

Calculation of the CD Spectrum of Class A β -Lactamase from *Escherichia coli* (TEM-1)

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Z. Naturforsch. **56 a**, 757–760 (2001); received September 12, 2001

The Circular Dichroism (CD) spectrum of β -lactamase from *Escherichia coli* (TEM-1) has been calculated with the matrix method on the basis of the x-ray diffraction structure. All known transitions in the peptide and side-chain groups, especially the aromatic and disulfide groups have been included. The calculations were performed with and without the tryptophan (Trp) residues. Rotational strengths calculated with the matrix method were combined with Gaussians to generate the CD spectrum. The calculated spectrum reproduces the signs and approximate magnitudes of the CD bands rather well only when the tryptophan side chains are included. However, the experimental negative double band at 208 and 222 nm, which is characteristic for α -helices, is absent in the calculated spectrum.

Key words: β -Lactamase; CD-spectrum; Matrix Method.