

Supporting Information

Identification and Optimization of a Novel Inhibitor of Mitochondrial Calpain 10

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and Rick G. Schnellmann ([†] Denotes an equal contribution to the completion of this work)

Contents: Analytical Purity of Compounds

Peptide	Mass (amu) expected	Mass (amu), found (M + H) ⁺	R.T.	R.T.
KAGYC-s-s-CYGAK ^a	1077.5	1077.8	17.5 ^d	20.0 ^e
CYGRKK ^b	753.9	753.2		
CYGRK ^b	625.8	625.4		
CYGAK ^b	540.4	540.7		
YGAK ^c	437.2	437.3		
C'YGAK ^c	554.4	554.5		
CVGAK ^b	476.6	476.3		
MeOPh-s-s-CYGAK ^c	678.3	678.5	22.0 ^f	28.0 ^g
Ethyl-s-s-CYGAK ^c	600.3	600.2	18 ^f	21 ^g
CAGAK ^b				

^aCYGAK dimer was analyzed for purity by two different HPLC methods and a single symmetric peak was detected in each case (purity > 98%). ^dAlltec Platinum C18 100A 3 μ , 33mm X 7mm, 0.7 mL/min, 4% acetonitrile/96% water + 0.1% TFA, linear gradient to 50% acetonitrile/50% water + 0.1% TFA after 50 min and then 100% acetonitrile/0% water after 60 min, U.V. detection at 220 nm. ^e4% methanol/96% water + 0.1% TFA, linear gradient to 30% methanol/70% water + 0.1% TFA after 15 min and then 100% methanol/0% water after 30 min, U.V. detection at 220 nm. ^f4% acetonitrile/96% water + 0.1% TFA, linear gradient to 60% acetonitrile /40% water + 0.1% TFA after 30 min and then 100% acetonitrile /0% water after 45 min, U.V. detection at 220 nm. ^g4% methanol/96% water + 0.1% TFA, linear gradient to 60% methanol/40% water + 0.1% TFA after 30 min and then 100% methanol/0% water after 45 min, U.V. detection at 220 nm.

^bThese peptides were obtained from commercial sources (purity > 90%). ^c

These peptides were prepared in the laboratory and each purified twice on Prep LC column (purity > 95%).