Supplementary Information

Navigating Protein Fitness Landscapes Through Simulated Evolutionary Jumps

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Content

Supplemental information Table S1-8, Figure S1-6.

Supplementary Information

Supplementary Table 1. TadA/ABE deaminase protein sequences for LoRA fine-tuning model

Name	Sequence
ABE7.10	MSEVEFSHEYWMRHALTLAKRARDEREVPVGAVLVLNNRVIGEGWNRAIGLHDPTAHAEIMALRQGGLVMQNYRLIDATLYVTFEPCVMCAGAMIHSRIGRVVFGVRNAKTGAAGSLMDVLHYPGMNHRVEITEGILADECAALLCYFFRMPRQVFNAQKKAQSSTD
ABE7.9	MSEVEFSHEYWMRHALTLAKRAWDEREVPVGAVLVHNNRVIGEGWNRPIGRHDPTAHAEIMALRQGGLVMQNYRLIDATLYVTFEPCVMCAGAMIHSRIGRVVFGVRNAKTGAAGSLMDVLHYPGMNHRVEITEGILADECNALLCYFFRMPRQVFNAQKKAQSSTD
ABE7.4	MSEVEFSHEYWMRHALTLAKRAWDEREVPVGAVLVHNNRVIGEGWNRPIGRHDPTAHAEIMALRQGGLVMQNYRLIDATLYVTFEPCVMCAGAMIHSRIGRVVFGVRNAKTGAAGSLMDVLHYPGMNHRVEITEGILADECAALLCYFFRMRRQVFNAQKKAQSSTD
ABE6.4	MSEVEFSHEYWMRHALTLAKRAWDEREVPVGAVLVHNNRVIGEGWNRPIGRHDPTAHAEIMALRQGGLVMQNYRLIDATLYVTFEPCVMCAGAMIHSRIGRVVFGVRNAKTGAAGSLMDVLHYPGMNHRVEITEGILADECNALLCYFFRMRRQVFNAQKKAQSSTD
ABE5.3	MSEVEFSHEYWMRHALTLAKRAWDEREVPVGAVLVHNNRVIGEGWNRPIGRHDPTAHAEIMALRQGGLVMQNYRLIDATLYVTFEPCVMCAGAMIHSRIGRVVFGVRNAKTGAAGSLMDVLHYPGMNHRVEITEGILADECAALLCYFFRMRRQVFNAQKKAQSSTD
ABE3.1	MSEVEFSHEYWMRHALTLAKRAWDEREVPVGAVLVHNNRVIGEGWNRPIGRHDPTAHAEIMALRQGGLVMQNYRLIDATLYVTFEPCVMCAGAMIHSRIGRVVFGVRNAKTGAAGSLMDVLHYPGMNHRVEITEGILADECAALLSYFFRMRRQVFKAQKKAQSSTD
ABE2.9	MSEVEFSHEYWMRHALTLAKRAWDEREVPVGAVLVHNNRVIGEGWNRPIGRHDPTAHAEIMALRQGGLVMQNYRLIDATLYVTLEPCVMCAGAMIHSRIGRVVFGVRNAKTGAAGSLMDVLHYPGMNHRVEITEGILADECAALLSYFFRMRRQVIKAQKKAQSSTD
TadA8e	MSEVEFSHEYWMRHALTLAKRARDEREVPVGAVLVLNNRVIGEGWNRAIGLHDPTAHAEIMALRQGGLVMQNYRLIDATLYVTFEPCVMCAGAMIHSRIGRVVFGVRNSKRGAAGSLMNVLNYPGMNHRVEITEGILADECAALLCDFYRMPRQVFNAQKKAQSSIN
TadA8e_V106W	MSEVEFSHEYWMRHALTLAKRARDEREVPVGAVLVLNNRVIGEGWNRAIGLHDPTAHAEIMALRQGGLVMQNYRLIDATLYVTFEPCVMCAGAMIHSRIGRVVFGWRNSKRGAAGSLMNVLNYPGMNHRVEITEGILADECAALLCDFYRMPRQVFNAQKKAQSSIN
TadA8e_N108Q	MSEVEFSHEYWMRHALTLAKRARDEREVPVGAVLVLNNRVIGEGWNRAIGLHDPTAHAEIMALRQGGLVMQNYRLIDATLYVTFEPCVMCAGAMIHSRIGRVVFGVRQSKRGAAGSLMNVLNYPGMNHRVEITEGILADECAALLCDFYRMPRQVFNAQKKAQSSIN

Supplementary Table 2. CcdA family antitoxin protein sequences for LoRA fine-tuning model

Uniport ID	Sequence
P62552	RRLRAERWKAENQEGMAEVARFIEMNGSFADENRDW
A0AAX1M1G6	RRLRAERWKAENQEGMVEVARFIEMNGSFADENRNW
A0A6N9SHB8	RRLRAERWQAENQEGMAEVARFIEMNGSFAEENRDW
A0A0B0VNF4	RRLRAERWKAENQEGMAEVARFIEMNGSFADENREW
A0AAN5UII2	RRLRAERWKAENQEGMAEVARFIEMNSSFADENRDW
A0A8S7BM37	RRLRAGRWKAENQEGMAEVARFIEMNGSFADENRDW
A0A828UFP5	RRLRAERWKVENQEGMVEVARFIEMNGSFADENRDW
A0A1W1EMI8	RRLRAERWKAENREGMAEVARFIEMNGSFADENRDW
A0A6D0XUY0	RRLRAERWLAENQEGMAEVARFIEMNGSFADENRDW
A0A0F6YRL5	RRLRAERWRAENQEGMAEVARFIEMNGSFADENRDW
Q46995	RRLRPERWKVANQEGMAEVARFIEMNGSFADENRDW
Q99Q95	RRLRAERWQAENQQGMAEIARFIEMNGSFADENRDW
A0A2X4T6S6	RRLRAKRWQAENQEGMAEVALFIETNGSFADENRDW
A0A0G4JQF2	RRIKAEQWKKENREGMEEVARFITQNGSFADENRNW
Q6D9V2	RRIKAEEWKKENRERMEDIARFIAKNVFFADENRNW
A0A0L7T4A9	RRIKAEQWKTENREGMEEVARFIAQNGSFADENRNW
A0A2I5TNW4	RRIKAEAWKKENREGMEEVARFITQNGSFADENRNW
A0A3D9UGR6	RRIKAEKWKADNHEGMTEVANFIAQHGSFAEENRNW
A0A4R3XSF1	RRIKAERWLAENQSALDEYNRRIEMRGTFSDGLRNW
B2TT52	RRLRAERWQAENQQGMAEIARFIEMNGSFADENRDW
D2TV55	RRLRAERWQEENREGMAEVASFIEANGSFADENRDW
A0A4R1NF65	RRIKAEQWKKENHEGMEEVARFIAQNGSFADENRNW

Supplementary Table 3. TadA variant sequences from the SPIN-JEvo first-round evolved sequences (n = 60) and SPIN-JEvo second-round evolved sequences (n=60) for experimental test.

Index	Protein Sequence
ecTadA	MLSEVEFSHEYWMRHALTLAKRAWDEREVPVGAVLVHNNRVIGEGWNRPIGRHDPTAHAEIMALRQGGLVMQNYRLIDATLYVTLEPCVMCAGAMIHSRIGRVVFGARDAKTGAAGSLMDVLHHPGMNHRVEITEGILADECAALLSDFFRMRRQEIKAQKKAQSSTD
jTadA-1	MAYTPEDERWMRLAIEEARAAAQRGEVPVGCVIVRNGQVIARAPNAVEATLKATQHAEILALESASRELISWRLQDTTCYVTLEPCAMCAGAMVLARIPRVVFGVPNPKAGAAGSVVNLLEWPHLNHRVEVHRGVLEEEARQLLMEFFKQRRAQKKARG
jTadA-2	MAYTPEDERWMRLAIEEARAAMQRGEVPVGCVIVRNGQVIARAPNAVEADLKATQHAEWLALELASRELNSWRLPDTTSYVTLEPCACCAGAIALARIPRVVFGVGNPKAGAAGSVVNLLDWPGLNHRVEVMRGVLEGEARQILMEFFKQRRAEKKARG
jTadA-3	MAYTPEDERWMRLAIEEARAAMQRGEVPVGCVIVRNGQVIARAPNAVEADLKATQHAEWLALELASRELNSWRSPDTTNYVTLEPCACCAGAIVLARIPRYVFGVPNPKAGAAGSVVNLLDWPGLNHRVEVHRGVLEEEARTLLMEFFKQRRAQKAARG
jTadA-4	MAYTPEDERWMFLDIEEARAAAQRGEVPVGCVIVRNGQVIARAPNAVEATLKATQHAEILALELASRELNSWRLPDTTCYVTLEPCAMCAGAMVLARIPRVVFGVPNPKAGAAGSVVNLLEWPHLNHRVEVHRGVLEEEARQLLMEFFKQRRAQKKARG
jTadA-5	MAYHPEDERWMRLAIEEARAAMQRGEVPVGCVIVRNGQVIARAPNAVEADLKATQHAEWLALDLASRQLNSWRLDDTTNYVTLEPCAMCAGAMVLARIPRVVFGVPNPKAGAAGMVVNLLDWPGLNHRVEVHRGVLEEEARQILMEFFKQRRAQKCARG
jTadA-6	MAYTPEDERWMRLAIEEAYAAKQRGEVPVGCVIVRNGQVIARGPNAAEETLKATMHAEWLAIELASRELGSWRLPETTMYVTLEPCAMCAGAMVSARIPRVVFGVPNPKAGAAGSVVNLLDWPQLNHRVQVHRGVLEEEARNLLMEFFKQRRAQKKAQL
jTadA-7	MAYTPEDERWMRLAIEEARAAMQRGEVPVGCVIVRNNQVIARAPNAVCATLSATQHAEWLAIELASRELNSWRLPDTTCYVTLEPCAMCAGAMVLARIPRVVFGVPNPKAGAAGSVVNILDWPGLNHRVEYHRGVLEEEARQILMEFFKQRRAQKKAQG

jTadA-8	MSEQAQPTDWMQLALEEAKRAMANGEVPVGAVIVRNGEVIARGFNAPEERKNATLHAEVWAIQAAAEKYRSWRLLECTGFVTVEPCIMCMGAVQMARIPRIIFGVANEKGGAAGSYYNLHQVDWFNQRITVEKGVEEERARELLAQFFRDRRAAKRGQA
jTadA-9	MSEQAQPVDWMQLALEEAKRAMANGEVPVGAVIVRNGEVIARGFNAPEERKNATLHAEVQAISAAAEKYRSWRLLDCTGFVTVEPCIMCMGAIQIARIPRIIFGVANPKAGAAGSYYNIHQVDWFNHRVTVEKGVMAERARELLAQFFRDRRAAKRGTA
jTadA-10	MSEQAQPTDWMQLALEEAKRAMANGEVPVGAVIVRNGEVIARGFNAPEERKNATLHAEVWAIQAAAEKYRSWRLLDCTGFVTVEPCIMCMGAVQMARIPRIIFGVANEKGGAAGSYYNLHQVDWFNQRITVEKGVEEERARELLAQFFRDRRAAKRGQA
jTadA-11	MSEQAQPTDWMRLALEEAKRAMANGEVPVGAVIVRNGEVIARGFNAPEERKNATLHAEVWAIQAAAEKYRSWRLLDCTGFVTEEPCIMCMGAVQMARIPRRIFGVANEKGGAAGSYLNLHQIDWFNHRVTVEKGVERERAKELLAQFFRDRRAAKRGQA
jTadA-12	MAYTEHDLRWMRLAIEQAREAARRWEVPVGAVIVRDGRVIATAFNEREAELNAYAHAEILAIQRASREWQDWRLWDATWYVALEPCVMCAGALVQAREKRVVNGVRNPKAGAAGSLVDLPQQPWFNHRVEIERGVAQEEAAEILRAFFRERRAQKRAQS
jTadA-13	MAYTEHDERWMRLAIEQAREAARRWEVPVGAVIVRDGRVIATAFNEREAELNAYAHAEILAIQRASREWQDWRLWDATWYVTLEPCIMCAGALVQAREKRVVFGVYNPKAGAAGSLVDLPQQPWFNHRVEIERGVAPEEAAEILRAFFRERRAQKRAQS
jTadA-14	MAYTEHDERWMRLAIEQAREAARRWEVPVGAVIVRDGRVIATAFNEREAELNAYAHAEILAIQRASREWQDWRLWDATWYVTLEPCVMCAGALVAAREKRVVFGVYNPKAGAAGSLVDLPQQPWFNHRVEIERGVAPEEAAEILRAFFRERRAQKRAQS
jTadA-15	MAYTAEDERWMRLAIELARRAMERFEVPVGAVIVRDGKLVATAFNEVEELLHPTKQAELLNIEEASKAYNSWRLYGCDDYVTLFPCVMCAGAIVNAWIPRVVFGVPNPKDGAAGFVVRLHDIPEINHRVTVERGVREQECRDLLTQFFRERRAQKRAQR
jTadA-16	MQHSAQDLQWMQRALELAKRAAAQGEVPVGAVLVRDNQKIGDGFNAVEQDAQPTGHAEQMAIQAGARAQQSWRLQGYTLFVMLEPCPMCMGAIHNARIARNVFGVHNEKGGADGSYYRLADDARFNHAVELHKGVADEAARAQLSDFFKAQRKAKRGDA
jTadA-17	MSHSAQDLQWMQRALELAKRAAAQGEVPVGAVLVRDNTLIGDSFNAYEQDAQPTGHAEQMAIQAGLAAQQSWRLQGYTLFVMLEPCPMCMGAIHNARIARNVFGVHNEKGGADVSYYRLADDARFNHQVELHSGVADEAARAQLSDFFKAQRAAKRGKA

