

**Investigation of the mechanism of action of chemical constituents of celery seed against
gout disease using network pharmacology, molecular docking and molecular dynamics
simulations**

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Table S1. 155 chemical constituents of celery seed

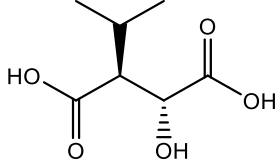
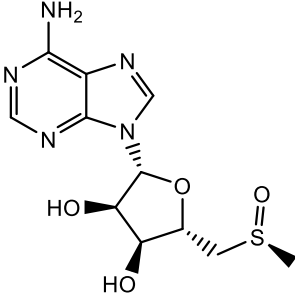
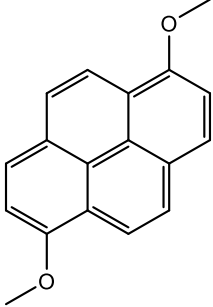
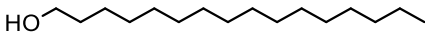
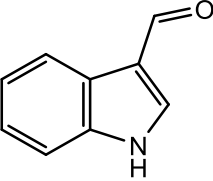
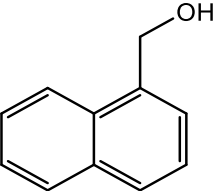
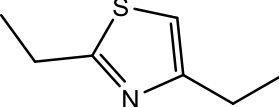
Table S2. 1551 genes related to gout

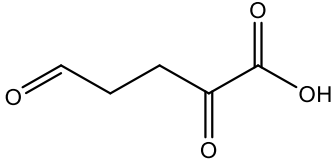
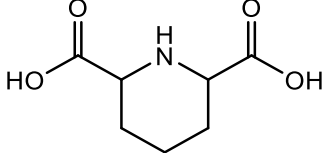
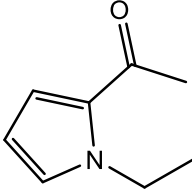
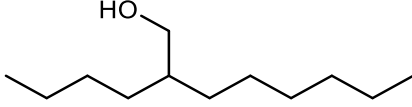
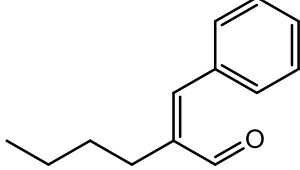
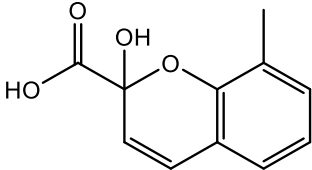
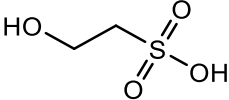
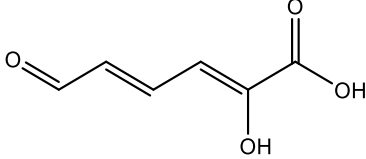
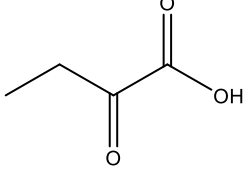
Table S3. 779 targets of celery seed

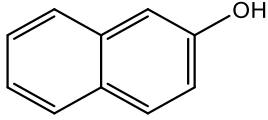
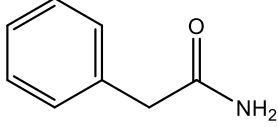
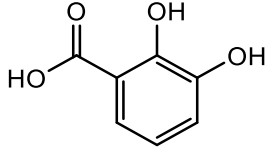
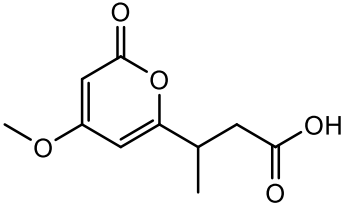
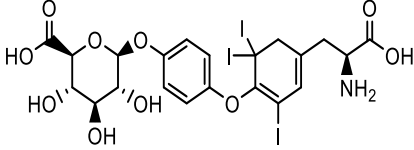
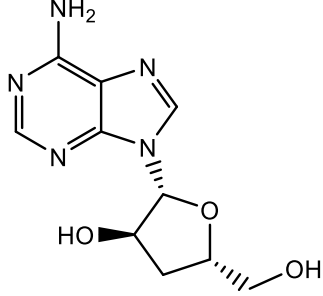
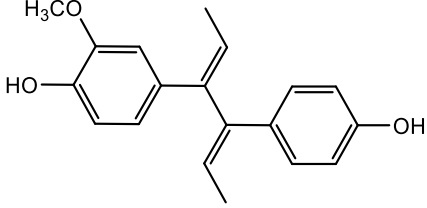
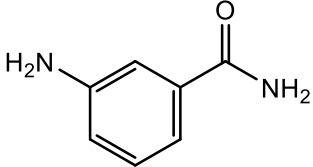
Table S4. Molecular interaction between the potent compounds of celery seed and core targets of gout disease

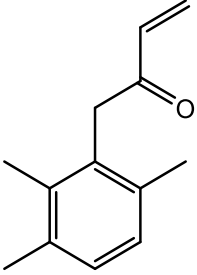
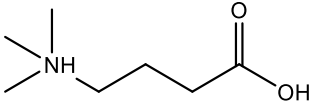
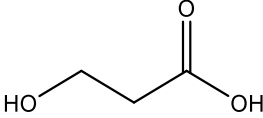
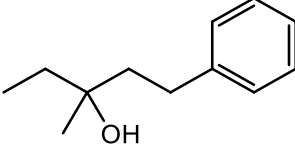
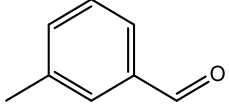
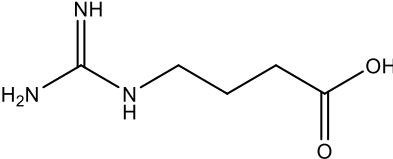
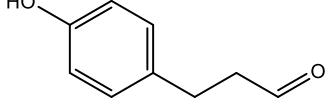
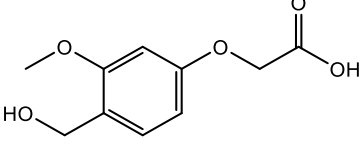
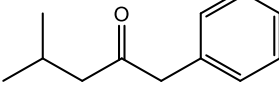
Figure S1. Interaction between C1 and HSP90 α (a), MAPK14-C1 (b) after molecular dynamics simulations. The interacted residues of HSP90 α were identified as Phe22, Gln23, Ile26, Met98, Leu103, Leu107, Gly108, Phe138, Tyr139, Trp162, and Phe170. The interacted residues of MAPK14 were identified as Tyr35, Val38, Ala51, Lys53, Leu108, Met109, Ala157, Leu167, and Phe169.

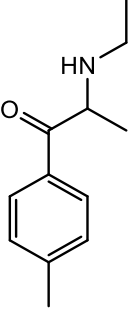
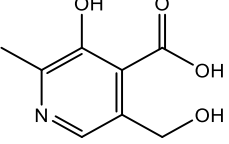
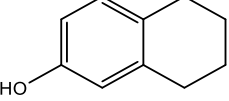
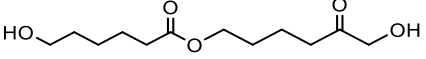
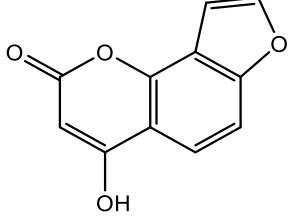
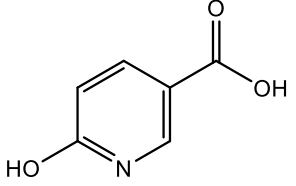
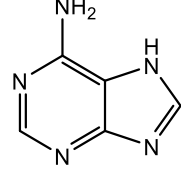
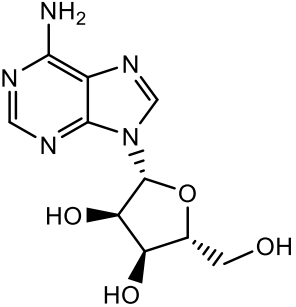
Table S1. 155 chemical constituents of celery seed

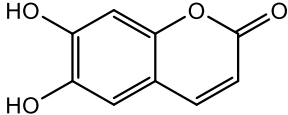
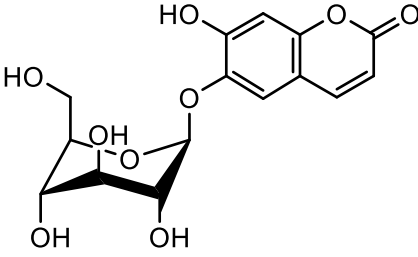
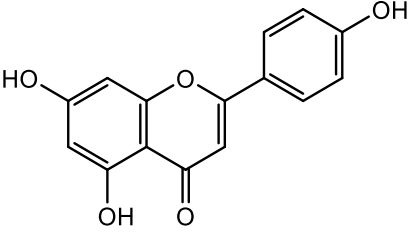
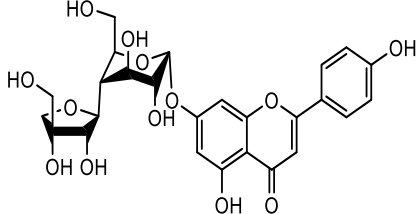
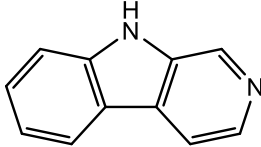
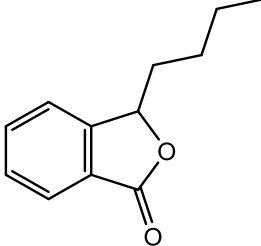
No.	Compound	Structure	F(30%)
1	(2R,3S)-2-Hydroxy-3-isopropylbutanedioic acid	 <p>The structure shows a four-carbon chain with two carboxylic acid groups at the ends. The second carbon has a hydroxyl group (OH) attached with a wedge bond, and the third carbon has an isopropyl group attached with a wedge bond.</p>	0.982
2	(S)-5'-deoxy-5'-(methylsulfinyl)adenosin	 <p>The structure consists of an adenine base attached to a ribose sugar ring. The sugar has hydroxyl groups at the 2' and 3' positions and a methylsulfinyl group (-S(=O)CH₃) at the 5' position. The adenine base has an amino group (-NH₂) at the 6-position.</p>	0.199
3	1,6-Dimethoxyppyren	 <p>The structure is a pyrene molecule with two methoxy groups (-OCH₃) attached at the 1 and 6 positions.</p>	0.783
4	1-Hexadecanol	 <p>The structure is a long-chain alcohol with a hydroxyl group (-OH) at the end of a 16-carbon alkyl chain.</p>	0.992
5	1H-indol-3-carboxaldehyd	 <p>The structure is an indole ring system with an aldehyde group (-CHO) attached at the 3-position.</p>	0.967
6	1-naphthylmethanol	 <p>The structure is a naphthalene ring system with a hydroxymethyl group (-CH₂OH) attached at the 1-position.</p>	0.142
7	2,4-Diethylthiazol	 <p>The structure is a five-membered thiazole ring with ethyl groups (-CH₂CH₃) attached at the 2 and 4 positions.</p>	0.674

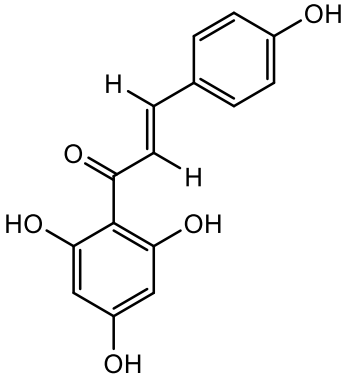
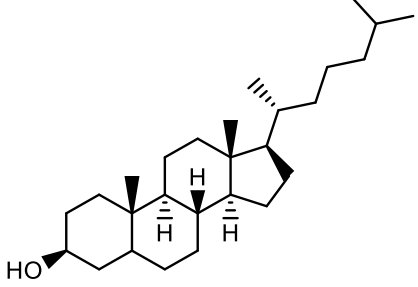
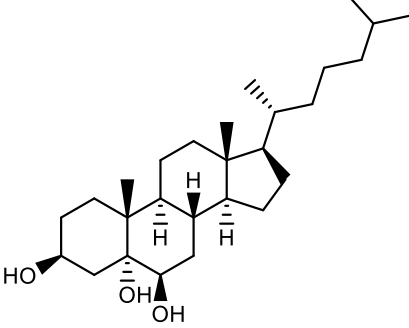
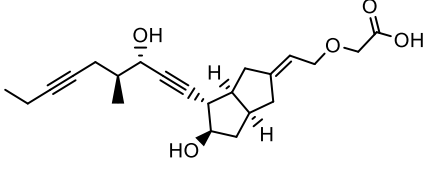
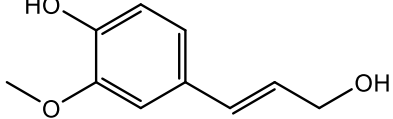
No.	Compound	Structure	F(30%)
8	2,5-Dioxopentanoat		0.222
9	2,6-Piperidinedicarboxylic acid		0.066
10	2-Acetyl-1-ethylpyrrol		0.003
11	2-Butyl-1-octanol		0.918
12	2-Butyl-3-phenyl-2-propen-1-al		0.018
13	2-Hydroxy-8-methylchromen-2-carboxylat		0.001
14	2-Hydroxyethanesulfonat		0.986
15	2-Hydroxymuconat semialdehyd		0.057
16	2-Ketobutyric acid		0.057

