

Metabolite	Name in KEGG	KEGG ID	Similarity	Tie	Selected	Pathway ID	Pathway Name
SM C16:0	Sphingomyelin	cpd:C00550	0.19	No	Yes	path:rno00600	Sphingolipid metabolism
SM C16:0	Sphingomyelin	cpd:C00550	0.19	No	Yes	path:rno04071	Sphingolipid signaling pathway
lysoPC a C16:0	1–Lysophosphatidylcholine	cpd:C04233	0.31	Yes	Yes	path:rno00564	Glycerophospholipid metabolism
lysoPC a C16:0	2–Lysophosphatidylcholine	cpd:C04230	0.31	Yes	No	NA	NA
PC aa C28:1	Phosphatidylcholine	cpd:C00157	0.13	No	Yes	path:rno00564	Glycerophospholipid metabolism
PC aa C28:1	Phosphatidylcholine	cpd:C00157	0.13	No	Yes	path:rno05231	Choline metabolism in cancer
Ala	L–Alanine	cpd:C00041	0.50	No	Yes	path:rno00250	Alanine, aspartate and glutamate metabolism
Carnosine	Carnosine	cpd:C00386	1.00	No	Yes	path:rno00410	beta–Alanine metabolism
Val	L–Valine	cpd:C00183	0.55	No	Yes	path:rno00290	Valine, leucine and isoleucine biosynthesis
Val	N–Hydroxy–L–valine	cpd:C20313	0.29	No	No	NA	NA