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Supporting information for article:

The structural basis of the Tle4–Tli4 complex reveals the self-protection mechanism of H2-T6SS in *Pseudomonas aeruginosa*

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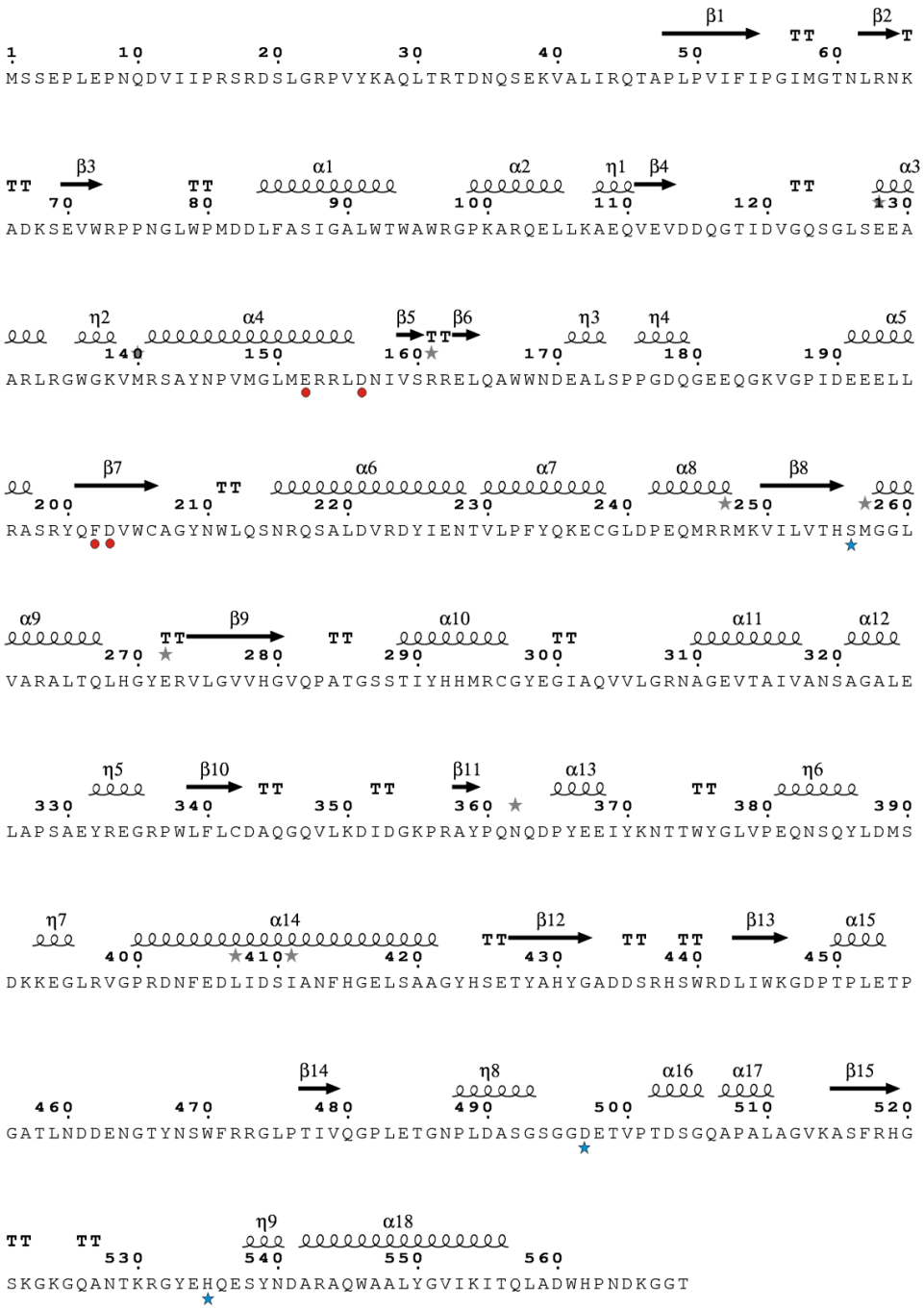

Figure S1 Secondary structure distribution of Tle4. α-helices and β-strands are represented by helical ribbons and schematic arrows; η stands for the 3_{10}-helix; TT represents for the turns. The residues in the calcium binding motif are labeled with red circles and the residues in catalytic triad are labeled with blue stars.