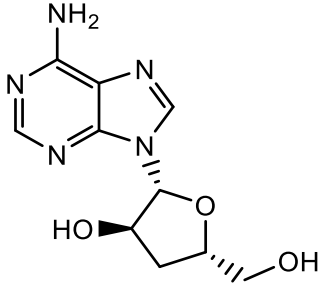
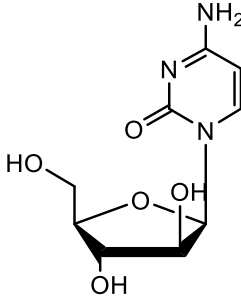
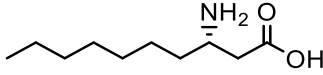
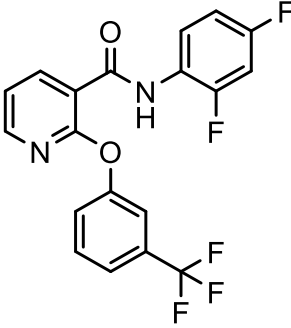
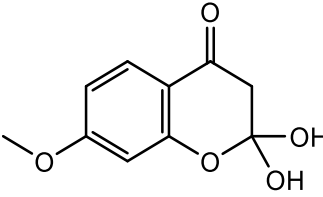
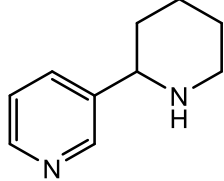
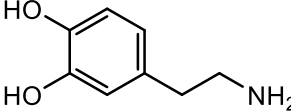
No.	Compound	Structure	F(30%)
17	2-Naphthol		0.803
18	2-Phenylacetamid		0.013
19	2-Pyrocatechuic acid		0.973
20	3-(4-methoxy-6-oxopyran-2-yl)butanoic acid		0.938
21	3,3,5-Triiodo-L-thyronine-beta-D-glucuronosid		0.001
22	3'-Deoxyadenosin		0.099
23	3'-Methoxy-E,E-dienoestrol		0.084
24	3-Aminobenzamid		0.988

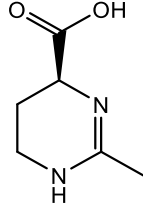
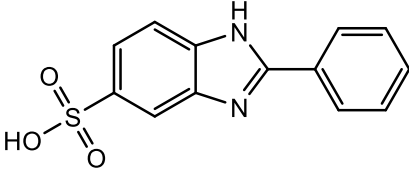
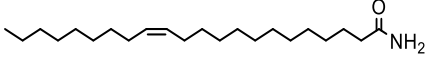
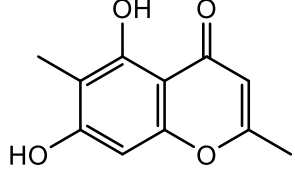
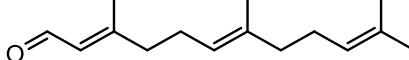
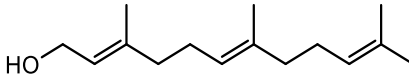
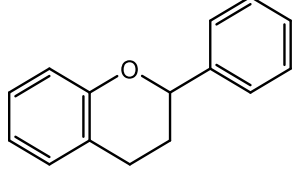
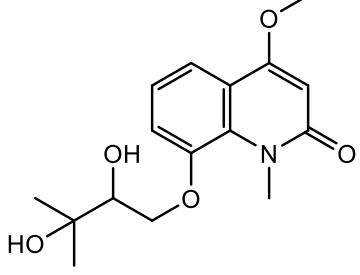
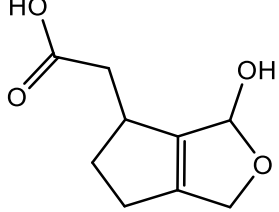
No.	Compound	Structure	F(30%)
25	3-Buten-2-on 1-(2,3,6-trimethyl phenyl)		0.002
26	3-Carboxypropyl trimethylammonium		0.98
27	3-Hydroxypropionic acid		0.985
28	3-Methyl-1-phenyl-3-pentanol		0.003
29	3-Methylbenzaldehyd		0.003
30	4-Guanidinobutanoic acid		0.842
31	4-Hydroxydihydrocinnamaldehyd		0.016
32	4-Hydroxymethyl-3-methoxyphenoxyacetic acid		0.208
33	4-Methyl-1-phenyl-2-pentanon		0.001

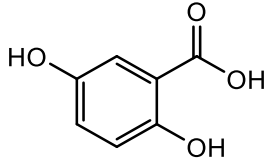
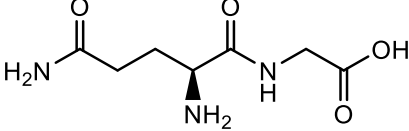
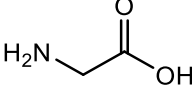
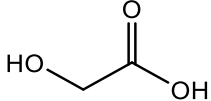
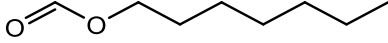
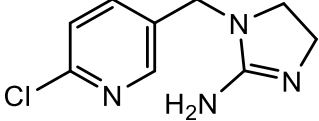
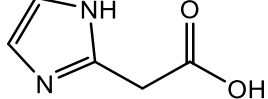
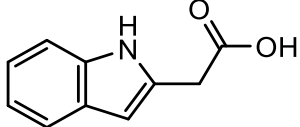
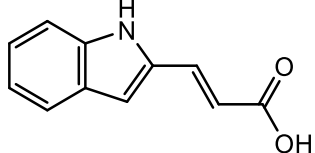
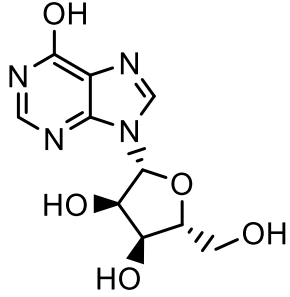
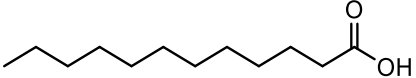
No.	Compound	Structure	F(30%)
34	4-Methyl-N-ethylcathinon		0.065
35	4-Pyridoxic acid		0.015
36	5,6,7,8-Tetrahydro-2-naphthol		0.995
37	6-Hydroxy caproic acid dimer		0.01
38	6-Hydroxyangelicin		0.995
39	6-Hydroxynicotinic acid		0.919
40	Adenin		0.379
41	Adenosin		0.64

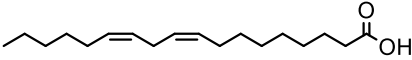
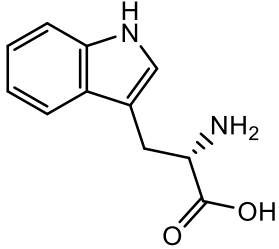
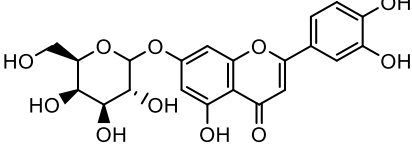
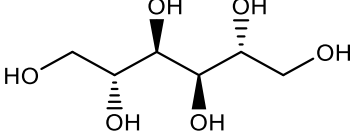
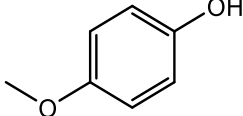
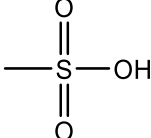
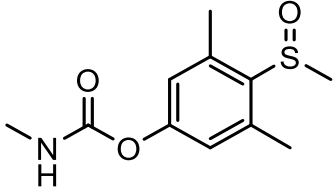
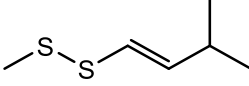
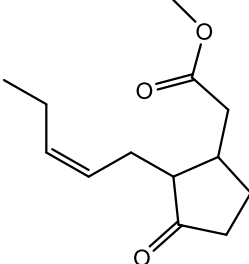
No.	Compound	Structure	F(30%)
42	Aesculetin		1
43	Aesculin		0.998
44	Apigenin		0.999
45	Apiin		0.999
46	Beta-carboline		0.399
47	Butylphthalid (3-n-Butylphthalid)		0.582

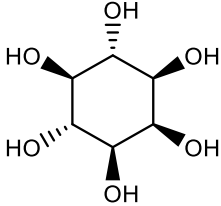
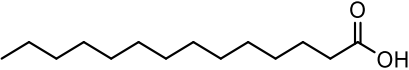
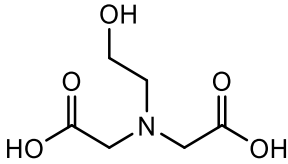
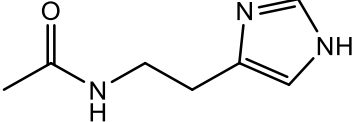
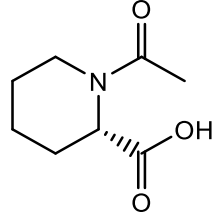
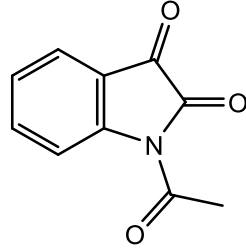
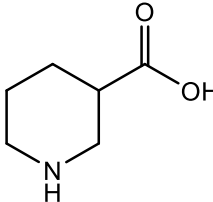
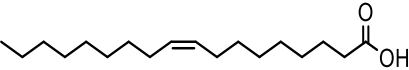
No.	Compound	Structure	F(30%)
48	Chalconaringenin		0.609
49	Cholestan-3beta-ol		0.732
50	Cholestane-3,5,6-triol, (3beta, 5alpha,6beta)-		0.614
51	Cicaprost		0.014
52	Coniferyl alcohol		0.742

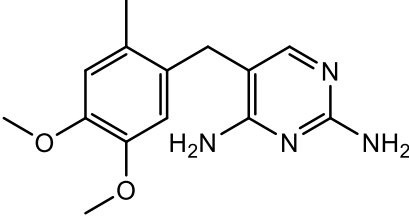
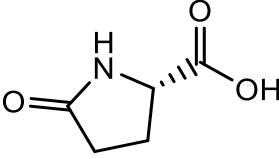
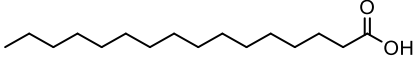
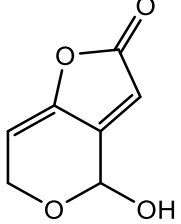
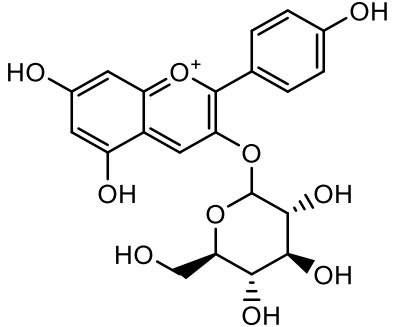
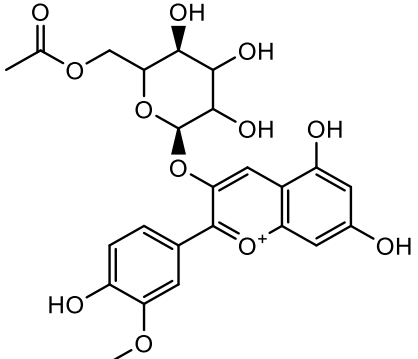
No.	Compound	Structure	F(30%)
53	Cordycepin		0.099
54	Cytarabine		0.921
55	(S)-3-Aminodecanoic Acid		0.127
56	Diflufenican		0.004
57	Dihydroxy-7-methoxy-2,3-dihydrochromen-4-on		0.06
58	DL-anabasin		0.564
59	Dopamin		0.971

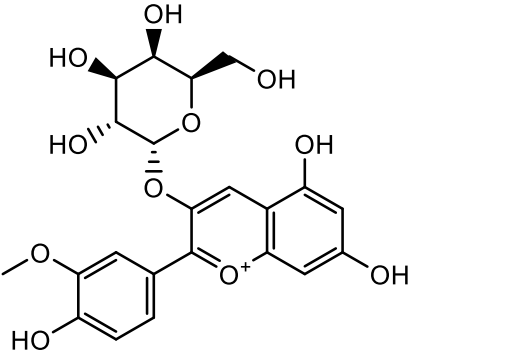
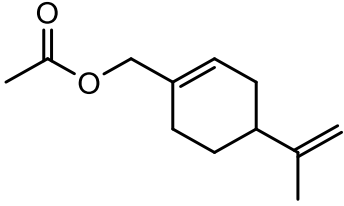
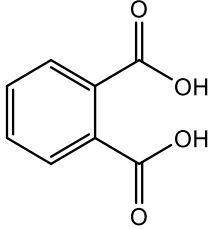
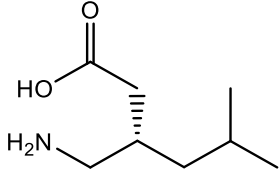
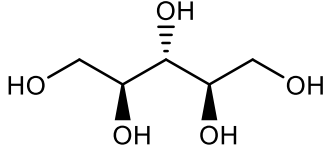
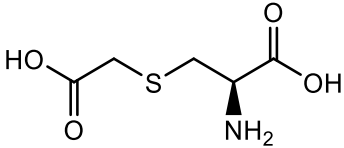
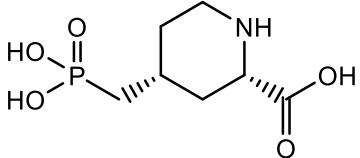
No.	Compound	Structure	F(30%)
60	Ectoin		0.003
61	Ensulizol		0.106
62	Erucamid		0.97
63	Eugenitol		0.838
64	Farnesal		0.685
65	Farnesol		0.995
66	Flavan skeleton		0.891
67	Foliosidin		0.094
68	Genipic acid		0.646

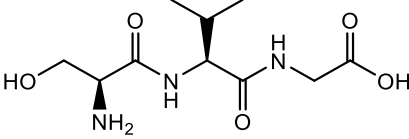
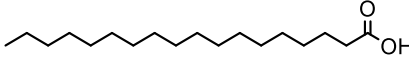
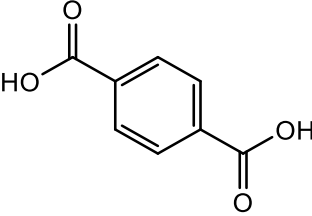
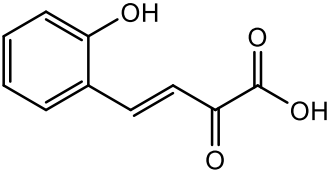
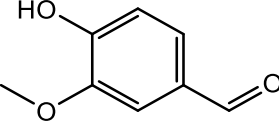
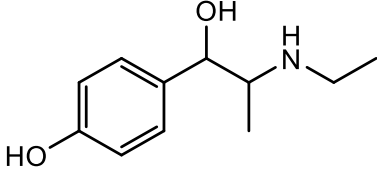
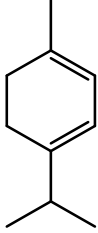
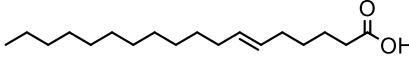
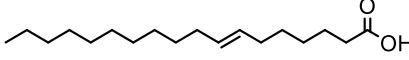
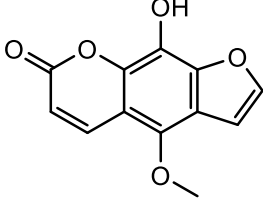
No.	Compound	Structure	F(30%)
69	Gentisic acid		0.988
70	Glycyl-glutamin		0.047
71	Glycin		0.001
72	Glycolic acid		0.007
73	Heptyl format		0.826
74	Imidacloprid-guanidin		0.004
75	Imidazoleacetic acid		0.004
76	Indoleacetic acid		0.008
77	Indoleacrylic acid		0.146
78	Inosin		0.266
79	Lauric acid		0.979

