

Flow Linear Dichroism of Some Prototypical Proteins

Benjamin M. Bulheller, Alison Rodger, Matthew R. Hicks, Timothy R. Dafforn, Louise C. Serpell, Karen Marshall, Elizabeth H. C. Bromley, Patrick J. S. King, Kevin J. Channon, Derek N. Woolfson and Jonathan D. Hirst

- (26) Rodger, A.; Rajendra, J.; Marrington, R.; Ardammar, M.; Nordén, B.; Hirst, J.D., Gilbert, A.T.B.; Dafforn, T.R.; Halsall, D.J.; Woolhead, C.A.; Robinson, C.; Pinheiro, T.J.T.; Kazlauskaitė, J.; Seymour, M.; Perez, N.; Hannon, M.J. *Phys. Chem. Chem. Phys.* **2002**, *4*, 4051–4057.

LD Calculation of 1fsz-z

The z axis is defined as *parallel* orientation, x and y as *perpendicular*. The protein is rotated with a certain rotation interval about the *rotation axis* until a full rotation has been carried out. For each rotation the LD spectrum is determined. After this, the protein and its rotation axis are tilted away from the initial position around the *tilt axis* about a given tilt interval and rotated again. This is repeated until a maximum tilt angle is reached.

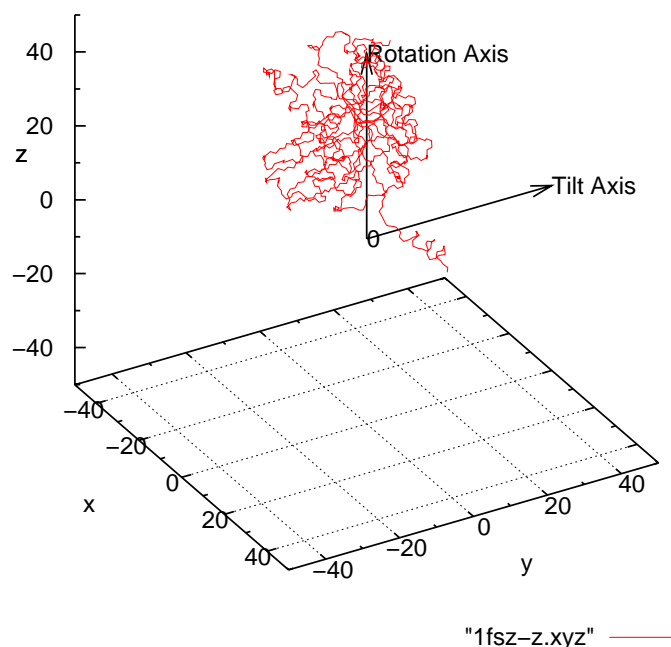
The spectra show the LD, calculated by the formula

$$LD = A_{\parallel} - A_{\perp} = \mu_z^2 - \frac{1}{2}(\mu_x^2 + \mu_y^2)$$

Parameters for this calculation

Tilt Axis:	y	Rotation Axis:	z
Tilt Interval:	30°	Rotation Interval:	60°
Tilt Angle:	90°	Rotation Angle:	360°

Original Orientation



This calculation was done using DichroCalc <http://comp.chem.nottingham.ac.uk/dichrocalc>

B.M. Bulheller & J.D. Hirst, DichroCalc – Circular and Linear Dichroism Online.

