

Supplementary Table. Computational approach to determining disulfide connectivity of cycloviolacin O14^a

set	Disulfide connectivity	DYANA target function ^b (Å ²)
1	I-II III-IV V-VI	7.85
2	I-II III-V IV-VI	6.80
3	I-II III-VI IV-V	10.38
4	I-III II-IV V-VI	8.60
5	I-III II-V IV-VI	5.96
6	I-III II-VI IV-V	10.04
7	I-IV II-III V-VI	5.65
8	I-IV II-V III-VI	4.90 ^c
9	I-IV II-VI III-V	5.11
10	I-V II-III IV-VI	10.88
11	I-V II-IV III-VI	14.09
12	I-V II-VI III-IV	10.70
13	I-VI II-III IV-V	8.77
14	I-VI II-IV III-V	5.71
15	I-VI II-V III-IV	5.32

^a Structures were calculated with each of the 15 alternative disulfide connectivities (sets 1-15) and the DYANA target functions were evaluated

^b Smaller numbers represent better fits amongst the ensemble of structures generated

^c Set 8 corresponds to the disulfide connectivity best fitting the restraint data and is the same connectivity determined experimentally for kalata B1 [38]