

Table S3: Combinational factors of the triplets in KaiC hexamer

Triplets centered by the transition state interface	N factor
$\mathbf{m}_{00}\text{-}\mathbf{m}_{00}\text{-}\mathbf{m}_{00}$	$f(\alpha, 1)f(\alpha - 1, 2)$
$\mathbf{m}_{00}\text{-}\mathbf{m}_{00}\text{-}\mathbf{m}_{01}$	$f(\alpha, 1)f(\alpha - 1, 1)f(\beta, 1)$
$\mathbf{m}_{00}\text{-}\mathbf{m}_{00}\text{-}\mathbf{m}_{10}$	$f(\alpha, 1)f(\alpha - 1, 1)f(\gamma, 1)$
$\mathbf{m}_{00}\text{-}\mathbf{m}_{00}\text{-}\mathbf{m}_{11}$	$f(\alpha, 1)f(\alpha - 1, 1)f(\delta, 1)$
$\mathbf{m}_{01}\text{-}\mathbf{m}_{00}\text{-}\mathbf{m}_{01}$	$f(\alpha, 1)f(\beta, 2)$
$\mathbf{m}_{01}\text{-}\mathbf{m}_{00}\text{-}\mathbf{m}_{10}$	$f(\alpha, 1)f(\beta, 1)f(\gamma, 1)$
$\mathbf{m}_{01}\text{-}\mathbf{m}_{00}\text{-}\mathbf{m}_{11}$	$f(\alpha, 1)f(\beta, 1)f(\delta, 1)$
$\mathbf{m}_{10}\text{-}\mathbf{m}_{00}\text{-}\mathbf{m}_{10}$	$f(\alpha, 1)f(\gamma, 2)$
$\mathbf{m}_{10}\text{-}\mathbf{m}_{00}\text{-}\mathbf{m}_{11}$	$f(\alpha, 1)f(\gamma, 1)f(\delta, 1)$
$\mathbf{m}_{11}\text{-}\mathbf{m}_{00}\text{-}\mathbf{m}_{11}$	$f(\alpha, 1)f(\delta, 2)$
$\mathbf{m}_{00}\text{-}\mathbf{m}_{01}\text{-}\mathbf{m}_{00}$	$f(\beta, 1)f(\alpha, 2)$
$\mathbf{m}_{00}\text{-}\mathbf{m}_{01}\text{-}\mathbf{m}_{01}$	$f(\beta, 1)f(\alpha, 1)f(\beta - 1, 1)$
$\mathbf{m}_{00}\text{-}\mathbf{m}_{01}\text{-}\mathbf{m}_{10}$	$f(\beta, 1)f(\alpha, 1)f(\gamma, 1)$
$\mathbf{m}_{00}\text{-}\mathbf{m}_{01}\text{-}\mathbf{m}_{11}$	$f(\beta, 1)f(\alpha, 1)f(\delta, 1)$
$\mathbf{m}_{01}\text{-}\mathbf{m}_{01}\text{-}\mathbf{m}_{01}$	$f(\beta, 1)f(\beta - 1, 2)$
$\mathbf{m}_{01}\text{-}\mathbf{m}_{01}\text{-}\mathbf{m}_{10}$	$f(\beta, 1)f(\beta - 1, 1)f(\gamma, 1)$
$\mathbf{m}_{01}\text{-}\mathbf{m}_{01}\text{-}\mathbf{m}_{11}$	$f(\beta, 1)f(\beta - 1, 1)f(\delta, 1)$
$\mathbf{m}_{10}\text{-}\mathbf{m}_{01}\text{-}\mathbf{m}_{10}$	$f(\beta, 1)f(\gamma, 2)$