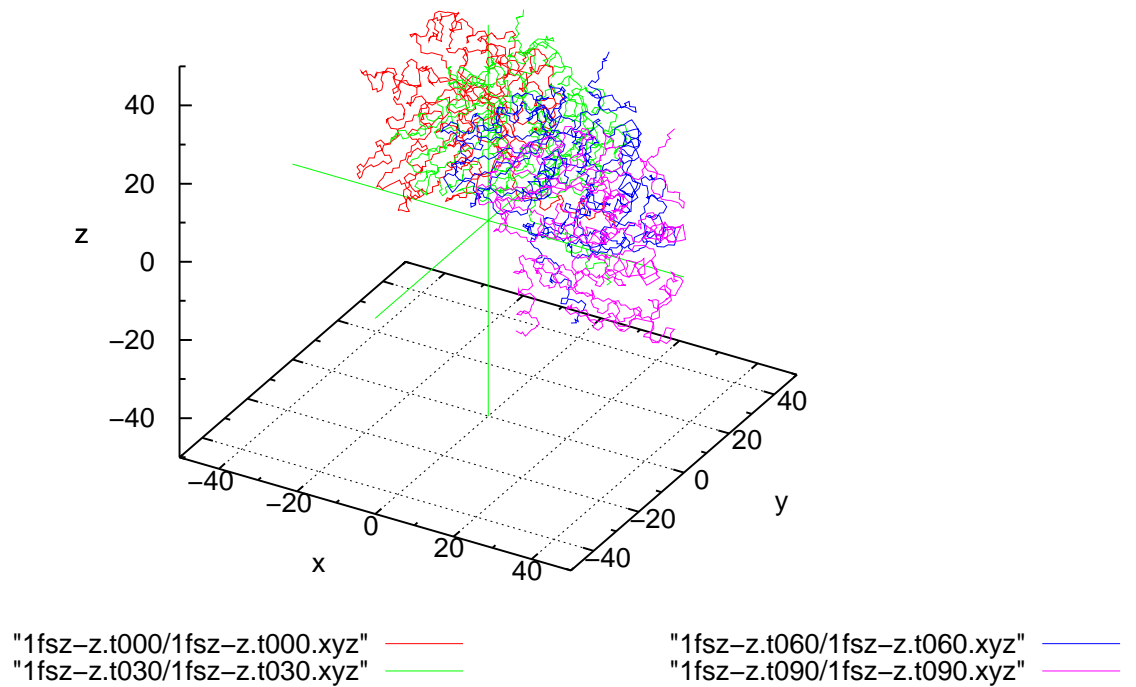
Bioinformatics, **25**, 539–540 (2009).

Plot of the Protein Orientations at All Angles

Initial Orientation at All Tilt Angles

The protein is rotated about the tilt axis using the tilt interval. Each of the structures shown in the next figure is then rotated about the rotation axis. The initial rotation axis is z and is tilted about the tilt axis with the protein.