jTadA-18	MSHSAQDLQWMSRALELAKRAAAQGEVPVGAVLVKDNTLIGDGFNAVEQDAQPTGHAEQMAIQAGARAQQSWRLQDYTLFVMLEPCPMCMGAIHNARIARNVFGVHNEKGGADGSYYRLADDARFDHQVELHKGVADEAARAQLSDFFKAQRKAKRGKA
jTadA-19	MSHSAQDLQWMSRALELAKRAAAQGEVPVGAVLVRDNTLIGDHFNAVEQDSQPTGHAEQMAIQAGARAQQSWRLQGYTLFVMLEPCPMCWGAIHNARIARVVMGVHNEKGGADGSYYRLADDARFNHQVELHNGVADEAARAQLSDFFKAQRKAKRGKA
jTadA-20	MSHSAQDLQWWQRALELAKRAAAQGEVPVGAVLVRDNTLIGDGFNAVEQDAQPGGHAEQMAIQAGARAQQSWRLQGYTLFVMLEPCPMCLGAIHNARKARVVFGVHNEKGGADGSYYRVADDARFNHQIELHNGVADEAARAQLSDFFKAQRAAKRGKA
jTadA-21	MSHSAQDLQWMQRALELAKRAAAQGEVPVGAVLVRDNTLIGDGFNAVEQDAQPTGHAEQNAIQHGQRAQQSWRLQGYTLFVMLEPCPMCMGAIHNARIARVVFGVHNEKGGADGSYYRLADDARFNHQVELHKGVADEAARAQLSDFFKAQRKAKRGKA
jTadA-22	MSHSAQDLCWMQRALELAKRAAAQGEVPVGAVLVRDNTLIGDGFNAVEQDAQPTGHAEQMAIQAGARAQQSWRLQGYTLFVMLEPCPMCMGAIHNARIARVVFGVHNEKGGADGSYYRLADDARFNHQVELHKGVADEAARAQLSDFFKAQRKAKRGKA
jTadA-23	MSHSAQDLQWMQRALELAKRAAAQGEVPVGAVLVRDNTLIGDSFNAYEQDAQPTGHAEQMAIQAGARAQQSWRLQGYTLFVMLEPCPMCMGAAHNARAARVVFGVHNEKGGADVSYYRLADDAHFNHQVELHSGVADEAARAQLSDFFKAQRAAKRGKA
jTadA-24	MSHSAQDLQWMSRALELAKRAAAQGEVPVGAVLVRDNTLIGDGFNAVEHDSQPTGHAEAMAIQAGARAQQSWRLQGYTLFVTLEPCPMCWGAIHNARIARVVFGVHNEKGGSDGSYLRLADDARFNHQVEWHKGVADEAARAQLSDFFKAQRAAKRGKA
jTadA-25	MSHSAQDLQWMSRALELAKRAAAQGEVPVGAVLVRDNTLIGDGFNAVEQDSQPTGHAEQMACCAGARAQQSWRLQGYTLFVTLEPCPMCWGAIHNARIARNVFGVHNEKGGADGSYYRLADDARFNHKVELHNGVADEAARAALSDFFKAQRKAKRGKA
jTadA-26	MSHSAQDLQWMQRALELAKRAAAQGEVPVGAVLVRDNTLIGDGFNAVEQDAQPSGHAEQMAIQAGARAQQSWRLMGYTLFVTLEPCPMCWGAIHNARIARPVFGVHNEKGGADGSYYRLADDARFNHQVELHNGVADEAARAYLSDFFKAQRAAKRGKA
jTadA-27	MSHSAQDLTWMQRALELAKRAAAQGEVPSGAVLVRDNTLIGDGFNAVEQDAQPTGHAEQMAIQAGKRAQQSWRLQGYTLFVMLEPCPMCMGAIHNARIARNVFGVHNEKGGADGSYYRLADDARFNHQVELHKGVAEEAARAQLSDFFKAQRKAKRGKA

jTadA-28	MSHSAQDLQWMSHALNLAKRAAAQGEVPVGAVLVRDNTLIGDGFNAVEQDAHPTGHAEQMAIQRGDRCQQSWRLQGYTLGVTLEPCPMCWGAVHNARIARVVFGVHNEKGGADGSYYRLADDARFNHQVELHAGVADEAARAQLSDFFKAQRAAKRGKA
jTadA-29	MSHSAQDLQWMSRALELAKRAAAQGEVPVGAVLVRDNTLIGDGFNAVEQDAQMTGHAELMAIQAGARAQQSWRLQGYHLFVTLEPCPMCWGAIHNARIGRVVFGVFNEKGGADGSYYRLADDARFNHQVELHKGVSDEFARAQLSDFFKAQRTAKRGKA
jTadA-30	MSDTALPQHWLQHAIEQAKLAADNWEVPVGCVIVQDGKVLATGFNAVEQLAEPCGHAEMVAKQQACKALNSWRLLDCHWFVSVEPCNMCAGALINSRIAQLHFGVPNDKMWAAGSYIDLAQGEWYNHRVQVHSGVNAEQCAELLKGFFKSQRAAKKAKG
jTadA-31	MSDTALPQHMLQQAIEQAKLAADNWEVPVGCVIVQDGKVLATGFNAVEQLAEPTGHAEMVAIQWACKALESWRLLDCHWFVSIEPCAMCAGALINSRIAQLHFGVWNDKMGAAGSLIDLAQGEWYNHRVQTHSGVQAEQCAELLKGFFKSQRAAKKAKG
jTadA-32	MSDTALPQHWLQQAIEQAKLAADNWEVPVGHVIVQDGKVLATGFNAVEQHAEPTGHAEMVAIQWACKALNSWRLLDCHMFVTLEPCAMCAGALINSRIKQCHFGVRNDKMGAAGSLIPLAQGEWYNHRVQTHSGEQAEQCAELLKGFFKSQRAAKKAKG
jTadA-33	MSDTALPAHWLQQACEQAKLAADNWEVPVGCVIVQDGKTLATGFNAVEQAREPTGHAEMVAIQWATKALESWRLLDCHIFVSIEPCAMCAGALINSRIAQLHFGVPNDKMGAAGSLIDLAQGEWYNHRVQTHSGQQAEQCAELLKGFFKGQRAARKAKG
jTadA-34	MSDTALPAHWLQQAIEQAKLAADNWEVPVGCVIVQDGKVLATGFNAVEQLAEPTGHAEMVAIQWSCKALNSWRLLDCHMFVTVEPCAMCAGALINSRIASLHFGVPNDKMGAAGSLDDLAQGEWNNHRAQTHSGVQAEQCAELLKGFFKSQRAAKKAKG
jTadA-35	MSQTAVPAHWLQQAIELAKLAADNWEVPVGCVIVQDGKVLATGFYAVEQLAEPTSHAEMVAIQWACKALNSWRLLDCHMFVTVEPCAMCAGALINSRIADLHFGVPNDKMGAAGSLIDLLQGEWYNHRVQTHSGVQAEQCAELLKGFFKSQRAAKKAKG
jTadA-36	MSATALPAHWLQQAIEQAKLAYDNWEVPVGCVIVQDGKVLAGGFNAVEQLREPTGHAEMVAIQWACKALNSWRLKECHWFVQVEGCAMCAGALINSRIAQLHFGVQNDKMGAAGSFIDLAQGEWYNHRVQTHSGVQAEQCAELLKGFFKSQRAAKKAKG
jTadA-37	MSDTALPQHWIQQAIEQAKLAADNWEVPVGCVIVQDGKVLATGFNAVEQAREPTGHAEMVADQWACKALNSWRLLDCHWFVSIEPCAMCAGALICSRIAQLHFGVINDKMGAAGSLIDLAQGEWYNHRVQTHSGWQAEQCAELNKGFFKSQRAAKKAKG

jTadA-38	MSDTALPAHWLQQACEQAKLAADNWEVPVGCVIVQDGKVLATGFNAVEQAREPTGHAEMVAIQWACKALESWRLLDCHIFVSIEPCAMCAGALINSRIAQLHFGVPNDKMGAAGSLIDLAQGEWYNHRVQTHSGQQAEQCAELLKGFFKGQRAARKAKG
jTadA-39	MSDTALPQHWLQQAIEQAKLAADNWEVPVGCVIVQDGKVLATGFNAVEQLAEPTGHAEMVAIQWACKALNSWRLLDCHWFVSIEPCAVCAGALINSRIAQLHFGVPNDKMGAAGSLIDLAQGEWYNHRVQTHSGVQEEQCAELLKGFFKSQRAAKKAKG
jTadA-40	MSDTALPAHWLQQACEQAKLAADNWEVPVGCVIVQDGKVLATGFNAVEQAREPTGHAEMVAIQWACKALESWRLLDCHIFVSIEPCAMCAGGLINSRIAQLHFGVPNDKMGAAGSLIDLAQGEWYNHRVQTHSGQQAEQCAELLKGFFKGQRAARKAKG
jTadA-41	MSDTALPQHWLQQAIEQAKLAADNWEVPVGCVIVQDGKVLATGFNAVEQLAEPTGHAEMVAIQWACKALESWRLLDCHWFVSIEPCAMCAGALINSRIAQLHFGVWNDKMGAAGSLIDLAQGEWYNHRVQTHSGVQAEQCAELLKGFFKSQRAAKKDKG
jTadA-42	MSDTQLPQHWLQQAIEQAKLAADNWEVPMGCVIVQDGKQLATGFNAVEQLAEPTGHAEMVAIQWACKALFSWRLLDCHMDVTVEPCAMCAGALINSRIRQDHFGVPNDKMGAAGSLIDLAQGEWYNHRVQTHSGVQAEQCAELLKGFFKSQRAAKKAKG
jTadA-43	MSDTALPAHWLQQAIEQAKLAADNWEVPVGCVIVQDGKVLATGFNAVEQAREPTGHAEMVAIQWACKALESWRLLDCHIFVSIEPCAMCAGALINSRIAQLHFGVPNDKMGAAGSLIDLAQGEWYNHRVQTHSGQQAEQCAELLKGFFKGQRAARKAKG
jTadA-44	MSDTALPAHWLQQAIETAKLAADNWEVPVGCVIVQEGKVLATGFNAVEQLAEPCGHAEMPPIQQACKHLNSWRLLDCHMFVSVEPCAMCAGALINSRIAQLHFGVGNDKMGAAGSLIDLAQGEWYNHRVQTHVGVQAEQCAELLKGFFKSQRAAKKAKG
jTadA-45	MSDTALPQHWLQQAIEQAKLAADNWEVPVGHVIVQDGKVLATGFNAVEQLAEPTGHAEMVAIQWACKALESWRLLDCHWFVSIEPCAMCAGALINSRIAQLHFGVPNDKMGAAGSLIDLCQGEWYNHRVQTHSGWQAEQCAELNKGFFKSQRAAKKAKG
jTadA-46	MSDTALPAHWLQQAIEQAKLAADNWEVPVGCVIVQDGKVLATGFNAVEQAREPTGHAECVAIQWACKALESWRLLDCHIFVSIEPCAMCAGALINSRIAQLHFGVPNDKMGAAGSLIDLAQGEWYNHRVQTHSGQQAEQCAELLKGFFKGQRAARKAKG
jTadA-47	MSDTQLPQHWLQQAIEQAKLAADNWEVPMGCVIVQDGKQLATGFNAVEQLAEPTGHAEMVAIQWACKALNSWRLLDCHMDVTVEPCAMCAGALINSRIRQDHFGVPNDKMGAAGSLIDLAQGEWYNHRVQTHSGVQAEQCAELLKGFFKSQRAAKKAKG

