3	0.500572176	-7.09	64-18-6	0.164027651	-1.25
50-28-2	0.493301823	-5.715	89-83-8	0.15911088	-4.075
64-17-5	0.491419382	-1.585	100-41-4	0.149185578	-3.18
480-40-0	0.470483615	-5.185	548-04-9	0.144001495	-7.825
69-72-7	0.467451365	-3.175	108-95-2	0.143659474	-2.655
961-29-5	0.46563675	-4.725	91-22-5	0.138185289	-3.375
491-67-8	0.446637417	-5.49	122-32-7	0.138080164	
508-02-1	0.439934436	-5.93	91-64-5	0.133825291	-3.585
104-46-1	0.438084544	-3.72	120-72-9	0.126144352	-3.1
111-14-8	0.436111788	-3.06	624-15-7	0.120026157	-4.32
57-88-5	0.427611334	-6.815	112-80-1	0.117534991	-5.23
64-19-7	0.408085471	-1.455	299-42-3	0.103496961	-3.725
74-90-8	0.394046101	-1.1	124-07-2	0.086613127	-3.31
120-08-1	0.381586835	-4.01	59803-98-4	0.086357692	-4.63
4852-22-6	0.381293935	-6.375	2463-53-8	0.083905509	-3.555
529-44-2	0.380812528	-5.995	505-57-7	0.063072176	-2.675
59-67-6	0.380072914	-2.695	76-22-2	0.056127731	-3.745
7770-78-7	0.379444581	-5.985	84-66-2	0.049437921	-4.39
27013-91-8	0.376716528	-5.42	78-70-6	0	-4.435
99-50-3	0.366215932	-3.315	544-63-8	0	
6917-35-7	0.361566638	-3.535	83-48-7	0	-6.775
5779-62-4	0.35196992	-7.555	10385-78-1	0	-3.935
77-95-2	0.350457741	-3.51	89-80-5	0	-4.205
150-86-7	0.34934975	-6.22	499-75-2	0	-4.29

11079-53-1	0.344735982	-7.795	29388-59-8	0	-5.755
512-04-9	0.342502241	-5.07	84-69-5	0	-5.295
482-36-0	0.339709008	-7.1	131-11-3	0	-3.455
481-72-1	0.339709008	-5.44	127-91-3	0	-3.675
520-34-3	0.339417081	-5.515	5187-84-8	0	-7.4
128-37-0	0.33700262	-6.215	5392-40-5	0	-4.205
2197-37-7	0.32937481	-5.365	144-68-3	0	-6.9
71-43-2	0.328583563	-2.435	71-41-0	0	-2.485
518-82-1	0.326021227	-5.45	110-15-6	0	-2.08
621-82-9	0.318221759	-3.365	78-83-1	0	-2.375
485-72-3	0.313414067	-5.26	543-39-5	0	-4.395
855-96-9	0.301716528	-5.495	90-19-7	0	-5.98
98-92-0	0.291603902	-2.84	82597-74-8	0	-6.14
120-46-7	0.288008828	-4.28	928-96-1	0	-2.865
4602-84-0	0.287052477	-5.355	18524-94-2	0	-6.05
13270-61-6	0.285144233	-6.11	14838-15-4	0	-3.54
121-34-6	0.280638657	-3.38	156-38-7	0	-3.435
632-85-9	0.278281838	-5.61	99-48-9	0	-4.085
123-51-3	0.276728789	-2.8	102-61-4	0	-4.575
97-53-0	0.270288583	-4.05	108-39-4	0	-3.255
63968-64-9	0.266930814	-5.245	79-83-4	0	-3.96
77-52-1	0.264304398	-5.415	68526-83-0	0	-3.6
108-38-3	0.260411558	-3.47	80-56-8	0	-3.705
20549-47-7	0.253024358	-4.01			