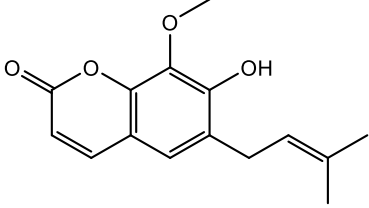
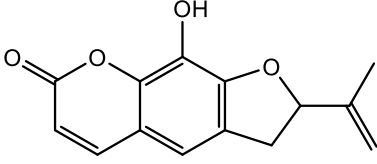
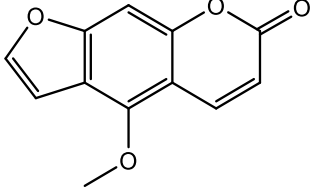
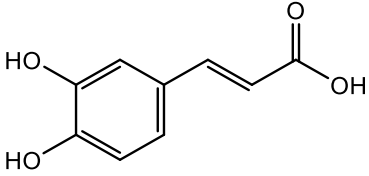
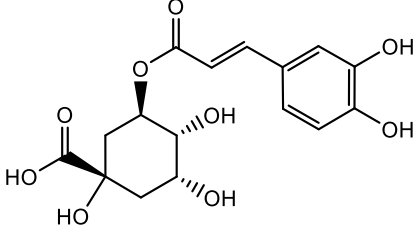
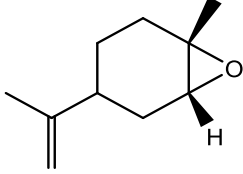
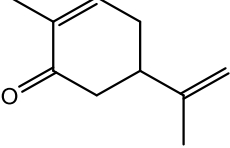
No.	Compound	Structure	F(30%)
80	Linoleic acid		0.549
81	L-tryptophan		0.001
82	Luteolin 7-galactosid		0.999
83	Mannitol		0.992
84	Mequinol		0.277
85	Mesylat		0.043
86	Methiocarb-sulfoxid		0.055
87	Methyl 3-methyl-1-butenyl disulfid		0.806
88	Methyl jasmonat		0.153

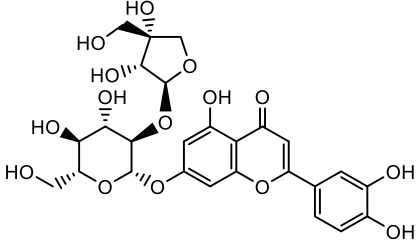
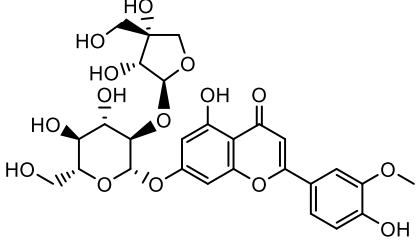
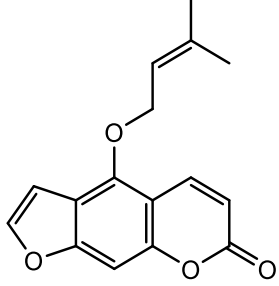
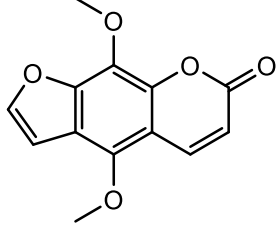
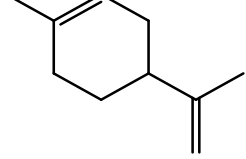
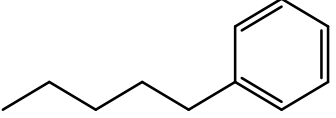
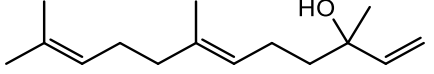
No.	Compound	Structure	F(30%)
89	Myo-inositol		0.999
90	Myristic acid		0.987
91	N-(2-hydroxyethyl)-iminodiacetic acid		0.991
92	N-acetylhistamin		0.35
93	N-Acetylhomoprolin		0.004
94	N-acetylisatin		0.114
95	Nipecotic acid		0.087
96	Oleic acid		0.658

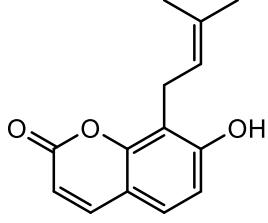
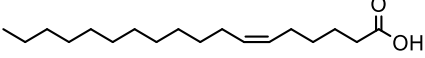
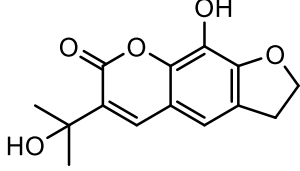
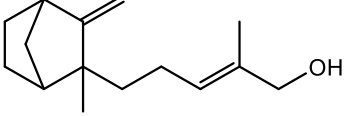
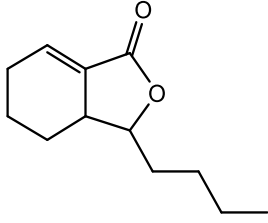
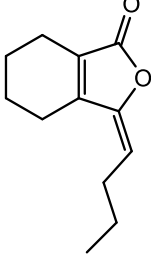
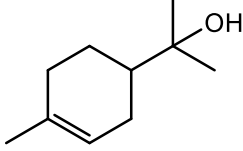
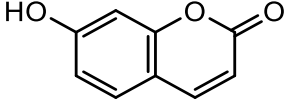
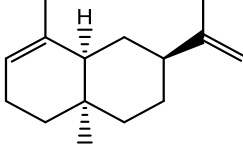
No.	Compound	Structure	F(30%)
97	Ormetoprim		0.006
98	Oxoprolin		0.971
99	Palmitic acid		0.991
100	Patulin		0.705
101	Pelargonidin 3-O-glucosid		0.996
102	Peonidin 3-(6''-acetylglucosid)		0.982

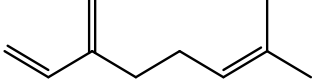
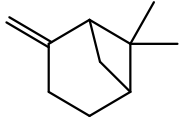
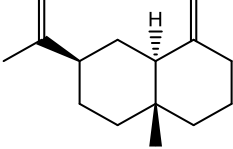
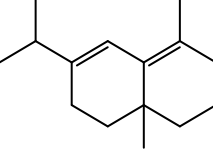
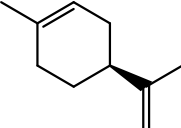
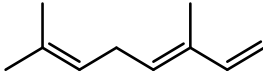
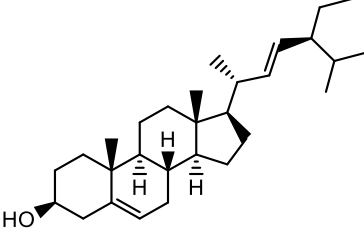
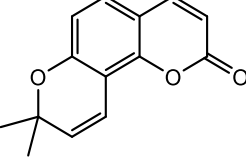
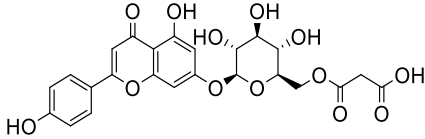
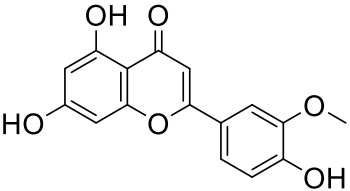
No.	Compound	Structure	F(30%)
103	Peonidin-3-O-beta galactopyranosid	 <p>The structure shows a beta-D-galactopyranoside ring attached to the 3-position of a peonidin cation. The peonidin core consists of a chromone ring system with a methoxy group at position 6, hydroxyl groups at positions 5 and 7, and a hydroxyl group at position 8. The galactose ring is in its pyranose form with hydroxyl groups at positions 2, 3, 4, and 6.</p>	0.993
104	Perillyl acetat	 <p>The structure shows a cyclohexene ring with an acetate group (-O-C(=O)-CH₃) attached to the allylic position (C1) and an isopropenyl group (-C(CH₃)=CH₂) attached to the ring (C4).</p>	0.816
105	Phthalic acid	 <p>The structure shows a benzene ring with two carboxylic acid groups (-COOH) attached to adjacent carbons (ortho position).</p>	0.897
106	Pregabalin	 <p>The structure shows a cyclohexane ring with a carboxylic acid group (-COOH) and an isopropylamino group (-NH-CH₂-CH₂-CH(CH₃)₂) attached to adjacent carbons.</p>	0
107	Ribitol	 <p>The structure shows a five-carbon polyhydroxy alcohol chain with hydroxyl groups at positions 2, 3, and 4. The hydroxyl groups at positions 2 and 4 are on wedges, and the hydroxyl group at position 3 is on a dash.</p>	0.991
108	S-carboxymethylcystein	 <p>The structure shows a cysteine derivative with a carboxymethyl group (-CH₂-COOH) attached to the sulfur atom and an amino group (-NH₂) attached to the alpha carbon.</p>	0.001
109	Selfotel	 <p>The structure shows a piperidine ring with a phosphate group (-P(=O)(OH)₂) attached to the 2-position and a carboxylic acid group (-COOH) attached to the 4-position.</p>	0.992

No.	Compound	Structure	F(30%)
110	Seryl-Valyl-Glycin		0.232
111	Stearic acid		0.994
112	Terephthalic acid		0.259
113	<i>Trans</i> -O-hydroxybenzylidenepyruvat		0.022
114	Vanillin		0.216
115	α -[1-(ethylamino)ethyl]-p-hydroxy-benzyl alcohol		0.009
116	α -Terpinen		0.103
117	Δ 6,7- octadecanoic acid		0.963
118	Δ 7,8-octadecanoic acid		0.963
119	8-hydroxyl-5-methoxypsoralen		0.392

No.	Compound	Structure	F(30%)
120	Apigravin		0.495
121	Apiumetin		0.042
122	Bergapten		0.989
123	Caffeic acid		0.454
124	Chlorogenic acid		0.996
125	<i>Cis</i> -limonen oxide		0.007
126	D-carvon		0.003

No.	Compound	Structure	F(30%)
127	Graveobioside A (luteolin - 7 - apiosylglucoside)		1
128	Graveobioside B (chrysoeriol - 7 - apiosylglucoside)		0.999
129	Isoimperatorin		0.988
130	Isopimpinellin		0.012
131	Limonen		0.798
132	N-amylobenzen		0.935
133	Nerolidol		0.829

No.	Compound	Structure	F(30%)
134	Osthenol		0.984
135	Petroselinic acid		0.658
136	Rutaretin		0.204
137	Santalol		0.233
138	Sedanolid		0.964
139	Sedanonic anhydride		0.991
140	Terpineol		0.014
141	Umbelliferon		0.999
142	α -selenin		0.284

No.	Compound	Structure	F(30%)
143	β -myrcen		0.011
144	β -pinen		0.004
145	β -selinen		0.012
146	D-selinen		0.881
147	D-limonen		0.798
148	Ocimen		0.075
149	Stigmasterol		0.185
150	Seselin		0.952
151	Apigenin 7-O-6''-malonylapiosyl-glucoside		0.998
152	Chrysoeriol		0.998

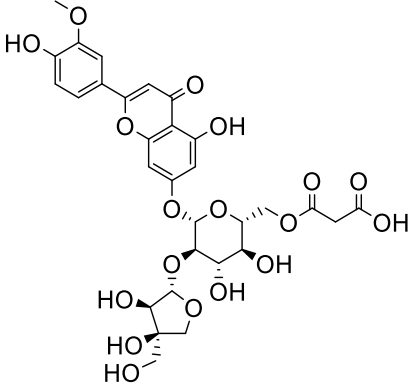
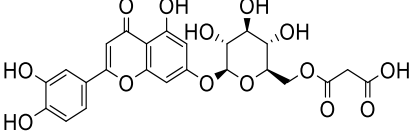
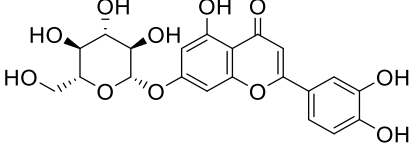
No.	Compound	Structure	F(30%)
153	Chrysoeriol 7- <i>O</i> -6"-malonyl-apiosyl-glucoside		0.999
154	Luteolin 7- <i>O</i> -6"-malonylglucoside		0.999
155	Luteolin-7- <i>O</i> -glucoside		0.999