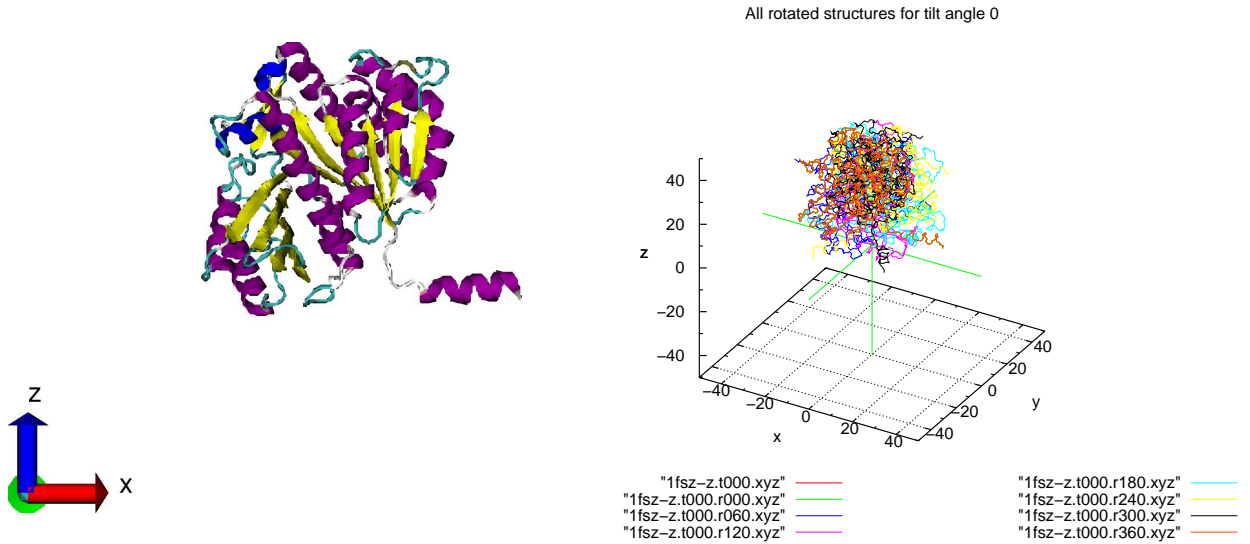
Structures for all tilt angles



Plot of the Rotations at All Tilt Angles

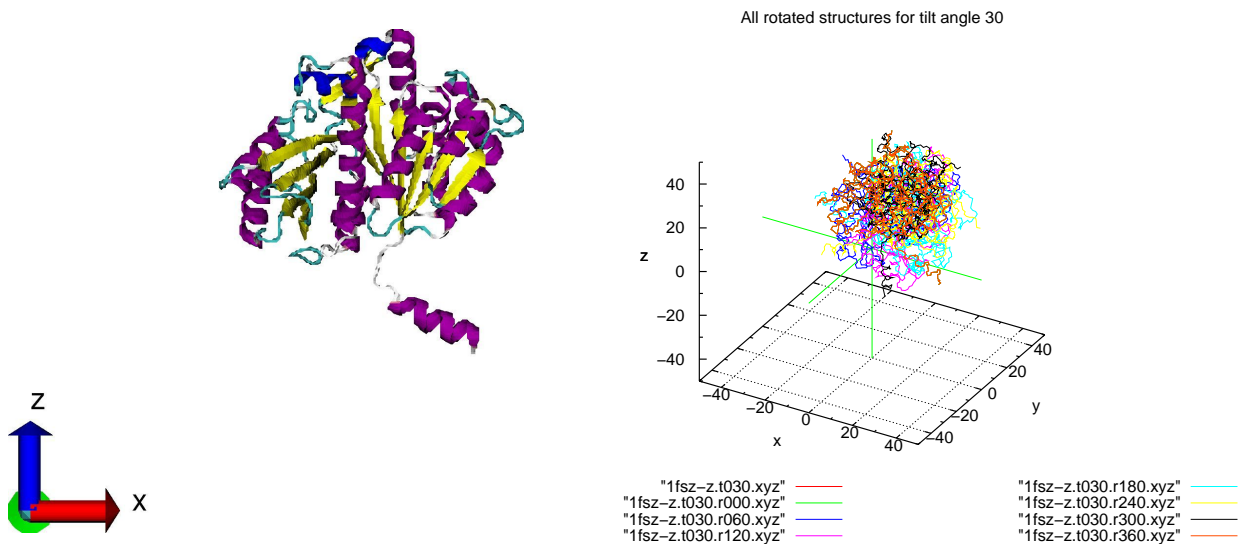
Tilt Angle 0°

After the protein has been tilted 0° about the tilt axis y , it is rotated in 60° intervals around the rotation axis until 360° are reached.



