Supporting Information

Dym *et al.* 10.1073/pnas.0801525105

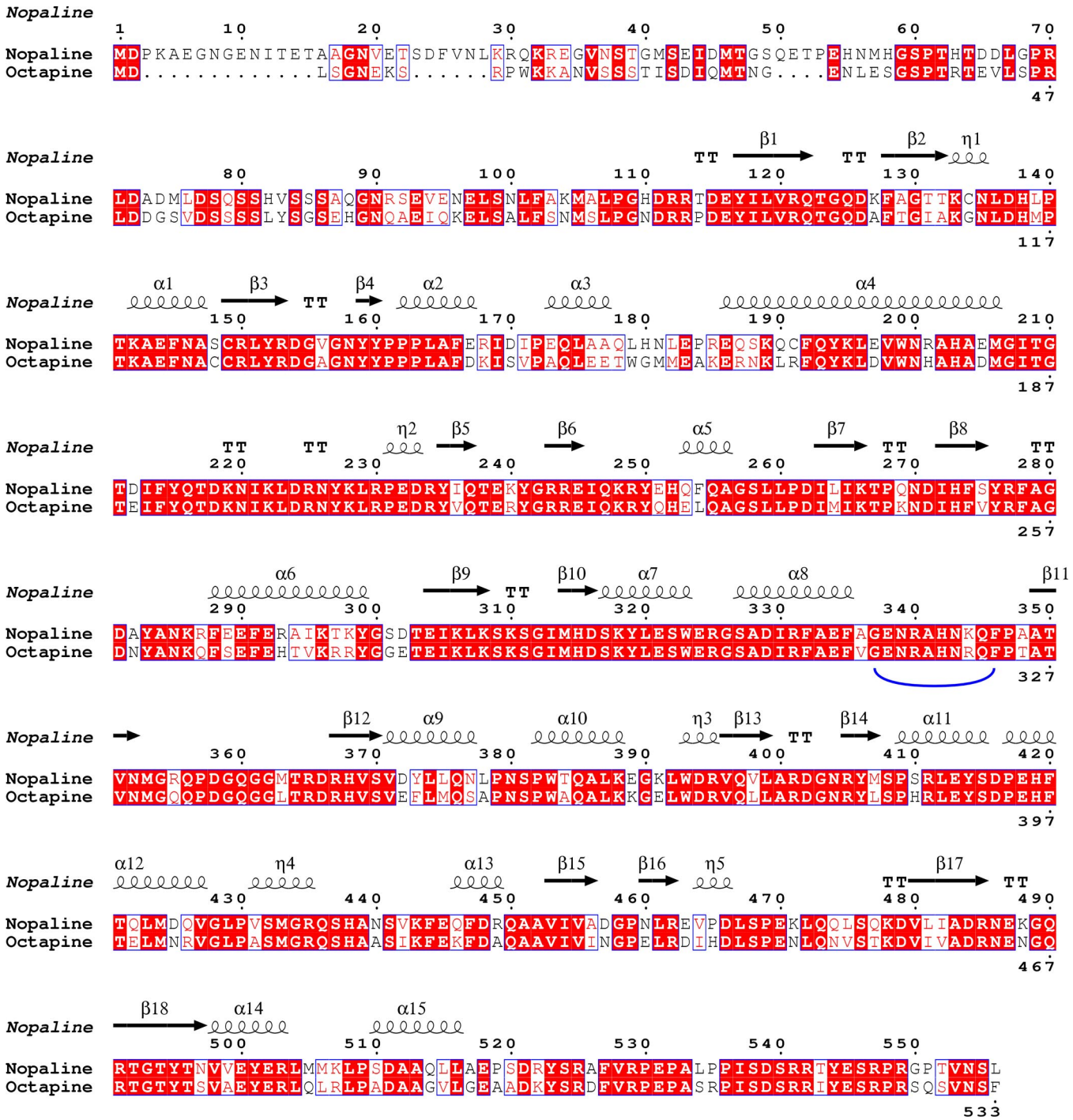

Fig. S1. Sequence and secondary structure alignment of VirE2. The sequence of nopaline VirE2 is compared with that of octapine VirE2 (numbering above sequence: nopaline; numbering below sequence: octopine). Secondary structure elements of VirE2 are labeled above the corresponding sequence; α-helices are indicated by spirals and β-strands by arrows. Numbering of elements matches Fig. 1*B* in the main text. The residues conserved in both proteins appear in red blocks. The flexible linker between residues 337 and 346, connecting the two VirE2 domains, is marked with a blue brace. The figure was created by using ESPript (Gouet P, Courcelle E, Stuart DI, Metoz F (1999) ESPript: multiple sequence alignments in PostScript. *Bioinformatics*. 15:305–8).

Table S1. Interacting residues between VirE1 and VirE2 (up to 3.5 Å)

VirE1	VirE2 N-terminal domain	VirE2 C-terminal domain
H31	K248	
Q32	E167	
N34	K248	
G35	Q247 S311	
F36	L164 Q247	
D40	S309 S311 H315	
E42	W323	K471
E45 L46		R367
E47	R168 Y319	
N48	R168	
V50		L378
H52	D170	
C53		M353 W383
P54		Q356 W383
L55		P382

Table S2. Data collection and refinement statistics

Data collection	
Resolution range, Å*	50.0–2.3 (2.38–2.3)
λ, Å	0.979
Space group	$P2_12_12_1$
Unit cell dimensions:	
a, Å	51.02
b, Å	96.27
c, Å	112.48
Number of molecules in the asymmetric unit	1
Number of reflections measured	179,275
Number of unique reflections*	25,250 (2,464)
R_{sym}*†	0.109 (0.386)
Completeness, %*	99.8 (99.9)
Redundancy	7.1 (6.6)
$\langle I\rangle/\langle\sigma(I)\rangle$	16.8 (4.6)
Refinement statistics	
Resolution limits, Å	48.1–2.3
R_{free}, %‡	21.0
R_{work}, %‡	25.3
Mean B factor, Å^2	32.38
Rms deviations	
Bond lengths, Å	0.025
Bond angles, °	2.16
Torsion angles, °	9.29
Ramachandran plot	
Most favored, %	90.5
Additional allowed, %	8.9
Generously allowed, %	0.3
Disallowed regions, %	0.3

* Values in parentheses are for the highest-resolution shells.

†$R_{sym} = \Sigma|\langle I_{hkl}\rangle - I_{hkl}|/|I_{hkl}|$, where $\langle I_{hkl}\rangle$ is the average intensity over symmetry-related reflections and I_{hkl} is the observed intensity.

‡$R = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$, where F_o denotes the observed structure factor amplitude and F_c the structure factor calculated from the model.