$\mathfrak{m}_{10}\text{-}\mathbf{m}_{01}\text{-}\mathfrak{m}_{11}$	$f(\beta,1)f(\gamma,1)f(\delta,1)$
$\mathfrak{m}_{11}\text{-}\mathbf{m}_{01}\text{-}\mathfrak{m}_{11}$	$f(\beta,1)f(\delta,2)$
$\mathfrak{m}_{00}\text{-}\mathbf{m}_{10}\text{-}\mathfrak{m}_{00}$	$f(\gamma,1)f(\alpha,2)$
$\mathfrak{m}_{00}\text{-}\mathbf{m}_{10}\text{-}\mathfrak{m}_{01}$	$f(\gamma,1)f(\alpha,1)f(\beta,1)$
$\mathfrak{m}_{00}\text{-}\mathbf{m}_{10}\text{-}\mathfrak{m}_{10}$	$f(\gamma,1)f(\alpha,1)f(\gamma-1,1)$
$\mathfrak{m}_{00}\text{-}\mathbf{m}_{10}\text{-}\mathfrak{m}_{11}$	$f(\gamma,1)f(\alpha,1)f(\delta,1)$
$\mathfrak{m}_{01}\text{-}\mathbf{m}_{10}\text{-}\mathfrak{m}_{01}$	$f(\gamma,1)f(\beta,2)$
$\mathfrak{m}_{01}\text{-}\mathbf{m}_{10}\text{-}\mathfrak{m}_{10}$	$f(\gamma,1)f(\beta,1)f(\gamma-1,1)$
$\mathfrak{m}_{01}\text{-}\mathbf{m}_{10}\text{-}\mathfrak{m}_{11}$	$f(\gamma,1)f(\beta,1)f(\delta,1)$
$\mathfrak{m}_{10}\text{-}\mathbf{m}_{10}\text{-}\mathfrak{m}_{10}$	$f(\gamma,1)f(\gamma-1,2)$
$\mathfrak{m}_{10}\text{-}\mathbf{m}_{10}\text{-}\mathfrak{m}_{11}$	$f(\gamma,1)f(\gamma-1,1)f(\delta,1)$
$\mathfrak{m}_{11}\text{-}\mathbf{m}_{10}\text{-}\mathfrak{m}_{11}$	$f(\gamma,1)f(\delta,2)$
$\mathfrak{m}_{00}\text{-}\mathbf{m}_{11}\text{-}\mathfrak{m}_{00}$	$f(\delta,1)f(\alpha,2)$
$\mathfrak{m}_{00}\text{-}\mathbf{m}_{11}\text{-}\mathfrak{m}_{01}$	$f(\delta,1)f(\alpha,1)f(\beta,1)$
$\mathfrak{m}_{00}\text{-}\mathbf{m}_{11}\text{-}\mathfrak{m}_{10}$	$f(\delta,1)f(\alpha,1)f(\gamma,1)$
$\mathfrak{m}_{00}\text{-}\mathbf{m}_{11}\text{-}\mathfrak{m}_{11}$	$f(\delta,1)f(\alpha,1)f(\delta-1,1)$
$\mathfrak{m}_{01}\text{-}\mathbf{m}_{11}\text{-}\mathfrak{m}_{01}$	$f(\delta,1)f(\beta,2)$
$\mathfrak{m}_{01}\text{-}\mathbf{m}_{11}\text{-}\mathfrak{m}_{10}$	$f(\delta,1)f(\beta,1)f(\gamma,1)$
$\mathfrak{m}_{01}\text{-}\mathbf{m}_{11}\text{-}\mathfrak{m}_{11}$	$f(\delta,1)f(\beta,1)f(\delta-1,1)$
$\mathfrak{m}_{10}\text{-}\mathbf{m}_{11}\text{-}\mathfrak{m}_{10}$	$f(\delta,1)f(\gamma,2)$

$m_{10}\text{-}\mathbf{m}_{11}\text{-}m_{11}$	$f(\delta,1)f(\gamma,1)f(\delta-1,1)$
$m_{11}\text{-}\mathbf{m}_{11}\text{-}m_{11}$	$f(\delta,1)f(\delta-1,2)$

It is defined: $f(n,k) = \begin{cases} \frac{n!}{k!(n-k)!} & \text{if } n \geq 1, 0 < k \leq n \\ 0 & \text{else} \end{cases}$. α , β , γ and δ are the

numbers of m_{00} , m_{01} , m_{10} and m_{11} in one KaiC hexamer, respectively. The m_{ij} marked bold is the reaction interface.