jTadA-48	MSDTALPQHWMQQAIEQAKLAADNWEVPVGCVIVQDGKVLATGFNAVEQLAEPTGHAEMVAIQWACKALESWRLLDCHWFVSIEPCAMCAGALINSRIAQPHFGVGNDKMGAAGSLIDLAQGEWYNHRVQTHSGVQAEQCAELLKGFFKSQRAAKKAKG
jTadA-49	MSTETWDERWMRLALEQARLAMDSWEVPVGAVIVRNNQVVATSFNEREQLRNPTAHAEMLAFERAARELGSWRCTDTTSYVTLEPCIMCAGAAHLARLDRIVFGVMNPKAGGVESWINIADEPRHNHRIEVRRGVLEEEARELLKAFFRQRRAEKARQS
jTadA-50	MATETWDERWMRLALEQARLAMDSWEVPVGAVIVRNNQVVATCFNDREQLDNPTAHAEMLAFERAARELGSWRCVDTTSYVTLEPCIMCAGAAHLARLDRIVFGVPNPKAGGVESWINITDEPRWNHRIEVRRGVLEEEAREPLKAFFRQRRAEKARQS
jTadA-51	MSEYEYMRHALTLAHDARDEFEPPVGAVNVWNNRTHNAGWNRLVGLDDPFTHAEIMALRYSGPVKTGHTLMWATLYMTFEPCVMCAGAMVTSRIGDVVFGVRNAKGSAAQGEMDVLHRPWYGARVIITEGKLDQECARSLCRFFISQRRRSTA
jTadA-52	MYEHEYWMRHALTLAHDAGDEFEVPVGAVQVMNTRTDRSSVFRTKGLDDLTTHAEIMALRQQGQVATGITLIWAHLYATFEPCVMCAGQTIASRLGDVVFGVRNAKGSAAQSEMDVLHRPQMGARVIITEGRLDQECARLLCRFFSRHRRVSKA
jTadA-53	MSEHEWMRHALTLAHDAATEFEIPVGAVNVWNNRTINSGWNDLKGLDDPTYHAEIMADRQSWDVMFGHTLMWATLYMTFEPCVMCAGAMVTSRIGDVVFGVRNAKGSAAQGEMDVLHRPWYGARVIITEGKLDQECARSLCRFFISQRRRSTA
jTadA-54	MGDDEHWLRHALTLAKRAHDEEEVPVGCVLVQNNKVIQEFHNNAFGRMDPTAHAEISILNQAQDQEQNLTLSDATLYTTLEPCVMCAMKMQLSRIDRVVFGVANPYTGAAGSLMDILDHPRQNHTVEIHAGILADECAQELAHYFRSKRPGK
jTadA-55	MADDEEHWLRHALTLAKRAHDEAEVPVGCVLVQNNKVIQEFHNNAFGRMDPTAHAEIDILNQCGDVEQNYQLSDATLYTTLEPCVMCAMAMQLSRIDRVVFGVANPKDGAAGSLMDILKHPVMNHRVEIHAGILADECAQALAMYFISKRPVK
jTadA-56	MADEEHWLSHALTLAKRAHAEAEVPVGCVLVQNNKVIQEFANNAFGRMDPTAHAEIDILNQCCDVEQNTQLSDATLYTTLEPCVMCAMAMQLSRIDRVVFGVANPKTGAAGSLMDILTHPRQNRRVNIHAGILADECAQELAHYFRSKRPGT
jTadA-57	MADDEHEHWLRHALTLAKRAHDEAEVPVGCVLVQNNKVIQEFHNNAFGRMDPTAHAEIDILNQCGDVEQNYQLSDATLYTTLEPCVMCAMAMQLSRIDRVVFGVANPKDGAAGSLMDILKHPVMNHRVEIHAGILADECCQALAHYFQSKRPVK

jTadA-58	MADDEEYHWLRHALTLAKRAHDEAEVPVGCVLVQNNKVIQEFHNNAFGRMDPTAHAEIDILNQCRDVEQNYQLSDATLYTTLEPCVMCAMAMQLSRIDRVVFGVANPKTGAAGSLMDILKHPRQNHRVEIHAGILRDECAQVLAHYFDSKRPGK
jTadA-59	MADDEHWLRHALTLAKRAHDIAEVPTGCVLVQNNKVIQEFHNNAFGRMDPTAHAEIDILNQCRDVEQNYQLSDATLYTTLEPCVMCAMAMQLSRIDRVVFGVANPKTGAAGSLMDILKHPRQNHRVEIHAGILADECAQVLAHYFDSKRTGKN
jTadA-60	MYEVEYWMRHALTLAHDAGDEFEGPVGAVQVMNTRTDRSSVFRTKGLDDLTTHAEIMALRQQGQVATGITLIWAHLYATFEPCVMCAGQTIASRLGDVVFGVRNAKGSAAQSEMDVLHRPQMGARVIITEGRLDQECARLLCRFFSRHRRVSKA
jTadA-2-1	MGKRMQNECKFMQKAIDEARKAFALKEVPIGAIICKGDEVIASANNELINGMLPSKHAEFIAIEMAAQRLDSWRLEGFDIYVSMEPCMMCADALLHSRIARVVFGVDNIKCGSMGMAQEIFKAPQNNKVVSVEKGVLGDECVNLLKDYFAHVRAKGGVKK
jTadA-2-2	MGKRMQNECKFMQKAIDEARKAFALKEVPIGAIICKGDEVIASANNELINNMLPSKHAEFIAIEMAAQRLDSWRLEGFDIYVSMEPCMMCADALLHSRIARVVYGVDNIKCGSMGMAQEIFKAPQNNKVVSVEKGVLGDECVNLLKDYFAHVRAKGGVKK
jTadA-2-3	MRYDMATDKKFMERAIAEAKKAYAGGEFPSGAIIVKNGEVIGTANNSYFTGMKPEMHCEKINIEDAANALHSYRLEGCTVYCTMEPCLMCAGTIVMSRIWRIVYGADDWKGGGAKVAATLIPQEGVNSRVIVEKGIFKDECDRLFMDFFSAGRDKWKHHY
jTadA-2-4	MRYDMATDKKFMERAIAEAKKAMAGGEFPSGAILVKNGEVIGAAYNSYRAGNKPEKHAEQICIEEACSMLHSYHLEGCTVYCTMEPCLMCAGTIVMSRIPHIVFGADDWRGGNHKVAANLIPQEGVNHRFMIEKGYYKDECDRLNADFFSNGRRKNKHEY
jTadA-2-5	MRYDMATDKKFMERAIAEAKKAFAMGEFPSGAILVKNGEVIGAAVNSYRAGNKPEKHAEQICIEEAANALHSYHLEGCTVYCTMEPCAMCAGTIVMSRIWHIVFGVDNWKGGGAKVAANLIPQEGVNHRVMVEKGAYKDECDRLNADFFSNGRRKWMHHS
jTadA-2-6	MGEEELRDRNYMRLAIEMAKKARELGEVPTGAIITLGDKVIAKSYNMYVGYHAPTAHAEVRTPLEASEVLKSWNLEGCVMYCTLEPCVMCAGAICHSRIKRVVFGVDNFKGGSAGSGMQILQCQNKNHDIIVDKGVMVDECKALLAGFFAGRRANKDYRY
jTadA-2-7	MGEQELRDRYYMRLAIEEAKKARELGEVPTGAIITLGDKVIAKSMNEYVGGCAPTAHAEVRAPLEASEVLKSWNLEGCVIYWTLEPCVMCAGAVQHSRIKRVIFGYDDFKGMAIGSGMKILSKGNHNHDIIVDKGVMVDECKALLAGFFAGRRANKTDRY

jTadA-2-8	MGEEELRDRNYMRLAIEMAKKARELGEVPTGAIITLGDKVIAKSYNEYVGYHAPTAHAEVRTPLEASEVLKSWNLEGCVMYCTLEPCVMCAGAICHSRIKRVVFGVDNFKGGSAGSGMQILQCQNKNHDIIVDKGVMVDECKALLAGFFAGRRANKTDRY
jTadA-2-9	MGYDMAKECEFMEFGIKEAASAMQNNDVPTGGVIFRGNKVIAMGHNAYEEDGIPSMHAEANIIKECTNALGNYDLEGCINVITLEPCPMCAGTIVHSRIAKVIYGCDDVKYGWAGVASELYRIKGNNSKVIVEKGIARDACERLLTGFFKKRRADKNGRY
jTadA-2-10	MGKAMAEDKYFMQLALENAKKAMINGDVPIGAIIVKNGEVIAVDGNAYATGMAPMGHAEFIAIKKAQNELKSWRLEGCTLYVSLEPCVMCAGATVQSRIERVVFGVDNAKGGALGCAMKIYEYAGANRKVMVEKGFLKDECDALLHAAFVSRRRYFKRNE
jTadA-2-11	RIPQGSDEYWMKKALELAKQARAAGERPYGAVLIKKGEEVGRGYNTRITERDPTAHAEIKALREAGRRLDDWLLDGATLKVTEQPCVMCAGALIHARVKRVVYGAPNIEFGAAVSYMDVLNHPGLGHRVEVVKGVYAAECAALIDDYKAVKEALKAADK
jTadA-2-12	EIDPGSDEYWMKQAIELAKIALQRGELPIGFVVVKNGEVVGKGFNERMTLNDPTAHAERLCLREAGERLGNPVLEDCTDYITPEPCVMCAGALINAKVARVVYGLRNEDFGASGSLMRVLDFPGNSHRVEVVRGVLAEECKALLEEYKAGHRKKKERLA
jTadA-2-13	VIDENSDEYWMRKALELAREAYKAGEYPVGAVFVKNNEIIGTGYNARIRHNDAPAHAEISAIREAAKKMENPFLEGATLYITLEPCVMCAGAMINKKIAKVVYGAPNVKHGACGSFMDVLNHPKNPWKTEVVKGVLADECAALLRTEFFKYKQMKGRN
jTadA-2-14	SYDDNSAEYWMLKALELAKIAYKLGEYPVGAVLVKDGQVIFEGYNAEVTLNDPTAHCEIIALREAGKKMKNFCLEGATLYITLEPCVMCACAMIAAKIAYVVYGADNISSGAAGNYMTVLDHPGNHHRVAVRRGVLAEEAAELLRKYKEDKAKAKKGSA
jTadA-2-15	ACDEGSDERWMQKAIELAKISLKKGEYPIGAVLVENGKVIGEGYPNRKVSNDPTAHDEIIALRKIGKSKGNYRLKGCTLYITEEPCVMCSGAMIAAKVDRVIYGADDPLHGALGTAMDVLHHPGNDNRVAVRRGVCADECRALREKYFRLIREEKKLVS
jTadA-2-16	RKDIDLDAAFLRRAKELAEKAYEAGEVPVGAVVVKDGVIVAEGYNQVVATRDTTAHNEVEAIREAAKHLGSHRIEGTVLYVTLEPCAMCCGWFVQARVARLIFGAPDPRAGAVGNVVNLCEDDSLNHQADVVGGVLENEASELLKKFFAKRRKKKAAEE
jTadA-2-17	EFPKNSDAYWMQRALDLAKQALAAGEYPVGRVLVKGNEVVGTMFNMRITEKDPTGHAEIKALREGGKTLKSPYLEDCVLYITREPCVMCAGALNNAKIASVVYGAVNNASGAAGSTMDVLNTPGNPFTVAVKRGVLADEAAALEAAYFAKKSKKKELFK

