

Supporting Information

Introduction of a α,β -unsaturated carbonyl conjugated pyrene-lactose hybrid as a fluorescent molecular probe for micro-scale anisotropic media

Ivy Sarkar^a, Arasappan Hemamalini^b, Thangamuthu Mohan Das^{*b,c}, Ashok Kumar Mishra^{*a}

^a Department of Chemistry, Indian Institute of Technology Madras, Chennai – 600 036, India

^b Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai - 600 025,
India

^c Department of Chemistry, School of Basic and Applied Sciences, Central University of Tamil
Nadu, Thiruvavur – 610 101, India

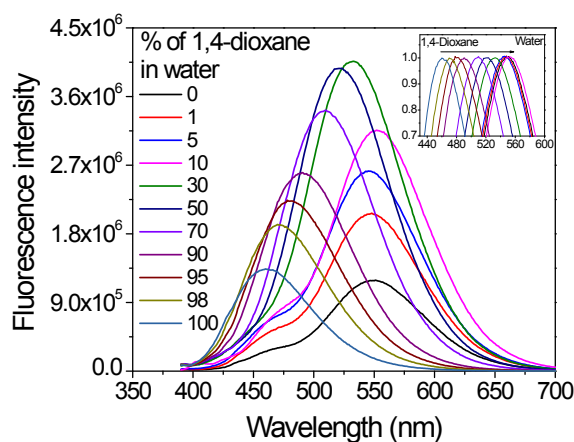


Figure S1: Fluorescence spectra of pyd-lact in water with increasing % of 1,4-dioxane and inset shows normalized fluorescence spectra, at λ_{ex} 380 nm.

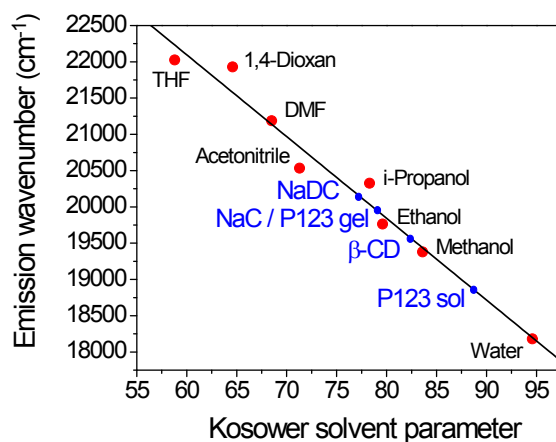


Figure S2: Determination of the medium polarity from λ_{em} value using Kosower Z scale for β -CD, bile salts (NaC, NaDC) and pluronics media.

