

Table S1: Related genes with the target metabolites in nicotinate and nicotinamide metabolism.

Input Compound	Compound ID	Compound Name	Input Gene	Entrez Gene ID	Gene Symbol	Gene Description
Yes	C00003	NAD+	No	142	PARP1	poly (ADP-ribose) polymerase 1
Yes	C00003	NAD+	No	143	PARP4	poly (ADP-ribose) polymerase family, member 4
Yes	C00003	NAD+	No	417	ART1	ADP-ribosyltransferase 1
Yes	C00003	NAD+	No	419	ART3	ADP-ribosyltransferase 3
Yes	C00003	NAD+	No	420	ART4	ADP-ribosyltransferase 4 (Dombrock blood group)
Yes	C00003	NAD+	No	683	BST1	bone marrow stromal cell antigen 1
Yes	C00003	NAD+	No	952	CD38	CD38 molecule
Yes	C00003	NAD+	No	1727	CYB5R3	cytochrome b5 reductase 3
Yes	C00003	NAD+	No	3248	HPGD	hydroxyprostaglandin dehydrogenase 15-(NAD)
Yes	C00003	NAD+	No	3283	HSD3B1	hydroxy-delta-5-steroid dehydrogenase, 3 beta- and steroid delta-isomerase 1
Yes	C00003	NAD+	No	3284	HSD3B2	hydroxy-delta-5-steroid dehydrogenase, 3 beta- and steroid delta-isomerase 2
Yes	C00003	NAD+	No	5167	ENPP1	ectonucleotide pyrophosphatase/phosphodiesterase 1
Yes	C00003	NAD+	No	5168	ENPP2	ectonucleotide pyrophosphatase/phosphodiesterase 2
Yes	C00003	NAD+	No	5169	ENPP3	ectonucleotide pyrophosphatase/phosphodiesterase 3
Yes	C00003	NAD+	No	8658	TNKS	tankyrase, TRF1-interacting ankyrin-related ADP-ribose polymerase
Yes	C00003	NAD+	No	10038	PARP2	poly (ADP-ribose) polymerase 2
Yes	C00003	NAD+	No	10039	PARP3	poly (ADP-ribose) polymerase family, member 3
Yes	C00003	NAD+	No	23057	NMNAT 2	nicotinamide nucleotide adenyltransferase 2
Yes	C00003	NAD+	No	25976	TIPARP	TCDD-inducible poly(ADP-ribose) polymerase
Yes	C00003	NAD+	No	23530	NNT	nicotinamide nucleotide transhydrogenase

Yes	C00003	NAD+	No	51548	SIRT6	sirtuin (silent mating type information regulation 2 homolog) 6 (<i>S. cerevisiae</i>)
Yes	C00003	NAD+	No	51706	CYB5R1	cytochrome b5 reductase 1
Yes	C00003	NAD+	No	54625	PARP14	poly (ADP-ribose) polymerase family, member 14
Yes	C00003	NAD+	No	54956	PARP16	poly (ADP-ribose) polymerase family, member 16
Yes	C00003	NAD+	No	55191	NADSY N1	NAD synthetase 1
Yes	C00003	NAD+	No	56965	PARP6	poly (ADP-ribose) polymerase family, member 6
Yes	C00003	NAD+	No	57097	PARP11	poly (ADP-ribose) polymerase family, member 11
Yes	C00003	NAD+	No	64761	PARP12	poly (ADP-ribose) polymerase family, member 12
Yes	C00003	NAD+	No	64802	NMNAT 1	nicotinamide nucleotide adenyltransferase 1
Yes	C00003	NAD+	No	65220	NADK	NAD kinase
Yes	C00003	NAD+	No	79668	PARP8	poly (ADP-ribose) polymerase family, member 8
Yes	C00003	NAD+	No	80351	TNKS2	tankyrase, TRF1-interacting ankyrin-related ADP-ribose polymerase 2
Yes	C00003	NAD+	No	83594	NUDT1 2	nudix (nucleoside diphosphate linked moiety X)-type motif 12
Yes	C00003	NAD+	No	83666	PARP9	poly (ADP-ribose) polymerase family, member 9
Yes	C00003	NAD+	No	84875	PARP10	poly (ADP-ribose) polymerase family, member 10
Yes	C00003	NAD+	No	11696 9	ART5	ADP-ribosyltransferase 5
Yes	C00003	NAD+	No	16563 1	PARP15	poly (ADP-ribose) polymerase family, member 15
Yes	C00003	NAD+	No	34956 5	NMNAT 3	nicotinamide nucleotide adenyltransferase 3
No	C00004	NADH	No	1727	CYB5R3	cytochrome b5 reductase 3
No	C00004	NADH	No	3248	HPGD	hydroxyprostaglandin dehydrogenase 15-(NAD)
No	C00004	NADH	No	3283	HSD3B1	hydroxy-delta-5-steroid dehydrogenase, 3 beta- and steroid delta-isomerase 1
No	C00004	NADH	No	3284	HSD3B2	hydroxy-delta-5-steroid dehydrogenase, 3 beta- and steroid delta-isomerase 2
No	C00004	NADH	No	51706	CYB5R1	cytochrome b5 reductase 1