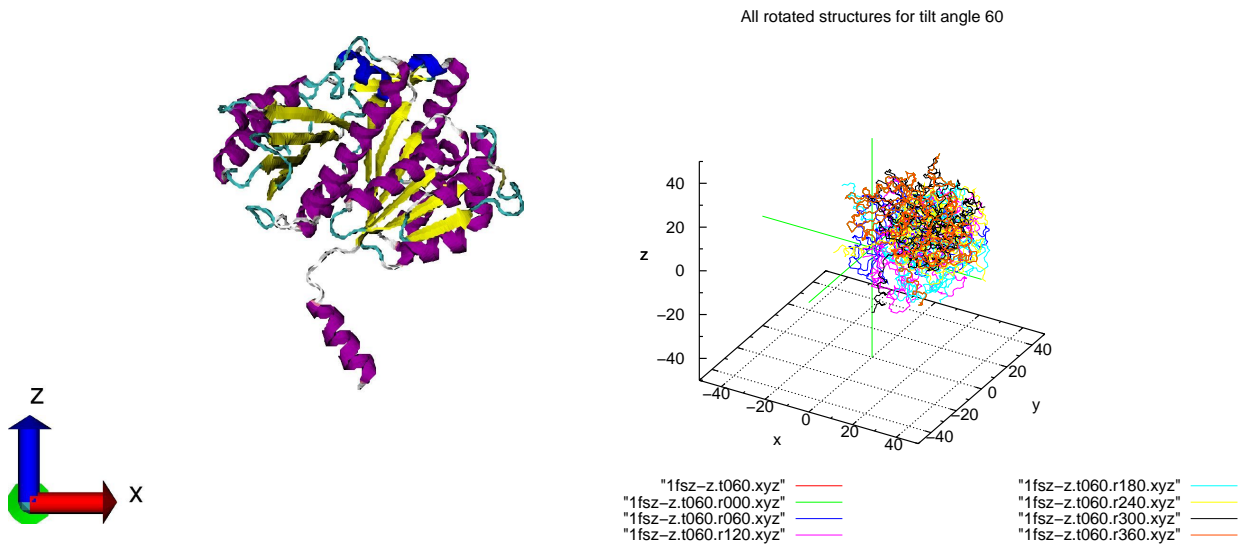
Tilt Angle 30°

After the protein has been tilted 30° about the tilt axis y , it is rotated in 60° intervals around the rotation axis until 360° are reached.



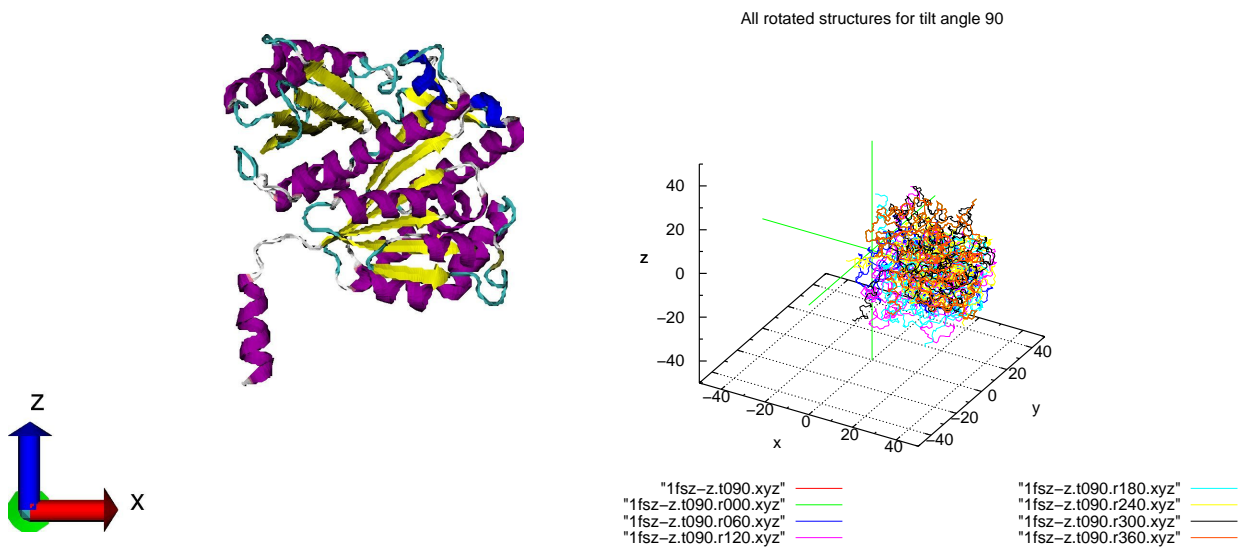
Tilt Angle 60°

After the protein has been tilted 60° about the tilt axis y , it is rotated in 60° intervals around the rotation axis until 360° are reached.