jTadA-2-18	REDIDLDEAYMERAISIAEQAYEAEEVPIGAIVVKDDMIVAEGYNQYIETNDPTAMAEDLADTEAAAKLDNHRLEGTVLFVTLEPCIMCAGAKLQARVKKIVYGAPDPKAGATGTVVNLLQDDRLNHKAENAGGVLKEDASELLKKFFCKRRKKKERFK
jTadA-2-19	EISKNSDEYWMSVAIEEAKKALADGEGPRGAVLIKDNKIIGRGYNARRKENDPTAHAEIIAYREDGKNLKNFELKDCTLYITQEPCVMCACAMINAKIAKVVYGAPNPNHGAVGSFMDVLNRPGNNHKVEVVRGVLAEECQALLDEYFVRKYAKYLRAR
jTadA-2-20	KNPADSDEYWMKKALEMARKALAAGEYPIGAVLVLDNEVIGEGYYSPTTKNDPYAHAEIENLRAAGQKRNDWRLEGATLYVTCEPCFMCAGAMNAAKIGRVVYGAENPRRGATGDYMDVLCHPGNPHRVEGVRGVLAEESKALLDYYFTKESQDKARQR
jTadA-2-21	MRDTDLDKEFMERAIAQAEKAYEAGEVPVGAIVVHDNEILAEGYNQFISTNDPTAHGQVEAMRMAAQALGNYRIENCVLYVTLEPCSMCTGAIVQARVARLIYGAPDPRAGAVGTVVNLVNDDSLNHHADVYCGVLEERASDLLKKFFKKLRKKKEGAH
jTadA-2-22	LKYEGSDAYYMKMALELANEALKAREYPVGAILCKDNELVGRGYNNTIVSMDATAHAEINALREGGKILKSWMLKNCTLYITCEPCVMCAGALIIWKIGKVVYGAPNPSWGAAGSLMDVLHMPGNDIQVEVVSGPYAEQCKALKDEFLAKRRKKKRELK
jTadA-2-23	MKDADLDAAFMERAIELAEKAYQAGEVPTGAVVVKDDKIVAEGYNQPVATNEPTAHEEIIAIREAAMALNNHRIEGTVLYVTLEPCIMCAGAITQARVKRLVYGAPDPRAGVVGTVVNLLNDPSLNHKATVIGGVLEERAREMLKAFFQTLRKKKAASK
jTadA-2-24	ATPEESDAYWMQLAFEEAEKARAGGEYPVFAVLVKDGEVVGTGWNNRVTRNDPTAHAEIVALREGGKSLKRWELNGCTLFITEEPCVMCAGALINAKVAKVVYGAPNPATGALGVYMDVLQHPGNPHRVEVVGGVLAEACAALKNAYKEAKAGAKYEAL
jTadA-2-25	MEDIALDEKFLFRAVEQARKAYEAGEVPIGRLIVHDGKELAEGYNQTVHTRDPTAFAEVEAPREAAAHLENFRLEGTVLYVTLEPCIMCTGALVQARVKKVIYGCPDPRAGAVGTVQNLVDDPRLNHQAQVIGGVLAEEASELLKKFFKKRRKKKAASE
jTadA-2-26	KIPDGSDEAWMDQALELAAVALQNGEHPVGAVLVKDNKVIGKGYNAKKILNDATAHAEIIALREAGKNMKSYWLEDATLYITEEQCVMCAGACINAKVKKVVYGAPNPKQGACGEFMDVLSHPGNMHKIETVKGVLAEKAAKLLEEYFKKKRKAKRAIA
jTadA-2-27	DIPEGSDEYWMCRALALAQKAYEAGELPIGAVLVKNGEVIGEGFNAITTLNDPTAHAEIMAIRKGGKTCKNPMLQGSTLYITREPCVMCAGAMIAAQIARVVYGAPDPASGAAGSAMDVYMAPGNKHKVEVVKGVLAEESAALIARYLKEKRNAKRRKA

jTadA-2-28	REDCDLDRAFLERAIAQARQAYEAGEVPIGALVVHDGEILATGYNQTVEINDPTWHAEVLAHRENARVLGNHRLEGTVLYVTLEPCIMCAGAIVQCRVARLIYGMPDPRAGAVGTVVKLVEDESLNHKAEVVGMVLEEEAMDLLKKFFQQRRKKKAASE
jTadA-2-29	MNDAELDDRFLARAIEHAEKAYIAWEVPVGAVVVKDGEKYAEGYNQTVATRDPTAHAEVLQIREAAAALGSHRLEGCVLYVTLEPCAMNTGALVQARIERLIYGAPDPKAGASGTVVKLVADERLNHKADVIGGVRAEEASELLKKFFKCLRKKKAASE
jTadA-2-30	MEDKKKDEEFMERAIEQAEKAYAAGEVPVGAIVVKDGKIVAEGYNKLIETRDPTAHAYVEAIREAAAALGNHRLEGTVLYTTLEPCIMCSGALMQQRVARLVFGARDPRAGAVGTAVNLVEDDRLNHKTDVVEGVLEEEASDLLKAFFKKRRIKKYASE
jTadA-2-31	PIPMNSDEYWMKKALEYAKKAYEEGERPIGAVLVKNGEIIGVGYNARVTENFPTAHAEIKAIREAGKRLGNFVLEGATLYITQEPCVMCAGAMIAAKVKRVCFGARNPRYGAAGSYMDVLMHPGNPWRVEIVDGVLADECKALLRNYFKEKRKGKPALK
jTadA-2-32	QGDYDLDDKFMERAIEQAEKAYEAKEVPIGAIVVKDGENLAYGYNQTVETRDCTAHAEMLAIREAAAKLGNHRLEGTVLYVTLEPCIMCTGAIVQARVARVVYGCPDTKAGAVGTVVNLVDNPSLNHQATVVGGVLEERASKLLKAFFAGRRKKYAASE
jTadA-2-33	EIDEGSDAYYMQKAIELAMKAKAAGEYPVGLVLVKNKEIIGEGYNAVSVLNDPTAHGEIVALRAAGKATYNPKLEGATLYITEEPCVMCAMAMINAKVARVVYGAPNADSGAAGGAMQVLHHPRNPHKVEVVKGVLADQCKHLRDEYFAKLEKKAEQVL
jTadA-2-34	RIDIGSDEYWMSKAIELAREAYRAKEIPVGAVLVKDGEVIGRGYNNFFTENDPTKHAEINALREAMKTSKNPFLENATLYITQEPCVMCAGALVAAKVKRVVFGATQPQTGATGSFMDVLHNPGNTHRVEVYRGVLADECAALMEIYFVGRKQDCLARK
jTadA-2-35	FNDIALDDDFMEKAISQAEKAYEAGEVPVGRVVVKDGEIVAEAYNQTIMTNDATAHAEIGAIRNAAAKLGNYRIEGCVLYVTLEPCIMCAGAIVQARVARLVFGAADPKAGAVGTVVNLFNDPKLNHQAKVIGGCREAEASEILKKFFKKLRKKKGAEQ
jTadA-2-36	LKDEDLDEEFMKRAIEFAEKAYEAGEVPIGAIVVKDGRVVATGYNQIAEYKDHTAHAEVEADREAAAALENHRLEGCVLYVTLEPCYMCAGAIVQARVARVVYGAADPRAGAVGTVVNLTNDESLNHQADVVGGVLEERASDLLKKFFKRLRKKKAESY
jTadA-2-37	KNDFDADDDFMRRAIAMAEKAYEAGEVPIGAVVVKDGMIVASGYNQTIEHNDATYHAENEAIREAAAALGNHRLPGYMLYVTLEPCIMCAGALVQARVKHVVYGAADPRAGAVGTVLDLVEDLRLNNKVDVVGGVLEEDASNLLKKFFKKRRKLSEDAA

jTadA-2-38	REYADTDEEFMEKAIELAEKAMEADEIPIGAIVVKDGTIVAEGYNQTIATRDPTAHAEVEAIRAAAAHLGRHRIEGTVIYVTLEPCIMCAGALCQARVKRLIFGAPDPRAGAAGTGVNLMEDPSLNRQAFVVGGVLEEEPRELLMKFFKKLRKKKAAAE
jTadA-2-39	LEDYDLDMDFMKRAIEIAEKAKEAGEVPIGEIVVKDGRIVATGYNQRIENNDCTAHAEVLAIREAAAHLGNHKLEGTVIYVTLEPCIMCSGACVQARVARVIYGAPDPRAGAAGTVVNLVNDDRLNTQAEVVGGVLEEQAKELLKAFFKSKRKKKPAEE
jTadA-2-40	REDIKEDQTFMRRAICQPEKAYEAGEVPIGAIVCRDGEIVAEGYNQTIETNDAWAHAEVLADREAALALGNHRLEETVLYTTLEPCIMCTGAIVQARVKRIVYGAYDPRAGAVGTVVNLTEDESLNHMADVVGGVYEEEISELLKKFFKTKRKKKAVSW
jTadA-2-41	GQAERDDLRYARMAYEEARKAYAMKEMPIGAIVVKDGAVIGAAHNDSFMQCTPHMHAELNVISQASAMLQDWRLEGCTLYVVAEPCAMCAGVIHMSRIPRVIYGIDDGKYGAVGSCYSLLQQNGVNHRVDVLKGVMRDAAMDNMRYYFAVRRAQNKAYI
jTadA-2-42	GQDMLDDLKYMKLAIEEAKFAAQNGEFPIGAIIVKDGKVIARAHNKNFNGSPNAHQEIECIEEAAKVLMSWDLNGVTNYVTTEPCLMCAGCIVHNRIKRVVYGCDDVKHGCMGSGMALYQCANVNHDVIVDKGYAKEACMALLAEAFAKRRAMKKRVF
jTadA-2-43	GFDMANEKRFMELAIEEAKKAMQNGELPIGAIITCNGKVIARNNNARIGDGQMFKHAEYELIEMAAKELGSWRLEGTTLYVTNEPCMMCAGTIYMSRIERVIYGCDDFKGGCSGKAFNILQAPNANHRAQVCKGVLKEECEHLLRDYFKARRKNVKSVH
jTadA-2-44	GFDMANDEKFMTAAIEEAKRAMQNGEVPAGAIIVKNNEIIIRCDNAFYTSGDMTGHCEHIAPLRAKEAKNDWKLYDCTLYVTVEPCVMCAAFICNSRIPRNVFGMDTPVKGAAGSCYNILNIHDNNHRVDVVKGYTKDECEHLLSAYFKGIRNGKYLKF
jTadA-2-45	GDRMKDDKRFMTLAYELAKKAFSEGEMPMGAIVVKNGCVIGEGLNGFMFNSDPSQHAEHNAPERASAVLGSWKLDGCDIYVTAEPCALCMGTIAMSRISRVVYGIDNETNGGAGSIIALAQLRDLNHRVQVDCGMLRADAYALMADYFKRRRKRFKGAI
jTadA-2-46	AEDDIRDARFMQMAYEEAMKAWEGGDNPAGAIIVKDDKVIARTFNYKELANNPIKHGEHIAVEMAAKELGNFYLDGCTLYVTLEPCVGCAGTIINSRIKRIYYGFDDDKGGCAGSVYNVLKDKNANHEVIVKKGMLSEACRALCENFFKRKRAMKKYNV
jTadA-2-47	GYDIRNEAEFMEKAIAQAEKAYEAGEVWIGAIVVKNDEIVATGYNQTVATNDPTAHAEVNAIREAAAALKNYRLEGTVLFVTLEPCIMCAGAIVQARVARVIFGAPEPRAGAVGSVVNLVNDPQLNHIADVIGGVLEEECIDLLKKFFKGRRKKKAGAE