No	C00006	NADP+	No	683	BST1	bone marrow stromal cell antigen 1
No	C00006	NADP+	No	952	CD38	CD38 molecule
No	C00006	NADP+	No	23530	NNT	nicotinamide nucleotide transhydrogenase
No	C00006	NADP+	No	65220	NADK	NAD kinase
No	C00062	L-Arginine	No	417	ART1	ADP-ribosyltransferase 1
No	C00062	L-Arginine	No	419	ART3	ADP-ribosyltransferase 3
No	C00062	L-Arginine	No	420	ART4	ADP-ribosyltransferase 4 (Dombrock blood group)
No	C00062	L-Arginine	No	51548	SIRT6	sirtuin (silent mating type information regulation 2 homolog) 6 (<i>S. cerevisiae</i>)
No	C00062	L-Arginine	No	116969	ART5	ADP-ribosyltransferase 5
No	C00064	L-Glutamine	No	55191	NADSYN1	NAD synthetase 1
Yes	C00153	Nicotinamide	No	142	PARP1	poly (ADP-ribose) polymerase 1
Yes	C00153	Nicotinamide	No	143	PARP4	poly (ADP-ribose) polymerase family, member 4
Yes	C00153	Nicotinamide	No	417	ART1	ADP-ribosyltransferase 1
Yes	C00153	Nicotinamide	No	419	ART3	ADP-ribosyltransferase 3
Yes	C00153	Nicotinamide	No	420	ART4	ADP-ribosyltransferase 4 (Dombrock blood group)
Yes	C00153	Nicotinamide	No	683	BST1	bone marrow stromal cell antigen 1
Yes	C00153	Nicotinamide	No	952	CD38	CD38 molecule
Yes	C00153	Nicotinamide	No	4837	NNMT	nicotinamide N-methyltransferase
Yes	C00153	Nicotinamide	No	4860	NP	purine nucleoside phosphorylase
Yes	C00153	Nicotinamide	No	8658	TNKS	tankyrase, TRF1-interacting ankyrin-related ADP-ribose polymerase
Yes	C00153	Nicotinamide	No	10038	PARP2	poly (ADP-ribose) polymerase 2
Yes	C00153	Nicotinamide	No	10039	PARP3	poly (ADP-ribose) polymerase family, member 3
Yes	C00153	Nicotinamide	No	10135	PBEF1	nicotinamide phosphoribosyltransferase
Yes	C00153	Nicotinamide	No	25976	TIPARP	TCDD-inducible poly(ADP-ribose) polymerase
Yes	C00153	Nicotinamide	No	51548	SIRT6	sirtuin (silent mating type information regulation 2 homolog) 6 (<i>S. cerevisiae</i>)
Yes	C00153	Nicotinamide	No	54625	PARP14	poly (ADP-ribose) polymerase family, member 14