Table S8 eHiTS scores of docking compounds into 1MX1 and 1VCU

Compound	Efficacy Index	1MX1_Score	1VCU_Score
480-11-5	0.635196992	-6.6	-4.33
480-10-4	0.586752766	-7.78	-6.35
520-36-5	0.569648189	-6.29	-4.52
153-18-4	0.568893751	-10.47	-7.07
20362-31-6	0.552149747	-6.8	-5.22
5373-11-5	0.552149747	-7.42	-6.91
491-70-3	0.551756186	-6.4	-4.77
4773-96-0	0.529132977	-5.98	-5.83
58749-22-7	0.528036619	-7.61	-5.26
60976-49-0	0.526728789	-7.68	#
15932-80-6	0.526728789	-4.99	-3.63
520-18-3	0.519763872	-6.48	-4.98
117-39-5	0.517647083	-6.21	-4.25
559-74-0	0.506048717	-7.69	-0.94
54-11-5	0.505550797	-4.65	-3.38
59870-68-7	0.504495668	-7.53	-4.17
92-61-5	0.504005231	-4.38	-3.96
515-13-9	0.501880007	-6.58	-4.34
112-31-2	0.501144352	-4.37	-3.06
706-14-9	0.501144352	-4.53	-3.18
61276-17-3	0.500572176	-6.76	-6.53
124-19-6	0.500572176	-4.05	-2.83
111-02-4	0.500572176	-8.51	-7.15
552-59-0	0.500572176	-6.69	-4.38
55954-61-5	0.500572176	-3.42	-7.31
111-71-7	0.500572176	-3.64	-2.63
494-90-6	0.500572176	-4.77	-3.58
2463-63-0	0.500572176	-3.36	-2.75
437-64-9	0.500572176	-6.47	-4.96
122021-74-3	0.500572176	-6.38	-7.8
50-28-2	0.493301823	-7.29	-4.14
64-17-5	0.491419382	-1.68	-1.49
480-40-0	0.470483615	-6.19	-4.18
69-72-7	0.467451365	-3.37	-2.98
961-29-5	0.46563675	-5.32	-4.13
491-67-8	0.446637417	-6.31	-4.67
508-02-1	0.439934436	-6.2	-5.66
104-46-1	0.438084544	-4.1	-3.34
111-14-8	0.436111788	-3.65	-2.47
57-88-5	0.427611334	-8.52	-5.11
64-19-7	0.408085471	-1.72	-1.19
74-90-8	0.394046101	-1.1	#
120-08-1	0.381586835	-4.6	-3.42
4852-22-6	0.381293935	-6.55	-6.2
529-44-2	0.380812528	-6.76	-5.23
59-67-6	0.380072914	-2.81	-2.58
7770-78-7	0.379444581	-6.86	-5.11
27013-91-8	0.376716528	-5.42	#
99-50-3	0.366215932	-3.42	-3.21
6917-35-7	0.361566638	-3.72	-3.35
5779-62-4	0.35196992	-9.57	-5.54
77-95-2	0.350457741	-3.83	-3.19
150-86-7	0.34934975	-7.49	-4.95

Table S8

11079-53-1	0.344735982	-8.86	-6.73
512-04-9	0.342502241	-5.96	-4.18
482-36-0	0.339709008	-7.26	-6.94
481-72-1	0.339709008	-6.3	-4.58
520-34-3	0.339417081	-6.28	-4.75
128-37-0	0.33700262	-7.69	-4.74
2197-37-7	0.32937481	-6.17	-4.56
71-43-2	0.328583563	-2.56	-2.31
518-82-1	0.326021227	-6.56	-4.34
621-82-9	0.318221759	-3.68	-3.05
485-72-3	0.313414067	-5.95	-4.57
855-96-9	0.301716528	-6.48	-4.51
98-92-0	0.291603902	-3.01	-2.67
120-46-7	0.288008828	-5.03	-3.53
4602-84-0	0.287052477	-6.32	-4.39
13270-61-6	0.285144233	-7	-5.22
121-34-6	0.280638657	-3.45	-3.31
632-85-9	0.278281838	-6.57	-4.65
123-51-3	0.276728789	-3.11	-2.49
97-53-0	0.270288583	-4.34	-3.76
63968-64-9	0.266930814	-6.52	-3.97
77-52-1	0.264304398	-6.36	-4.47
108-38-3	0.260411558	-3.75	-3.19
20549-47-7	0.253024358	-4.78	-3.24
334-48-5	0.251716528	-4.39	-3.05
64-67-5	0.251716528	-4.07	-2.87
480-44-4	0.250572176	-5.77	-4.75
470-82-6	0.250572176	-4.78	-3.15
3913-71-1	0.250572176	-4.25	-2.95
472-70-8	0.250572176	-8.73	#
80466-34-8	0.250572176	-3.09	-2.56
522-12-3	0.250572176	-8.13	-6.3
34334-69-5	0.250572176	-6.92	-5.19
143-07-7	0.250351479	-4.84	-3.57
463-40-1	0.24976062	-6.2	-4.47
327-97-9	0.242709473	-5.36	-4.17
53-16-7	0.229482606	-7.31	-3.89
97-42-7	0.229482606	-5.46	-4
331-39-5	0.224104325	-3.83	-3.63
1921-70-6	0.221233565	-7.38	-4.91
1617-53-4	0.206375674	-3.57	-6.27
491-71-4	0.201144352	-6.29	-4.87
84-74-2	0.199926086	-5.9	-4.32
138-86-3	0.194237561	-4.54	-3.21
57-11-4	0.187522793	#	#
112-05-0	0.180684976	-4.32	-2.9
21967-41-9	0.172486513	-7.6	-6.85
19894-97-4	0.169691025	-4.24	-3.07
2111-75-3	0.169691025	-4.35	-3.17
91-20-3	0.168426863	-3.91	-3.42
2363-88-4	0.167238843	-4.18	-3.2
74-84-0	0.167238843	#	#
2091-29-4	0.167238843	-5.92	-5.11
64-18-6	0.164027651	-0.92	-1.58
89-83-8	0.15911088	-4.79	-3.36