jTadA-2-48	GEEELRDRNYMRLAIEMAKKARELGEVPTGAIITLGDKVIAKSYNEYVGYHAPTAHAEVRTPLEASEVLKSWNLEGCVMYCTLEPCVNCAGAICHSRIKRVVYGYDCFKGGSAGSGMQILQCQNKNHDIIVDKGVMVDECKALLAGFFAGRRANKTDRY
jTadA-2-49	GYDMENDERYLNLAIENAEKAFRNRDFPMGAIVVKDGAVIASAENYYECTHKPNVPAEYECIERAGEALNSWRLEGCVLYVTLEPCVMCAGTIVMSRIPRVIYGIDDDKMGCVSSAVNILQSKDNNHKIFIDRGVLKGRCEELLRSFFRNVRGQKYNHR
jTadA-2-50	GFDMADDRKYMERAIEIAKKAAQNGEVPIGRIIVKDGAVIAEAFNNNEMTSSPCAHAECEQIELAAKVLGKWTLEGCTMYVTLEPCVMCAGTIHMRRIQRIVYGVDDMKGGCAGSVMNLFKNKGINREAIVEKCVLKHACETLLRDFFKAKRKEYKYIR
jTadA-2-51	GYDMAEDERFAHDAIEEAKKAFAQGEVPIGAIICRDGKVIIRAFNNAETDAKPTAHPEYLMIERAKEELHSWRLEGCTLYVTIEPCVQCAGIIIMSRIERIVFGCDDDKYGCIGSIVKLLAQKHMNHRVKVDKGVLKDECMTLLKDFFVRLRSGKIYIR
jTadA-2-52	GEAMKDDKRFMMLALEEAEKARQNGDFPVGAIICKDGAVLVKANNAQYENAKPTKHAECEIQDEAANVLGMYALEGCTLYVTHEPCPMCAGIFHWSRIGKVIYGMDDIKNGCVGCVVNLLNDAKANHRVDVYKDVLKEANMALLSAYFAAKRAGKKKTF
jTadA-2-53	GDDMLADKRYMELAIEESKRAFAKGEVPTGAVIVKGKEVIARAENLCYEDGIPAKHAENIELETASKALNEFHLEGTTIYVTLEPCVQCAGAISMSRIDRIVYGLDDEKGGAYGQTMNLLKANRCNRREVIHGYLCDAGKDLIKAYFAMRRRNYKHHY
jTadA-2-54	GFDMANDEQFMKLAIENAKRGKARPEVPIGAIIVKNNELIMSADNYCEGNTDPTRPAEHIAIEEAAKRLNNWRLEGCTNYVTQEPCVMCAGTIVMSRIERIIYGADNIKMGAIGSVMALLQAKNANHRVQVIKGVLKEACEHLLADYFRGLRKNKDRNR
jTadA-2-55	VYDMANDERFCRKAIEEAEKAFALGETPQGAIIVKWNELICGAYNGNCDNGCPTAHADMRHIELAKKALGCYALEGCTLFVTTEPCVMCAGTIMQSKIGRVVYGCDDVKVGAVGKCVNLLQFANVNNRIEVKKGYAQDKCRDLCRKYFANIRKDKYGHK
jTadA-2-56	GEFKESDAYWMARALEMARRAFACGEYPIGAVLVKDGEVVGEGYNCRISSHDPTAHAEQIDLREAGARLRSPELTGAVLYVTKEPCVMCAGALIAARVARVVYGAPDPLYGAVGSAMDVLHHPGNPHRVNVVKGVLADESIALLKAYAKYERRRLLGLE
jTadA-2-57	RNDLDLDRTFLERAREQAEQAYELGEVPIGAIVVRDGEIVATGYNQVVTTNDPTAHAIVEAIREAARRLGKHRLEGTVLYVTLEPCIMCAGALVQARVKRVVFGAPDPRAGAWGTVVNLLNDESLNHQADVVKGVLEEEAFALLKKFFAVRRKQEAASE

jTadA-2-58	MYDIDNDACFMERAIEQAEKAYRAGENPIGAIMVKGDEIVGTGYNQTMATNDPTVHAEVEAIREAAAALGNHRLEGTVLFVTLEPCIMCAGAIVQARVARVIFGLPEPRAGAYGSVYNLVNQPQLNHMADVIGGVLEERASDLLKKFFANIRKDKYGHK
jTadA-2-59	REDTDLDMEFMERAIALSEKAYEAREVPVGAIVVHDNEILAEGYNNTIYTNDPTAHREVEAIREAAQALGNHRIENCVLYVTLEPCIMCTGAIVQARVRRLIYGAPDPRAGAVGTVVNLVRDDSLNHIADVYRGVLEEDASDLLKKFFKQLRKKKEGAE
jTadA-2-60	NYPKDSDEYWMSKAIELALKALAANEYPVGAVNAKDNQVVGEGYNARTGLNDATEHAEIRCLRQAGKTLNNMFLEDTTLYITEEPCVMCAGAMIEWKIKRVVYGADNPLRGAAGSFMDVLNHPGNPHKVEVKRGVLAEKCRGLIEEYFARERKKRLAEK

Supplementary Table 4. First-round TadA variants: mean colony counts, activity, and enzyme-catalyzed base-substitution rates (μ)

Index	Mean colony count (10 mL)	Activity (resistant plate colonies / colony count)	Enzyme-catalyzed base-substitution rate, $\mu_{s.p.b.}$
ecTadA	4.00E+09	6.39E-08	1.42E-8
jTadA-1	2.40E+10	3.70E-09	8.222E-10
jTadA-2	1.15E+11	4.83E-10	1.073E-10
jTadA-5	1.35E+10	3.29E-09	7.311E-10
jTadA-6	1.00E+12	4.11E-10	9.133E-11
jTadA-7	1.30E+10	3.42E-09	7.600E-10
jTadA-10	6.00E+09	1.11E-08	2.467E-09
jTadA-15	7.50E+09	1.93E-08	4.289E-09
jTadA-16	1.20E+10	4.63E-09	1.029E-09
jTadA-17	2.05E+10	2.17E-09	4.822E-10
jTadA-18	4.50E+11	5.68E-10	1.262E-10
jTadA-21	1.65E+10	2.69E-09	5.978E-10
jTadA-22	2.50E+11	1.33E-10	2.956E-11
jTadA-23	7.00E+09	4.13E-08	9.178E-09
jTadA-25	1.05E+10	3.17E-09	7.044E-10
jTadA-27	1.20E+10	1.02E-08	2.267E-09
jTadA-43	1.00E+11	7.78E-10	1.729E-10
jTadA-44	2.50E+11	2.67E-10	5.933E-11
jTadA-45	2.00E+11	9.44E-10	2.098E-10
jTadA-49	1.30E+10	2.56E-09	5.689E-10
jTadA-55	1.75E+9	3.95E-07	8.778E-08
jTadA-56	1.4E+9	1.14E-07	2.533E-08
jTadA-59	1.3E+9	1.58E-08	3.511E-09
jTadA-60	3.25 E+9	5.13E-08	1.140E-08

Supplementary Table 5: Second-round TadA variants: mean colony counts, activity, and enzyme-catalyzed base-substitution rates (μ)

Index	Mean colony count (10 mL)	Activity (resistant plate colonies / colony count)	Enzyme-catalyzed base-substitution rate, μs.p.b.
ecTadA	4.00E+09	6.39E-08	1.420E-08
jTadA-2-02	8.00E+08	2.36E-07	5.247E-08
jTadA-2-04	2.50E+09	3.11E-08	6.914E-09
jTadA-2-05	2.00E+09	7.22E-08	1.605E-08
jTadA-2-09	1.50E+09	1.26E-07	2.798E-08
jTadA-2-11	2.00E+09	2.81E-07	6.173E-08
jTadA-2-12	3.50E+09	4.23E-08	9.407E-09
jTadA-2-14	8.00E+08	5.83E-07	1.296E-07
jTadA-2-15	2.00E+09	1.61E-07	3.580E-08
jTadA-2-17	3.50E+09	6.19E-08	1.375E-08
jTadA-2-18	3.50E+08	3.17E-07	7.055E-08
jTadA-2-19	8.50E+08	1.96E-07	4.347E-08
jTadA-2-22	3.00E+09	1.11E-07	2.469E-08
jTadA-2-23	4.00E+09	5.00E-08	1.111E-08
jTadA-2-26	1.50E+09	6.91E-08	1.535E-08
jTadA-2-27	6.00E+08	2.96E-07	6.584E-08
jTadA-2-28	1.50E+09	3.70E-08	8.230E-09
jTadA-2-29	2.50E+09	2.96E-08	6.584E-09
jTadA-2-32	2.50E+09	3.70E-08	8.230E-09
jTadA-2-35	8.00E+08	5.42E-07	1.204E-07
jTadA-2-36	1.45E+09	1.15E-07	2.556E-08
jTadA-2-37	8.50E+08	1.70E-07	3.769E-08
jTadA-2-39	4.50E+08	2.22E-07	4.938E-08
jTadA-2-43	4.50E+08	6.17E-08	1.371E-08
jTadA-2-48	1.50E+09	4.94E-08	1.097E-08
jTadA-2-50	7.50E+08	1.48E-07	3.292E-08
jTadA-2-51	8.50E+08	2.72E-07	6.035E-08

jTadA-2-52	4.50E+08	1.98E-07	4.389E-08
jTadA-2-55	4.00E+08	5.56E-08	1.235E-08
jTadA-2-56	8.00E+08	6.48E-08	1.440E-08
jTadA-2-57	1.00E+09	5.19E-08	1.152E-08
jTadA-2-60	3.00E+09	1.85E-07	4.115E-08

Supplementary Table 6. The sequence of pUC57-Kan-ccdA/B, pUC57-Kan-2BspQI-ccdB and primers

pUC57-Kan-ccdA/B	TGCAGCTCTGGCCCGTGTCTCAAAATCTCTGATGTTACATTGCACAAGATAAAAATATATCATCATGAACAATAAAACTGTCTGCTTACATAAACAGTAATACAAGGGGTGTTATGAGCCATATTCAACGGGAAACGTCGAGGCCGCGATTAAATTCCAACATGGATGCTGATTTATATGGGTATAAATGGGCTCGCGATAATGTCGGGCAATCAGGTGCGACAATCTATCGCTTGTATGGGAAGCCCGATGCGCCAGAGTTGTTTCTGAAACATGGCAAAGGTAGCGTTGCCAATGATGTTACAGATGAGATGGTCAGACTAAACTGGCTGACGGAATTTATGCCTCTTCCGACCATCAAGCATTTTATCCGTACTCCTGATGATGCATGGTTACTCACCACTGCGATCCCCGGAAAAACAGCATTCCAGGTATTAGAAGAATATCCTGATTCAGGTGAAAATATTGTTGATGCGCTGGCAGTGTTCCTGCGCCGGTTGCATTCGATTCCTGTTTGTAATTGTCCTTTTAACAGCGATCGCGTATTTCGTCTCGCTCAGGCGCAATCACGAATGAATAACGGTTTGGTTGATGCGAGTGATTTTGATGACGAGCGTAATGGCTGGCCTGTTGAACAAGTCTGGAAAGAAATGCATAAACTTTTGCCATTCTCACCGGATTCAGTCGTCACTCATGGTGATTTCTCACTTGATAACCTTATTTTTGACGAGGGGAAATTAATAGGTTGTATTGATGTTGGACGAGTCGGAATCGCAGACCGATACCAGGATCTTGCCATCCTATGGAACTGCCTCGGTGAGTTTTCTCCTTCATTACAGAAACGGCTTTTTCAAAAATATGGTATTGATAATCCTGATATGAATAAATTGCAGTTTCATTTGATGCTCGATGAGTTTTTCTAATCAGAATTGGTTAATTGGTTGTAACATTATTCAGATTGGGCTTGATTTAAAACTTCATTTTTAATTTAAAAGGATCTAGGTGAAGATCCTTTTTGATAATCTCATGACCAAAATCCCTTAACGTGAGTTTTCGTTCCACTGAGCGTCAGACCCCGTAGAAAAGATCAAAGGATCTTCTTGAGATCCTTTTTTTCTGCGCGTAATCTGCTGCTTGCAAACAAAAAAACCACCGCTACCAGCGGTGGTTTGTTTGCCGGATCAAGAGCTACCAACTCTTTTTCCGAAGGTAACTGGCTTCAGCAGAGCGCAGATACCAAATACTGTTCTTCTAGTGTAGCCGTAGTTAGGCCACCACTTCAAGAACTCTGTAGCACCGCCTACATACCTCGCTCTGCTAATCCTGTTACCAGTGGCTGCTGCCAGTGGCGATAAGTCGTGTCTTACCGGGTTGGACTCAAGACGATAGTTACCGGATAAGGCGCAGCGGTCGGGCTGAACGGGGGGTTCGTGCACACAGCCCAGCTTGGAGCGAACGACCTACACCGAACTGAGATACCTACAGCGTGAGCTATGAGAAAGCGCCACGCTTCCCGAAGGGAGAAAGGCGGACAGGTATCCGGTAAGCGGCAGGGTCGGAACAGGAGAGCGCACGAGGGAGCTTCCAGGGGGAAACGCCTGGTATCTTTATAGTCCTGTCGGGTTTCGCCACCTCTGACTTGAGCGTCGATTTTTGTGATGCTCGTCAGGGGGGCGGAGCCTATGGAAAAACGCCAGCAACGCGGCCTTTTTACGGTTCCTGGCCTTTTGCTGGCCTTTTGCTCACATGTttgacagctagctcagtcctaggtataatgctagctactagagaaagaggagaaatactagATGCGTCGTCTGCGCGCAGAACGTTGGAAAGCAGAAAATCAGGAAGGCATGGCAGAAGTGGCCCGTTTTATTGAAATGAATGGCAGCTTTGCCGATGAAAATCGTGATTGGtaaAAGCTTgcacaggtcGTCGACTTAAATGCCCCAAAACATCAGGTTAATGGCATTCTTAATATCATTTTCACGATGACTCAGATCTGCCAC