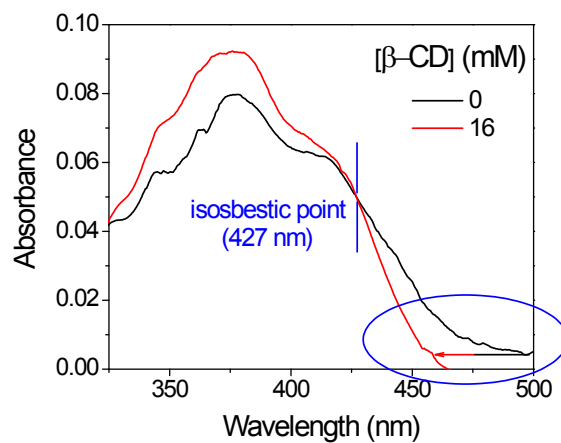
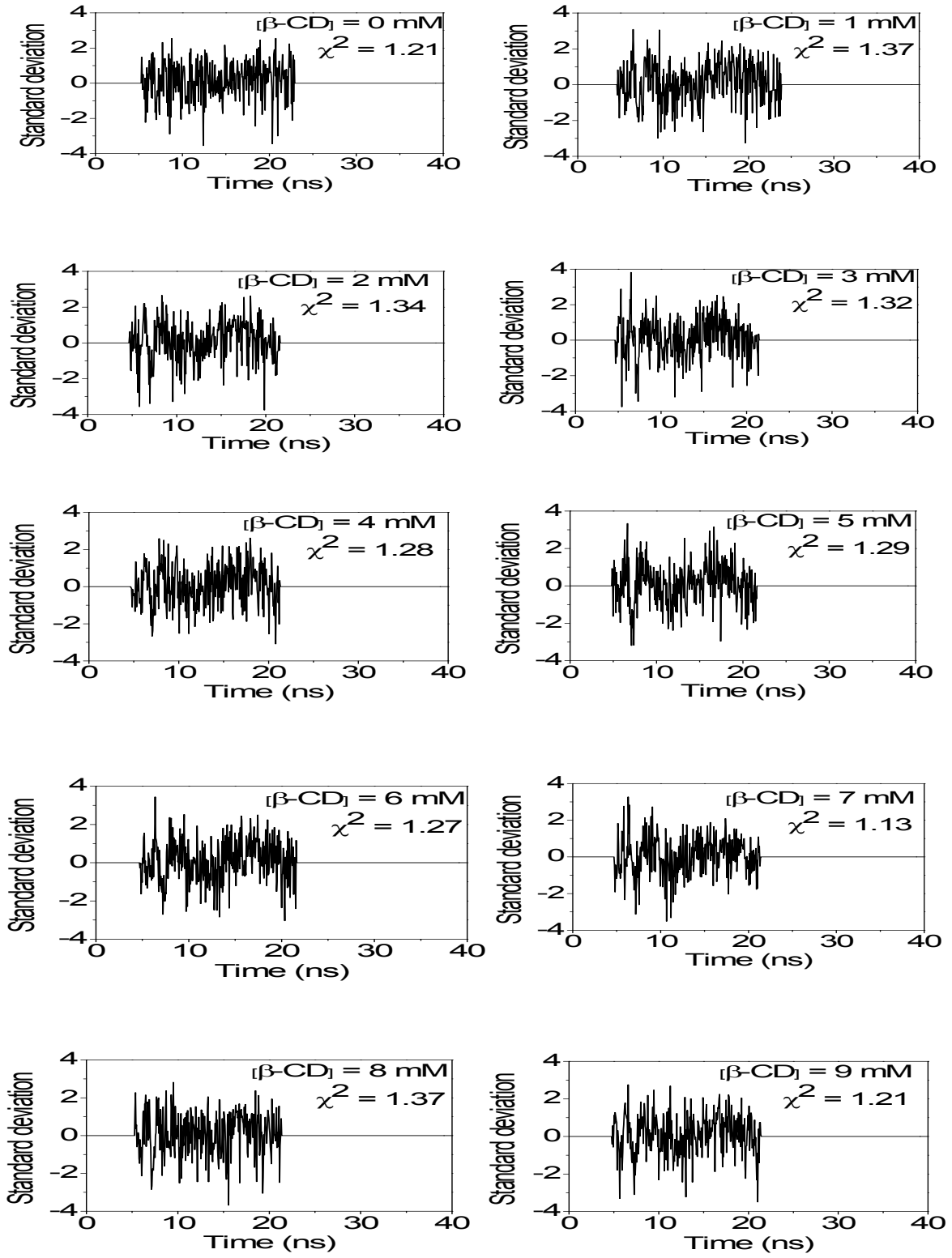


Figure S3: Absorbance spectra of pyd-lact in water and 16 mM β -CD concentration.

Table S1: Fluorescence lifetime data of pyd-lact with increasing β -CD concentration, $\lambda_{\text{ex}} = 370$ nm.

$[\beta\text{-CD}]$ (mM)	τ_1 (β_1)	τ_2 (β_2)	τ_{avg} (ns)	χ^2
0	0.52 (0.99)	3.65 (0.01)	0.55	1.21
1	0.54 (0.89)	1.92 (0.11)	0.69	1.37
2	0.56 (0.81)	1.82 (0.19)	0.80	1.34
3	0.61 (0.77)	1.82 (0.23)	0.89	1.32
4	0.62 (0.75)	1.80 (0.25)	0.91	1.28
5	0.72 (0.75)	1.87 (0.25)	1.01	1.29
6	0.71 (0.74)	1.86 (0.26)	1.01	1.27
7	0.74 (0.74)	1.85 (0.26)	1.03	1.13
8	0.90 (0.78)	1.97 (0.22)	1.13	1.37
9	0.75 (0.74)	1.82 (0.26)	1.03	1.21
10	0.76 (0.74)	1.82 (0.26)	1.04	1.18
12	0.78 (0.74)	1.81 (0.26)	1.05	1.26
14	0.93 (0.83)	2.03 (0.17)	1.12	1.37
16	0.96 (0.84)	2.06 (0.16)	1.14	1.21



