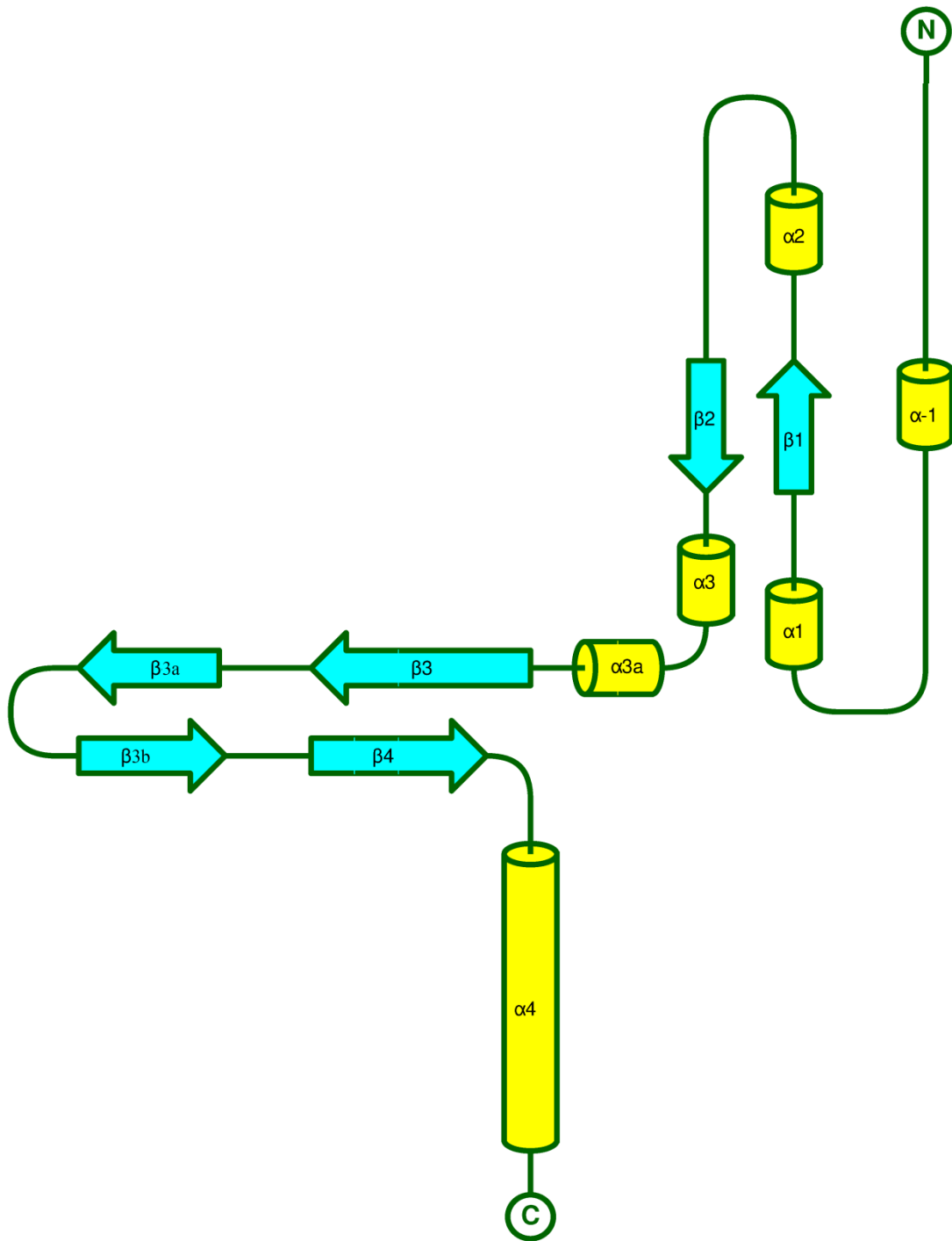


## Supplementary Materials:

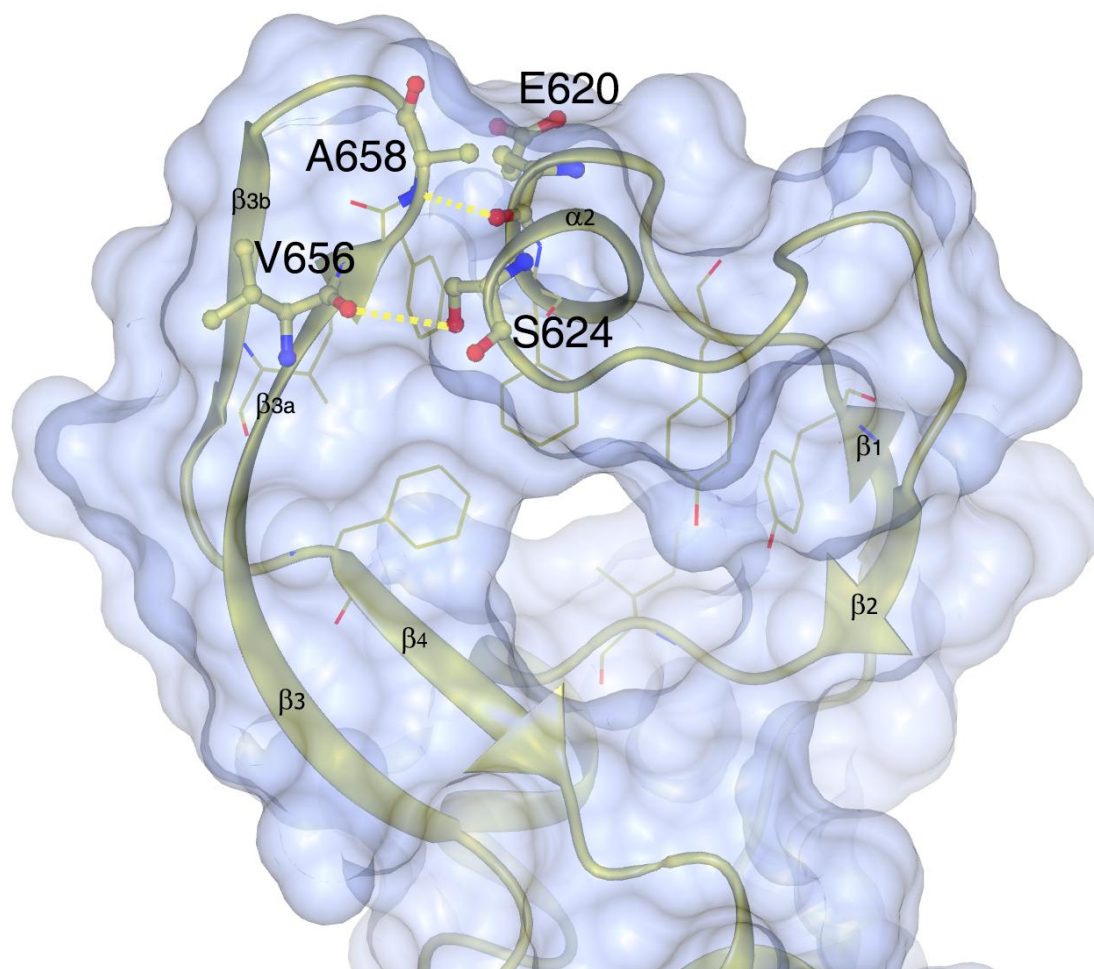
### **Crystal structure of the MyRF ICA domain with its upstream $\beta$ -helical stalk reveals the molecular mechanisms underlying its trimerization and self-cleavage**

Pei Wu<sup>1,3</sup>, Xiangkai Zhen<sup>1#</sup>, Bowen Li<sup>1</sup>, Qian Yu<sup>1</sup>, Xiaochen Huang<sup>1</sup>, Ning Shi<sup>1,2\*</sup>