Table S2. 1551 genes related to gout

No.	Target	No.	Target	No.	Target
1	HPRT1	518	PVALEF	1035	S100A12
2	UMOD	519	RFX3-AS1	1036	ZFP57
3	ABCG2	520	TBX2-AS1	1037	CELA3B
4	PRPS1	521	LHFPL3-AS1	1038	ERAP2
5	DARS2	522	CASC17	1039	G6PC2
6	LDHD	523	AADAACL2-AS1	1040	KCNK16
7	SLC2A9	524	LOC101927855	1041	IER3IP1
8	SLC22A12	525	DST-AS1	1042	MIA2
9	LOC107032760	526	EIF3IP1	1043	NFKBIL1
10	SLC17A3	527	LINC01398	1044	ZFAND3
11	XDH	528	TOLLIP-DT	1045	CCL18
12	HNF1B	529	LOC100128993	1046	EXOSC4
13	MUC1	530	ANKRD20A9P	1047	GCC1
14	INS	531	GPR199P	1048	PPP1R3B
15	SLC17A1	532	LINC02724	1049	CDC123
16	SLC22A11	533	FAAHP1	1050	KIF12
17	HNFJ3	534	MIR6761	1051	ZNHIT3
18	IL1B	535	SLC25A51P4	1052	LACC1
19	PDZK1	536	LOC100287896	1053	OLAH
20	SLC16A9	537	FTH1P22	1054	SP6
21	TNF	538	LINC02372	1055	KLF14
22	APRT	539	RPL18AP11	1056	ANKS4B
23	ALPK1	540	RPS10P1	1057	R3HDML
24	ADSL	541	ENSG00000254739	1058	FABP12
25	ALDH2	542	ENSG00000259290	1059	C2CD4A
26	NLRP3	543	ENSG00000250132	1060	C2CD4B
27	SLC22A6	544	ENSG00000246982	1061	CLTRN
28	IL6	545	ENSG00000261490	1062	H19
29	MEFV	546	ENSG00000250829	1063	MACIR
30	P2RX7	547	ENSG00000257767	1064	TBC1D3G
31	CXCL8	548	ENSG00000272462	1065	HYMAI
32	ALDH16A1	549	LARP1P1	1066	MIR150

No.	Target	No.	Target	No.	Target
33	IL1R1	550	H2AC10P	1067	PLUT
34	CARMIL1	551	MRPS36P2	1068	LOC108251801
35	G6PC1	552	ENSG00000256706	1069	MAP3K7
36	IL18	553	ENSG00000257086	1070	NFKBIA
37	S100A9	554	ENSG00000271857	1071	HCK
38	TLR4	555	ENSG00000272218	1072	CAT
39	SEC61A1	556	ARMC10P1	1073	ITGAM
40	ALB	557	H2AC9P	1074	FADD
41	SLC22A8	558	CYB5AP4	1075	PIK3C2A
42	SLC37A4	559	H1-12P	1076	TSHR
43	PYCARD	560	OR6M2P	1077	EPHA3
44	GAA	561	RNU6-1270P	1078	PLAA
45	SLC22A13	562	RNU7-185P	1079	COX5A
46	MC3R	563	LOC105369980	1080	MB
47	GCKR	564	ENSG00000248245	1081	CDH10
48	ANKH	565	ENSG00000242798	1082	DCDC2
49	DNAJB11	566	ENSG00000257261	1083	DCBLD2
50	HNF1A	567	ENSG00000261584	1084	VPS45
51	APOE	568	CYP4F34P	1085	CCN2
52	PFKM	569	LINC02689	1086	MYO18B
53	OTULIN	570	MRPS33P3	1087	MRPS30
54	LOC100130744	571	RN7SKP93	1088	KLHL5
55	MAOA	572	RN7SL496P	1089	PRPSAP2
56	PPAT	573	RPL31P24	1090	VSTM4
57	RELN	574	RPF2P2	1091	ISCA1P1
58	KCNJ11	575	SNX18P26	1092	ASS1P7
59	ABCC8	576	ENSG00000249219	1093	IL2RA
60	REN	577	ENSG00000260743	1094	PRL
61	PRPS1L1	578	ENSG00000287898	1095	CLEC12A
62	SYK	579	Inc-DRD5-4	1096	RHOD
63	HNF4A	580	Inc-ATG2B-2	1097	PPARGC1B
64	PAX2	581	ENSG00000273015	1098	RPS6KB1
65	XPNPEP3	582	ENSG00000286894	1099	HMOX1
66	BLK	583	NONHSAG009952.2	1100	PLAU

No.	Target	No.	Target	No.	Target
67	GCK	584	piR-42491-087	1101	BCL2
68	PDX1	585	MK280607-090	1102	MAPT
69	NEUROD1	586	piR-38051-196	1103	MAPK8
70	PAX4	587	NONHSAG022975.2	1104	PTPRF
71	KLF11	588	NONHSAG047833.2	1105	SERPINE1
72	LRP6	589	piR-32214-100	1106	TUBB
73	SLC12A3	590	RF00017-5046	1107	VIM
74	SLC4A1	591	HSALNG0033332	1108	MVK
75	SPTA1	592	ENSG00000273088	1109	NFE2L2
76	CLCNKB	593	ENSG00000287935	1110	PLD1
77	ANK1	594	lnc-SLC37A2-4	1111	PLA2G6
78	SPTB	595	lnc-SLC38A2-2	1112	RHOA
79	EPB42	596	lnc-SMYD3-6	1113	SCN1A
80	PRPS2	597	lnc-TMEM105-1	1114	ACHE
81	PRKG2	598	lnc-WDR1-8	1115	KIF5B
82	APOA1	599	lnc-RHEB-3	1116	KNG1
83	IL4	600	lnc-RTKN2-4	1117	GAL
84	JAK2	601	lnc-VKORC1L1-2	1118	S100A4
85	COMT	602	L13714-395	1119	SELE
86	PTGS2	603	lnc-ADIPOR2-3	1120	DUSP19
87	LEP	604	lnc-ATE1-7	1121	KIF16B
88	CARD8	605	lnc-HIST1H2BF-1	1122	HCP5
89	SHLD2	606	lnc-COL21A1-8	1123	PSORS1C1
90	LPL	607	lnc-GLUD1-1	1124	LOC102724058
91	GRHPR	608	lnc-KRTCAP2-1	1125	RPS6KB2
92	NT5C2	609	HSALNG0062380	1126	MAPK1
93	MSMB	610	ENSG00000272166	1127	INPP5D
94	LRP2	611	ENSG00000274591	1128	ARHGAP26
95	LDLR	612	ENSG00000282988	1129	ADSS2
96	PNP	613	GPATCH11P1	1130	MIR155
97	NPHP1	614	CTB-49A3.2	1131	SH3KBP1
98	MOCOS	615	MN309129	1132	FUT2
99	AMPD1	616	NONHSAG003206.2	1133	ACE
100	CCL2	617	piR-43408-017	1134	TYMS

No.	Target	No.	Target	No.	Target
101	ATM	618	piR-46852	1135	CHKA
102	LIPC	619	piR-54765-015	1136	CXCL2
103	BCAS3	620	piR-39098-249	1137	CREBRF
104	CPT2	621	piR-52680-322	1138	URAD
105	CEL	622	HSALNG0084800	1139	COASY
106	MPL	623	lnc-UBASH3A-6	1140	PIK3R1
107	APPL1	624	lnc-PDZK1-2	1141	CBL
108	TET2	625	lnc-RUNX2-6	1142	CD79A
109	MLKL	626	lnc-TFF3-2	1143	IL12A
110	FAM167A	627	HSALNG0032849	1144	SH3GL3
111	INSL6	628	lnc-GLUD1-6	1145	PHGDH
112	C12orf43	629	lnc-KCNJ11-4	1146	CD4
113	INS-IGF2	630	lnc-HIST1H2AD-2	1147	SLCO1B1
114	ADA	631	HSALNG0090693	1148	TF
115	TGFB1	632	HSALNG0062381	1149	KLKB1
116	PYGM	633	HSALNG0082950	1150	AKR1C3
117	SLC12A1	634	HSALNG0094020	1151	C5
118	INSR	635	HSALNG0024737-002	1152	BMP2
119	TNFSF11	636	HSALNG0007818	1153	LCAT
120	NGF	637	HSALNG0024737-001	1154	ARRB2
121	MAF	638	piR-41405-125	1155	IVD
122	SLC17A2	639	MN309171	1156	FADS1
123	WDR1	640	piR-33804-159	1157	RBP4
124	PRTFDC1	641	piR-49423-021	1158	REV3L
125	CD14	642	piR-31313	1159	UGT1A9
126	CNTN5	643	piR-57138-043	1160	CYP4A11
127	ZNF724	644	RF00017-4964	1161	SLC7A6
128	MIR302F	645	piR-47223	1162	NAT2
129	NPHP4	646	piR-57461-011	1163	PPID
130	SCARF1	647	piR-60513	1164	SLC10A2
131	RMND1	648	piR-59316-017	1165	ALMS1
132	SHROOM3	649	piR-52594	1166	GLS2
133	SPATA5L1	650	RF00017-3993	1167	GPAA1
134	CST9	651	HSALNG0049690	1168	PKD2L1

No.	Target	No.	Target	No.	Target
135	CCDC160	652	lnc-TUBA3C-17	1169	UGT1A6
136	PKD2	653	lnc-UBASH3A-7	1170	UGT1A4
137	CD160	654	HSALNG0032847	1171	CNTN4
138	NIPAL1	655	HSALNG0032851	1172	ELOVL2
139	APOB	656	lnc-MBLAC1-2	1173	UGT1A10
140	NRXN2	657	lnc-ACSM1-3	1174	FFAR4
141	TLR2	658	lnc-HIST1H3D-1	1175	FFAR1
142	APP	659	lnc-KCNJ11-1	1176	HPS5
143	ADK	660	lnc-KMT2E-7	1177	PDXDC1
144	SLC6A3	661	HSALNG0035738	1178	UGT1A7
145	FGA	662	HSALNG0038925	1179	UGT1A3
146	ATIC	663	HSALNG0035741	1180	ABO
147	ERCC6	664	HSALNG0060278	1181	UNC119B
148	DGUOK	665	HSALNG0094021	1182	METTL6
149	RAPGEF3	666	HSALNG0050335	1183	TRIM4
150	RAPGEF4	667	HSALNG0050337	1184	UGT1A5
151	GDA	668	HSALNG0054805	1185	DGCR5
152	EN1	669	HSALNG0073411	1186	UOX
153	THAP1	670	HSALNG0012164-001	1187	LINC01428
154	VDR	671	piR-48209-523	1188	MTOR
155	PPARA	672	Hsa-Mir-95-P2_5p-007	1189	FCN1
156	CYP2C8	673	HSALNG0110062	1190	PIK3R2
157	PRKAG2	674	HSALNG0056912	1191	WAS
158	ADRB3	675	HSALNG0013825	1192	EPHA2
159	ZNF518B	676	HSALNG0030963	1193	NT5E
160	HLA-B	677	FLT3	1194	THRB
161	CLNK	678	NOD2	1195	ALPL
162	IL37	679	UCP2	1196	PTK2B
163	CSF2	680	NR0B2	1197	AHR
164	R3HDM2	681	SST	1198	IGF1
165	CYP2E1	682	MTHFR	1199	ITPR1
166	SLC2A6	683	CHUK	1200	IRAK4
167	IL10	684	HLA-A	1201	SCD
168	APOC3	685	ARID1B	1202	ASS1

No.	Target	No.	Target	No.	Target
169	IL17A	686	HLA-C	1203	MASP1
170	IL1RAPL2	687	SCGN	1204	HSP90AA1
171	HP	688	PIK3CG	1205	TXNRD1
172	MEN1	689	NR1H3	1206	TXNRD2
173	CDC42BPG	690	TREM1	1207	PTK2
174	GPT	691	CCL3	1208	CPS1
175	HRH2	692	YY1	1209	AMPD2
176	CSF1	693	VEGFA	1210	ACADM
177	FGF5	694	MC4R	1211	ACADS
178	TERT	695	FYN	1212	ETFDH
179	LPA	696	CTSB	1213	MASP2
180	MAP4K2	697	KIT	1214	SLC6A8
181	RASGRP2	698	IRS1	1215	TXN
182	SF1	699	HHEX	1216	PRODH
183	KCNJ16	700	TAGAP	1217	PTH
184	AICF	701	CASR	1218	CD27
185	RREB1	702	AGT	1219	HDC
186	PKLR	703	ACTB	1220	IL2
187	SLC22A7	704	SLC12A2	1221	ENPEP
188	INHBC	705	CTCF	1222	AKR1A1
189	TFAP2A	706	CETP	1223	CASP5
190	ADIPOQ	707	PAX5	1224	ITM2B
191	LRP1	708	PRDX2	1225	CXCL10
192	KTN1	709	WNK1	1226	NFIB
193	GYG1	710	ABCB11	1227	CCL5
194	AGL	711	AQP1	1228	BMP6
195	GBE1	712	EPB41	1229	IGFBP1
196	EGF	713	HBB	1230	CABIN1
197	CD44	714	KLF1	1231	COG2
198	IL12B	715	RHAG	1232	OPLAH
199	ADH1B	716	TRPM6	1233	NLRP2
200	SLC28A2	717	AOX1	1234	KIF3A
201	S100A8	718	ADCY10	1235	LGALS9
202	OIT3	719	KCNJ10	1236	EYA3

No.	Target	No.	Target	No.	Target
203	CST3	720	GYPA	1237	FLT3LG
204	CXCL16	721	STK39	1238	IL1F10
205	ABCC4	722	SUOX	1239	SLC16A10
206	PON1	723	THBS1	1240	NAT8
207	SLC17A5	724	STK24	1241	NUDT15
208	BTF3P7	725	SNCAIP	1242	LECT2
209	POMC	726	SPTBN1	1243	NLRP4
210	TNFRSF1A	727	WNK4	1244	LILRA1
211	HLA-DRB1	728	APOA5	1245	SUGT1
212	PPARG	729	BCL11A	1246	ADSS1
213	SIRT1	730	USF1	1247	NBPF3
214	IL23R	731	RPS3	1248	EMC4
215	NRBP1	732	SEC23B	1249	CNMD
216	SRC	733	CD34	1250	LILRA3
217	RELA	734	CD47	1251	MIR302B
218	MYD88	735	HBG1	1252	MIR488
219	SLC2A5	736	GYPC	1253	ELOVL2-AS1
220	PDK2	737	KLHL3	1254	MIR920
221	TRPM2	738	RPS27A	1255	MIR3936HG
222	PCBD1	739	SDC1	1256	MIR4700
223	LHX1	740	SRI	1257	URAHP
224	CDH4	741	ANK2	1258	UGT1A
225	UFM1	742	ADD2	1259	RAD17P1
226	CDK5RAP3	743	ANXA7	1260	KRT18P30
227	DDRGK1	744	CLDN16	1261	RPL29P5
228	UFL1	745	OSGEP	1262	BTK
229	MYH9	746	HS2ST1	1263	PIK3CA
230	IL6R	747	HS3ST1	1264	GRB2
231	CD40LG	748	HS6ST1	1265	FCN2
232	MYO9A	749	RHBDF2	1266	PLEK
233	TFRC	750	RHD	1267	DNM1
234	GCG	751	RPS3A	1268	RPS6KA2
235	TBXAS1	752	CTCFL	1269	SLC7A11
236	CYP4B1	753	BSND	1270	FCN3