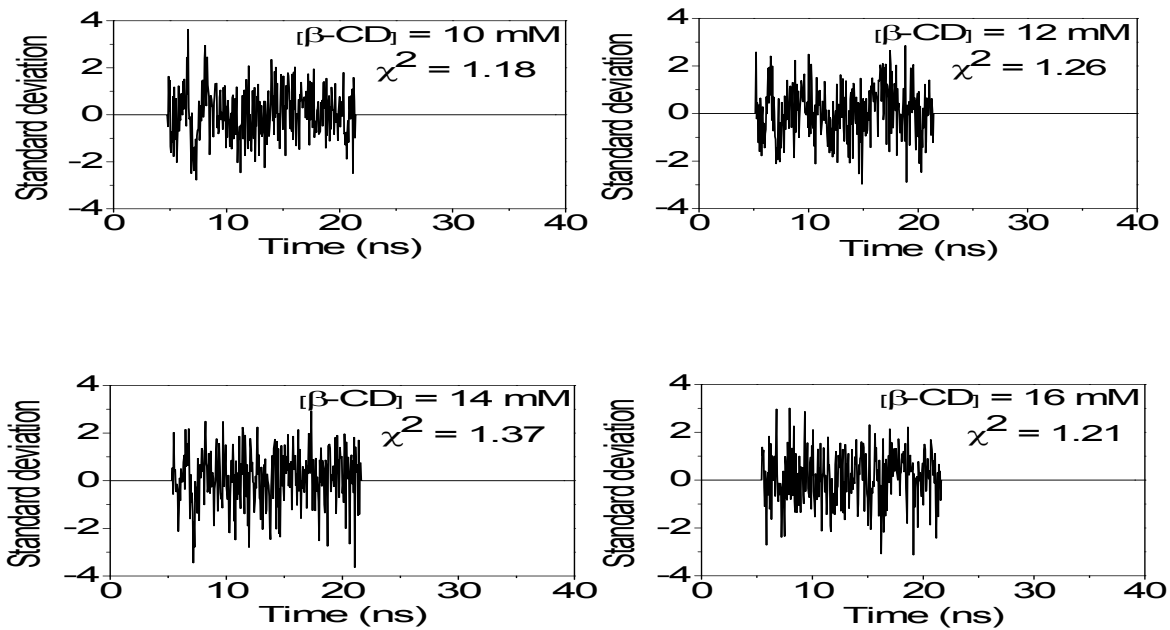


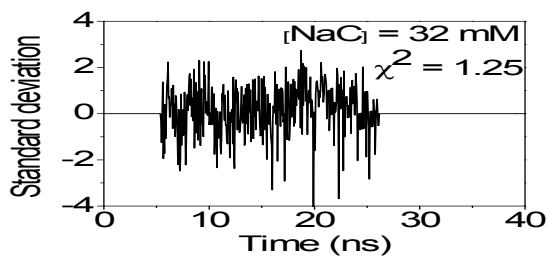
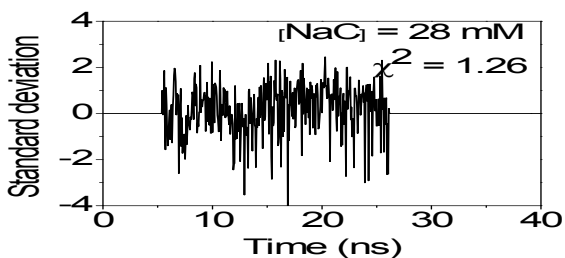
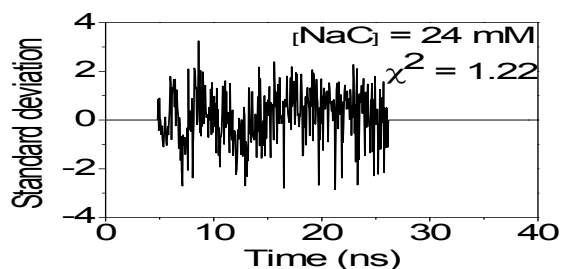
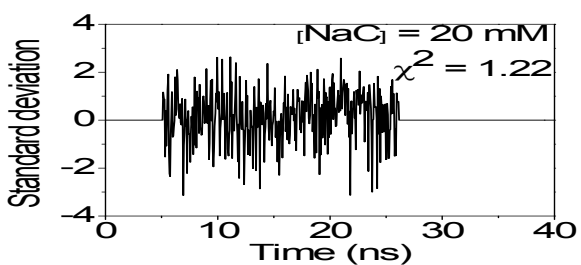
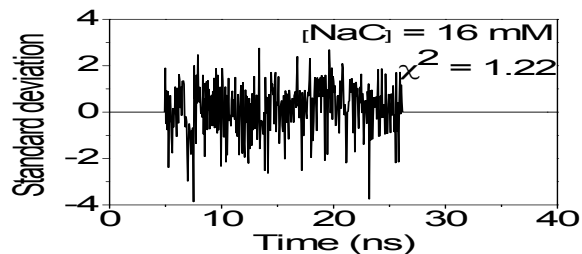
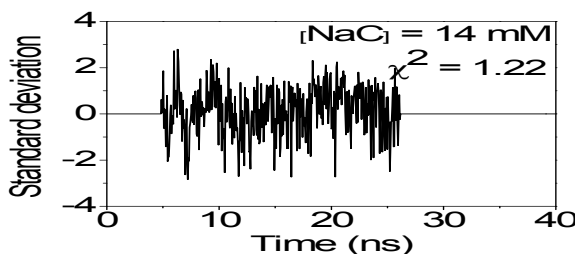
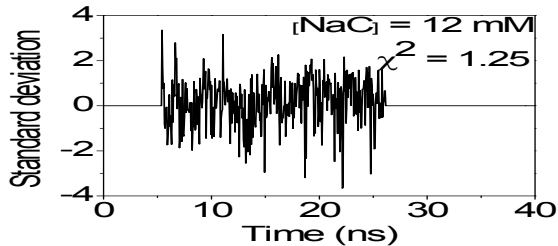