Yes	C00153	Nicotinamide	No	54956	PARP16	poly (ADP-ribose) polymerase family, member 16
Yes	C00153	Nicotinamide	No	56965	PARP6	poly (ADP-ribose) polymerase family, member 6
Yes	C00153	Nicotinamide	No	57097	PARP11	poly (ADP-ribose) polymerase family, member 11
Yes	C00153	Nicotinamide	No	64761	PARP12	poly (ADP-ribose) polymerase family, member 12
Yes	C00153	Nicotinamide	No	79668	PARP8	poly (ADP-ribose) polymerase family, member 8
Yes	C00153	Nicotinamide	No	80351	TNKS2	tankyrase, TRF1-interacting ankyrin-related ADP-ribose polymerase 2
Yes	C00153	Nicotinamide	No	83666	PARP9	poly (ADP-ribose) polymerase family, member 9
Yes	C00153	Nicotinamide	No	84875	PARP10	poly (ADP-ribose) polymerase family, member 10
Yes	C00153	Nicotinamide	No	116969	ART5	ADP-ribosyltransferase 5
Yes	C00153	Nicotinamide	No	165631	PARP15	poly (ADP-ribose) polymerase family, member 15
No	C00222	3-Oxopropanoate	No	18	ABAT	4-aminobutyrate aminotransferase
Yes	C00455	Nicotinamide D-ribonucleotide	No	4877	NT3	3'-nucleotidase
Yes	C00455	Nicotinamide D-ribonucleotide	No	4907	NT5E	5'-nucleotidase, ecto (CD73)
Yes	C00455	Nicotinamide D-ribonucleotide	No	5167	ENPP1	ectonucleotide pyrophosphatase/phosphodiesterase 1
Yes	C00455	Nicotinamide D-ribonucleotide	No	5168	ENPP2	ectonucleotide pyrophosphatase/phosphodiesterase 2
Yes	C00455	Nicotinamide D-ribonucleotide	No	5169	ENPP3	ectonucleotide pyrophosphatase/phosphodiesterase 3
Yes	C00455	Nicotinamide D-ribonucleotide	No	10135	PBEF1	nicotinamide phosphoribosyltransferase
Yes	C00455	Nicotinamide D-ribonucleotide	No	22978	NT5C2	5'-nucleotidase, cytosolic II
Yes	C00455	Nicotinamide D-ribonucleotide	No	23057	NMNAT2	nicotinamide nucleotide adenyltransferase 2
Yes	C00455	Nicotinamide D-ribonucleotide	No	30833	NT5C	5', 3'-nucleotidase, cytosolic
Yes	C00455	Nicotinamide D-ribonucleotide	No	51251	NT5C3	5'-nucleotidase, cytosolic III

Yes	C00455	Nicotinamide D-ribonucleotide	No	56953	NT5M	5',3'-nucleotidase, mitochondrial
Yes	C00455	Nicotinamide D-ribonucleotide	No	64802	NMNAT1	nicotinamide nucleotide adenyltransferase 1
Yes	C00455	Nicotinamide D-ribonucleotide	No	83594	NUDT12	nudix (nucleoside diphosphate linked moiety X)-type motif 12
Yes	C00455	Nicotinamide D-ribonucleotide	No	84618	NT5C1A	5'-nucleotidase, cytosolic IA
Yes	C00455	Nicotinamide D-ribonucleotide	No	93034	NT5C1B	5'-nucleotidase, cytosolic IB
Yes	C00455	Nicotinamide D-ribonucleotide	No	349565	NMNAT3	nicotinamide nucleotide adenyltransferase 3
No	C00584	Prostaglandin E2	No	3248	HPGD	hydroxyprostaglandin dehydrogenase 15-(NAD)
No	C00627	Pyridoxine phosphate	No	8566	PDXK	pyridoxal (pyridoxine, vitamin B6) kinase
No	C00857	Deamino-NAD+	No	55191	NADSYN1	NAD synthetase 1
No	C00996	Ferricytochrome b5	No	1727	CYB5R3	cytochrome b5 reductase 3
No	C00996	Ferricytochrome b5	No	51706	CYB5R1	cytochrome b5 reductase 1
No	C00999	Ferrocycytochrome b5	No	1727	CYB5R3	cytochrome b5 reductase 3
Input Compound	Compound ID	Compound Name	Input Gene	Entrez Gene ID	Gene Symbol	Gene Description
No	C00999	Ferrocycytochrome b5	No	51706	CYB5R1	cytochrome b5 reductase 1
No	C01034	3-Oxo-delta5-steroid	No	3283	HSD3B1	hydroxy-delta-5-steroid dehydrogenase, 3 beta- and steroid delta-isomerase 1
No	C01034	3-Oxo-delta5-steroid	No	3284	HSD3B2	hydroxy-delta-5-steroid dehydrogenase, 3 beta- and steroid delta-isomerase 2
No	C01161	3,4-Dihydroxyphenylacetate	No	218	ALDH3A1	aldehyde dehydrogenase 3 family, member A1
No	C01161	3,4-Dihydroxyphenylacetate	No	220	ALDH1A3	aldehyde dehydrogenase 1 family, member A3
No	C01161	3,4-Dihydroxyphenylacetate	No	221	ALDH3B1	aldehyde dehydrogenase 3 family, member B1
No	C01161	3,4-Dihydroxyphenylacetate	No	222	ALDH3B2	aldehyde dehydrogenase 3 family, member B2
No	C01201	N(omega)-(ADP-D-ribosyl)-L-arginine	No	417	ART1	ADP-ribosyltransferase 1