No.	Target	No.	Target	No.	Target
237	PANX1	754	CLCNKA	1271	MET
238	HMGCR	755	PGLYRP1	1272	PTEN
239	FGFR2	756	USF2	1273	PLCG1
240	SFMBT1	757	ST8SIA4	1274	PIK3C2B
241	TRIM46	758	RPS23	1275	IL7R
242	MLXIP	759	RPS16	1276	SLC34A2
243	SGK1	760	WNK3	1277	WWP2
244	LPXN	761	HS3ST2	1278	DNM3
245	LINC01010	762	HBE1	1279	RPS6
246	CT69	763	BLOC1S6	1280	WWP1
247	PPARGC1A	764	LDB2	1281	GLMN
248	HGF	765	LDB1	1282	SGO1
249	KCNQ1	766	GLCE	1283	ZNHIT6
250	FOXA2	767	HS3ST3B1	1284	FGFR1
251	JAZF1	768	PIEZO1	1285	FGFR3
252	MMP2	769	SACM1L	1286	ITK
253	PTPN11	770	ZFPM1	1287	ZAP70
254	ABCB1	771	DMTN	1288	EP300
255	GYS1	772	GYPB	1289	MERTK
256	FBP1	773	NPRL3	1290	PDPK1
257	GAPDH	774	HS3ST3A1	1291	KAT2B
258	PC	775	GTF3C1	1292	CYP24A1
259	NCOA3	776	HS3ST6	1293	IFIH1
260	PHKA2	777	HS3ST4	1294	MTR
261	PHKB	778	VEZF1	1295	MALT1
262	APOC2	779	HS3ST5	1296	PRLR
263	NCOA1	780	DPH3	1297	XPO1
264	NCOA2	781	PYDC1	1298	ITCH
265	FXYD2	782	OR51V1	1299	WASF1
266	HFE	783	OR51M1	1300	ADM
267	NFE2	784	H3-2	1301	EOMES
268	G6PC3	785	MMP2-AS1	1302	SAE1
269	SLC37A3	786	IGHV4-38-2	1303	PVR
270	SLC37A1	787	ABL1	1304	S1PR1

No.	Target	No.	Target	No.	Target
271	PAGR1	788	TYK2	1305	S1PR2
272	LIME1	789	STAT1	1306	STRADA
273	H2AC18	790	CSF1R	1307	SP1
274	MIR142	791	MYC	1308	KCNH7
275	CRP	792	BCL2L1	1309	CALCA
276	IGF1R	793	CR1	1310	CD86
277	MMP3	794	LAMA5	1311	CDKN3
278	HNF4G	795	CLEC16A	1312	MANBA
279	PTX3	796	FCRL3	1313	RGS14
280	G6PD	797	BMPR2	1314	PRPF31
281	GATA1	798	CASP1	1315	ZFP36L1
282	HBG2	799	ACVRL1	1316	AHI1
283	TP53	800	ACVR1B	1317	BACH2
284	B2M	801	TUBB1	1318	BIRC6
285	F2	802	ACVR2A	1319	CXCR5
286	GPI	803	FRK	1320	BATF
287	TNFRSF11A	804	HDAC7	1321	ASAP1
288	TEC	805	B4GALT1	1322	GCA
289	FCGR3A	806	USP2	1323	TNFSF14
290	ATG16L1	807	ARNT	1324	GPR65
291	ABCF1	808	DAB2	1325	SLC15A2
292	IL17REL	809	ATXN2	1326	MYNN
293	MMP1	810	MLXIPL	1327	SLC30A7
294	IFNG	811	NFAT5	1328	TMPRSS5
295	PTGS1	812	ADPGK	1329	SOX8
296	NR5A2	813	INHBB	1330	PRAME
297	AMPD3	814	ORC4	1331	KIF15
298	PRPSAP1	815	LTBP3	1332	NDFIP1
299	SLC22A1	816	P2RY6	1333	PPP1R14C
300	TNFRSF1B	817	UBE2Q2	1334	SP140
301	KCNJ1	818	BAZ1B	1335	ARHGEF25
302	TNFRSF10B	819	ASAH2	1336	ANKRD17
303	SLC2A9-AS1	820	HLF	1337	ERGIC3
304	MMP9	821	STC1	1338	DKKL1

No.	Target	No.	Target	No.	Target
305	MMP14	822	DACH1	1339	PLEKHA8
306	SAA1	823	AKT1S1	1340	NFKBIZ
307	GATA4	824	NRG4	1341	CEP85L
308	ENO3	825	INHBE	1342	MPV17L2
309	HADH	826	OVOL1	1343	ZBTB46
310	PARK7	827	SLC48A1	1344	CALML4
311	PFKP	828	B3GNT4	1345	CLECL1
312	PFKL	829	ANKRD55	1346	ODF3B
313	PGAM2	830	MUSTN1	1347	SEPTIN1
314	FHL3	831	QRICH2	1348	PVT1
315	MYOZ3	832	TMEM171	1349	ERBB2
316	PPP1R3D	833	MIR146A	1350	MAP2K1
317	PDGFRB	834	LINC02875	1351	RAF1
318	STAT3	835	C5orf67	1352	AKT1
319	UGT1A1	836	B4GALT1-AS1	1353	BRAF
320	UGT1A8	837	ADPGK-AS1	1354	EGFR
321	PRKCA	838	LYN	1355	CSNK2A1
322	HMGB1	839	KDR	1356	NFKB1
323	GLUD1	840	MAPK14	1357	CDH1
324	RHEB	841	CYP3A4	1358	ITGB1
325	VCAM1	842	NOS2	1359	MYB
326	VWF	843	TNFRSF11B	1360	MAP3K1
327	GAD1	844	CTSL	1361	PIM1
328	IL1RN	845	IDO1	1362	RPS6KA1
329	SLC22A4	846	NOD1	1363	TSC2
330	IL1A	847	CALCB	1364	CBS
331	TBX21	848	TXNIP	1365	ITGA6
332	NTRK2	849	LACTB	1366	CSNK2B
333	CFTR	850	EZH2	1367	GATA2
334	RARB	851	PDGFRA	1368	MAPK3
335	KCNJ2	852	JAK1	1369	PIK3CB
336	MYL2	853	DNMT3A	1370	PRKCE
337	ALDH1A2	854	JAK3	1371	RAC1
338	DRD5	855	IDH2	1372	XIAP

No.	Target	No.	Target	No.	Target
339	MITF	856	IDH1	1373	FGR
340	MAP3K11	857	TH	1374	PRKACG
341	RUNX2	858	ADAM17	1375	ARF1
342	ABCA1	859	CALR	1376	CD40
343	ETV1	860	ITGB3	1377	BIRC3
344	PPARD	861	MPO	1378	CSK
345	PTGDR	862	MMP13	1379	BRD4
346	WWOX	863	NR2F2	1380	HDAC9
347	PDE1C	864	PTPRC	1381	ITGA3
348	MYH11	865	COL2A1	1382	CYP27B1
349	TOP2B	866	DPP4	1383	NCF2
350	TRPA1	867	ADCY5	1384	MBL2
351	TACR1	868	ANXA1	1385	NEDD4
352	PTPRD	869	OPRM1	1386	RASA1
353	SPP1	870	MIF	1387	TTN
354	ABCC9	871	PLA2G4A	1388	TSC1
355	BDKRB2	872	MMP7	1389	IRF8
356	MAPKAPK5	873	MMP8	1390	PKD1
357	MAPK6	874	SLC2A2	1391	PDK1
358	SOX6	875	SLC16A1	1392	PRDX5
359	WNT5B	876	TTR	1393	TRIO
360	CASQ1	877	RIPK1	1394	PTGER4
361	ABCG1	878	STAT5B	1395	VDAC1
362	SLC13A3	879	PTPN6	1396	VAV1
363	SMARCC1	880	COMP	1397	CORIN
364	CACNA2D4	881	FOXO1	1398	CBX5
365	CD2	882	GATA6	1399	CRHR1
366	BAIAP2	883	GGT1	1400	BAG3
367	BRSK2	884	PAX6	1401	BCL10
368	ADIPOR2	885	PCK1	1402	KIF2C
369	CLIC5	886	NR1H2	1403	PANK2
370	DST	887	MMP19	1404	NCK1
371	NDE1	888	PTPN22	1405	MAP3K14
372	SLC38A1	889	SERPINC1	1406	S1PR3

No.	Target	No.	Target	No.	Target
373	TOLLIP	890	ACAN	1407	PTPRK
374	ADAM15	891	CSF3R	1408	SHC1
375	ARID5B	892	ETV6	1409	TCF7
376	CDK13	893	EPOR	1410	TMPRSS2
377	ERC1	894	IRF5	1411	RIPK4
378	FANCE	895	IL6ST	1412	SCO2
379	HIBADH	896	GLP1R	1413	HPN
380	CUX2	897	FOXP3	1414	HAAO
381	NTNG2	898	HK2	1415	FABP4
382	OPN4	899	IGF2	1416	TRIM33
383	MFN1	900	HSPA5	1417	DDAH1
384	RAD52	901	HSPD1	1418	ALCAM
385	SLC38A2	902	PCK2	1419	CFP
386	SNCG	903	PCSK1	1420	EEF1D
387	SMYD3	904	MTNR1B	1421	EIF4A3
388	CACNA2D3	905	MMP10	1422	GLUD2
389	ARID2	906	NR4A2	1423	GRB10
390	ALX4	907	SLC11A1	1424	CYFIP2
391	ATP1A4	908	SLC5A2	1425	KRT7
392	ASH1L	909	PRKAB1	1426	PLA2G4C
393	GABPA	910	STAT4	1427	RBX1
394	GRID1	911	TLR1	1428	TNFRSF25
395	GREM2	912	DGKB	1429	SP3
396	NALCN	913	BAD	1430	SFTPD
397	PIBF1	914	ANXA5	1431	TMPRSS3
398	POLD3	915	F5	1432	WASF2
399	RFX3	916	GAD2	1433	AGK
400	SLC28A3	917	ISL1	1434	ARHGEF11
401	TFF3	918	KCNJ3	1435	ADCYAP1
402	TPST1	919	FTO	1436	KRT20
403	SUCNR1	920	MMP12	1437	IL7
404	SUPT3H	921	MMP15	1438	PKIA
405	SV2B	922	RELB	1439	TNFRSF8
406	TAX1BP1	923	SLC19A2	1440	TPD52

No.	Target	No.	Target	No.	Target
407	TAF6	924	TCF7L2	1441	CD6
408	ACSM1	925	REL	1442	CD5
409	BTN3A1	926	STAT5A	1443	CDC37
410	KMT2E	927	SERPINH1	1444	AGAP2
411	TAF11	928	TRPV1	1445	HNRNPF
412	ACSM5	929	WFS1	1446	SLC16A4
413	ACAD10	930	CCR6	1447	SRSF2
414	AP4M1	931	ALDOB	1448	PSMC6
415	AATK	932	ALOX5AP	1449	ZMIZ1
416	BTN2A1	933	CCR2	1450	AP2A1
417	ARL4A	934	CTLA4	1451	CENPA
418	GALNTL5	935	CIITA	1452	BLZF1
419	KCTD7	936	FOXM1	1453	CRHBP
420	RBFOX1	937	IRS2	1454	CHST12
421	RAB27B	938	IGF2BP2	1455	HBS1L
422	PTGFRN	939	HMGA2	1456	NCKAP1
423	THEM4	940	HAMP	1457	MLANA
424	WDR4	941	NLRP1	1458	SAFB
425	DHX15	942	HGD	1459	SESN3
426	NSUN3	943	SELP	1460	ARF3
427	WDR11	944	PMPCA	1461	CD58
428	ACSM2A	945	PSTPIP1	1462	CLIC6
429	ANO2	946	PTPRN	1463	EXTL2
430	BTN2A2	947	SOCS2	1464	EDC4
431	BTN3A2	948	KITLG	1465	EVI5
432	ASB10	949	IGFBP2	1466	IL22RA2
433	COL21A1	950	IL17RA	1467	OLIG3
434	CNIH2	951	MMP17	1468	MAGEA1
435	EI24	952	IL13	1469	PLCL2
436	H1-4	953	THBD	1470	RGS1
437	NAP1L5	954	PRKCSH	1471	THEMIS
438	MED27	955	TIMP1	1472	AP2A2
439	NAA25	956	SOCS3	1473	COPG2
440	KIF26B	957	SEC63	1474	IL20RA

