## SUPPORTING INFORMATION

	PDB ID	Protein name	Description	Z-score	RMSD (Å)
1	4XRT	StfQ	Aromatase/cyclase	12.0	3.6
2	3RT2	PYL10	Abscisic acid receptor	11.8	4.2
3	2RER	TcmN	Aromatase/cyclase	11.6	3.7
4	5UR5	PYR1	Abscisic acid receptor	11.6	3.6
5	3JRS	PYL1	Abscisic acid receptor	11.5	3.4
6	3TFZ	ZhuI	Aromatase/cyclase	11.3	3.3
7	5Z8O	MSMEG0129	Aromatase/cyclase	11.2	3.3
8	3IE5	HYP-1	Phenolic oxidative coupling protein	11.2	3.7
9	3TVR	WhiE	Aromatase/cyclase	11.0	3.6

**Table S1.** Structure similarity analysis of CGL2373 using Dali. The proteins were ranked according to the similarity score (Z-score) with CGL2373.



**Figure S1.** Rotational correlation time ( $\tau_c$ ) estimate for CGL2373. Average <sup>15</sup>N  $T_1$  (A) and  $T_2$  (B) relaxation times were determined for NC CGL2373 from 1D <sup>15</sup>N-edited  $T_1$  and  $T_2$  (CPMG) experiments recorded on a Varian Inova 600 MHz spectrometer at 298 K. C, linear fit of  $\tau_c$  (ns) versus protein molecular weight (kDa) for a series of standard proteins studied by the NESG consortium, including Ubiquitin (5.1 ns, 9.1 kDa), NsR143 (5.9 ns, 7.5 kDa), ShR105F (6.8 ns, 13.4 kDa), TaR80B (8.6 ns, 12.2 kDa), AhR99 (8.9 ns, 17.1 kDa), ReR242 (9.1 ns, 17.8 kDa), SgR171 (9.2 ns, 13.9 kDa), CrR115 (9.9 ns, 17.0 kDa), ChR152 (11.1 ns, 20.3 kDa), CgR157 (11.5 ns, 18.0 kDa), and SpR104 (12.3 ns, 19.4 kDa). The overall  $\tau_c$  was 11.5 ns for NC CGL2373 (corresponding to a fitted MW of 20.2 kDa) indicated by the solid circle, which suggested that CGL2373 under the NMR study conditions was predominantly monomeric (expected MW = 19.9 kDa, including C-terminal His-tag).



**Figure S2.** Internal pocket of CGL2373. A, electrostatic surface potential diagram of CGL2373 colored by electrostatic potential (-76.53 kT/e, red to + 76.53 kT/e, blue). Black arrow indicates the entrance of the internal pocket in typical polyketide cyclase. B, the residues involved in forming the pocket of CGL2373 are shown with sticks in the cartoon model of CGL2373 structure (top) as the same orientation in (A), and are highlighted with green color in the sequence of CGL2373 (bottom).



**Figure S3.** Comparison of CGL2373 with three abscisic acid (ABA) receptors from *Arabidopsis* including PYR1, PYL1 and PYL10. A, Sequence alignment of CGL2373 with the three ABA receptors. Alignment was rendered using ESPript 3.0 with default settings for similarity calculations. Secondary structural elements of CGL2373 are indicated above the amino acid residue number in the sequence. Identical (white letters filled with red color) and similar (red letters with blue box) amino acids are denoted. The residues essential for ABA binding of PYR1 are labeled with blue circles below the sequence. The residues labeled with green and violet circles are additionally involved in ABA binding for PYL1 and PYL10, respectively. B, C, and D, Superposition of the structure of CGL2373 (cyan) with those of PYR1 (green), PYL1 (magenta), and PYL10 (yellow), respectively. Black arrows denote the marked differences between CGL2373 structure and those of the three ABA receptors.