The anthracyclines, a family of organic compounds of general formula I and analogs thereof, two members, daunomycin, Ia, and adriamycin, Ib, have found extensive clinical use as cancer chemotherapeutic agents. Both produce serious side effects including cumulative cardiotoxicity. Consequently considerable effort has been and is being invested toward the discovery of new analogs that are either active chemotherapeutic agents at much lower dose or are much less cardiotoxic.

The mechanisms of activity (chemotherapeutic and cardiotoxic) are topics of active current debate. The role that X-ray crystallography will play in helping to understand the mechanisms and in establishing structure-activity relationships at the molecular level remains to be determined.

This report presents the crystal structure determinations for two very different anthracyclines: 9-deacetyl daunomycin, Ic (as the hydrochloride), and 7-deoxyxorugol, Id (free base). Their respective space groups and lattice parameters are: P21_21_21, a=23.899(3), b=4,879(1), c=25,831(3) \( \beta = 97.231(9) \) and \( \beta = 102.1(6) \), \( a=24.282(6) \), \( b=9.110(2) \), \( c=53.007(10) \). The associated R-values are 0.073 (760 parameters, 30 data) and 0.019 (775 parameters, 4622 data). Both structures contain disordered solvent.

A comparison of these structures with others determined in our laboratory and from the literature will be presented.