No.	Target	No.	Target	No.	Target
441	SLC17A4	958	ADAMTS4	1475	NCOA5
442	TRMT112	959	ADAMTS5	1476	MAGEA3
443	PKNOX2	960	ASXL1	1477	TIMMDC1
444	PRDM8	961	GHRL	1478	XPO6
445	CCDC68	962	FABP1	1479	BRK1
446	ACSM2B	963	FOXA1	1480	ANKRD30A
447	NIPSNAP3B	964	PADI4	1481	EFS
448	SCAF11	965	MIPEP	1482	MMEL1
449	THEM5	966	MAFB	1483	SVEP1
450	RTKN2	967	HLA-DQB1	1484	ALPK2
451	BTN3A3	968	IL3	1485	MRPS26
452	ABT1	969	SLC30A8	1486	KIF21B
453	FSTL4	970	SLC30A10	1487	PPIL4
454	EVA1A	971	U2AF1	1488	CSN1S1
455	LHFPL3	972	PSMD9	1489	NUTM1
456	MMRN2	973	CAMK1D	1490	SH3BGRL2
457	UHRF1BP1	974	CAPN10	1491	RGCC
458	PXDNL	975	BMP3	1492	ZNF746
459	ZMYM6	976	CILP	1493	TMEM39A
460	ZMYM1	977	HSPA4	1494	CTAG1B
461	ZFPL1	978	IAPP	1495	H3-4
462	CNPY4	979	GSTM1	1496	SH2D4B
463	HMGN4	980	FABP2	1497	MAMSTR
464	KRTCAP2	981	IFNA2	1498	ZNF438
465	SSUH2	982	OSM	1499	DLEU1
466	PRDM15	983	MNX1	1500	INAVA
467	ZNF639	984	MAFA	1501	H3C14
468	DMBX1	985	LTA	1502	ST13P4
469	GPR89A	986	PADI2	1503	IL12A-AS1
470	FRMD4B	987	NEUROG3	1504	ZNF767P
471	FBXL14	988	KDM4C	1505	MIR548AW
472	NCKAP5	989	TNFAIP6	1506	MIR5699
473	FAM53A	990	PTGES	1507	LOC285626
474	ADIRF	991	THPO	1508	MIR5702

No.	Target	No.	Target	No.	Target
475	H1-3	992	PTF1A	1509	MIR5696
476	H3C4	993	ARAP1	1510	LINC01147
477	OR8D4	994	CYB5R4	1511	MIR5685
478	OR13C8	995	BCAM	1512	MIR5687
479	H2BC5	996	EPO	1513	MIR5694
480	H4C8	997	FSTL1	1514	MIR5703
481	H4C3	998	FOLR2	1515	MIR5706
482	SLC22A18AS	999	IFNB1	1516	MIR5707
483	ZNF322	1000	ONECUT1	1517	MIR548AT
484	OR4D5	1001	NKX2-2	1518	MIR5695
485	OR6M1	1002	NKX6-1	1519	MIR5680
486	OR6T1	1003	MICB	1520	MIR5684
487	H4C5	1004	TNIP1	1521	MIR5690
488	MBLAC1	1005	REG1A	1522	MIR5688
489	SMIM21	1006	RFX6	1523	MIR5692C2
490	TMEM225	1007	PPY	1524	MIR5705
491	C2orf16	1008	STEAP4	1525	MIR548AX
492	DMAC1	1009	PF4	1526	MIR5692B
493	H2AC7	1010	ADAMTS12	1527	MIR5692C1
494	MALRD1	1011	APOM	1528	MIR5697
495	H2BC7	1012	CCRL2	1529	MIR5700
496	FAM25A	1013	CDKAL1	1530	MIR5681A
497	REXO5	1014	IL15	1531	MIR5681B
498	BTN2A3P	1015	GLIS3	1532	MIR5682
499	CLDN24	1016	IL19	1533	MIR5691
500	TMEM35B	1017	RBP1	1534	MIR5689
501	NUTM2D	1018	TSPAN8	1535	MIR5693
502	HCG11	1019	BTNL2	1536	MIR5704
503	GUSBP2	1020	BTLA	1537	MIR5708
504	MIR1250	1021	CD177	1538	MIR5698
505	GBAP1	1022	CSF3	1539	MIR5701-1
506	LINC01405	1023	FIP1L1	1540	MIR4666B
507	LINC02903	1024	IL23A	1541	MIR5683
508	NUTM2A-AS1	1025	CTRB1	1542	CFHR3

No.	Target	No.	Target	No.	Target
509	MIR3679	1026	IFNA1	1543	CFHR1
510	MSC-AS1	1027	IMMP2L	1544	GSR
511	BAIAP2-DT	1028	GIP	1545	MAT1A
512	LMCD1-AS1	1029	NKX6-2	1546	GPATCH8
513	LINC00940	1030	MICA	1547	UAQTL5
514	LINC00944	1031	MAEA	1548	UAQTL6
515	MIR5701-2	1032	MIR5692A1	1549	LMNA
516	MRPS17P5	1033	MIR5692A2	1550	TBX19
517	MIR5701-3	1034	GDI2P1	1551	HMCN1

Table S3. 779 targets of celery seed

No.	Target	No.	Target	No.	Target
1	ABAT	261	ESRRB	521	NMUR2
2	ABCB1	262	F10	522	NOS1
3	ABCC1	263	F2	523	NOS2
4	ABCC9	264	F2R	524	NOS3
5	ABCG2	265	F3	525	NOTUM
6	ABHD6	266	F9	526	NPC1L1
7	ACACB	267	FAAH	527	NPY5R
8	ACE	268	FABP1	528	NQO1
9	ACE2	269	FABP2	529	NQO2
10	ACHE	270	FABP3	530	NR1H2
11	ACLY	271	FABP4	531	NR1H3
12	ACP1	272	FABP5	532	NR1H4
13	ACPP	273	FADS1	533	NR1I2
14	ACR	274	FAP	534	NR1I3
15	ACVRL1	275	FBP1	535	NR3C1
16	ADA	276	FDFT1	536	NR3C2
17	ADAM17	277	FDPS	537	NT5E
18	ADAM9	278	FFAR1	538	NTRK1
19	ADAMTS5	279	FGFR1	539	NTRK2
20	ADH1A	280	FGFR3	540	NTRK3
21	ADH1B	281	FGFR4	541	NTSR1
22	ADH1C	282	FGR	542	NUAK1
23	ADH7	283	FKBP1A	543	OAT
24	ADK	284	FLT1	544	OGA
25	ADORA1	285	FLT3	545	OPRD1
26	ADORA2A	286	FLT4	546	OPRK1
27	ADORA2B	287	FNTA	547	OPRL1
28	ADORA3	288	FNTB	548	OPRM1
29	ADRA1A	289	FOLH1	549	P2RX3
30	ADRA1B	290	FOS	550	P2RX7
31	ADRA1D	291	FPR2	551	P4HTM
32	ADRA2A	292	FTO	552	PABPC1

No.	Target	No.	Target	No.	Target
33	ADRA2B	293	FUCA1	553	PAM
34	ADRA2C	294	FURIN	554	PAOX
35	ADRB1	295	FUT4	555	PARP1
36	ADRB2	296	FUT7	556	PARP10
37	ADRB3	297	FYN	557	PARP2
38	AGPAT2	298	G6PD	558	PCSK6
39	AGTR1	299	GAA	559	PDCD4
40	AHCY	300	GABBR1	560	PDE10A
41	AKR1B1	301	GABBR2	561	PDE2A
42	AKR1B10	302	GABRA1	562	PDE4A
43	AKR1C3	303	GABRA2	563	PDE4B
44	AKT1	304	GABRA3	564	PDE4D
45	ALDH1A1	305	GABRA4	565	PDE5A
46	ALDH2	306	GABRA5	566	PDE6D
47	ALDH3A1	307	GABRA6	567	PDE7A
48	ALDH5A1	308	GABRB2	568	PDE9A
49	ALK	309	GABRB3	569	PDF
50	ALOX15	310	GABRG2	570	PDGFRA
51	ALOX15B	311	GABRR1	571	PDGFRB
52	ALOX5	312	GALR3	572	PDPK1
53	ALPG	313	GAPDH	573	PEPD
54	ALPL	314	GBA	574	PER2
55	AMPD1	315	GBA2	575	PGA5
56	AMPD2	316	GCGR	576	PGC
57	AMPD3	317	GFPT1	577	PGD
58	ANPEP	318	GLI1	578	PGF
59	AOC3	319	GLI2	579	PGGT1B
60	APH1A	320	GLO1	580	PGR
61	APH1B	321	GLRA1	581	PHF8
62	APP	322	GPBAR1	582	PHLPP2
63	AR	323	GPR139	583	PIK3C3
64	ARG1	324	GPR17	584	PIK3CA
65	ATP12A	325	GPR35	585	PIK3CB
66	AURKA	326	GPR84	586	PIK3CD

No.	Target	No.	Target	No.	Target
67	AURKB	327	GRIA1	587	PIK3CG
68	BACE1	328	GRIA2	588	PIK3R1
69	BACE2	329	GRIA4	589	PIM1
70	BAZ2A	330	GRIK1	590	PIM2
71	BAZ2B	331	GRIK2	591	PIM3
72	BBOX1	332	GRIK3	592	PIN1
73	BCHE	333	GRIK5	593	PIP4K2C
74	BCL2	334	GRIN1	594	PLA2G10
75	BDKRB1	335	GRIN2A	595	PLA2G1B
76	BMP1	336	GRIN2B	596	PLA2G2A
77	BMX	337	GRK2	597	PLA2G2C
78	BRAF	338	GRK6	598	PLA2G5
79	BRD4	339	GRM1	599	PLAA
80	C5AR1	340	GRM2	600	PLAT
81	CA1	341	GRM3	601	PLAU
82	CA12	342	GRM4	602	PLEC
83	CA13	343	GRM5	603	PLG
84	CA14	344	GRM6	604	PLK1
85	CA2	345	GRM7	605	PLK4
86	CA3	346	GRM8	606	PNMT
87	CA4	347	GSK3A	607	PNP
88	CA5A	348	GSK3B	608	POLA1
89	CA5B	349	GSR	609	POLB
90	CA6	350	GZMB	610	PPARA
91	CA7	351	HAO1	611	PPARD
92	CA9	352	HCAR2	612	PPARG
93	CACNA1B	353	HCAR3	613	PPIA
94	CACNA2D1	354	HCRTR1	614	PPP1CA
95	CACNA2D2	355	HCRTR2	615	PREP
96	CAPN1	356	HDAC2	616	PRKCA
97	CAPN2	357	HDAC3	617	PRKCB
98	CASP1	358	HDAC4	618	PRKCD
99	CASP3	359	HDAC5	619	PRKCE
100	CASP4	360	HDAC6	620	PRKCG

No.	Target	No.	Target	No.	Target
101	CASP6	361	HDAC7	621	PRKCH
102	CASP7	362	HDAC8	622	PRKD1
103	CASP8	363	HDAC9	623	PRKDC
104	CASP9	364	HEXA	624	PRMT3
105	CASR	365	HEXB	625	PRSS1
106	CBFB	366	HIF1A	626	PSEN1
107	CBR1	367	HLA-A	627	PSEN2
108	CCKBR	368	HLA-DRB3	628	PSENE1
109	CCNA1	369	HLCS	629	PSMB1
110	CCNA2	370	HMGCR	630	PSMB2
111	CCNB1	371	HMOX1	631	PTAFR
112	CCNB2	372	HPRT1	632	PTGDR
113	CCNB3	373	HRH1	633	PTGDR2
114	CCNC	374	HRH2	634	PTGER1
115	CCND1	375	HRH3	635	PTGER2
116	CCND2	376	HRH4	636	PTGER3
117	CCND3	377	HSD11B1	637	PTGER4
118	CCNE1	378	HSD11B2	638	PTGES
119	CCNE2	379	HSD17B1	639	PTGFR
120	CCNH	380	HSD17B2	640	PTGIR
121	CCNT1	381	HSD17B3	641	PTGIS
122	CCR1	382	HSP90AA1	642	PTGS1
123	CCR2	383	HSP90AB1	643	PTGS2
124	CCR5	384	HSPA1A	644	PTK2
125	CD38	385	HSPA5	645	PTPN1
126	CD81	386	HSPA8	646	PTPN11
127	CDA	387	HTR1A	647	PTPN2
128	CDC25A	388	HTR1B	648	PTPN6
129	CDC25B	389	HTR1D	649	PTPRA
130	CDC42	390	HTR1E	650	PTPRC
131	CDC45	391	HTR2A	651	PTPRF
132	CDC7	392	HTR2B	652	PYGL
133	CDK1	393	HTR2C	653	PYGM
134	CDK2	394	HTR3A	654	QPCT

No.	Target	No.	Target	No.	Target
135	CDK4	395	HTR4	655	RAC1
136	CDK5	396	HTR5A	656	RAD51
137	CDK5R1	397	HTR6	657	RAF1
138	CDK6	398	HTR7	658	RBP4
139	CDK7	399	ICAM1	659	RELA
140	CDK8	400	ICMT	660	REN
141	CDK9	401	IDH1	661	RET
142	CECR2	402	IDO1	662	RGS4
143	CENPE	403	IGF1R	663	RIPK2
144	CES1	404	IKBKB	664	RNPEP
145	CES2	405	IL2	665	ROCK1
146	CETP	406	IMPDH1	666	ROCK2
147	CHEK1	407	IMPDH2	667	RORA
148	CHRM1	408	INSR	668	RORC
149	CHRM2	409	ITGA2B	669	ROS1
150	CHRM3	410	ITGA4	670	RPS6KA3
151	CHRM4	411	ITGA5	671	RPS6KB1
152	CHRM5	412	ITGAL	672	RXRA
153	CHRNA2	413	ITGAV	673	S1PR3
154	CHRNA3	414	ITGB1	674	S1PR4
155	CHRNA4	415	ITGB2	675	S1PR5
156	CHRNA7	416	ITGB3	676	SAE1
157	CHRNB2	417	ITGB7	677	SCD
158	CHRNB4	418	JAK1	678	SCN10A
159	CLK1	419	JAK2	679	SCN2A
160	CLK4	420	JAK3	680	SCN4A
161	CMA1	421	JUN	681	SCN5A
162	CNR1	422	KAT2B	682	SELE
163	CNR2	423	KCNA3	683	SERPINA6
164	COMT	424	KCNA5	684	SERPINE1
165	CPA1	425	KCNE1	685	SETD7
166	CPA3	426	KCNH2	686	SHBG
167	CPB1	427	KCNJ11	687	SHH
168	CPB2	428	KCNJ3	688	SIGMAR1

