

Table II Target metabolites for *CARCINOSCOPE*

No	Annotation	KEGG ID	No	Annotation	KEGG ID
1	2,3-Diphosphoglyceric acid	C01159	59	Guanosine	C00387
2	2-Hydroxyglutaric acid	C01087,C02630,C03196	60	Guanosine 5-diphosphate	C00035
3	2-Oxoglutaric acid	C00026	61	Guanosine 5-monophosphate	C00144
4	2-Oxoisovaleric acid	C00141	62	Guanosine 5-triphosphate	C00044
5	2-Phosphoglyceric acid	C00631	63	Histidine	C00135,C00768,C06419
6	3-Phosphoglyceric acid	C00197	64	Homocysteine	C00155
7	6-Phosphogluconic acid	C00345	65	Homoserine	C00263
8	Acetoacetyl coenzyme A	C00332	66	Hydroxymethylglutaryl coenzyme A	C00356
9	Acetyl coenzyme A	C00024	67	Hydroxyproline	C01015,C01157
10	Adenine	C00147	68	Hypoxanthine	C00262
11	Adenosine	C00212	69	Inosine	C00294
12	Adenosine 5-diphosphate	C00008	70	Inosine 5-monophosphate	C00130
13	Adenosine 5-monophosphate	C00020	71	Isocitric acid	C00311
14	Adenosine 5-triphosphate	C00002	72	Isoleucine	C00407,C06418,C16434
15	Adenylosuccinic acid	C03794	73	Lactic acid	C00186,C00256,C01432
16	ADP-ribose	C00301	74	Leucine	C00123,C01570,C16439
17	Alanine	C00041,C00133,C01401	75	Lysine	C00047,C00739,C16440
18	Arginine	C00062,C00792	76	Malic acid	C00149,C00497,C00711
19	Argininosuccinic acid	C03406	77	Malonyl coenzyme A	C00083
20	Asparagine	C00152,C01905,C16438	78	Methionine	C00073,C00855,C01733
21	Asparaginic acid	C00049,C00402,C16433	79	Mevalonic acid	C00418
22	Betaine	C00719	80	N,N-Dimethylglycine	C01026
23	Betaine aldehyde	C00576	81	N-Acetylglutamic acid	C00624
24	Carbamoyl aspartic acid	C00438	82	Nicotinamide adenine dinucleotide (oxidized form)	C00003
25	Carbamoyl phosphate	C00169	83	Nicotinamide adenine dinucleotide (reduced form)	C00004
26	Carnitine	C00318,C00487	84	Nicotinamide adenine dinucleotide phosphate (oxidized form)	C00006
27	Carnosine	C00386	85	Nicotinamide adenine dinucleotide phosphate (reduced form)	C00005
28	Choline	C00114	86	Ornithine	C00077,C00515,C01602
29	cis-Aconitic acid	C00417	87	Phenylalanine	C00079,C02057,C02265
30	Citric acid	C00158	88	Phosphocreatine	C02305
31	Citrulline	C00327	89	Phosphoenolpyruvic acid	C00074
32	Coenzyme A	C00010	90	Phosphoribosyl pyrophosphate	C00119
33	Creatine	C00300	91	Proline	C00148,C00763,C16435
34	Creatinine	C00791	92	Putrescine	C00134
35	Cyclic adenosine 5-monophosphate	C00360	93	Pyruvic acid	C00022
36	Cyclic guanosine 5-monophosphate	C00942	94	Ribose 1-phosphate	C00620
37	Cystathionine	C00542,C02291	95	Ribose 5-phosphate	C00117
38	Cysteine	C00097,C00736,C00793	96	Ribulose 5-phosphate	C00199,C01101
39	Dihydroxyacetone phosphate	C00111	97	S-Adenosylhomocysteine	C00021
40	Erythrose 4-phosphate	C00279	98	S-Adenosylmethionine	C00019
41	Folate	C00504	99	Sarcosine	C00213
42	Fructose 1,6-diphosphate	C00354	100	Sedoheptulose 7-phosphate	C05382
43	Fructose 1-phosphate	C01094,C05001	101	Serine	C00065,C00716,C00740
44	Fructose 6-phosphate	C00085	102	Spermidine	C00315
45	Fumaric acid	C00122	103	Spermine	C00750
46	Galactose 1-phosphate	C00446	104	Succinic acid	C00042
47	Glucose 1-phosphate	C00103	105	Threonine	C00188,C00820
48	Glucose 6-phosphate	C00092	106	Tryptophan	C00078,C00525,C00806
49	Glutamic acid	C00025,C00217,C00302	107	Tyrosine	C00082,C01536,C06420
50	Glutamine	C00064,C00303,C00819	108	UDP-glucose	C00029
51	Glutathione (oxidized form)	C00127	109	Urea	C00077,C00515,C01603
52	Glutathione (reduced form)	C00051	110	Uric acid	C00366
53	Glyceraldehyde 3-phosphate	C00118	111	Valine	C00183,C06417,C16436
54	Glycerol 3-phosphate	C00093	112	Xanthine	C00385
55	Glycine	C00037	113	Xanthosine 5-monophosphate	C00655
56	Glycolic acid	C00160	114	Xylulose 5-phosphate	C00231,C03291
57	Glyoxylic acid	C00048	115	β -Alanine	C00099
58	Guanine	C00242	116	γ -Aminobutyric acid	C00334