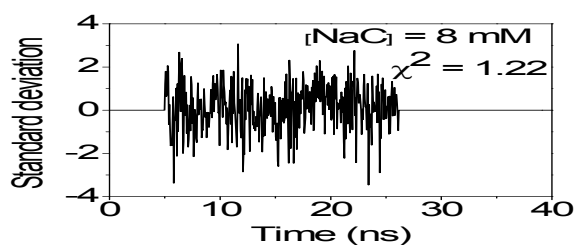
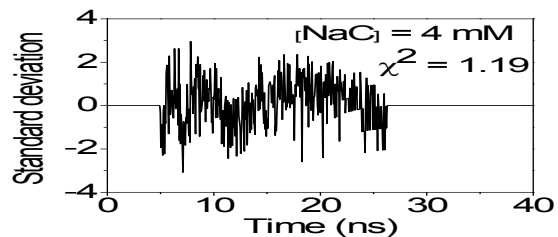
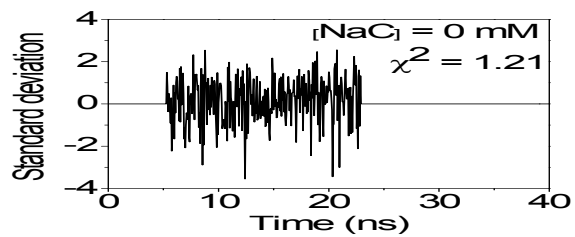
Figure S4: Residue distribution plots of pyd-lact in β -CD (corresponds to Table S1).

Table S2: Fluorescence lifetime data of pyd-lact with increasing NaC concentration, at $\lambda_{\text{ex}} = 370 \text{ nm}$.