Table S8

100-41-4	0.149185578	-3.45	-2.91
548-04-9	0.144001495	-7.95	-7.7
108-95-2	0.143659474	-2.82	-2.49
91-22-5	0.138185289	-3.8	-2.95
122-32-7	0.138080164	#	#
91-64-5	0.133825291	-3.85	-3.32
120-72-9	0.126144352	-3.38	-2.82
624-15-7	0.120026157	-4.76	-3.88
112-80-1	0.117534991	-6.21	-4.25
299-42-3	0.103496961	-3.88	-3.57
124-07-2	0.086613127	-3.92	-2.7
59803-98-4	0.086357692	-5.25	-4.01
2463-53-8	0.083905509	-4.03	-3.08
505-57-7	0.063072176	-2.94	-2.41
76-22-2	0.056127731	-4.62	-2.87
84-66-2	0.049437921	-4.87	-3.91
78-70-6	0	-4.9	-3.97
544-63-8	0	#	#
83-48-7	0	-8.31	-5.24
10385-78-1	0	-4.76	-3.11
89-80-5	0	-4.96	-3.45
499-75-2	0	-4.97	-3.61
29388-59-8	0	-6.45	-5.06
84-69-5	0	-6.08	-4.51
131-11-3	0	-3.9	-3.01
127-91-3	0	-4.46	-2.89
5187-84-8	0	-7.99	-6.81
5392-40-5	0	-4.77	-3.64
144-68-3	0	-6.9	#
71-41-0	0	-2.76	-2.21
110-15-6	0	-2.35	-1.81
78-83-1	0	-2.55	-2.2
543-39-5	0	-4.8	-3.99
90-19-7	0	-6.73	-5.23
82597-74-8	0	-8.32	-3.96
928-96-1	0	-3.07	-2.66
18524-94-2	0	-6.98	-5.12
14838-15-4	0	-3.8	-3.28
156-38-7	0	-3.48	-3.39
99-48-9	0	-4.73	-3.44
102-61-4	0	-5.32	-3.83
108-39-4	0	-3.49	-3.02
79-83-4	0	-4.55	-3.37
68526-83-0	0	-4.2	-3
80-56-8	0	-4.5	-2.91

indicates that there is no solution for this case in eHiTS.

Talbe S9 Active Component–Gene Target Interaction. In this table, the predicted active compounds, gene targets, active component interactions and corresponding STITCH confidence scores are presented. Compounds and genes are presented in the form of compound name and gene name. Totally, 16 active components, 29 gene targets and 162 active component–gene target interactions are predicted.