Tilt Angle 90°

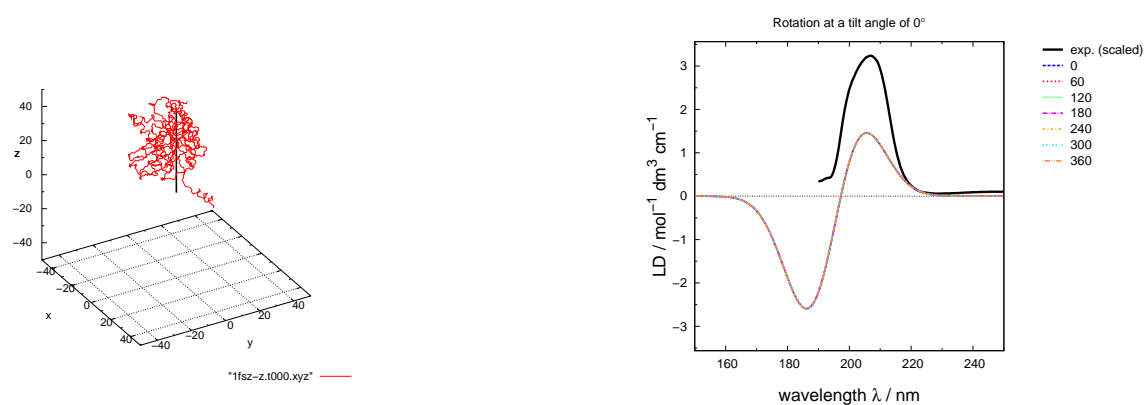
After the protein has been tilted 90° about the tilt axis y , it is rotated in 60° intervals around the rotation axis until 360° are reached.



