SUPPORTING INFORMATION

Solution structures of cyclosporin A and its complex with dysprosium(III) in SDS micelles: NMR and molecular dynamics studies

Francesca Bernardi, Nicola D'Amelio, Elena Gaggelli, Elena Molteni, Gianni Valensin

Table S1: List of the NOE-derived distance restraints used for structure determination of free CsA in H_2O/SDS, in the form of "upper limit" (upl) constraints; the corresponding "lower limits" are 0.02 nm smaller

res1 number	res1 name	atom1 name	res2 number	res2 name	atom2 name	distance (Å)
1	MeBmt	HN	1	MeBmt	Hβ	4.05
1	MeBmt	Hα	2	Abu	HN	2.43
1	MeBmt	Hβ	2	Abu	HN	2.03
1	MeBmt	Hδ11	1	MeBmt	HN	3.42
1	MeBmt	Hδ11	1	MeBmt	Hβ	3.22
1	MeBmt	Hδ11	1	MeBmt	Hδ21	3.67
1	MeBmt	Hζ	1	MeBmt	Hδ21	2.41
1	MeBmt	Hζ	1	MeBmt	Hδ22	2.44
1	MeBmt	Hδ21	1	MeBmt	Hβ	2.70
1	MeBmt	Hδ22	1	MeBmt	Hβ	2.58
1	MeBmt	Hδ22	1	MeBmt	Hδ11	3.40
1	MeBmt	Hδ22	1	MeBmt	Hδ21	1.98
1	MeBmt	Hγ2	1	MeBmt	Hδ11	2.98
2	Abu	Hα	2	Abu	HN	3.25
2	Abu	Hα	2	Abu	Hβ2	3.10
2	Abu	Hα	2	Abu	Hβ3	3.02
2	Abu	Hβ2	3	Sar	HN	4.00
2	Abu	Hβ3	2	Abu	HN	2.32
2	Abu	Hβ3	3	Sar	HN	3.99
2	Abu	Hγ1	2	Abu	HN	3.72
2	Abu	Hγ1	3	Sar	HN	3.62
3	Sar	HN	3	Sar	Hα2	3.31
3	Sar	Hα1	3	Sar	HN	2.55
3	Sar	Hα1	3	Sar	Hα2	2.23
3	Sar	Hα1	4	MeLeu	HN	2.82
4	MeLeu	HN	3	Sar	Hα2	3.38
4	MeLeu	HN	4	MeLeu	Hβ2	3.26
4	MeLeu	HN	4	MeLeu	Hβ3	3.80
4	MeLeu	HN	4	MeLeu	Hγ	3.29
4	MeLeu	HN	5	Val	HN	3.58
4	MeLeu	Hα	4	MeLeu	HN	3.43
4	MeLeu	Hα	4	MeLeu	Hβ2	3.07
4	MeLeu	Hα	5	Val	HN	2.51
5	Val	Hα	5	Val	HN	3.02
5	Val	Hα	5	Val	Hβ	2.64
5	Val	Hα	6	MeLeu	HN	2.63
5	Val	Hβ	5	Val	HN	2.10
5	Val	Hγ11	5	Val	HN	3.41
5	Val	Hγ21	5	Val	HN	3.95
6	MeLeu	HN	6	MeLeu	Hβ2	3.09
6	MeLeu	HN	6	MeLeu	Hγ	4.32
6	MeLeu	Hα	6	MeLeu	Hβ2	3.37
6	MeLeu	Hα	6	MeLeu	Hβ3	3.15
6	MeLeu	Hα	6	MeLeu	Hγ	2.55
6	MeLeu	Hα	7	Ala	HN	2.31
6	MeLeu	Hα	8	D-Ala	HN	3.35
6	MeLeu	Hβ2	6	MeLeu	Hβ3	1.87
6	MeLeu	Hβ2	6	MeLeu	Hγ	2.41
6	MeLeu	Hβ3	6	MeLeu	HN	2.88
6	MeLeu	Hδ21	7	Ala	HN	3.45