[NaC] (mM)	τ_1 (β_1)	τ_2 (β_2)	τ_{avg} (ns)	χ^2
0	0.52 (0.99)	3.65 (0.01)	0.55	1.21
4	0.63 (0.88)	2.09 (0.12)	0.81	1.19
8	1.03 (0.78)	2.51 (0.22)	1.36	1.22
12	1.02 (0.81)	2.51 (0.19)	1.30	1.25
14	0.88 (0.79)	2.32 (0.21)	1.18	1.22
16	0.79 (0.75)	2.17 (0.25)	1.13	1.22
20	0.89 (0.81)	2.36 (0.19)	1.17	1.22
24	0.80 (0.79)	2.20 (0.21)	1.09	1.22
28	0.88 (0.78)	2.23 (0.22)	1.18	1.26
32	0.82 (0.78)	2.19 (0.22)	1.12	1.25
36	0.86 (0.80)	2.26 (0.20)	1.14	1.24
40	0.77 (0.78)	2.14 (0.22)	1.07	1.19
44	0.81 (0.80)	2.25 (0.20)	1.10	1.21
48	0.77 (0.79)	2.18 (0.21)	1.07	1.20

Table S3: Fluorescence lifetime data of pyd-lact with increasing NaDC concentration, at $\lambda_{\text{ex}} = 370$ nm.

[NaDC] (mM)	τ_1 (β_1)	τ_2 (β_2)	τ_{avg} (ns)	χ^2
0	0.52 (0.99)	3.65 (0.01)	0.55	1.21
1	0.61 (0.92)	2.76 (0.08)	0.78	1.25
2	0.66 (0.89)	2.55 (0.11)	0.87	1.36
3	0.92 (0.84)	2.53 (0.16)	1.18	1.21
4	0.86 (0.83)	2.32 (0.17)	1.11	1.31
5	0.82 (0.81)	2.13 (0.19)	1.07	1.22
6	0.84 (0.81)	2.08 (0.19)	1.08	1.20
7	0.87 (0.83)	2.19 (0.17)	1.09	1.27
8	0.86 (0.82)	2.16 (0.18)	1.09	1.21
10	0.85 (0.82)	2.13 (0.18)	1.08	1.11
12	0.88 (0.83)	2.20 (0.17)	1.10	1.29
14	0.88 (0.84)	2.24 (0.16)	1.10	1.18
16	0.84 (0.79)	2.07 (0.21)	1.10	1.19
18	0.85 (0.81)	2.11 (0.19)	1.09	1.09