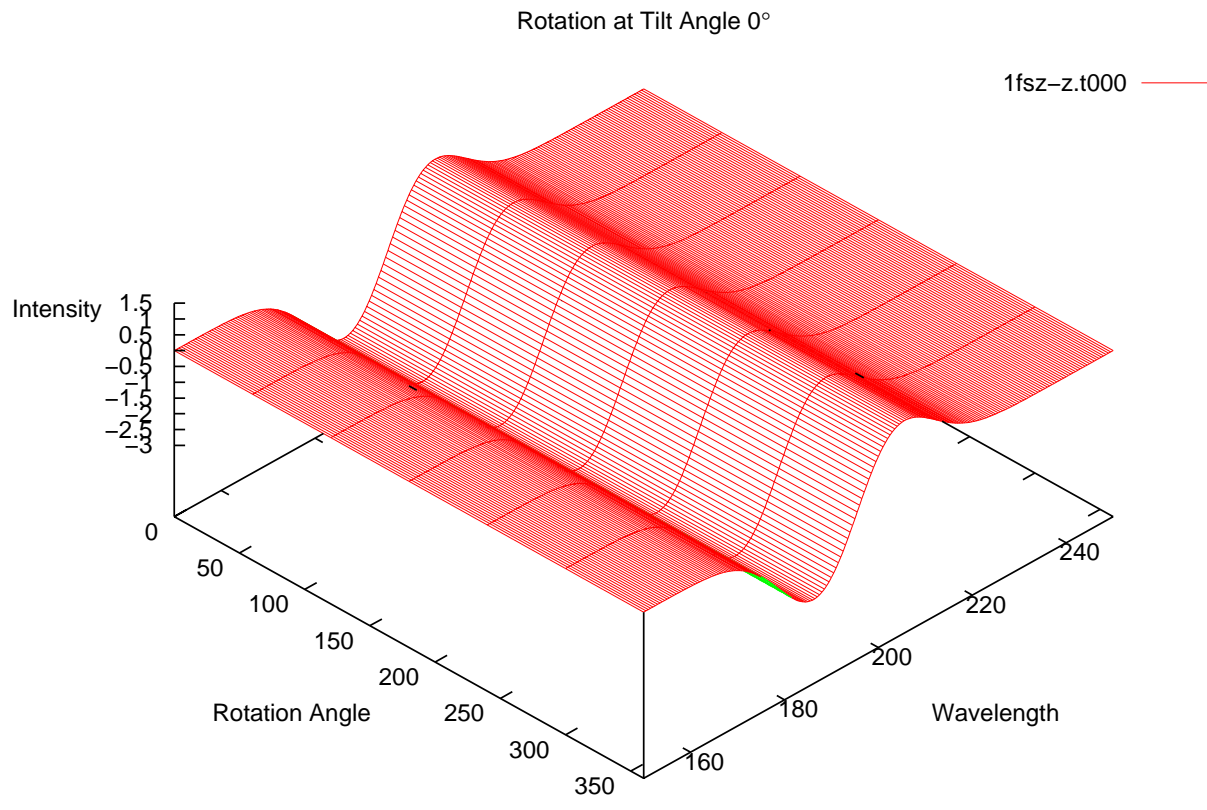
Tilt Angle 0°

Directory: 1fsz-z.t000
Rotation Axis: $x = 0.000$
 $y = 0.000$
 $z = 1.000$

Single Spectra of Rotations



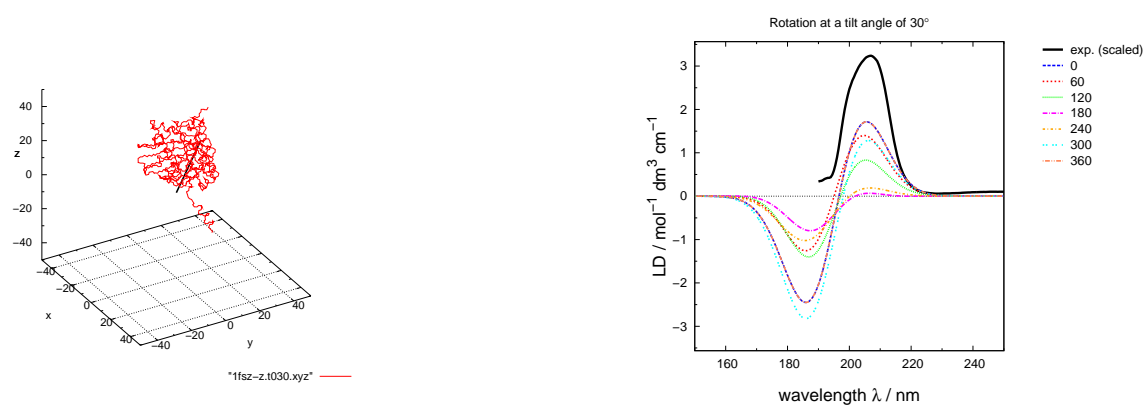
3D View



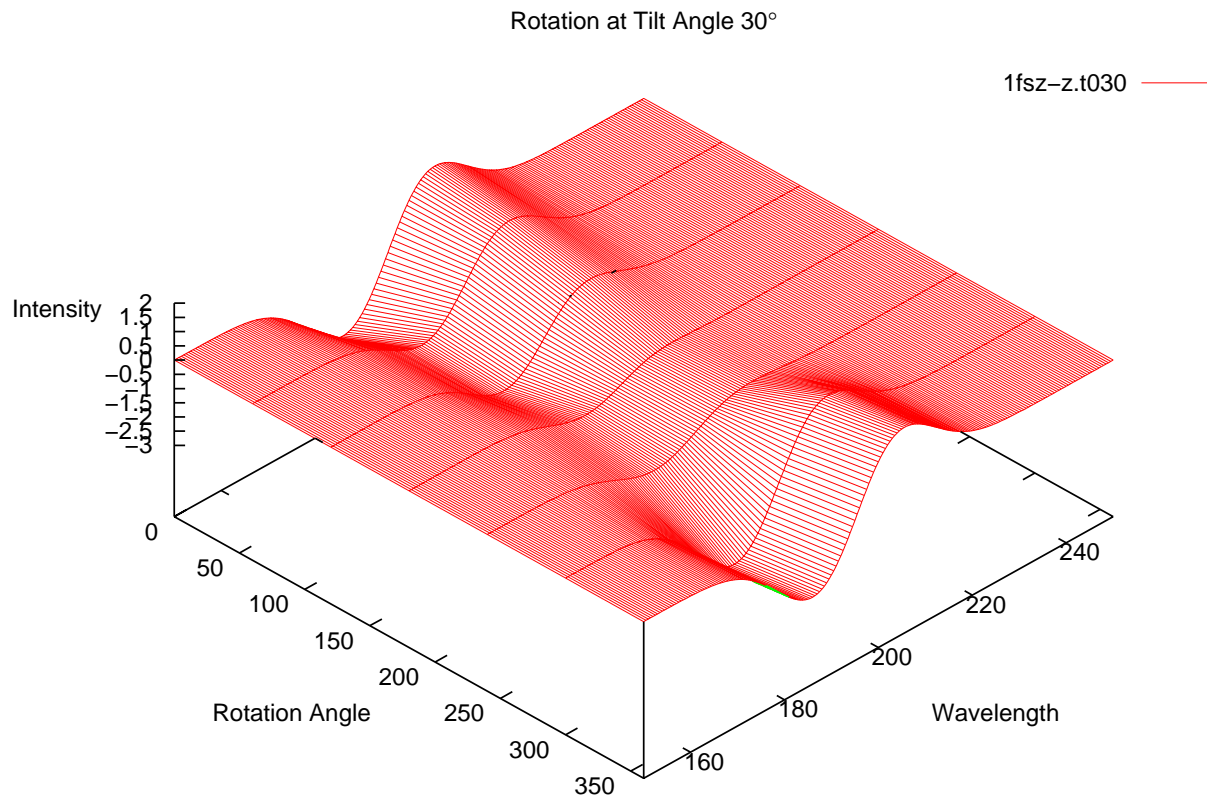