STITCH			STITCH		
Compound Name	Gene Name	Confidence Score	Compound Name	Gene Name	Confidence Score
quercetin	TNF	0. 91	apigenin	NFKBIA	0. 214
quercetin	NOS2	0. 36	apigenin	MAPK3	
quercetin	IL1B	0. 943	apigenin	RELA	0. 356
quercetin	IL6	0. 976	apigenin	AKT1	0. 928
quercetin	MAPK3		apigenin	CASP9	0. 7
quercetin	CASP3	0. 852	apigenin	FOS	0. 818
quercetin	MAPK1	0. 715	apigenin	JUN	0. 395
quercetin	IFNG	0. 226	apigenin	TP53	0. 888
quercetin	RELA		apigenin	CASP8	
quercetin	CCL2	0. 965	apigenin	CYCS	0. 573
quercetin	FOS	0. 824	apigenin	FAS	
quercetin	NFKBIA	0. 761	apigenin	IL10	
quercetin	AKT1	0. 983	apigenin	NFKB1	0. 88
quercetin	IL8	0. 195	arctiin	IL6	
quercetin	TP53	0. 954	arctiin	TNF	
quercetin	CASP9	0. 7	astragalin	NOS2	
quercetin	JUN	0. 976	astragalin	CCL2	
quercetin	TGFB1		astragalin	IL1B	
quercetin	NFKB1	0. 526	astragalin	IL6	
quercetin	CCL5		astragalin	NFKBIA	
quercetin	MAPK8	0. 942	astragalin	RELA	
quercetin	CASP8		astragalin	TNF	
quercetin	CASP1		luteolin-7-glucoside	IL6	
quercetin	CYCS	0. 573	luteolin-7-glucoside	TNF	
quercetin	GSK3B	0. 925	licochalcone-A	IL1B	
quercetin	IL1A		oroxylin	NOS2	
quercetin	FAS		oroxylin	IL1B	
quercetin	IL10		oroxylin	IL6	0. 81
quercetin	TNFRSF1A		oroxylin	TNF	
rutin	IL1B		oroxylin	NFKBIA	
rutin	TNF		oroxylin	RELA	
rutin	IL6		mangiferin	TNF	0. 87
rutin	NOS2		mangiferin	IFNG	
rutin	CASP3		mangiferin	RELA	0. 278
rutin	CASP9		mangiferin	NOS2	
rutin	IL8		mangiferin	IL6	
rutin	TP53		mangiferin	TGFB1	
rutin	MAPK1		mangiferin	IL8	
rutin	MAPK3		mangiferin	MAPK1	
rutin	NFKBIA		mangiferin	MAPK3	
rutin	RELA		mangiferin	NFKBIA	
kampferol	NOS2	0. 465	mangiferin	IL1B	

kampferol	TNF		mangiferin	AKT1	
kampferol	TP53		mangiferin	CASP3	
kampferol	IL1B		mangiferin	CCL2	
kampferol	CASP3	0. 733	mangiferin	CCL5	
kampferol	CCL2	0. 815	mangiferin	FAS	
kampferol	CYCS	0. 573	mangiferin	IL1A	
kampferol	FOS		mangiferin	MAPK8	
kampferol	IL6	0. 8	mangiferin	NFKB1	
kampferol	JUN		friedelin	CASP3	
kampferol	MAPK1	0. 7	geraniin	TNF	
kampferol	MAPK3		glabridin	CYCS	
kampferol	RELA		pulegone	TNF	
kampferol	AKT1	0. 226	nicotine	MAPK3	
kampferol	CASP9	0. 718	nicotine	MAPK1	
kampferol	CCL5		nicotine	CASP3	
kampferol	NFKBIA	0. 733	nicotine	TP53	
luteolin	TNF	0. 935	nicotine	IL1B	
luteolin	IL1B		nicotine	AKT1	0. 8
luteolin	IFNG		nicotine	FOS	0. 994
luteolin	NFKBIA		nicotine	IL8	0. 8
luteolin	CASP3	0. 818	nicotine	NOS2	0. 502
luteolin	IL6	0. 86	nicotine	RELA	
luteolin	JUN	0. 821	nicotine	TNF	0. 818
luteolin	NOS2	0. 675	nicotine	MAPK8	
luteolin	RELA		nicotine	CYCS	
luteolin	FOS	0. 715	nicotine	NFKB1	0. 336
luteolin	MAPK1	0. 7	nicotine	CCL2	
luteolin	CASP8		nicotine	FAS	
luteolin	CASP9	0. 721	nicotine	JUN	0. 818
luteolin	MAPK3		nicotine	CASP1	
luteolin	MAPK8	0. 936	nicotine	IL6	0. 841
luteolin	NFKB1	0. 85	nicotine	NFKBIA	
luteolin	IL10		nicotine	TNFRSF1A	0. 291
apigenin	TNF	0. 872	nicotine	CASP8	
apigenin	IL1B		nicotine	CASP9	
apigenin	CASP3	0. 941	nicotine	CCL5	
apigenin	IFNG		nicotine	GSK3B	
apigenin	NOS2		nicotine	IL10	0. 15
apigenin	MAPK1		nicotine	IL1A	0. 824