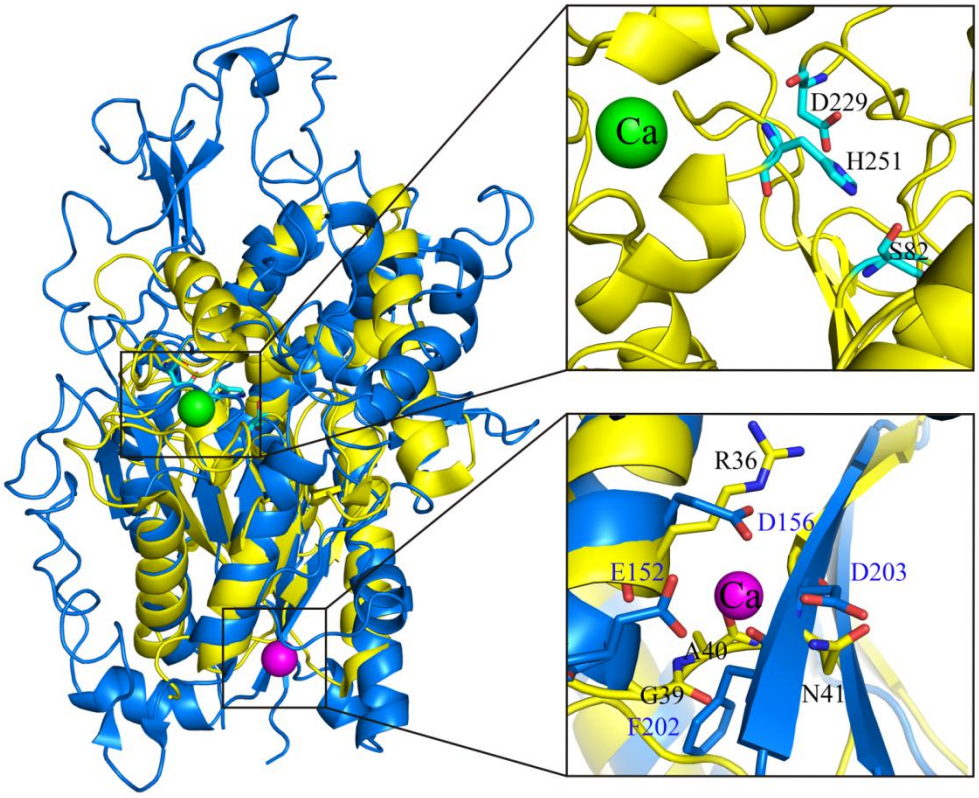

Figure S2 The comparison of calcium binding motifs in Tle4 and lipase PAL (PDB code: 1EX9). Tle4 and PAL are represented in cartoon and colored in marine blue and yellow respectively. The calcium ions in Tle4 and PAL are shown in sphere model in magenta and green color respectively. The left panel shows the structural alignment between Tle4 and PAL. The top panel in the right shows the spatial relationship between calcium binding motif and catalytic triad in PAL. The bottom panel in the right shows the non-conserved residues forming the calcium binding motif in Tle4 and the corresponding residues in PAL. The residues are shown in stick-and-ball model, and labeled in black and blue color for PAL and Tle4 respectively.