Tilt Angle 30°

Directory: 1fsz-z.t030
Rotation Axis: $x = 0.500$
 $y = 0.000$
 $z = 0.866$

Single Spectra of Rotations



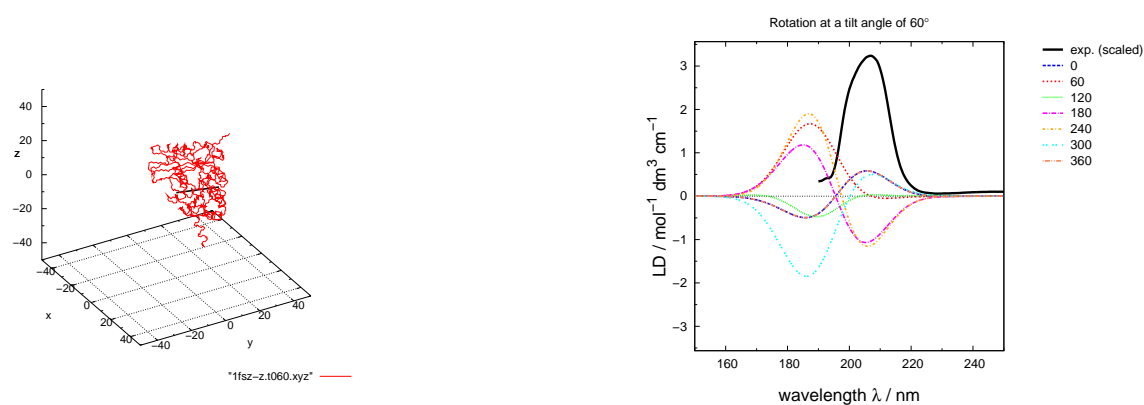
3D View



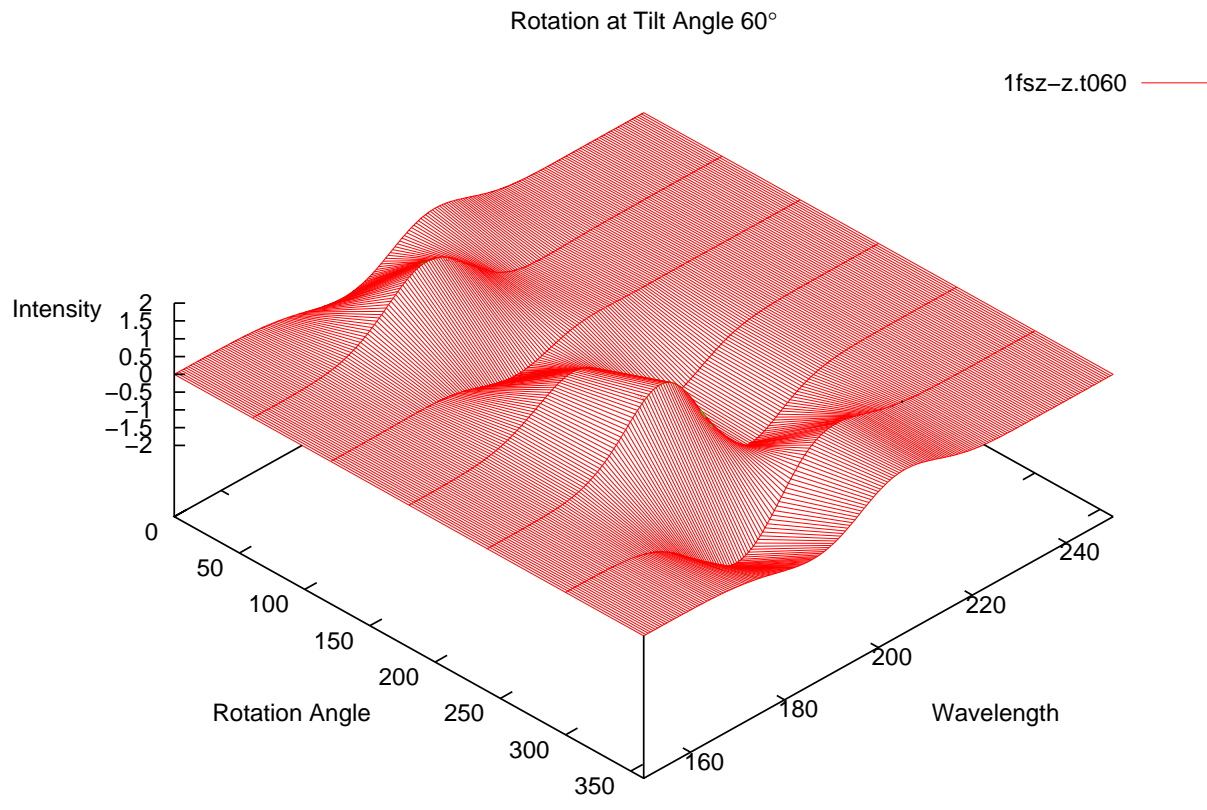
Tilt Angle 60°

Directory: 1fsz-z.t060