7	Ala	Hα	7	Ala	HN	2.96
7	Ala	Hα	7	Ala	Hβ1	2.93
7	Ala	Hα	8	D-Ala	HN	3.01
7	Ala	Hβ1	7	Ala	HN	2.99
7	Ala	Hβ1	8	D-Ala	HN	3.63
8	D-Ala	Hα	8	D-Ala	HN	2.90
8	D-Ala	Hα	9	MeLeu	HN	2.51
8	D-Ala	Hβ1	9	MeLeu	HN	2.69
9	MeLeu	HN	9	MeLeu	Hβ2	2.99
9	MeLeu	HN	10	MeLeu	Hβ2	3.85
9	MeLeu	Hα	9	MeLeu	HN	3.70
9	MeLeu	Hα	9	MeLeu	Hβ2	3.27
9	MeLeu	Hβ2	9	MeLeu	Hβ3	1.87
9	MeLeu	Hβ2	9	MeLeu	Hγ	2.26
9	MeLeu	Hγ	9	MeLeu	Hδ11	3.02
9	MeLeu	Hγ	9	MeLeu	Hδ21	2.80
9	MeLeu	Hδ21	9	MeLeu	Hα	3.24
10	MeLeu	HN	10	MeLeu	Hβ2	3.30
10	MeLeu	Hα	9	MeLeu	Hα	2.35
10	MeLeu	Hα	10	MeLeu	Hδ11	3.18
10	MeLeu	Hδ11	10	MeLeu	Hβ2	2.65
11	MeVal	HN	8	D-Ala	HN	3.74
11	MeVal	HN	11	MeVal	Hβ	2.97
11	MeVal	Hα	1	MeBmt	HN	2.53
11	MeVal	Hα	11	MeVal	Hγ11	3.00
11	MeVal	Hβ	11	MeVal	Hγ21	2.74
11	MeVal	Hγ11	1	MeBmt	HN	2.90
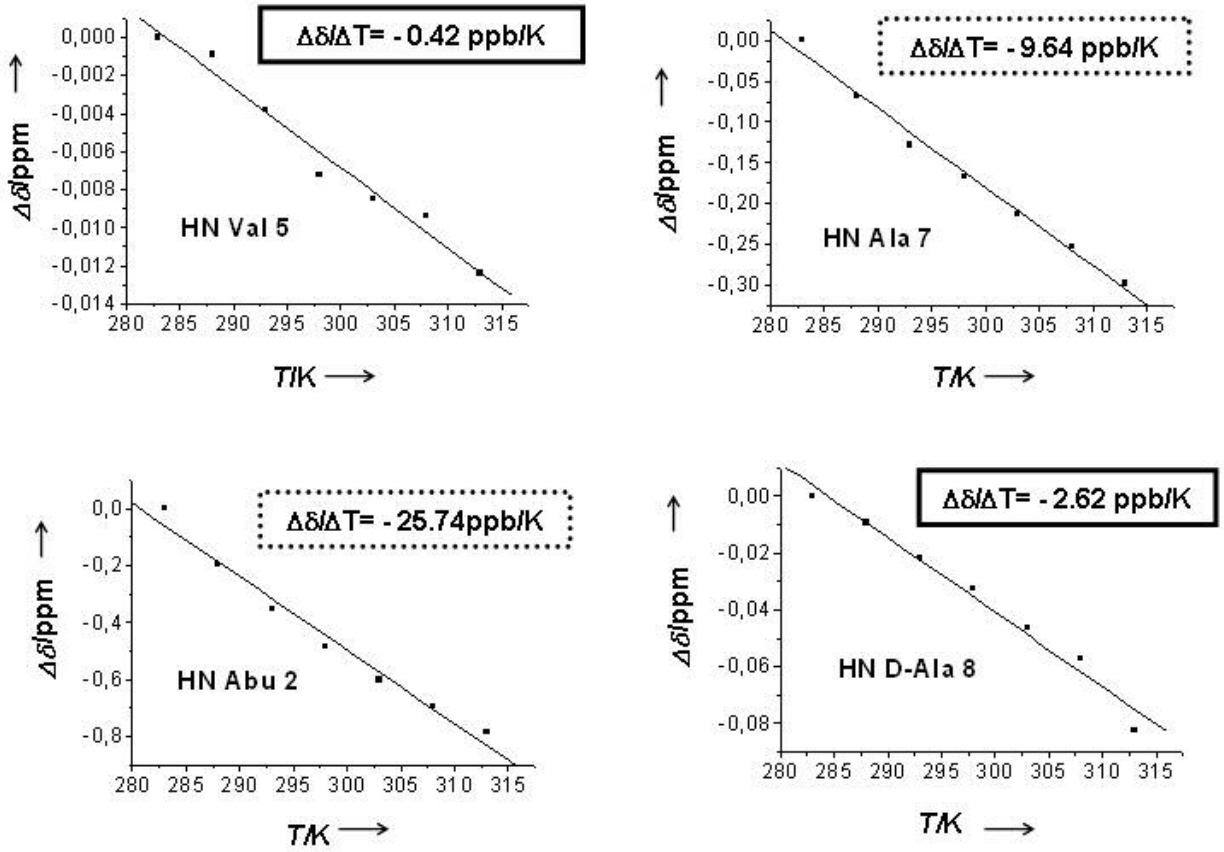
Figure S1. Plots of the chemical shift variations as a function of temperature for the mobile protons of free CsA in micelles, with the temperature coefficients obtained by the linear fitting.