No	C01201	N(omega)-(ADP-D-ribose)-L-arginine	No	419	ART3	ADP-ribosyltransferase 3
No	C01201	N(omega)-(ADP-D-ribose)-L-arginine	No	420	ART4	ADP-ribosyltransferase 4 (Dombrock blood group)
No	C01201	N(omega)-(ADP-D-ribose)-L-arginine	No	51548	SIRT6	sirtuin (silent mating type information regulation 2 homolog) 6 (<i>S. cerevisiae</i>)
No	C01201	N(omega)-(ADP-D-ribose)-L-arginine	No	116969	ART5	ADP-ribosyltransferase 5
Yes	C01586	Hippurate	No	1312	COMT	catechol-O-methyltransferase
No	C02642	3-Ureidopropionate	No	51733	UPB1	ureidopropionase, beta
No	C02918	1-Methylnicotinamide	No	4837	NNMT	nicotinamide N-methyltransferase
No	C03150	N-Ribosylnicotinamide	No	4860	NP	purine nucleoside phosphorylase
No	C03150	N-Ribosylnicotinamide	No	4877	NT3	3'-nucleotidase
Input Compound	Compound ID	Compound Name	Input Gene	Entrez Gene ID	Gene Symbol	Gene Description
No	C03150	N-Ribosylnicotinamide	No	4907	NT5E	5'-nucleotidase, ecto (CD73)
No	C03150	N-Ribosylnicotinamide	No	22978	NT5C2	5'-nucleotidase, cytosolic II
No	C03150	N-Ribosylnicotinamide	No	30833	NT5C	5', 3'-nucleotidase, cytosolic
No	C03150	N-Ribosylnicotinamide	No	51251	NT5C3	5'-nucleotidase, cytosolic III
No	C03150	N-Ribosylnicotinamide	No	56953	NT5M	5',3'-nucleotidase, mitochondrial
No	C03150	N-Ribosylnicotinamide	No	84618	NT5C1A	5'-nucleotidase, cytosolic IA
No	C03150	N-Ribosylnicotinamide	No	93034	NT5C1B	5'-nucleotidase, cytosolic IB
No	C03245	ADP-D-ribose-acceptor	No	142	PARP1	poly (ADP-ribose) polymerase 1
No	C03245	ADP-D-ribose-acceptor	No	143	PARP4	poly (ADP-ribose) polymerase family, member 4
No	C03245	ADP-D-ribose-acceptor	No	8658	TNKS	tankyrase, TRF1-interacting ankyrin-related ADP-ribose polymerase
No	C03245	ADP-D-ribose-acceptor	No	10038	PARP2	poly (ADP-ribose) polymerase 2
No	C03245	ADP-D-ribose-acceptor	No	10039	PARP3	poly (ADP-ribose) polymerase family, member 3
No	C03245	ADP-D-ribose-acceptor	No	25976	TIPARP	TCDD-inducible poly(ADP-ribose) polymerase

