



## Interfacing medicinal chemistry with structural bioinformatics

Jentzsch, Franziska; Hines, Jennifer V

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## Interfacing medicinal chemistry with structural bioinformatics: Implications for T box riboswitch RNA drug discovery

Franziska Jentzsch, Jennifer V. Hines

*Additional File 1*

**Table 1.** Predicted  $\Delta G$  values for aaRS T box terminators and antiterminators

Aminoacyl-tRNA synthetase gene <sup>a</sup>	$\Delta G$ Terminator <sup>b</sup> (kcal/mol)	$\Delta G$ Antiterminator <sup>b</sup> (kcal/mol)	$\Delta\Delta G^c$ (kcal/mol)
BS_ALAS	-18	-12.1	-5.9
BC_ALAS	-21.6	-8.6	-13
SA_ALAS	-13.1	-6.9	-6.2
CB_ALAS	-12.7	-6.6	-6.1
BC_ARGS2	-17.1	-6.1	-11
CB_ARGS	-16.4	-5.7	-10.7
CPE_ARGS	-14.5	-6.3	-8.2
BC_ASNS2	-16.1	-4.7	-11.4
BC_ASNS3	-21	-6.8	-14.2
CB_ASNS2	-19.3	-4.8	-14.5
CB_ASNS3	-11.8	-1.4	-10.4
CDF_ASNS2	-21.1	-10	-11.1
CPE_ASNS2	-15.3	-7.4	-7.9
BS_GLYQ	-29.5	-10.9	-18.6
BC_GLYS2	-29.4	-14.8	-14.6
SAG_GLYQ	-34.7	-9.3	-25.4
SPY_GLYQ	-30.3	-8.6	-21.7
BS_HISS	-28.2	-8.2	-20
BC_HISS	-22.6	-7.7	-14.9
BS_ILES	-23.1	-11	-12.1
BC_ILES	-27.8	-8.4	-19.4
BC_ILES2	-21.6	-12.2	-9.4
CB_ILES	-12.6	-5.3	-7.3
CPE_ILES	-12.1	-2.9	-9.2
SAG_ILES	-11.7	-2	-9.7
SPY_ILES	-8.7	-2	-6.7
BS_LEUS	-20.4	-13.3	-7.1
BC_LEUS	-24	-8	-16
CB_LEUS	-13.7	-5.7	-8
CPE_LEUS	-17.8	-7.1	-10.7
BC_LYSS	-24.7	-6.1	-18.6
BC_METS	-31.1	-8.3	-22.8
CB_METS	-17.1	-3.8	-13.3
CDF_METS	-16.5	-6.3	-10.2
CPE_METS	-17.5	-6.8	-10.7
BS_PHE5	-18.4	-4.7	-13.7
BC_PHE5	-15.7	-5	-10.7

SA_PHEs	-23.2	-4.7	-18.5
CB_PHEs	-14.8	-6	-8.8
CDF_PHEs	-17.6	-6.8	-10.8
CPE_PHEs	-22.1	-5.9	-16.2
SAG_PHEs	-20.9	-6.8	-14.1
SPY_PHEs	-25.7	-6.8	-18.9
BC_PROs	-20.5	-8.5	-12
CDF_PROs	-24.6	-5.8	-18.8
CPE_PROs	-16.7	-5.7	-11
BS_SERs	-26.7	-9	-17.7
BC_SERs	-24.8	-9.5	-15.3
SA_SERs	-21.7	-4.9	-16.8
CB_SERs2	-21.9	-5	-16.9
CB_SERs1	-15.6	-9.3	-6.3
CPE_SERs	-17.4	-3.3	-14.1
BS_THRs	-20.4	-4.6	-15.8
BS_THRz	-21.3	-5.6	-15.7
BS_THRz*	-21.1	-7.3	-13.8
BC_THRs	-18.7	-5.1	-13.6
BC_THRz	-25.5	-7.1	-18.4
BC_THRz*	-29.4	-6.9	-22.5
SA_THRs	-16.9	-4.7	-12.2
CB_THRz	-16.5	-5.1	-11.4
CDF_THRz	-14.4	-5.7	-8.7
CPE_THRz	-28.7	-7	-21.7
SAG_THRz	-17.9	-3.6	-14.3
SPY_THRz	-6.3	-5.1	-1.2
BS_TRPs	-20.6	-4.7	-15.9
BC_TRPs	-20.4	-5.7	-14.7
BC_TRPs2	-15.1	-6	-9.1
CB_TRPs	-11.9	-7.7	-4.2
SPY_TRPs	-11.9	-9.6	-2.3
BS_TYRs	-18.8	-6.4	-12.4
BS_TYRz	-18.9	-7.8	-11.1
BC_TYRs	-16.7	-6.1	-10.6
BC_TYRs2	-12.2	-4.8	-7.4
BS_VALs	-24.4	-5.1	-19.3
BC_VALs	-23.3	-3.8	-19.5
SA_VALs	-18	-6.6	-11.4
CB_Y5-VALs	-19.8	-4.8	-15
CPE_VALs	-13.1	-4.1	-9
SAG_Y1VALs	-13.7	-7.5	-6.2
SPY_Y1VALs	-20.6	-9.6	-11

<sup>a</sup>Abbreviation as defined in reference [2].

<sup>b</sup> $\Delta G$  values determined using DINAMelt (Quickfold RNA 3.0), see Methods for details.

<sup>c</sup> $\Delta\Delta G = \Delta G_{\text{terminator}} - \Delta G_{\text{antiterminator}}$