	TTCTTCACCAATAACACTAACCGGCACACTTGCCATATCGGTGGTCATCATACGCCAACTTTCATCGCCAATATGCACAACCGGATACAGTTCACGACTCACTTTATCACTCAGCAGGCGGGCGCTGGCCAGCGGAATAACCATACGGCGACCCGGGGTATCAATAATATCGCTCTGCACATCCACAAACAGACGATAACGGCTTTCACGCTTATAGGTGTAAACCTTAAACTGCATactcttcctttttcaatattattgaagcatttatcagggttattgtctcatgagcggatacatatttgaatgtatttagaaaaataaacaaaCATATGGTGCACTCTCAGTACAATCTGCTCTGATGCCGCATAGTTAAGCCAGCCCCGACACCCGCCAACACCCGCTGACGCGCCCTGACGGGCTTGTCTGCTCCCGGCATCCGCTTACAGACAAGCTGTGACCGTCTCCGGGAGCTGCATGTGTCAGAGGTTTTCACCGTCATCACCGAAACGCGCGA

For pUC57-Kan-ccdA/B, the J23119 promoter, ccdA$^{36-72}$, ccdB and AmpR promoter sequence are highlighted in red, green, blue, and purple, respectively. The plasmid backbone is pUC57-Kan.

pUC57-Kan-2BspQI-ccdB	TGCAGCTCTGGCCCGTGTCTCAAAATCTCTGATGTTACATTGCACAAGATAAAAATATATCATCATGAACAATAAAACTGTCTGCTTACATAAACAGTAATACAAGGGGTGTTATGAGCCATATTCAACGGGAAACGTCGAGGCCGCGATTAAATTCCAACATGGATGCTGATTTATATGGGTATAAATGGGCTCGCGATAATGTCGGGCAATCAGGTGCGACAATCTATCGCTTGTATGGGAAGCCCGATGCGCCAGAGTTGTTTCTGAAACATGGCAAAGGTAGCGTTGCCAATGATGTTACAGATGAGATGGTCAGACTAAACTGGCTGACGGAATTTATGCCTCTTCCGACCATCAAGCATTTTATCCGTACTCCTGATGATGCATGGTTACTCACCACTGCGATCCCCGGAAAAACAGCATTCCAGGTATTAGAAGAATATCCTGATTCAGGTGAAAATATTGTTGATGCGCTGGCAGTGTTCCTGCGCCGGTTGCATTCGATTCCTGTTTGTAATTGTCCTTTTAACAGCGATCGCGTATTTCGTCTCGCTCAGGCGCAATCACGAATGAATAACGGTTTGGTTGATGCGAGTGATTTTGATGACGAGCGTAATGGCTGGCCTGTTGAACAAGTCTGGAAAGAAATGCATAAACTTTTGCCATTCTCACCGGATTCAGTCGTCACTCATGGTGATTTCTCACTTGATAACCTTATTTTTGACGAGGGGAAATTAATAGGTTGTATTGATGTTGGACGAGTCGGAATCGCAGACCGATACCAGGATCTTGCCATCCTATGGAACTGCCTCGGTGAGTTTTCTCCTTCATTACAGAAACGGCTTTTTCAAAAATATGGTATTGATAATCCTGATATGAATAAATTGCAGTTTCATTTGATGCTCGATGAGTTTTTCTAATCAGAATTGGTTAATTGGTTGTAACATTATTCAGATTGGGCTTGATTTAAAACTTCATTTTTAATTTAAAAGGATCTAGGTGAAGATCCTTTTTGATAATCTCATGACCAAAATCCCTTAACGTGAGTTTTCGTTCCACTGAGCGTCAGACCCCGTAGAAAAGATCAAAGGATCTTCTTGAGATCCTTTTTTTCTGCGCGTAATCTGCTGCTTGCAAACAAAAAAACCACCGCTACCAGCGGTGGTTTGTTTGCCGGATCAAGAGCTACCAACTCTTTTTCCGAAGGTAACTGGCTTCAGCAGAGCGCAGATACCAAATACTGTTCTTCTAGTGTAGCCGTAGTTAGGCCACCACTTCAAGAACTCTGTAGCACCGCCTACATACCTCGCTCTGCTAATCCTGTTACCAGTGGCTGCTGCCAGTGGCGATAAGTCGTGTCTTACCGGGTTGGACTCAAGACGATAGTTACCGGATAAGGCGCAGCGGTCGGGCTGAACGGGGGGTTCGTGCACACAGCCCAGCTTGGAGCGAACGA

	CCTACACCGAACTGAGATACCTACAGCGTGAGCTATGAGAAAGCGCCA CGCTTCCCGAAGGGAGAAAGGCGGACAGGTATCCGGTAAGCGGCAGG GTCGGAACAGGAGAGCGCACGAGGGAGCTTCCAGGGGGAAACGCCT GGTATCTTTATAGTCCTGTCGGGTTTCGCCACCTCTGACTTGAGCGTCG ATTTTTGTGATGCTCGTCAGGGGGGCGGAGCCTATGGAAAAACGCCAG CAACGCGGCCTTTTTACGGTTCCTGGCCTTTTGCTGGCCTTTTGCTCAC ATGTttgacagctagctcagtcctaggtataatgctagctactagagaaagaggagaaatactagATGAGA AGAGCACGTCCGATTGCTCTTCGtaaAAGCTTgcacaggtcGTCGACTTAAAT GCCCCAAAACATCAGGTTAATGGCATTCTTAATATCATTTTCACGATGA CTCAGATCTGCCACTTCTTCACCAATAACACTAACCGGCACACTTGCC ATATCGGTGGTCATCATACGCCAACTTTCATCGCCAATATGCACAACCG GATACAGTTCACGACTCACTTTATCACTCAGCAGGCGGGCGCTGGCCA GCGGAATAACCATACGGCGACCCGGGGTATCAATAATATCGCTCTGCAC ATCCACAAACAGACGATAACGGCTTTCACGCTTATAGGTGTAAACCTT AAACTGCATactcttcctttttcaatattattgaagcatttatcagggttattgtctcatgagcggatacatatttga atgtatttagaaaaataaacaaaCATATGGTGCACTCTCAGTACAATCTGCTCTGATG CCGCATAGTTAAGCCAGCCCCGACACCCGCCAACACCCGCTGACGCG CCCTGACGGGCTTGTCTGCTCCCGGCATCCGCTTACAGACAAGCTGTG ACCGTCTCCGGGAGCTGCATGTGTCAGAGGTTTTCACCGTCATCACCG AAACGCGCGA

For pUC57-Kan-2BspQI-ccdB, the J23119 promoter, BspQI site, ccdB and AmpR promoter sequence are highlighted in red, green, blue, and purple, respectively. The plasmid backbone is pUC57-Kan.

BspQI-FP	GATTGCTCTTCGtaaAAGCTTgcacaggtcGTCGACTTAAAT
BspQI-RP	GGACGTGCTCTTCTCATctagtatttctcctctttctctagtagctagc

Supplementary Table 7. Cloning and sequence verification of selected CcdA variants.

Name	Protein sequence	Log2 F	AF3 ipTM	Sequence identity to WT	DNA sequence
WT	MRRLRAERWKAENQEGMAEVARFIEMNGSFADENRDW	8.46	0.973	1.0	ATGCGTCGTCTGCGCGCAGAACGTTGGAAAGCAGAAAATCAGGAAGGCATGGCAGAAGTGGCCCGTTTTATTGAAATGAATGGCAGCTTTGCCGATGAAAATCGTGATTGGTAA
878	MRRIEAEEFREKNKEGLKEVAEFIKKEGSFAEENRDW	5.31	0.91	0.65	ATGCGTCGTATTGAAGCGGAAGAATTTCGCGAAAAAAACAAAGAAGGCCTGAAAGAAGTGGCGGAATTTATTAAAAAAGAAGGCAGCTTTGCGGAAGAAAACCGCGATTGGTAA
854	MRRISAEEFREKNKEGLKEIAEFIKEEGSFAEENRDW	3.28	0.9	0.62	ATGCGTCGTATTAGCGCGGAAGAATTTCGCGAAAAAAACAAAGAAGGCCTGAAAGAAATTGCGGAATTTATTAAAGAAGAAGGCAGCTTTGCGGAAGAAAACCGCGATTGGTAA
903	MRRISAEEFREKNKEGLEEIARFIEEEGSFAEDNRDW	3.30	0.9	0.65	ATGCGTCGTATTAGCGCGGAAGAATTTCGCGAAAAAAACAAAGAAGGCCTGGAAGAAATTGCGCGCTTTATTGAAGAAGAAGGCAGCTTTGCGGAAGATAACCGCGATTGGTAA
924	MRRLEAEAFREKNKEGLAEVAKFIEEEGSFSEENRDW	3.23	0.9	0.68	ATGCGTCGTCTGGAAGCGGAAGCGTTTCGTGAAAAAAACAAAGAAGGCCTGGCGGAAGTGGCGAAATTTATTGAAGAAGAAGGCAGCTTTAGCGAAGAAAACCGCGATTGGTAA
1654	MRQARAERWKTENREGMAEVQHFIAENGSFCDENREW	3.04	0.91	0.73	ATGCGTCAGGCGCGTGCGGAACGTTGGAAAACCGAAAACCGTGAAGGCATGGCGGAAGTGCAGCATTTTATTGCGGAAAACGGCAGCTTTTGCGATGAAAACCGTGAATGGTAA

Table S8. Identity-to-reference versus predicted divergence time from TimeTree-calibrated fits

Family	Reference	Identity to reference	Predicted divergence (Ma)
TadA	*E. coli* TadA (UniProt P68398)	0.8	1.4049
		0.7	231.7360
		0.6	561.3701
		0.5	1148.1288
CcdA	*E. coli* CcdA (UniProt P62552)	0.9	4.6449
		0.8	20.3885
		0.7	40.2859
		0.6	67.3466
		0.5	109.8419
		0.4	215.5726

Notes: Values are derived from TimeTree-calibrated timetrees and MSA-based identities using a saturating decay fit. They are intended as approximate, order-of-magnitude mappings rather than strict molecular-clock estimates.