No	C03245	ADP-D-ribosyl-acceptor	No	54625	PARP14	poly (ADP-ribose) polymerase family, member 14
No	C03245	ADP-D-ribosyl-acceptor	No	54956	PARP16	poly (ADP-ribose) polymerase family, member 16
No	C03245	ADP-D-ribosyl-acceptor	No	56965	PARP6	poly (ADP-ribose) polymerase family, member 6
No	C03245	ADP-D-ribosyl-acceptor	No	57097	PARP11	poly (ADP-ribose) polymerase family, member 11
No	C03245	ADP-D-ribosyl-acceptor	No	64761	PARP12	poly (ADP-ribose) polymerase family, member 12
No	C03245	ADP-D-ribosyl-acceptor	No	79668	PARP8	poly (ADP-ribose) polymerase family, member 8
No	C03245	ADP-D-ribosyl-acceptor	No	80351	TNKS2	tankyrase, TRF1-interacting ankyrin-related ADP-ribose polymerase 2
No	C03245	ADP-D-ribosyl-acceptor	No	83666	PARP9	poly (ADP-ribose) polymerase family, member 9
No	C03245	ADP-D-ribosyl-acceptor	No	84875	PARP10	poly (ADP-ribose) polymerase family, member 10
No	C03245	ADP-D-ribosyl-acceptor	No	16563 1	PARP15	poly (ADP-ribose) polymerase family, member 15
No	C03758	4-(2-Aminoethyl)-1,2-benzenediol	No	26	ABP1	amiloride binding protein 1 (amine oxidase (copper-containing))
No	C03758	4-(2-Aminoethyl)-1,2-benzenediol	No	314	AOC2	amine oxidase, copper containing 2 (retina-specific)
No	C03758	4-(2-Aminoethyl)-1,2-benzenediol	No	4128	MAOA	monoamine oxidase A
No	C03758	4-(2-Aminoethyl)-1,2-benzenediol	No	4129	MAOB	monoamine oxidase B
No	C03758	4-(2-Aminoethyl)-1,2-benzenediol	No	8639	AOC3	amine oxidase, copper containing 3 (vascular adhesion protein 1)
No	C03836	3beta-Hydroxy-delta5-steroid	No	3283	HSD3B1	hydroxy-delta-5-steroid dehydrogenase, 3 beta- and steroid delta-isomerase 1
No	C03836	3beta-Hydroxy-delta5-steroid	No	3284	HSD3B2	hydroxy-delta-5-steroid dehydrogenase, 3 beta- and steroid delta-isomerase 2
No	C04707	(5Z,13E)-11alpha-Hydroxy-9,15-dioxoprost-13-enoate	No	3248	HPGD	hydroxyprostaglandin dehydrogenase 15-(NAD)
No	C05653	Formylanthranilate	No	12506 1	AFMID	arylformamidase
No	C05665	beta-Aminopropion aldehyde	No	217	ALDH2	aldehyde dehydrogenase 2 family (mitochondrial)

No	C05665	beta-Aminopropion aldehyde	No	218	ALDH3A 1	aldehyde dehydrogenase 3 family, member A1
No	C05665	beta-Aminopropion aldehyde	No	219	ALDH1B 1	aldehyde dehydrogenase 1 family, member B1
No	C05665	beta-Aminopropion aldehyde	No	220	ALDH1A 3	aldehyde dehydrogenase 1 family, member A3
No	C05665	beta-Aminopropion aldehyde	No	223	ALDH9A 1	aldehyde dehydrogenase 9 family, member A1
No	C05665	beta-Aminopropion aldehyde	No	224	ALDH3A 2	aldehyde dehydrogenase 3 family, member A2
No	C05665	beta-Aminopropion aldehyde	No	501	ALDH7A 1	aldehyde dehydrogenase 7 family, member A1
No	CE2934	o-methylhippurate	No	1312	COMT	catechol-O-methyltransferase