Table S1: The putative molecular targets of the khat constituents cathine and cathinone, obtained based on both canonical and isomeric SMILES from the PubChem Database. The target list also shows the associated target classes identified by Swiss Target Prediction.

SwissTargetPrediction							
		Cathine	Cathinone				
No.	Uniprot ID	Target Class	Uniprot ID	Target Class			
1	P08913	Family A G protein-coupled receptor	P25103	Family A G protein-coupled receptor			
2	P18089	Family A G protein-coupled receptor	P31645	Electrochemical transporter			
3	P35348	Family A G protein-coupled receptor	Q01959	Electrochemical transporter			
4	P31645	Electrochemical transporter	P23975	Electrochemical transporter			
5	Q96RJ0	Family A G protein-coupled receptor	Q96RJ0	Family A G protein-coupled receptor			
6	Q01959	Electrochemical transporter	P27338	Oxidoreductase			
7	P23975	Electrochemical transporter	P23141	Enzyme			
8	P28223	Family A G protein-coupled receptor	O00748	Enzyme			
9	P15144	Protease	P28223	Family A G protein-coupled receptor			
10	P46098	Ligand-gated ion channel	Q05940	Electrochemical transporter			
11	Q05940	Electrochemical transporter	P54289	Calcium channel auxiliary subunit alpha2delta family			
12	P54289	Calcium channel auxiliary subunit alpha2delta family	Q03405	Membrane receptor			
13	O60341	Eraser	Q6V1X1	Protease			
14	P28221	Family A G protein-coupled receptor	P32297 P30926	Ligand-gated ion channel			
15	P14416	Family A G protein-coupled receptor	P43681	Ligand-gated ion channel			
16	P21397	Oxidoreductase	P29475	Enzyme			
17	P27338	Oxidoreductase	P35228	Enzyme			
18	P07550	Family A G protein-coupled receptor	P29474	Enzyme			
19	Q9H3N8	Family A G protein-coupled receptor	Q99720	Membrane receptor			
20	P25103	Family A G protein-coupled receptor	P11086	Enzyme			
21	Q969F8	Family A G protein-coupled receptor	Q92831	Writer			
22	P11509	Cytochrome P450	P08253	Protease			
23	P11086	Enzyme	Q969F8	Family A G protein-coupled receptor			
24	Q16853	Enzyme	P21397	Oxidoreductase			
25	P08588	Family A G protein-coupled receptor	P25021	Family A G protein-coupled receptor			
26	P35228	Enzyme	Q9H3N8	Family A G protein-coupled receptor			
27	P30926 P43681	Ligand-gated ion channel	Q9Y2I1	Other cytosolic protein			
28	P30926 Q15822	Ligand-gated ion channel	P32297 P17787	Ligand-gated ion channel			
29	P00390	Oxidoreductase	P33261	Cytochrome P450			
30	P18825	Family A G protein-coupled receptor	P11509	Cytochrome P450			
31	P28335	Family A G protein-coupled receptor	P30542	Family A G protein-coupled receptor			
32	Q9H228	Family A G protein-coupled receptor	P36544	Ligand-gated ion channel			
33	O95977	Family A G protein-coupled receptor	P43166	Lyase			
34	Q99500	Family A G protein-coupled receptor	P00915	Lyase			
35	P21453	Family A G protein-coupled receptor	P23280	Lyase			
36	P16662	Enzyme	O43570	Lyase			
37	P29475	Enzyme	Q9ULX7	Lyase			
38	Q9GZQ4	Family A G protein-coupled receptor	Q16790	Lyase			
39	Q9UHL4	Protease	Q9Y2D0	Lyase			
40	Q13126	Enzyme	P35218	Lyase			

1	41	Q01650	Electrochemical transporter	Q8N1Q1	Lyase
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44					
P00491				_	
P35462				_	
PS2732					
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83P29275Family A G protein-coupled receptorQ86V86Kinase84P50579ProteaseQ92769Eraser85Q8NET8Voltage-gated ion channelP04818Transferase86P37058EnzymeO60341Eraser					
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				`	Family A G protein-coupled receptor
89 Q13418 Kinase O00311 Kinase			· · · · · · · · ·		<i>i</i> 1 1 1

90	O75899	Family C G protein-coupled receptor	P31751	Kinase
	Q9UBS5			
91	B2RXH2	Eraser	P28838	Protease
92	P06241	Kinase	Q8IXJ6	Eraser
93	P41146	Family A G protein-coupled receptor	Q96EB6	Eraser
94	P06239	Kinase	Q96PY6	Kinase
95	P14867 P47870	Ligand-gated ion channel	O75899	Family C G protein-coupled receptor
	P18507		Q9UBS5	
96	P21554	Family A G protein-coupled receptor	P49841	Kinase
97	P34972	Family A G protein-coupled receptor	P06241	Kinase
98	P63316 P45379	Unclassified protein	P06239	Kinase
	P19429			
99	O00311	Kinase	P46059	Electrochemical transporter
100	P41595	Family A G protein-coupled receptor	Q02750	Kinase