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**Selective Treatment of Cancer:
Synthesis, Biological Evaluation and Structural Elucidation of Novel
Analogues of the Antibiotic CC-1065 and the Duocarmycins**

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Experimental Section

CD measurements: CD investigations of (+)-*anti*-**5** were performed on a J-715 spectrometer (Jasco) in a 0.2 mm quartz cuvette at room temperature within the range of 200–400 nm. CD spectra were measured in acetonitrile ($c = 2.07 \text{ mmol mL}^{-1}$), methanol ($c = 2.04 \text{ mmol mL}^{-1}$) and ethanol ($c = 2.07 \text{ mmol mL}^{-1}$) (Figure S1).

Figure S1. CD spectra of (+)-*anti*-**5** measured in acetonitrile, methanol, and ethanol.

Computational details:

Table S1. Defined dihedral angles and heats of formation of the 16 minimum conformers found within the AM1 based conformational analysis of (1*S*,10*R*)-**5**.

Conformer	[ABCD] [°]	[EFGH] [°]	[IJKL] [°]	[MNOP] [°]	[QRST] [°]	$\Delta\Delta H_f$ [kcal/mol]
(1 <i>S</i> ,10 <i>R</i>)- 5 _{conf1}	172.2	-22.7	171.0	82.4	49.8	0.00
(1 <i>S</i> ,10 <i>R</i>)- 5 _{conf2}	172.3	-23.0	177.4	-177.3	25.5	0.56
(1 <i>S</i> ,10 <i>R</i>)- 5 _{conf3}	172.4	159.6	172.7	83.5	27.7	1.00
(1 <i>S</i> ,10 <i>R</i>)- 5 _{conf4}	172.5	160.6	-179.8	-178.2	30.3	1.44
(1 <i>S</i> ,10 <i>R</i>)- 5 _{conf5}	172.4	160.8	178.9	-179.0	-27.7	1.48
(1 <i>S</i> ,10 <i>R</i>)- 5 _{conf6}	-16.0	-21.3	172.9	81.2	49.5	1.72
(1 <i>S</i> ,10 <i>R</i>)- 5 _{conf7}	-16.2	-21.4	-179.1	179.6	-23.3	2.23
(1 <i>S</i> ,10 <i>R</i>)- 5 _{conf8}	-16.2	-21.4	179.6	-178.9	23.7	2.25
(1 <i>S</i> ,10 <i>R</i>)- 5 _{conf9}	-164.0	-22.9	171.2	82.9	50.0	2.28
(1 <i>S</i> ,10 <i>R</i>)- 5 _{conf10}	172.6	-23.5	80.9	83.9	31.1	2.37
(1 <i>S</i> ,10 <i>R</i>)- 5 _{conf11}	-15.2	158.4	174.0	82.4	25.3	2.68
(1 <i>S</i> ,10 <i>R</i>)- 5 _{conf12}	173.1	158.9	76.5	87.8	35.6	2.78
(1 <i>S</i> ,10 <i>R</i>)- 5 _{conf13}	-164.0	-23.2	177.4	-177.3	-25.1	2.86
(1 <i>S</i> ,10 <i>R</i>)- 5 _{conf14}	-15.5	158.8	-177.4	180.0	29.5	3.12
(1 <i>S</i> ,10 <i>R</i>)- 5 _{conf15}	-15.5	159.0	-178.4	179.0	-28.7	3.13
(1 <i>S</i> ,10 <i>R</i>)- 5 _{conf16}	-163.3	160.6	172.2	84.2	24.4	3.21

Figure S2. Comparison of the experimental CD curve of (+)-**5** (in acetonitrile) with the CD spectra calculated by a) the OM2^[20] based method, and b) by using the TDDFT/B3LYP/TZVP^[21–23] approach. The B3LYP based calculations for (1*S*,10*R*)-**5** have predicted very precisely all the excitation energies, but unexpectedly, the rotatory strength value of the transition at 250 nm (marked with a gray background) was calculated with a wrong sign.

¹H/¹³C-NMR: Numbering

(+)-(1*S*,10*R*)-**12a**: