Supporting Information

Symersky et al. 10.1073/pnas.1207912109

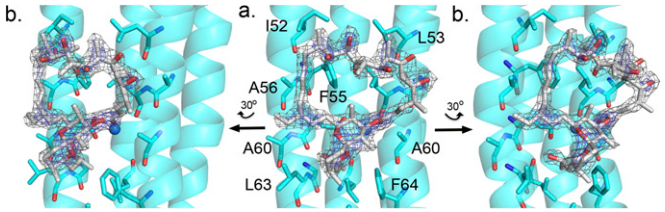


Fig. S1. Electron density map for oligomycin 1. (*A*) The electron density map (2Fo-Fc) is colored in gray (contoured at 1.3σ) and blue (contoured at 2.0σ). (*B*) As in *A*, but rotated 30° as indicated.

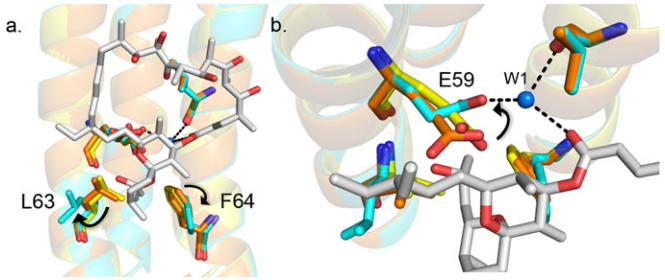


Fig. S2. Conformational changes caused by oligomycin binding. (*A*) Chains O and N for the oligomycin-bound structure (cyan) were superimposed onto chains D and C (yellow) (see Fig. 1) and also superimposed onto chains O and N from the structure of the c-ring without oligomycin (orange) (Protein Data Bank ID, 3UD0). (*B*) Top view of *A* showing the rotation of the side-chain carboxyl of Glu59 with oligomycin binding.

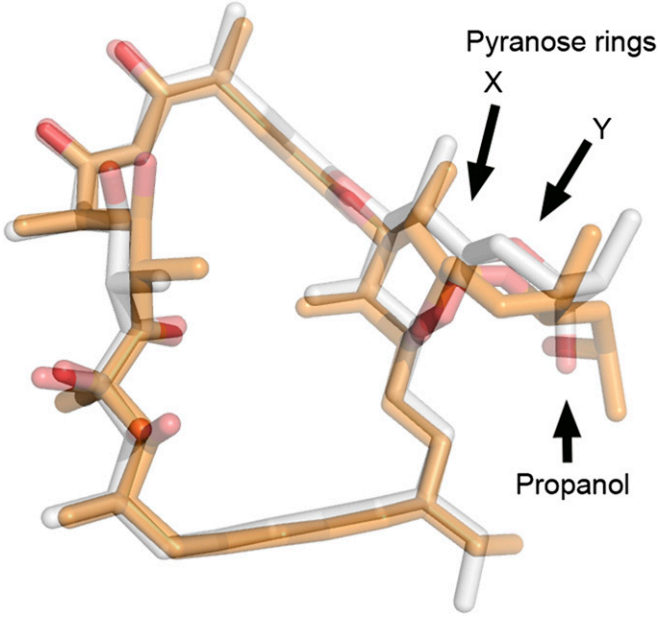
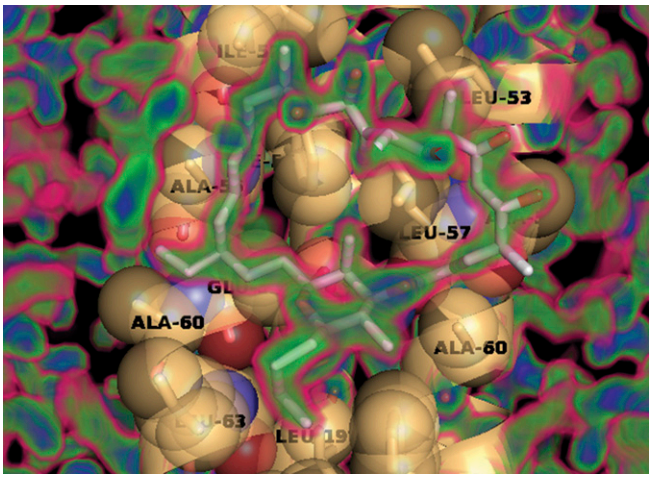


Fig. S3. Comparison of oligomycin 1 with the crystal structure of oligomycin. The crystal structure of oligomycin 1 is shown in gray and that of oligomycin A is in orange. Oligomycin consists of a 26-member macrocyclic ring with spiro-linked pyranose rings, labeled "X" and "Y." The structure of the macrocyclic ring is nearly identical in oligomycin 1 and oligomycin A. The greatest differences are in the pyranose rings where the propanol group interacts with Leu63 and Phe64.

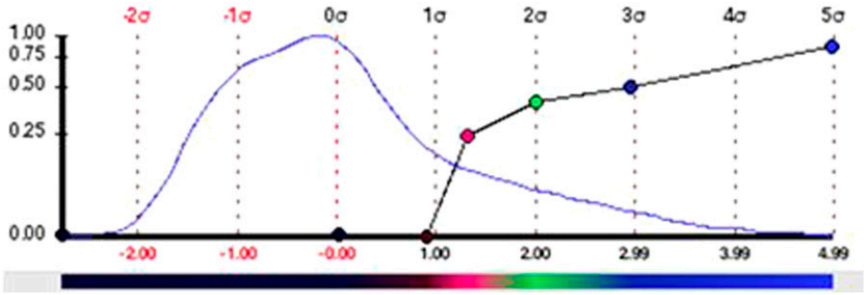
Table S1. Data collection and refinement statistics from a single crystal

Data collection	
Space group	$I4_122$
Cell dimensions	
a, b, c (Å)	76.7, 76.7, 488.2
α, β, γ (°)	90.0, 90.0, 90.0
Resolution (Å)	30–1.9 (1.97–1.9)*
R_{merge}	0.084 (0.652)
I /σI	20.8 (1.8)
Completeness (%)	98.1 (90.6)
Redundancy	20.8 (1.8)
Matthews coefficient (Å^3/Da)	2.11
Solvent content (%)	41.6
Refinement	
Resolution (Å)	30–1.9 (1.95–1.9)
No. reflections	53035
R_{work} /R_{free}	0.202/0.228
No. atoms	
Protein	5,494
Ligand	392
Water	150
B-factors (Å^2)	
Protein	26.0
Ligand	41.3
Water	34.2
Average	26.8
rms deviations	
Bond lengths (Å)	0.010
Bond angles (°)	1.181
Ramachandran most favored (%)	97.2
Ramachandran additional (%)	2.8
No. c-subunits per asymmetrical unit	10

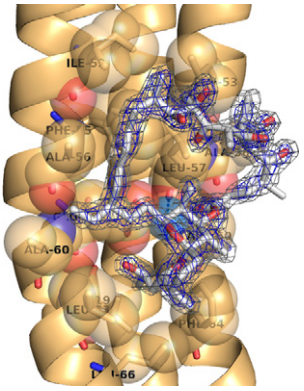
*Values in parentheses are for highest-resolution shell.



Movie S1. Electron density map for oligomycin 1 using a volume representation. The 2Fo-Fc map is shown colored as a gradient as shown below.



Movie S1



Movie S2. Binding site for oligomycin 1 with electron density for 2Fo-Fc contoured at 1.3σ (gray mesh) and 2.0σ (blue mesh).

Movie S2