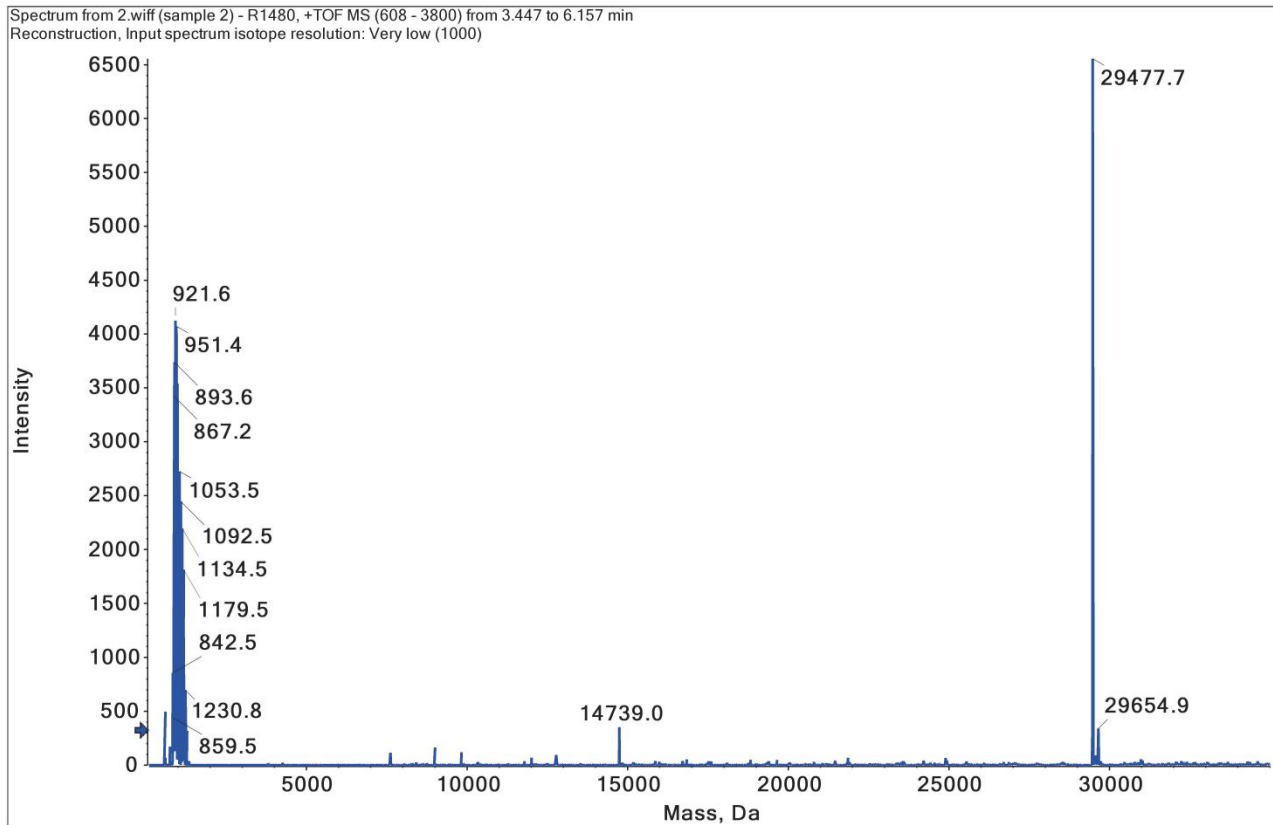
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**Figure S1.** Topology diagram of the MyRF ICA domain. The topology diagram gives an overview of the consecutive secondary structure elements found in the MyRF ICA domain.



