

Figure S7 Alignment of BECa/CPILE-ab amino acid sequences

(a) Amino acid sequence alignment of BECa (CPILE-a) (1) and BECb (CPILE-b) (2) of strains OS1, TS1, W5052 (GenBank accession nos. AP013033, AP13034, AB921559, respectively) and CP653 analyzed in the present study. Amino acids in CP653 proteins which are different from those of other three strains are shown in red, while asterisk indicates identical amino acid. A short loop sequence (residue 210-216) linking structurally homologous N-terminal domain and C-terminal domain is represented by shading above the sequence. Positions marked in yellow below the sequences represent common structural traits in ADP-ribosylating toxin (ADPRT)-family proteins, i.e., an aromatic residue (Y)-R/H, S-T-S motif (S-T-T in BECa/CPILE-a), an E-X-E motif in the ADP-ribosylating turn-turn (ARTT) loop underlined. Conserved amino acids associated with NADH recognition [26] are indicated by blue bars above the sequences. Loop I-V, and two protruding loops PT-I and PT-II associated with binding to actin [27] are indicated by green and red boxes, respectively.

(1) BECa / CPILE-a

CP653	MLDDNRPMDFAKDKNSATLWAKKRKQVWLNLSKAESTSIDNYIKNSSEINSYSIKKKFA	60
OS1	MLDDNRPMDFAKDKNSATLWAKKRKQVWLNLSKAESTSINNYIKNSSEINSYSIKKKFA	60
TS-1	MLDDNRPMDFAKDKNSATLWAKKRKQVWLNLSKAESTSINNYIKNSSEINSYSIKKKFA	60
W5052	MLDDNRPMDFAKDKNSATLWAKKRKQVWLNLSKAESTSINNYIKNSSEINSYSIKKKFA	60
	*****:*****:*****	
	α1 α2	
CP653	LDNYEGIETLNEDLKNISTSVKKSMLTKPLYVYYYETNDKFGFNQNLLESSLDSNIIDDEA	120
OS1	LDNYEGIETLNEDLKNISTAVKKSMLTKPLYVYYYEANDKFGFNQNLLESSLDSNIIDEEA	120
TS-1	LDNYEGIETLNEDLKNISTAVKKSMLTKPLYVYYYEANDKFGFNQNLLESSLDSNIIDEEA	120
W5052	LDNYEGIETLNEDLKNISTAVKKSMLTKPLYVYYYEANDKFGFNQNLLESSLDSNIIDEEA	120
	*****:*****:*****	
	loop I α3 β1	
CP653	INNFAKKISDTNFIQDGFKDVNMTEPDINSKLPILVHLKLPTNTPAASYGNDEENLRVLI	180
OS1	INNFAKKISDTNFIQDGFKDVMTTEPDINSKLPILVHLKLPTNTPAASYGNDEENLRVLI	180
TS-1	INNFAKKISDTNFIQDGFKDVMTTEPDINSKLPILVHLKLPTNTPAASYGNDEENLRVLI	180
W5052	INNFAKKISDTNFIQDGFKDVMTTEPDINSKLPILVHLKLPTNTPAASYGNDEENLRVLI	180
	*****:*****:*****	
	α4 β2 β3 β4	
	N-terminal domain ← → C-terminal domain	
CP653	DQGYSLKATGLSIVTIKKGQYAKVDADLIKQLNFENDVISASQWGEENYAPWLKELTSNE	240
OS1	DQGYSLKATGLSIVTIKKGQYAKVDADLIKQLNFENDVISASQWGEENYAPWLKELTSNE	240
TS-1	DQGYSLKATGLSIVTIKKGQYAKVDADLIKQLNFENDVISASQWGEENYAPWLKELTSNE	240
W5052	DQGYSLKATGLSIVTIKKGQYAKVDADLIKQLNFENDVISASQWGEENYAPWLKELTSNE	240
	*****:*****:*****	
CP653	LRDINNYLGGGYTAINKYLLDGTIGENTSKEDEEEKISNISSALKKKKIPEDIITYRRMG	300
OS1	LRDINNYLGGGYTAINKYLLDGTIGENTSKEDEEEKISNISSALKKKRKIPEDIITYRRMG	300
TS-1	LRDINNYLGGGYTAINKYLLDGTIGENTSKEDEEEKISNISSALKKKRKIPEDIITYRRMG	300
W5052	LRDINNYLGGGYTAINKYLLDGTIGENTSKEDEEEKISNISSALKKKRKIPEDIITYRRMG	300
	*****:*****:*****	
	loop II PT-I Aromatic residue (Y)-R/H	
CP653	PNEFGLDLNSPDYDFNKVENVSKFKEKWLGKTIPVKTFISTTVLSNNISAFAKRKLILRL	360
OS1	PNEFGLDLNSPDYDFNKVENVSKFKEKWLGKTIPVKTFISTTVLSNNISAFAKRKLILRL	360
TS-1	PNEFGLDLNSPDYDFNKVENVSKFKEKWLGKTIPVKTFISTTVLSNNISAFAKRKLILRL	360
W5052	PNEFGLDLNSPDYDFNKVENVSKFKEKWLGKTIPVKTFISTTVLSNNISAFAKRKLILRL	360
	*****:*****:*****	
	loop III S-T-S motif loop IV	
CP653	HLPNGSNAAYVSVAEGYKNEYEVLIDHGYSYKIDNITEYDESSLGGKTNKLIIDATLI	419
OS1	HLPNGSNAAYVSVAEGYKNEYEVLIDHGYSYKIDNITEYDESSLGGKTNKLIIDATLI	419
TS-1	HLPNGSNAAYVSVAEGYKNEYEVLIDHGYSYKIDNITEYDESSLGGKTNKLIIDATLI	419
W5052	HLPNGSNAAYVSVAEGYKNEYEVLIDHGYSYKIDNITEYDESSLGGKTNKLIIDATLI	419
	:**:*****	
	ARTT loop (E-X-E motif) / loop V PT-II	

CP653	IPYLKYFPKIGLRAFVNGIYKDLGLRFKNHDGHKTI LPTDYTDSPVKIDQFEVYVIDQY	780
TS1	IPFLKYFPQIGLRAFVNGIYKDLGLRLRNHDGYKTIITPADYTNSPVQIDQFEVYVIDQY	780
OS1	IPFLKYFPQIGLRAFVNGIYKDLGLRLRNHDGYKTIITPADYTNSPVQIDQFEVYVIDQY	780
W5052	IPFLKYFPQIGLRAFVNGIYKDLGLRLRNHDGYKTIITPADYTNSPVQIDQFEVYVIDQY	780

:***:*****:*****:*****:***:***:***:***:*****

CP653	GDPLTLFTSKDTIVLKYPF	799
TS1	GDPLTLFTSKDTIVLEYPF	799
OS1	GDPLTLFTSKDTIVLEYPF	799
W5052	GDPLTLFTSKDTIVLEYPF	799

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