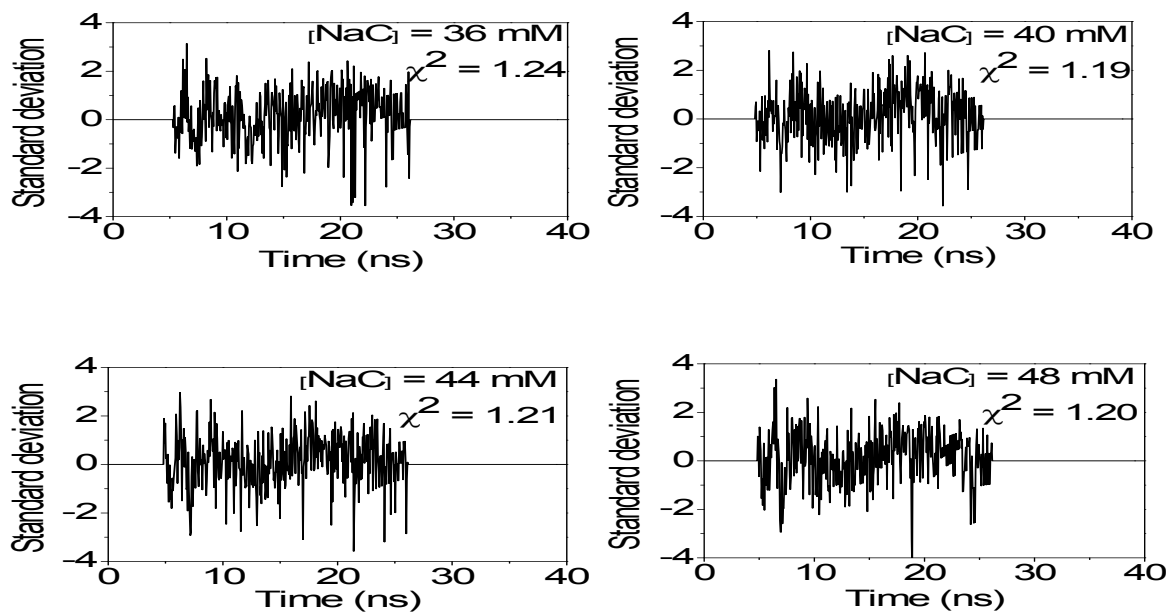
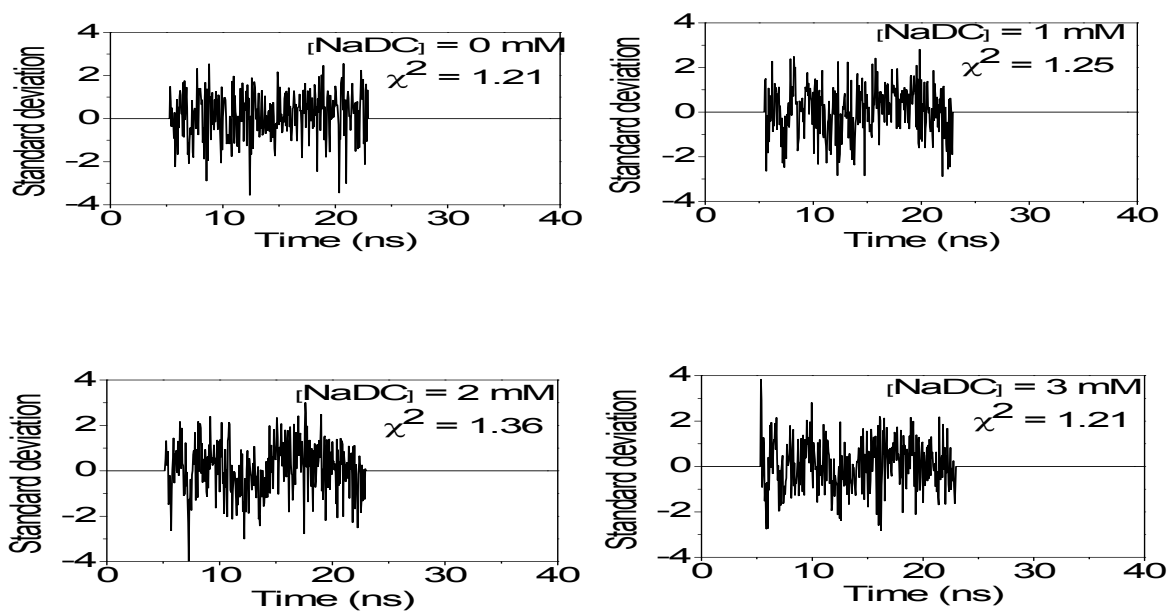


Figure S5: Residue distribution plots of pyd-lact in NaC (corresponds to Table S2).



