Cholic Acid Derivatives Containing Both 2-Naphthylcarbamate and 3,5-Dinitrophenylcarbamate Groups: A Combined Circular Dichroism-Molecular Mechanics Approach to the Definition of their Molecular Conformation

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Figure S6: Minimum energy conformations of compound **2** (**2a=black, 2b=green, 2c=magenta, 2d=orange, 2e=cyan, 2f=red, 2g=yellow**), whose theoretical CD spectrum agreed acceptably well (as far as sign, number position and order of magnitude of the dichroic bands are concerned) with the experimental one, superimposed on the iso-oriented cholestanic backbone. For the sake of clarity, hydrogen atoms and the alkyl chain at 17-position are not displayed.

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Mol.	Range	Area		Width	Height	λ_0
1 Exp.	[237.2, 248.6]	606.1	243.8	9.0	99.3	234.3
1a	[238.0, 250.7]	730.9	241.6	6.4	99.6	238.0
1b	[236.4, 249.1]	1016.7	240.4	6.4	138.7	236.4
1c	[238.2, 251.0]	682.8	241.6	6.5	93.2	238.2
1d	[231.9, 248.8]	722.1	239.2	9.2	78.3	231.9
1f	[237.9, 254.7]	753.7	243.9	9.0	78.6	237.9
2 Exp.	[240.6, 248.7]	673.5	244.4	6.0	149.1	236.8
2a	[237.2, 250.1]	1211.4	241.6	7.6	163.3	237.2
2b	[237.2, 250.4]	1169.9	241.0	7.6	155.4	237.2
2c	[237.2, 250.2]	972.5	241.6	7.6	131.3	237.2
2d	[236.6, 250.1]	930.9	241.0	7.6	121.6	236.6
2e	[237.2, 250.2]	1152.3	241.0	5.8	154.7	237.2
2f	[237.0, 250.3]	931.4	241.6	7.6	124.3	237.0
2g	[236.2, 249.9]	1105.2	241.0	8.2	142.7	236.1
3 Exp.	[236.6, 248.6]	213.5	243.2	9.6	32.6	231.4
3a	[236.8, 250.0]	344.2	241.0	7.6	45.5	236.8
3b	[237.9, 250.0]	432.3	241.6	7.0	62.1	238.0
3c	[238.0, 250.5]	247.1	241.6	7.6	35.2	238.0
3d	[235.0, 258.0]	358.2	244.5	10.8	28.7	235.0
3e	[236.9, 249.6]	364.4	241.0	6.4	49.9	236.8
4 Exp.	[240.4, 248.5]	1122.7	244.2	6.2	254.4	237.7
4a	[239.6, 255.4]	2211.3	245.1	7.8	243.9	239.5
4b	[238.6, 251.8]	1856.2	242.7	5.9	244.7	238.6
4c	[237.8, 252.7]	1888.9	242.7	8.3	220.6	237.7
4d	[237.9, 251.4]	1815.4	241.6	7.6	242.1	238.0
4e	[238.4, 252.2]	1665.9	242.7	6.5	210.7	238.5
4f	[238.8, 252.6]	1841.4	243.3	6.5	231.3	238.7

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