Sequence sampling of baseline models: ProteinMPNN and Pinal

ProteinMPNN

A structure-templated baseline library was generated using ProteinMPNN in fixed-backbone design mode with the experimental TadA reference structure as the input template (PDB: **2B3J**, Chain **A**). The structure file was preprocessed to retain only the designed protein chain (non-protein atoms were removed) and was provided to ProteinMPNN to compute per-position amino-acid distributions conditioned on the backbone coordinates. 1,000 sequences were then sampled stochastically from the model using temperature-controlled decoding (temperature = 0.1) with otherwise default ProteinMPNN settings. Sampled sequences were post-processed to remove exact duplicates and were written to FASTA for downstream structure prediction and evaluation.

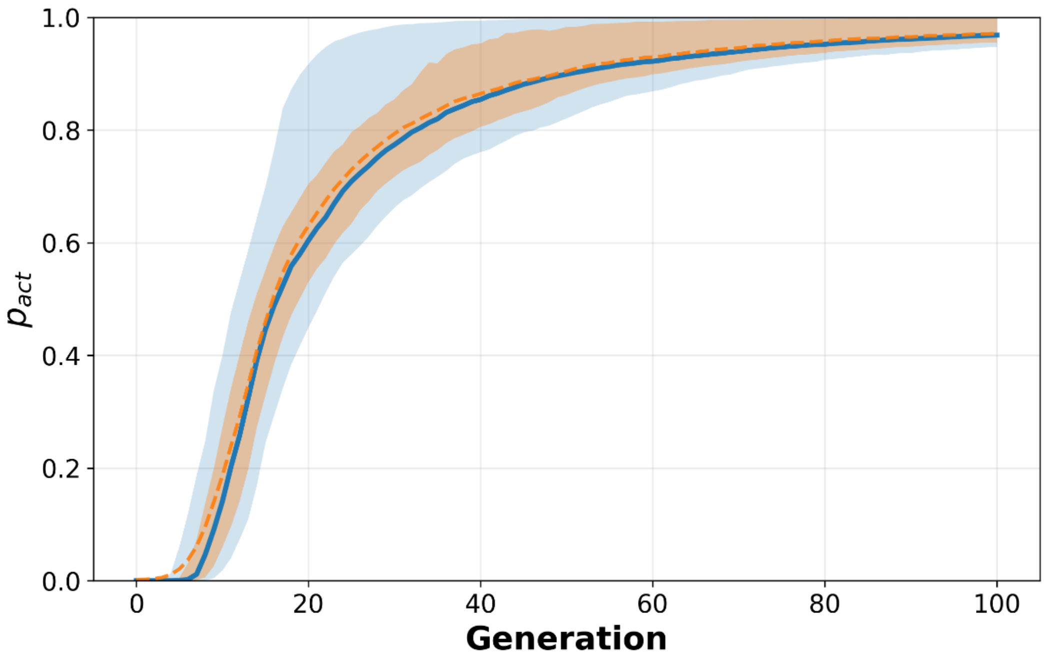
Prompt for Pinal Sequence Generation

Pinal sequences were generated using the official Pinal web server with default sampling/decoding parameters (all server defaults; no additional tuning).

TadA Prompt：TadA (tRNA adenosine deaminase) is an enzyme that catalyzes the deamination of adenosine to inosine at the wobble position (A34) of tRNA molecules, thereby expanding codon recognition during translation, adenosine$_{34}$ in tRNA + H2O + H^{+} = inosine$_{34}$ in tRNA + NH4^{+}. EC:3.5.4.33. Through the introduction of two key mutations, A106V and D108N, the substrate specificity of *E.coli* TadA has been reprogrammed, enabling the enzyme to catalyze adenosine and cytosine deamination directly on DNA substrates. These engineered TadA variants are incorporated into adenine base editors (ABEs), facilitating the precise conversion of A•T base pairs to G•C in DNA without introducing double-strand breaks. This strategy offers an efficient and high-fidelity tool for genome editing, particularly for the correction of disease-associated point mutations.

CcdA Prompt：CcdA is a bacterial antitoxin protein that functions as part of the CcdA–CcdB type II toxin-antitoxin system encoded by the F plasmid in *Escherichia coli*. The CcdA protein comprises 72 amino acids and adopts a two-domain structure: an N-terminal dimerization and DNA-binding domain, followed by a C-terminal domain that binds to the CcdB toxin. In the absence of CcdB, the C-terminal domain of CcdA is intrinsically disordered. Upon binding to CcdB, CcdA undergoes a conformational change, forming a stable CcdA–CcdB complex that neutralizes the toxicity of CcdB. This complex also acts as a transcriptional repressor of the ccd operon by binding to the operator region. The CcdA–CcdB interaction is dynamic, with varying stoichiometries leading to different complex formations, including (CcdA)2–(CcdB)2 and (CcdA)2–(CcdB)4 complexes. The balance between CcdA and CcdB concentrations regulates the stability of the complex and the repression of the operon. CcdA is subject to degradation by the Lon protease, which modulates the levels of the antitoxin and, consequently, the activity of the toxin.",

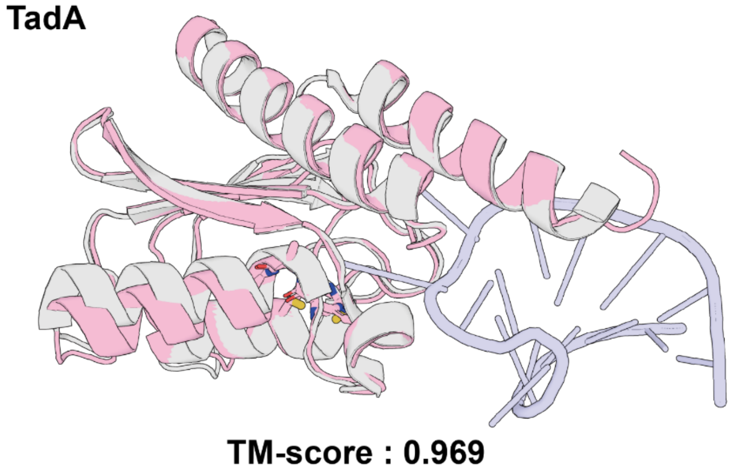
Supplementary Fig. 1



Supplementary Fig. 1. Trajectory of classifier scores under continuous selection during SPIN-JEvo sampling.

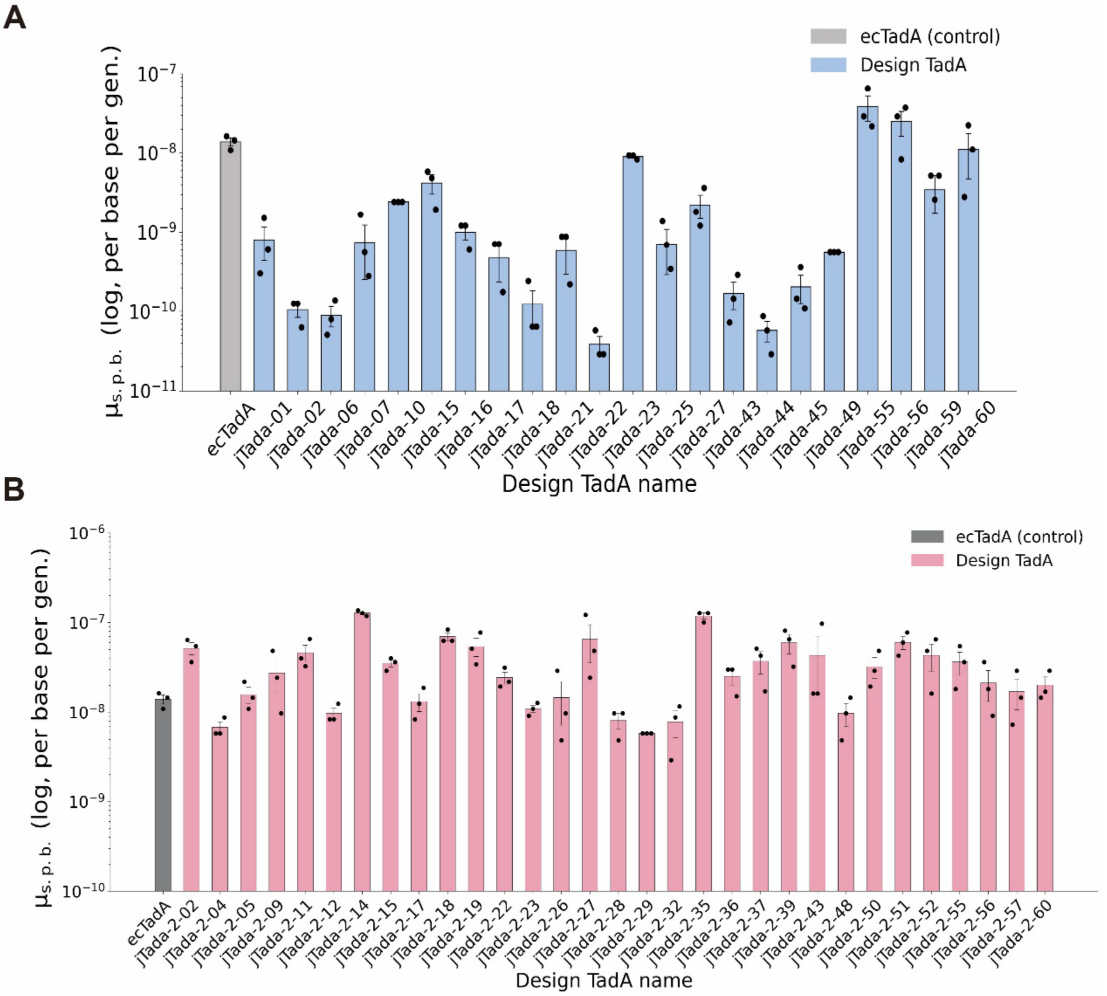
Across 20 independent genetic-algorithm runs, we tracked the population-wide activity score p_{act} at each generation (computed by the LoRA-adapted ESM-2 classifier). The solid curve shows the across-run mean p_{act} per generation and the dashed curve shows the median; shaded bands indicate between-run variability of the population distribution at each generation (interquartile range). The smooth upward shift and eventual saturation demonstrate that SPIN-JEvo applies a continuous, score-based selection pressure rather than a hard survival cutoff.

Supplementary Fig. 2



Supplementary Fig. 2. One illustrative example of the OmegaFold-predicted structure, superimposed on the corresponding wild-type structure (PDB ID: 2B3J). Gray, wild-type; light pink, a SPIN-JEvo-evolved variant.

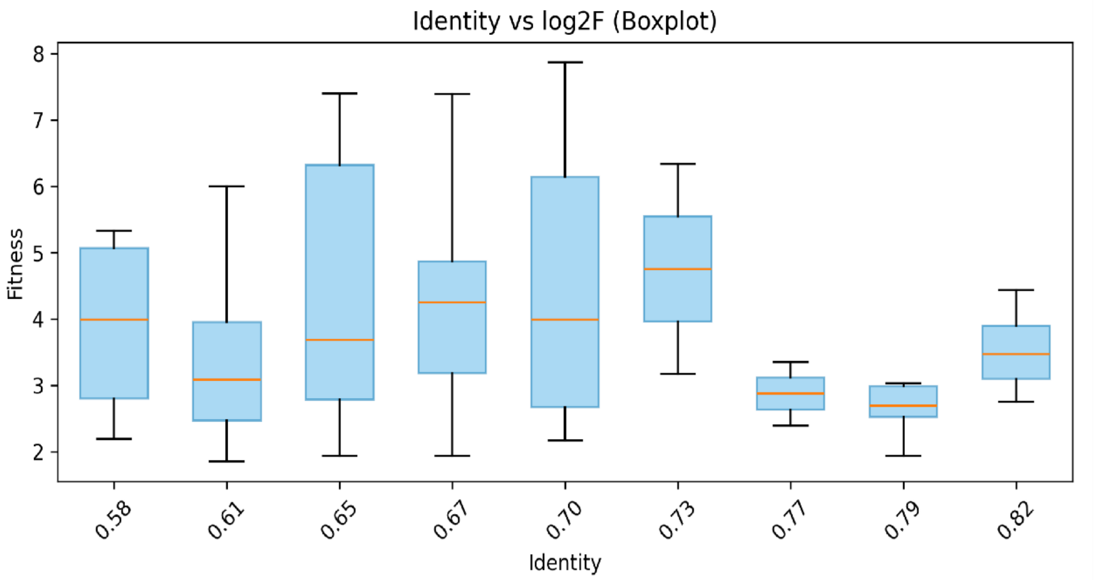
Supplementary Fig. 3



Supplementary Fig. 3. DNA-editing activity of SPIN-JEvo evolved sequences across two rounds.