No.	Target	No.	Target	No.	Target
169	CPN1	429	KCNJ5	689	SIRT1
170	CPT1A	430	KCNJ6	690	SIRT2
171	CPT1B	431	KCNMA1	691	SLC13A5
172	CPT2	432	KCNN4	692	SLC15A1
173	CREBBP	433	KCNQ1	693	SLC18A3
174	CRHR1	434	KDM1A	694	SLC1A1
175	CSF1R	435	KDM2A	695	SLC1A2
176	CSNK1D	436	KDM3A	696	SLC22A6
177	CSNK1G2	437	KDM4A	697	SLC27A1
178	CSNK2A1	438	KDM4B	698	SLC2A1
179	CTBP2	439	KDM4C	699	SLC5A1
180	CTRB1	440	KDM4E	700	SLC6A1
181	CTSA	441	KDM5A	701	SLC6A11
182	CTSB	442	KDM5B	702	SLC6A12
183	CTSC	443	KDM5C	703	SLC6A13
184	CTSD	444	KDM6B	704	SLC6A2
185	CTSE	445	KDM7A	705	SLC6A3
186	CTSF	446	KDR	706	SLC6A4
187	CTSG	447	KIF11	707	SLC6A7
188	CTSH	448	KISS1R	708	SLC7A5
189	CTSK	449	KIT	709	SLC9A1
190	CTSL	450	KLK1	710	SQLE
191	CTSS	451	KLK2	711	SRC
192	CTSV	452	KLKB1	712	SRD5A1
193	CXCR2	453	KMO	713	SRD5A2
194	CYP11B1	454	KYNU	714	SREBF2
195	CYP11B2	455	LAP3	715	SRM
196	CYP17A1	456	LCK	716	ST3GAL3
197	CYP19A1	457	LIG1	717	STAT1
198	CYP1A2	458	LIPA	718	STAT3
199	CYP1B1	459	LIPE	719	STK26
200	CYP27A1	460	LRRK2	720	STK3
201	CYP2C19	461	LSS	721	STK4
202	CYP2C9	462	LTA4H	722	SYK

No.	Target	No.	Target	No.	Target
203	CYP2D6	463	LTB4R	723	TAAR1
204	CYP51A1	464	LYN	724	TACR1
205	DAO	465	MAOA	725	TACR2
206	DBH	466	MAOB	726	TAS2R31
207	DCTPP1	467	MAP2	727	TBXA2R
208	DHCR7	468	MAP2K1	728	TBXAS1
209	DHFR	469	MAP2K7	729	TDO2
210	DLG4	470	MAP3K14	730	TDP1
211	DNMT3A	471	MAP3K8	731	TDP2
212	DNMT3B	472	MAP4K4	732	TERT
213	DNPEP	473	MAPK1	733	TGFBR1
214	DPP4	474	MAPK10	734	TGM2
215	DPP8	475	MAPK14	735	TH
216	DPP9	476	MAPK3	736	THRA
217	DRD1	477	MAPK8	737	THRB
218	DRD2	478	MAPK9	738	TIE1
219	DRD3	479	MAPKAPK2	739	TK1
220	DRD4	480	MB	740	TKT
221	DUSP3	481	MC1R	741	TLR4
222	DYRK1A	482	MC4R	742	TLR9
223	DYRK1B	483	MCHR1	743	TNFRSF10A
224	EBP	484	MCL1	744	TNKS
225	ECE1	485	MDM2	745	TNKS2
226	EDNRA	486	MERTK	746	TNNC1
227	EDNRB	487	MET	747	TNNI3
228	EGFR	488	METAP1	748	TNNT2
229	EGLN1	489	MGLL	749	TOP1
230	EGLN3	490	MIF	750	TOP2A
231	EHMT1	491	MKNK1	751	TPMT
232	EHMT2	492	MKNK2	752	TPO
233	EIF2AK1	493	MME	753	TRAP1
234	EIF4E	494	MMEL1	754	TRPA1
235	ELANE	495	MMP1	755	TRPM8
236	ELOVL6	496	MMP10	756	TRPV1

No.	Target	No.	Target	No.	Target
237	ENPEP	497	MMP12	757	TRPV3
238	EP300	498	MMP13	758	TSPO
239	EPAS1	499	MMP14	759	TTK
240	EPHA1	500	MMP2	760	TTL
241	EPHA2	501	MMP3	761	TTR
242	EPHA3	502	MMP7	762	TUBB1
243	EPHA4	503	MMP8	763	TYK2
244	EPHA5	504	MMP9	764	TYMP
245	EPHA6	505	MPI	765	TYMS
246	EPHA7	506	MPO	766	TYR
247	EPHA8	507	MST1R	767	UBA2
248	EPHB1	508	MTAP	768	UGCG
249	EPHB2	509	MT-ND4	769	UGT2B7
250	EPHB3	510	MTNR1A	770	UPP1
251	EPHB4	511	MTNR1B	771	UTS2R
252	EPHB6	512	MTOR	772	VDR
253	EPHX1	513	MYLK	773	VEGFA
254	EPHX2	514	NAAA	774	WDR5
255	ERAP2	515	NAMPT	775	XDH
256	ERBB2	516	NAT1	776	XIAP
257	ERBB4	517	NCSTN	777	XPO1
258	ERN1	518	NEK1	778	YARS
259	ESR1	519	NGFR	779	ZAP70
260	ESR2	520	NISCH		

Table S4. Molecular interaction between the potent compounds of celery seed and core targets of gout disease

Potent compounds	Core targets	Free binding energy (kcal/mol)	Interacted residues	
			Hydrogen bond	Other interactions
C1	AKT1	-7.6	Thr291, Asp292	Val164, Ala177, Lys179, Met281
	EGFR kinase	-7.9	-	Leu718, Val726, Leu844, Ala743, Lys745, Leu777, Leu788, Met766
	ERK1	-7.3	Asp128	Leu173, Ile48, Val56, Ala69, Cys183, Ile101
	ERK2	-7.0	Asp165, Gln103	Val37, Ala50, Ile29, Met106, Leu105, Leu154
	HSP90 α	-9.2	Tyr139	Trp162, Phe138, Leu107, Met98, Val150, Val186
	Integrin β 1	-5.9	Lys334	Ile363, Pro333, Leu428
	JNK1	-7.9	Arg69	Leu168, Val40, Ala53, Met108, Ile32, Ile86, Val158, Met111
	MAPK14	-9.6	Thr106, His107	Lys53, Phe169, Ala51, Val38, Val30, Tyr35, Leu108
	NF- κ B p65	-6.7	Thr60, His58, Gln114	Ile24
	NO synthase	-9.0	Val352, Asn370	Val352, Tyr373, Glu377, Pro350
PI3K α	-7.7	Arg818, Gln630	Phe666, Arg662, Lys271	

Potent compounds	Core targets	Free binding energy (kcal/mol)	Interacted residues	
			Hydrogen bond	Other interactions
	PPAR α	-8.4	Tyr334	Thr279, Val324, Met220, Met320
C2	AKT1	-7.5	Lys158	Phe161, Leu181, Ile186
	EGFR kinase	-7.0	Tyr998, Asp800, Gly796	Leu792, Leu844, Leu718
	ERK1	-6.6	Met125	Cys183
	ERK2	-7.0	Glu69, Gln103	Val37, Lys52
	HSP90 α	-7.1	Ser52, Gly135	Phe138, Leu107, Met98, Ala55
	Integrin β 1	-4.9	Asn330	Leu428
	JNK1	-7.0	Ser155, Met111	Ala36, Val40, Leu168
	MAPK14	-7.1	Thr106, Met109	Tyr35, Val30
	NF- κ B p65	-5.0	Ser112	Arg108
	NO synthase	-7.5	Gly371, Asn370, Glu377, Arg381	Ala262
	PI3K α	-6.9	Lys271, Asn170, Pro835	Phe666
	PPAR α	-7.3	Tyr334, Met320, Tyr214	Ile317, Val324, Met220
C3	AKT1	-5.9	Leu295	Phe161, Lys179, Glu191
	EGFR kinase	-6.7	Thr854, Asp855	Cys775, Thr790, Ala743, Val726, Lys745
	ERK1	-5.7	Met125	Ile173, Cys183, Ala69, Val56
	ERK2	-5.3	-	Leu154, Ala50, Ile29, Val37
	HSP90 α	-7.4	Tyr139, Gly108	Ile26, Val150, Trp162, Leu103, Phe138
	Integrin β 1	-4.3	Leu86, Lys85	Leu86

Potent compounds	Core targets	Free binding energy (kcal/mol)	Interacted residues	
			Hydrogen bond	Other interactions
	JNK1	-5.7	Asn114	Val40, Ala53, Leu168, Val158
	MAPK14	-6.9	-	Phe169, Tyr35, Val38, Ala51, Leu75
	NF- κ B p65	-5.0	Tyr100	Lys93, Phe113, His111
	NO synthase	-6.8	-	Pro350, Tyr373
	PI3K α	-5.9	-	Leu839, Phe666
	PPAR α	-6.6	Ser280	Cys276, Ile354, Val444, Tyr464, Phe273, Leu456
	C4	AKT1	-6.0	Glu234
EGFR kinase		-6.5	Thr854, Lys745, Asp855	Val726, Leu718, Leu844, Ala743
ERK1		-6.1	Thr127, Met125, Cys183	Val56, Leu173
ERK2		-6.0	-	Ile82, Leu14, Ala50, Val37
HSP90 α		-7.4	Leu103, Asn51, Tyr139	Met98, Phe138, Leu107, Ala111, Tyr139
Integrin β 1		-5.0	Thr388, Asn391, Lys394	Lys394
JNK1		-6.2	Glu109	Val40, Met108, Leu168, Ala53
MAPK14		-6.1	Arg67, Gly170	Asp168, Leu74, Leu75
NF- κ B p65		-5.0	Gln114, Arg108	His111
NO synthase		-7.0	Pro350, Gln262, Val352	Pro350, Tyr373, Glu377, Val352

Potent compounds	Core targets	Free binding energy (kcal/mol)	Interacted residues	
			Hydrogen bond	Other interactions
	PI3K α	-6.7	Cys838	Arg818, Phe666, Leu839, His670
	PPAR α	-7.1	Thr283, Ala333, Tyr334	Val324, Leu321, Met330, Tyr334
C5	AKT1	-9.6	Lys158, Gly162, Glu191, Gly294	Phe161, Lys179, Glu198, Leu295
	EGFR kinase	-8.7	Thr854, Asp855, Asn842, Arg841, Gly719, Ser720	Leu718, Ala743, Leu844, Lys745, Val726, Cys797
	ERK1	-8.2	Lys71, Tyr53, Arg84, Asp184, Glu88	Asp184, Ala52
	ERK2	-8.5	Lys52, Gln103, Cys164, Glu69, Met106	Lys52, Cys164, Val37, Leu154, Ala50
	HSP90 α	-9.6	Gly135, Asn51, Leu107	Phe138, Val150, Leu103, Trp162, Met98, Leu107, Ile110
	Integrin β 1	-6.8	Phe262, Val324	Pro228, Phe262
	JNK1	-7.9	Ser155, Arg69	Lys153, Ser34, Leu168, Val40, Met108
	MAPK14	-8.2	Asp168, Arg67	Leu74, Arg70, Arg149
	NF- κ B p65	-6.8	Tyr100, Gln114, Asn115, Cys105, His111, Asp103	Phe113, Val72, Ala102, Lys93
	NO synthase	-10.1	Gln263, Arg388, Arg266, Gly371, Trp372	Arg381, Pro350
	PI3K α	-8.8	Cys838, Gln630	Lys271, Phe666, Arg818, Leu839

Potent compounds	Core targets	Free binding energy (kcal/mol)	Interacted residues	
			Hydrogen bond	Other interactions
	PPAR α	-9.6	Tyr464, Tyr314, Ser280	Leu460, Val444, Phe273, His440, Cys276, Thr279, Leu321, Met355
C6	AKT1	-6.4	Asp292	Val164, Ala177, Met281
	EGFR kinase	-7.0	Thr854	Val726, Ala743, Lys745
	ERK1	-6.3	Met125, Glu126	Ile48, Leu173, Val56
	ERK2	-5.9	Met106, Glu107	Leu154
	HSP90 α	-7.1	Tyr139	Phe138, Leu107
	Integrin β 1	-6.4	Ser335, Lys329, Lys334, Pro333	Ile363
	JNK1	-6.4	Met111, Glu109	Val158, Ile32
	MAPK14	-7.1	Asp168, Thr106	Lys53, Ala51, Val38
	NF- κ B p65	-6.4	Ser112, Thr60, His58, Arg50	-
	NO synthase	-7.7	Gln262, Tyr347, Asp382, Tyr373	Glu377
	PI3K α	-6.9	His670, Cys838	Arg818, Phe666
PPAR α	-7.1	Glu286, Asn219, Thr283	Val324	
C7	AKT1	-5.4	-	Val164, Lys179
	EGFR kinase	-6.6	Thr854, Asp855, Met766	Leu844, Ala743, Val726
	ERK1	-5.7	Asp128	Ile48
	ERK2	-5.6	Met106	Lys52, Val37
	HSP90 α	-6.7	Tyr139, Leu103	Trp162, Val150, Phe138
	Integrin β 1	-3.8	-	Ile363, Arg393
	JNK1	-5.6	-	Ile32
	MAPK14	-6.7	Asp168, Thr106	Leu108, Ala51

Potent compounds	Core targets	Free binding energy (kcal/mol)	Interacted residues	
			Hydrogen bond	Other interactions
	NF-κB p65	-5.2	Tyr100, Arg108	Ser112, Val72, Phe113, Ala102, Tyr100
	NO synthase	-6.3	Asp382, Tyr347	Gln263, Val352
	PI3K α	-6.2	Leu632, Ser629	Ile633, Phe666
	PPAR α	-6.2	Thr283, Met220	Met320, Ile317
C8	AKT1	-6.0	Glu191	Phe161, Lys179, Leu181, Glu191, Leu295
	EGFR kinase	-6.3	Lys745	Val726, Ala743, Leu844, Leu858, Met766
	ERK1	-6.0	Tyr53, Ala52, Gly54	Glu88, Lys71, Ile73
	ERK2	-5.6	-	Leu154, Ala50, Ile29, Lys52, Val37
	HSP90 α	-6.9	-	Val186, Met98, Trp162, Leu103, Leu107, Phe138
	Integrin β 1	-5.1	-	Ile363, Lys394
	JNK1	-6.0	Asn114	Val40, Met111, Ile86, Ala53, Leu168, Val158
	MAPK14	-7.3	Thr106	Lys53, Tyr35, Val30
	NF-κB p65	-5.2	Tyr100	Lys93
	NO synthase	-6.9		Val352, Pro350
	PI3K α	-6.1	Arg818	Leu755, Leu839, Phe666, His670, Leu632
PPAR α	-6.9	Tyr464	Val444, Phe273, Ile354, Phe351, Ile272	
C9	AKT1	-5.9	Arg241, Asp439	Glu234

