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Article

Posttranslational acylations of the rat brain transketolase discriminate the enzyme responses to inhibitors of ThDP-dependent enzymes or thiamine transport

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Supplementary data

Table S1. The peptides (up to four per protein, marked as p1-p4), used for the relative quantification by MS and the forms of acylatable peptides of the transketolase (TKT) are summarized in this table. Dependent on the number of the lysine, arginine and histidine residues in a peptide, several charged precursor variants (2+, 3+ or 4+) with monoisotopic precursor mass and the C13-isotopomepic variants ([M+1] and [M+2]) have been detected to increase the quantification accuracy. ox – Met oxidation (+16), cam – Cys carbamidomethylation (+57), n.a. – not analyzed.

Peptide	Specification	C13-isotopomepic variants of the precursors		
		monoisotopic	[M+1]	[M+2]
SK(mal)DDQVTVIGAGVTLHEALAAAEM(ox)LKK	TKT Mal-K499	966.5023+++	966.8366+++	967.1708+++
		725.1286++++	n.a.	n.a.
SKDDQVTVIGAGVTLHEALAAAEM(ox)LKK	TKT K499-deac	703.6285++++	703.8792++++	704.1298++++
		563.1042; +5	563.3048; +5	563.5053; +5
K(ac)ISSDLDGHPVPK	TKT Ac-K102	717.8830++	718.3845++	718.8858++
		478.9244+++	479.2587+++	479.5930+++
ISSDLDGHPVPK	TKT K102-deac	632.8302++	633.3317++	633.8330++
		422.2226+++	422.5569+++	422.8911+++
M(ox)EGYHK(ac)PDQQKLQALKDTANR	TKT Ac-K6	843.7553+++	844.0896+++	844.4237+++
QAFTDVATGSLGQGLGAAC(cam)GM(ox)AYTGK	TKT p1	1274.5940++	1275.0954++	1275.5963++
LGQSDPAPLQHQVDVYQK	TKT p2	1012.0158++	1012.5172++	1013.0186++
		675.0130+++	675.3473+++	675.6815+++
TSRPENAIIYSNNEDFQVGQAK	TKT p3	1241.1039++	1241.6053++	1242.1067++
		827.7383+++	828.0726+++	828.4069+++
SVPM(ox)STVFYPSDGVATEK	TKT p4	965.9588++	966.4603++	966.9613++
VAPEEHPVLLTEAPLNPK	ActB p1	977.5358++	978.0373++	978.5387++
		652.0263+++	652.3606+++	652.6949+++
DLYANTVLSGGTTM(ox)YPGIADR	ActB p2	1116.0361++	1116.5375++	1117.0386++
QEYDESGPSIVHR	ActB p3	758.8550++	759.3564++	759.8577++
		506.2391+++	506.5734+++	506.9076+++
EVDEQM(ox)LAIQSK	Tubb3 p1	703.8452++	704.3467++	704.8474++
LATPTYGDLNHLVSATM(ox)SGVTTSLR	Tubb3 p2	1311.1656++	1311.6670++	1312.1682++
		874.4462+++	874.7805+++	875.1146+++
YLTVATVFR	Tubb3 p3	535.3057++	535.8071++	536.3085++