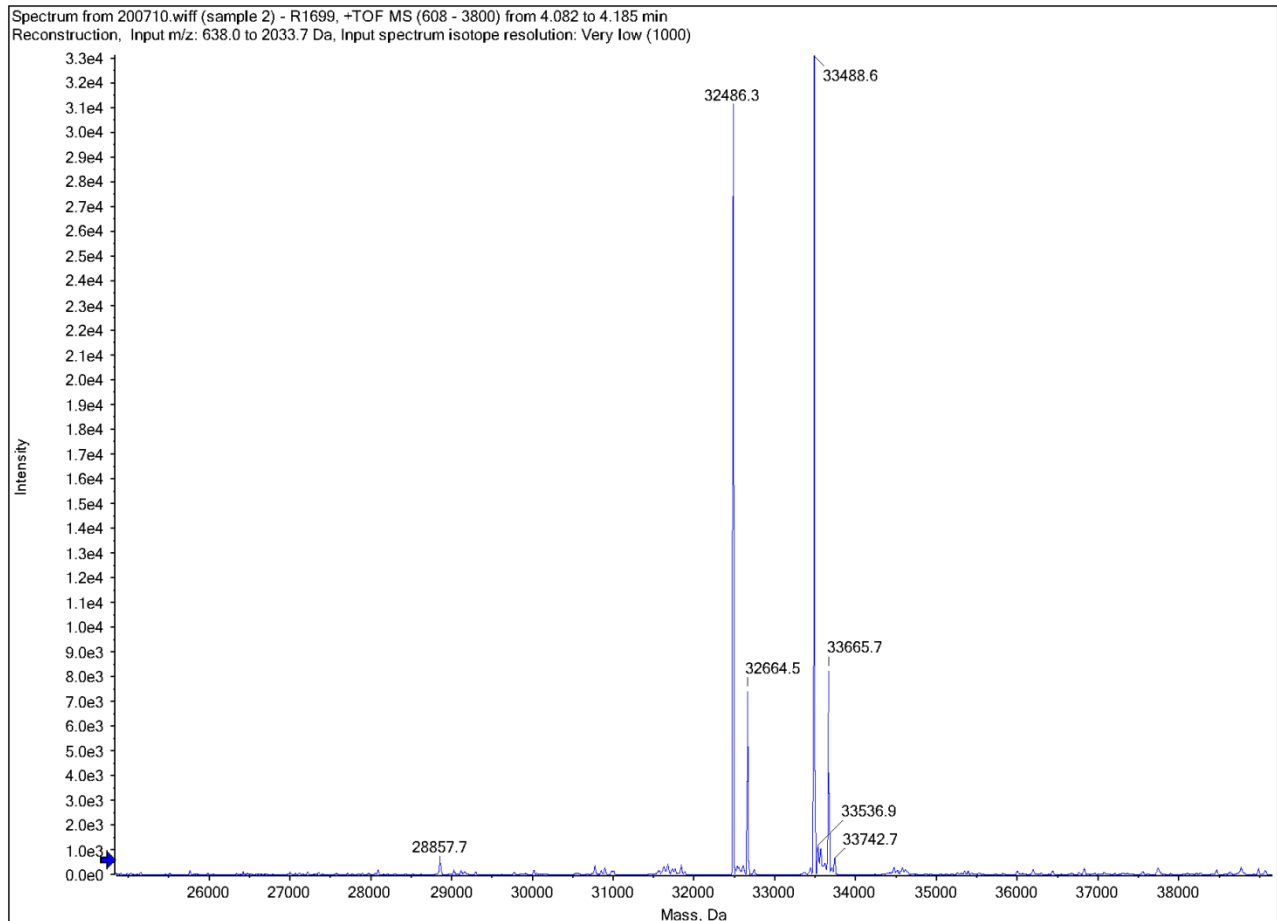
**Figure S2.** The hydrogen bonds were formed at the top of the “donut” which was formed of the  $\beta 3$ - $\beta 4$  and  $\beta 1$ - $\beta 2$  strands in MyRF. E620, S624 of the helix  $\alpha 2$  (between the stands of  $\beta 1$  and  $\beta 2$ ) and A658, V656 of the loop (between the stands of  $\beta 3a$  and  $\beta 3b$ ) were represented as sticks. The hydrogen bonds were formed between them and were showed as the yellow lines.



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**Figure S3.** Mass Spectrometric Analysis of MyRF<sub>wt</sub> (351-717) product

The result of MALDI-TOF-Mass spectrometry shows the molecular weight of MyRF DBD after auto-cleavage which matches the sequence 351-586 of MyRF (plus his tag and the linker residues) with calculated MW 29,477 Dalton.



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**Figure S4.** Mass Spectrometric Analysis of MyRFY<sub>Y615A&Y617A</sub> product

The result of MALDI-TOF-Mass spectrometry shows the molecular weight of MyRF DBD after auto-cleavage which matches the sequence 351-611 and 351-620 of MyRF (plus his tag and the linker residues) with calculated MW 32,486 Dalton and 33,488 Dalton.