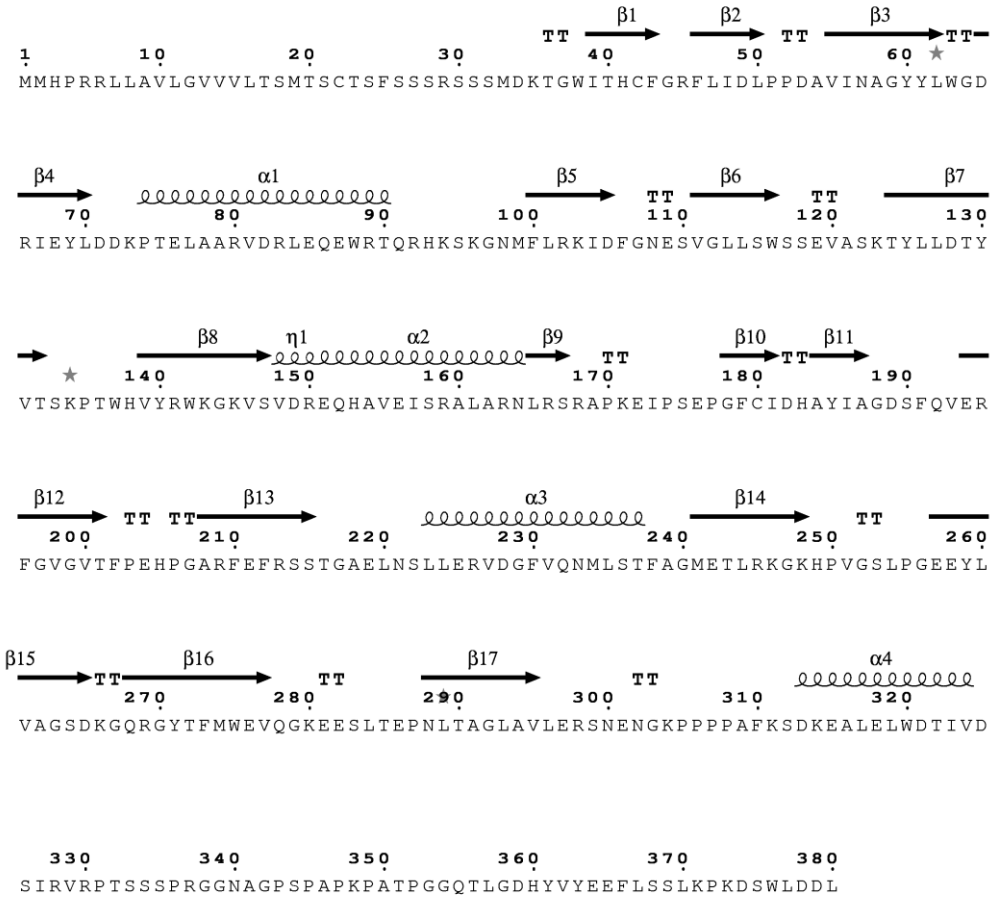

Figure S3 Secondary structure distribution of Tli4. α-helices and β-strands are represented by helical ribbons and schematic arrows; η stands for the 3_{10}-helix; TT represents for the turns.

Table S1 Details of Tle4-Tsi4 interactions

Hydrogen bonds (≤3.3 Å)		
Tle4	Tli4	Distance (Å)
Asn64 (ND2)	Tyr61 (OH)	3.21
Asn64 (OD1)	Tyr61 (OH)	3.28
Asp67 (OD1)	Arg213(NH2)	3.16
Asp67 (OD2)	Arg213 (NH1)	2.79
Ser69 (OG)	Glu211 (OE1)	2.70
Glu70 (OE1)	Arg209 (NE)	3.13
Glu70 (OE2)	Arg209 (NE)	3.23
Glu70 (OE2)	Arg209 (NH2)	3.01
Trp96 (O)	Arg226 (NH1)	2.79
Arg97 (NH1)	Glu211 (OE2)	2.87
Arg97 (NH2)	Glu211 (OE1)	2.97
Lys100 (N)	Glu219 (OE1)	2.91
Lys100 (NZ)	Gly217 (O)	2.73
Ala101 (N)	Glu219 (OE2)	3.07
Glu104 (OE2)	Ser215 (OG)	2.38
Lys107(NZ)	Gly64 (O)	3.18
Gln110 (NE2)	Gly64 (O)	2.76
Gln110 (OE1)	Arg195 (NH2)	2.93
Lys393 (O)	Arg150 (NH1)	2.66
Gly395 (O)	His153 (NE2)	3.19

Arg397 (NH2)	Asp65 (OD2)	2.84
Leu396 (O)	Arg150 (NH1)	3.13
Arg397 (O)	Ser147 (N)	2.93
Gly399 (N)	Ser147 (OG)	2.81
Asp402 (OD2)	Ser147 (OG)	2.42
Asp406 (OD1)	Ser122 (N)	3.07
Asp406 (OD2)	Thr124 (N)	2.73
Asp406 (OD2)	Thr124 (OG1)	2.68
Asp406 (OD2)	Lys123 (N)	2.97
Salt bridges (≤4 Å)		
Tle4	Tli4	
Asp67	Arg213	
Glu70	Arg209	
Arg97	Glu211	
Glu104	Arg195	
Arg141	Glu297	
Arg397	Asp65	
Glu405	Lys123	