Rotation Axis: $x = 0.866$
 $y = 0.000$
 $z = 0.500$

Single Spectra of Rotations



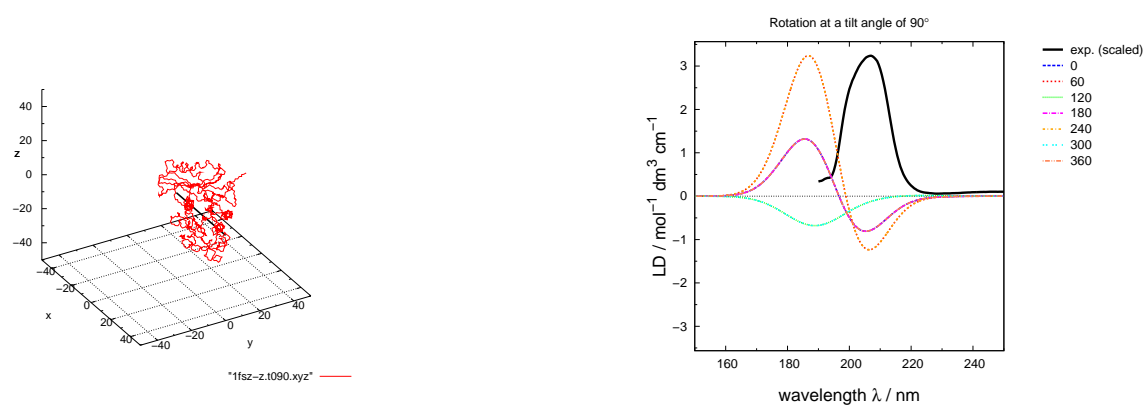
3D View



Tilt Angle 90°

Directory: 1fsz-z.t090
Rotation Axis: $x = 1.000$
 $y = 0.000$
 $z = 0.000$

Single Spectra of Rotations



3D View