(**A**) DNA-editing activity reported as mutation frequency and expressed as $\mu_{s.p.b.}$ for 60 selected variants from SPIN-JEvo, along with the activity of *E. coli* TadA as a reference. Data are from Table S4 (**B**) DNA-editing activity reported as mutation frequency and expressed as $\mu_{s.p.b}$ for 60 second-round jTadA variants after LoRA retraining on first-round data. Data are from Table S5.

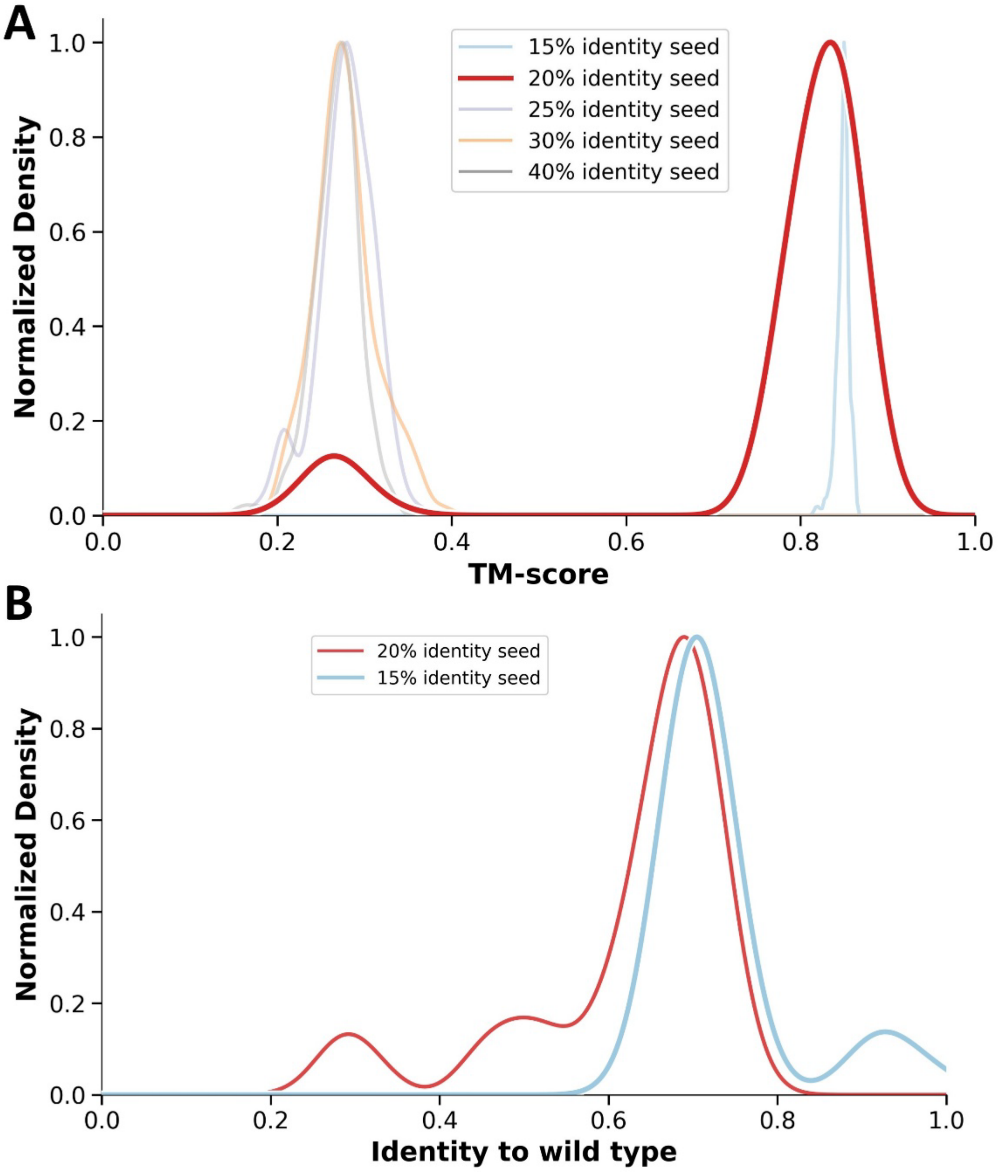
Supplementary Fig. 4



Supplementary Fig. 4. Relationship between divergence from wild-type CcdA and activity among functional hits.

Boxplots show the distribution of $\log_2$ fitness for variants with $\log_2$ fitness > 3, grouped by sequence identity bins relative to wild-type CcdA.

Supplementary Fig. 5



Supplementary Fig. 5. Seed identity trade-off for TadA sampling.

(**A**) Peak-normalized kernel density estimates of TM-scores between OmegaFold-predicted structures of sampled TadA variants and the *E. coli* TadA reference (structure alignment by TM-align). (**B**) Corresponding distributions of global sequence identity to *E. coli* TadA. Variants were generated from seeds initialized at different divergence levels (15–40% substitutions). A 20% mutation seed provides a balanced regime: it shifts designs to lower identity (greater diversity) while largely retaining a near-native fold distribution (high TM-score), whereas more aggressive initialization increases sequence novelty but yields more off-fold samples.

Joint phylogenetic analysis of natural homologs and evolved variants

For each target (TadA and CcdA), we constructed a single "mixed" phylogeny containing both natural homologs and experimentally validated positive evolved variants. For TadA, we used 1000 natural homologs from ref.[1] For CcdA, we collected 100 UniProtKB homologs by BLAST against the E. coli CcdA sequence (UniProt ID: P62552) as in ref.[2] Natural homologs and evolved sequences were combined and aligned with MAFFT[3]. Poorly aligned columns were optionally trimmed to reduce alignment noise. Maximum-likelihood trees were inferred from the trimmed alignments using IQ-TREE2[4] with automated model selection (ModelFinder) and branch-support estimation by bootstrap. Evolved sequences were renamed with a consistent prefix (jTadA_* or jCcda_*) and natural homologs were renamed to compact UniProt-style labels (accession_mnemonic) to enable unambiguous parsing and visualization. Novelty was assessed directly on the resulting tree topology by whether evolved sequences formed evolv-enriched clades distinct from the natural-homolog structure and by identifying the split point of the evolved clade as the parent node of the evolved sequences' MRCA, with the nearest natural lineage defined as the sister clade at that split.

Identity–time calibration for TadA and CcdA[5-7]

To provide a rough evolutionary scale for sequence exploration, we performed coarse identity–time calibrations within the TadA and CcdA families using the same procedure. For TadA, the ~1,000 orthologous sequences were taken from Supplementary Data 2 of the referenced study[1]. For CcdA, ~100 sequences were collected from UniProtKB by searching the keyword "Antitoxin CcdA" and retaining representative hits.

For each family, we computed identity to the *E. coli* reference from a multiple sequence alignment (MSA), and obtained approximate lineage divergence times by building a TimeTree 5[5] timetree for the subset of taxa recognized by the database and downloading the resulting Newick tree.

TimeTree branch lengths are in absolute time (Ma), so for each species we estimated its divergence from *Escherichia coli* as

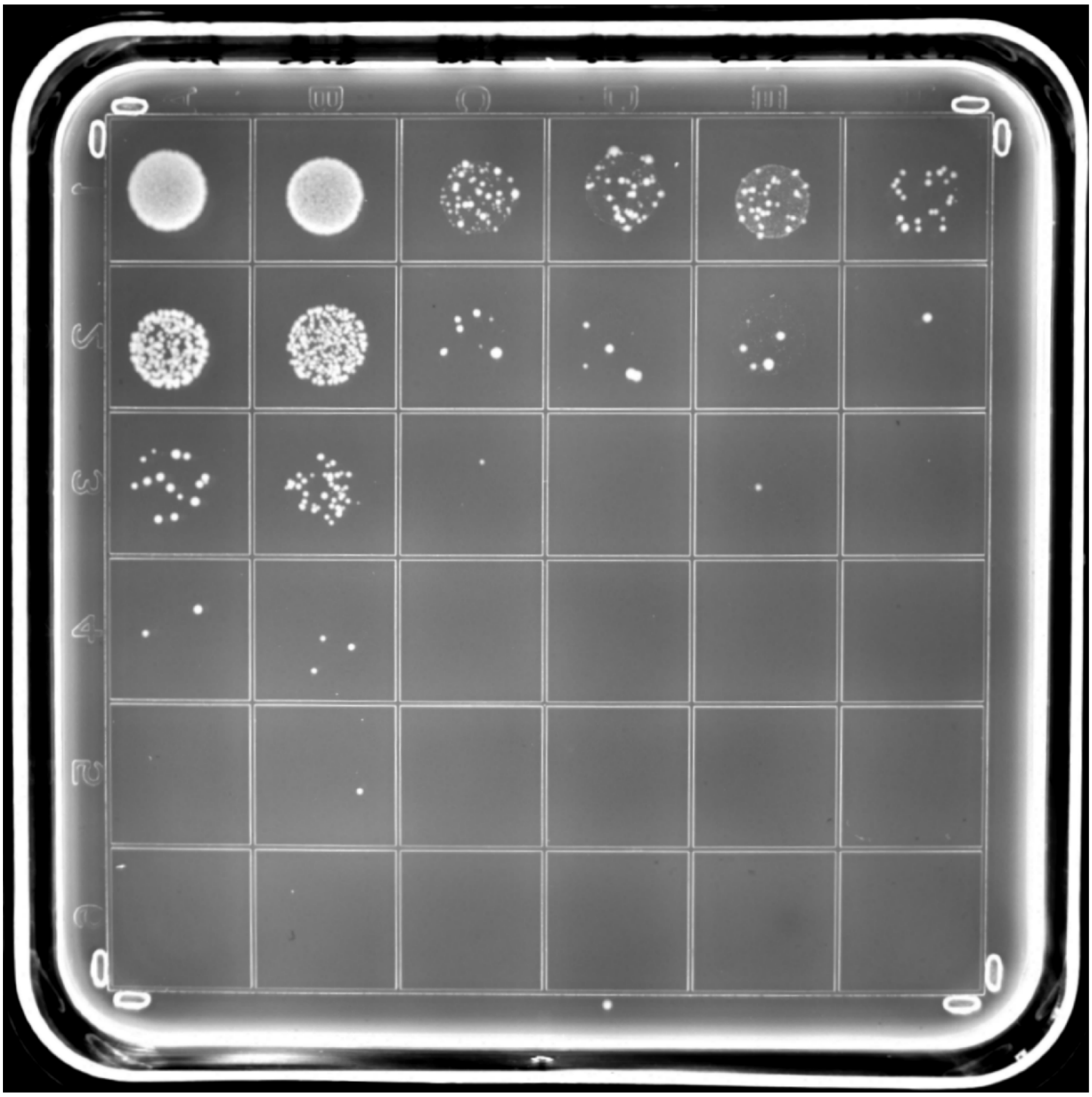
$$T_{div}(species, E.coli) = \frac{1}{2} d_{timetree(}species, E.coli)$$

where d_{timetree} is the patristic distance (sum of branch lengths) between the two leaves in the TimeTree timetree. Species times were mapped onto TadA sequences by matching normalized organism names, and we fit a simple empirical saturating exponential

$$I(T) = I_\infty + (I_0 - I_\infty)e^{-kT}$$

to relate identity I to divergence time T.

Supplementary Fig. 6



Supplementary Fig.6. Full CcdA spot-assay plates.

Uncropped images of the serial 10-fold dilution spot assays for CcdA SPIN-JEvo-evolved sequences tested in Fig. 3E. Overnight cultures were normalized, serially diluted (10^2–10^5), and spotted onto the corresponding selective agar used for the CcdA–CcdB growth assay. Growth across dilutions indicates functional CcdA variants that rescue viability under the assay condition, whereas reduced/no growth is consistent with non-functional variants. Negative and positive controls and variant identities are labeled on the plate.

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