

Human embryonic and induced pluripotent stem cells maintain phenotype but alter their metabolism after exposure to ROCK inhibitor

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Supplementary information

SUPPLEMENTARY FILE: The metabolite peaks detected in the MS-reconstructed chromatogram

PKM Name	METABOLITE	Molecular Weight	Retention time (min)	Chemical Category	FMO	Peak ID																									
						PK1	PK2	PK3	PK4	PK5	PK6	PK7	PK8	PK9	PK10	PK11	PK12	PK13	PK14	PK15	PK16	PK17	PK18	PK19	PK20	PK21	PK22	PK23	PK24	PK25	PK26
PK1	Acetylcholine	146	5.26	Cholinergic	1			
PK2	Acetylcholine	146	5.26	Cholinergic	1			
PK26	Acetylcholine	146	5.26	Cholinergic	1			
PK27	Acetylcholine	146	5.26	Cholinergic	1			
PK28	Acetylcholine	146	5.26	Cholinergic	1			

Note 1: Chemical category 1, 2 and 3 as used as defined in Kurnat and Kläber, 2017. Category 10 is assigned to peaks that are considered artifacts due to column bleed-through. 10 is assigned to category 1 metabolites that form only one derivative. 10 is assigned to those detection compound (in the case listed) which a category 1 metabolite. 10 is assigned to several detection compound in the case 1-10 (2) please which a category 2 metabolite.

Note 2: A peak is defined 'PK ID', respectively, if it has been qualified at least one of the assigned metabolite profile. (PK ID) if a peak is detected in at least one of the assigned metabolite profiles for a compound (one peak due to the shape of the peak).