Potent compounds	Core targets	Free binding energy (kcal/mol)	Interacted residues	
			Hydrogen bond	Other interactions
	EGFR kinase	-6.6	Thr854	Phe856, Thr790, Ala743, Val726, Lys745, Asp855
	ERK1	-5.9	-	Ile73
	ERK2	-5.6	-	Val37, Ala50, Lys52
	HSP90 α	-7.8	Trp162, Leu103	Met98, Leu107, Val150, Phe138
	Integrin β 1	-5.1	Ser33	Ile363, Lys394
	JNK1	-6.0	Gln117, Asn114	Met108, Ala53, Val158, Leu168
	MAPK14	-7.1	Lys53	Val38, Tyr35, Phe169, Ala51
	NF- κ B p65	-5.3	Asp103, Cys105, Tyr100	Tyr100
	NO synthase	-7.0	-	Pro350, Glu377, Val352
	PI3K α	-6.5	Cys838	Phe666
	PPAR α	-6.8		Ile354, Cys276, Ile272
	C10	AKT1	-7.2	Asp292, Gly294
EGFR kinase		-7.1	Arg841, Asn842, Asp855, Thr854, Lys745	Val726, Ala743, Leu844, Lys745
ERK1		-6.8	Cys183, Glu126, Asp128	Lys71, Val56, Ala69, Leu173, Ile48, Leu124, Met125
ERK2		-6.7	Met106, Asp104, Asp109, Cys164	Ala50, Ile29, Leu154, Lys152, Val37
HSP90 α		-8.3	Tyr139, Leu107, Asn51, Asp102	Trp162, Phe138, Val150, Met98
Integrin β 1		-6.2	Ser335, Lys329, Ile332, Lys394	Ile363, Pro333

Potent compounds	Core targets	Free binding energy (kcal/mol)	Interacted residues	
			Hydrogen bond	Other interactions
	JNK1	-6.5	Ser155, Ser34, Ile32	Leu168, Val40, Met108
	MAPK14	-7.3	Asp168, Glu71, Arg67	Arg70, Glu71, Leu75, Leu74
	NF- κ B p65	-6.3	Tyr100, Gln14, Asn115, Ser112	Ala102
	NO synthase	-7.4	Tyr347, Gln263, Tyr373, Glu377, Phe369, Trp372	Pro350, Val352
	PI3K α	-7.3	Met811, Arg818, Cys838	Arg818, Met811, Leu632, Phe666, His670
	PPAR α	-7.5	Ile317, Met320, Thr283, Val332, Ala333	Leu321, Val324, Met220, Tyr334, Thr279
	C11	AKT1	-7.9	Lys179, Glu198, Gly294
EGFR kinase		-7.9	Met793	Leu844, Ala743, Val726, Lys745
ERK1		-7.0	Met125	Leu173, Ile48, Val56, Asp184
ERK2		-7.5	Ser151, Asp109	Leu154, Ala50, Ile29, Ile82, Val37, Lys52, Cys164
HSP90 α		-7.9	Ser52	Leu107, Val150, Val186, Phe138, Met98
Integrin β 1		-5.7	Leu331	Glu390, Arg393, Ile363, Pro333
JNK1		-6.9	Ser155, Lys153, Ser34	Leu168, Val40, Met108, Ile32

Potent compounds	Core targets	Free binding energy (kcal/mol)	Interacted residues	
			Hydrogen bond	Other interactions
	MAPK14	-7.0	Arg149	Met78, Leu74, Ile141, Ile146, His148
	NF- κ B p65	-6.1	Asn115, Gln114	Ala102, Val72, Phe113
	NO synthase	-8.4	Arg388, Arg266, Tyr347, Gln263	Glu377, Asp382, Val352, Arg381
	PI3K α	-7.8	Gly837	Phe666, Leu632, His670, Met811
	PPAR α	-7.4	Met220, Tyr334, Thr279	Val324, Leu321, Met320, Leu331
	C12	AKT1	-6.0	Glu191
EGFR kinase		-5.7	Thr854, Asn842	Asp855, Lys745
ERK1		-6.1	Tyr53, Gly54, Ala52, Asp184, Gly51, Arg84	-
ERK2		-5.1	Gln103, Met106	-
HSP90 α		-5.6	Ser52, Leu48, Asn51, Thr184	-
Integrin β 1		-5.1	Lys334, Ser335, Glu361, Ser357	Lys329
JNK1		-4.9	Ser155, Arg69, Ser34	-
MAPK14		-6.1	Asp168, Glu71	-
NF- κ B p65		-5.2	Cys105, Tyr100, Gln114, Ser112	Gln114
NO synthase		-6.4	Tyr347, Glu377, Tyr373	-
PI3K α		-6.2	Asn822, Glu172, Arg274, Ser275	-
PPAR α		-5.9	Thr283, Asn219	Thr279
C13	AKT1	-6.8	Glu191, Thr195, Asp292	Lys179

Potent compounds	Core targets	Free binding energy (kcal/mol)	Interacted residues		
			Hydrogen bond	Other interactions	
	EGFR kinase	-6.5	Lys745	Val726, Ala743, Leu718, Leu844	
	ERK1	-6.6	Asp123, Gln122	Ile48, Ala69, Val56, Leu173	
	ERK2	-5.7	Asp109	Val37, Leu154, Ala50	
	HSP90 α	-7.9	Tyr139, Gly108, Leu103	Phe138, Trp162, Val150, Met98	
	Integrin β 1	-4.6	Ser396, Asn386, Cys395	Val385	
	JNK1	-6.3	Ser155	Leu168, Ala53, Ile32, Val158, Met108	
	MAPK14	-7.1	Thr106	Ala51, Val38, Lys53, Ile84, Thr106	
	NF- κ B p65	-5.4	Tyr100, Arg108, Gln114	Tyr100	
	NO synthase	-6.9	Tyr347, Tyr373, Glu377	Glu377, Val352	
	PI3K α	-7.3	Arg818	Phe666	
	PPAR α	-7.0	Tyr314, Tyr464, Ser280, Cys276	Ile354, Met355	
	C14	AKT1	-5.3	Glu191, Thr195	His194, Leu295
		EGFR kinase	-5.7	Thr854, Asp855, Phe856, Thr790, Arg776	-
ERK1		-4.4	Asp128	Val56	
ERK2		-4.2	Gln103, Ala50, Lys52, Ile51	Met106, Leu154, Ala50	
HSP90 α		-5.7	Asp93, Thr184	Trp162, Phe138	
Integrin β 1		-3.3	Phe262	Phe264	
JNK1		-4.7	Gln37, Arg69	Ile32, Val158	
MAPK14		-5.7	Asp168	Leu108, Val30, Val38, Tyr35, Ala51	

Potent compounds	Core targets	Free binding energy (kcal/mol)	Interacted residues	
			Hydrogen bond	Other interactions
	NF- κ B p65	-4.4	Tyr100	Cys105, His111
	NO synthase	-5.7	Tyr373, Asp382, Tyr347, Gln263, Glu377	Glu377, Val352
	PI3K α	-5.3	Gln630	Phe666, Leu839, Leu755
	PPAR α	-5.4	Leu331, Gly335	Met320, Phe218
C15	AKT1	-5.7	Asp292	Leu156, Val164, Ala177, Tyr229, Met281, Phe438
	EGFR kinase	-5.9	Thr854	Asp855, Ala743, Val726, Lys745, Leu844
	ERK1	-6.0	-	Val56, Ala69, Leu173, Ile48
	ERK2	-5.4	-	Ala50, Ile29, Leu154, Leu105
	HSP90 α	-7.5	Leu103, Trp162	Met98, Phe138, Val150, Leu107
	Integrin β 1	-4.6	-	Glu365, Glu308, Arg426, Gly367
	JNK1	-5.9	-	Ala53, Met111, Ile32, Val158, Ile86, Leu168
	MAPK14	-7.0	Thr106	Phe169, Ala51, Tyr35, Val38
	NF- κ B p65	-5.0	Asn115, Gln114	Tyr100
	NO synthase	-6.6	Pro350	Val352
	PI3K α	-6.3	Cys838	Phe666, Leu632, His670
	PPAR α	-6.1	-	His440, Leu456, Val444, Tyr464, Phe273

Potent compounds	Core targets	Free binding energy (kcal/mol)	Interacted residues	
			Hydrogen bond	Other interactions
C16	AKT1	-5.5	Gly294	Phe161, Leu181
	EGFR kinase	-5.7	Asp855, Thr854	Lys745, Ala743, Val726
	ERK1	-5.7	Tyr53, Gly54, Ala52	Tyr53, Lys71, Ile73
	ERK2	-5.0	Met106	Ala50, Val37
	HSP90 α	-5.6	Tyr139	Met98, Val150, Trp162, Phe138
	Integrin β 1	-3.9	Arg426	Arg426, Lys424
	JNK1	-5.3	Met111	Ala53, Leu168, Val40
	MAPK14	-6.1	His148	Val83, Ile141, Met78
	NF- κ B p65	-4.9	His111, Arg108, Tyr100	-
	NO synthase	-5.8	Ala351	Val352, Glu377
	PI3K α	-5.7	Arg818, Cys838	Phe666
PPAR α	-6.0	Thr283, Asn219	Leu321, Val324	

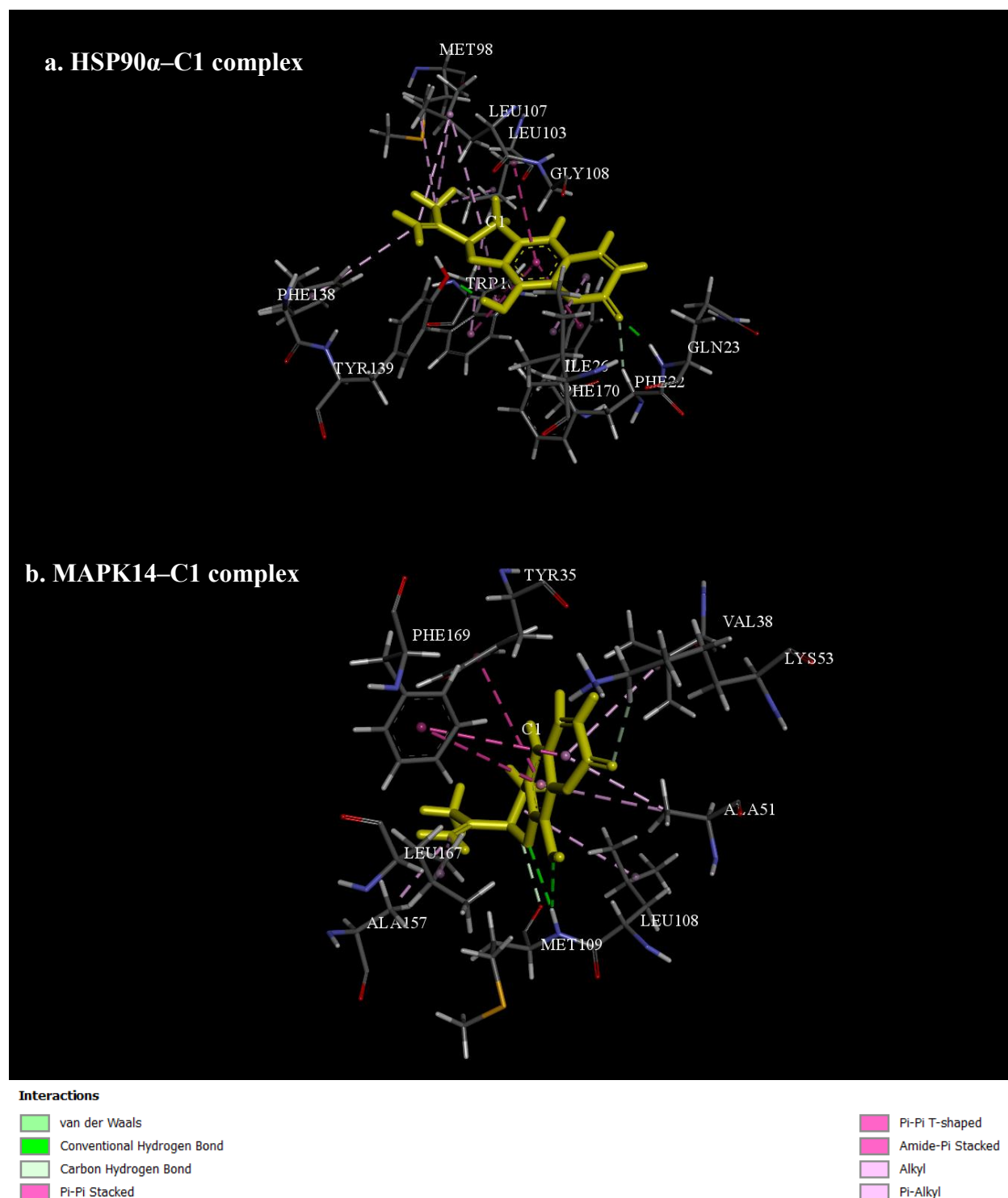


Figure S1. Interaction between C1 and HSP90 α (a), MAPK14-C1 (b) after molecular dynamics simulations. The interacted residues of HSP90 α were identified as Phe22, Gln23, Ile26, Met98, Leu103, Leu107, Gly108, Phe138, Tyr139, Trp162, and Phe170. The interacted residues of MAPK14 were identified as Tyr35, Val38, Ala51, Lys53, Leu108, Met109, Ala157, Leu167, and Phe169.