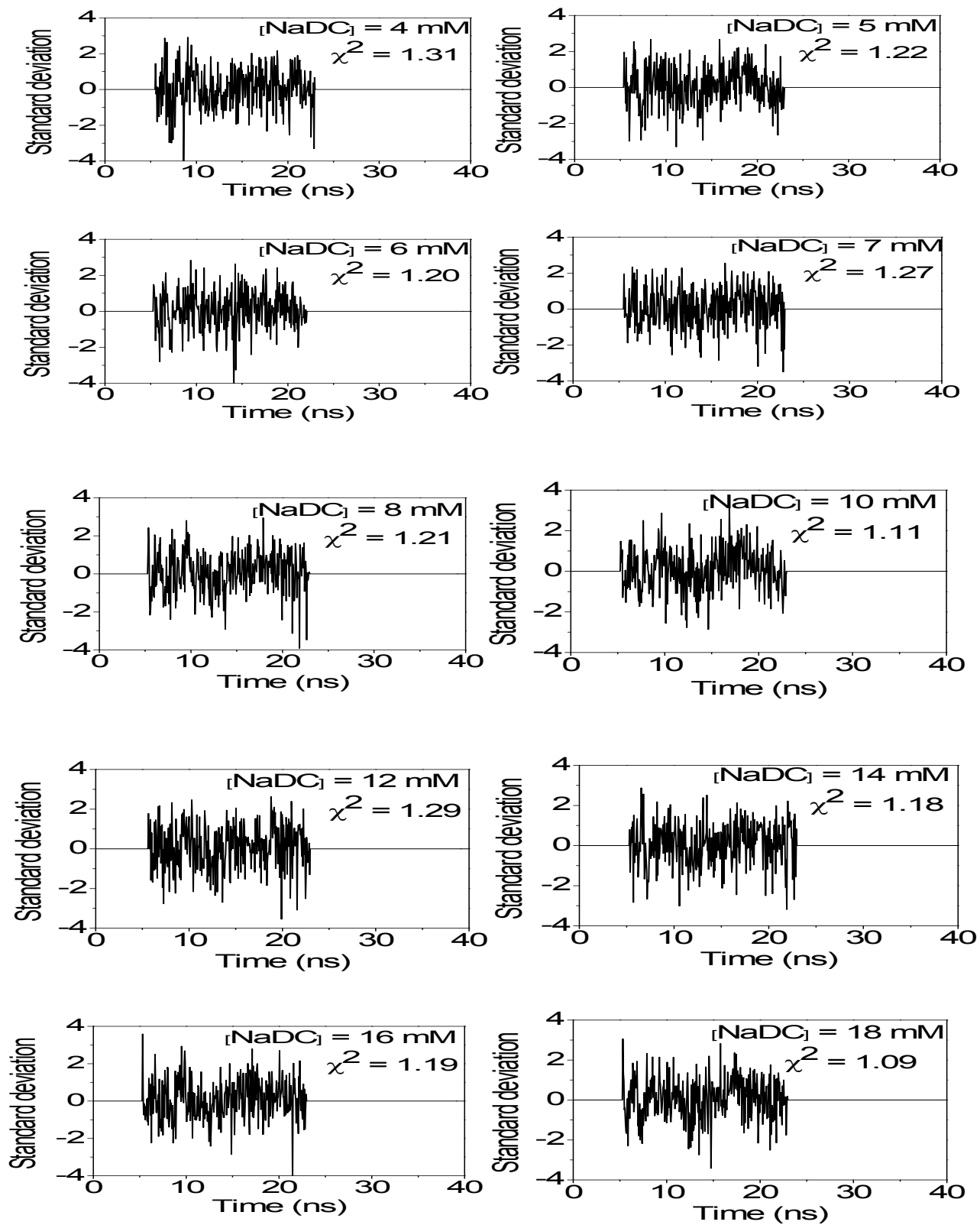


Figure S6: Residue distribution plots of pyd-lact in NaDC (corresponds to Table S3).

Table S4: Fluorescence lifetime data of pyd-lact in water and 10% pluronic P123 with increasing temperature, at $\lambda_{\text{ex}} = 370$ nm.

Sample	Temperature (°C)	τ_1 (β_1)	τ_2 (β_2)	τ_{avg} (ns)	χ^2
Water	5	0.80 (0.99)	4.27 (0.01)	0.83	1.14
	11	0.71 (0.98)	4.03 (0.02)	0.78	1.27
	15	0.66 (0.98)	3.76 (0.02)	0.72	1.21
	20	0.57 (0.98)	3.73 (0.02)	0.63	1.25
	24	0.60 (0.98)	4.09 (0.02)	0.67	1.32
P123 10%	5	1.37 (0.26)	2.60 (0.74)	2.28	1.22
	11	1.07 (0.31)	2.39 (0.69)	1.98	1.20
	15	1.08 (0.38)	2.19 (0.62)	1.77	1.27
	20	0.97 (0.67)	2.08 (0.33)	1.34	1.27
	24	1.02 (0.77)	2.11 (0.23)	1.27	1.32

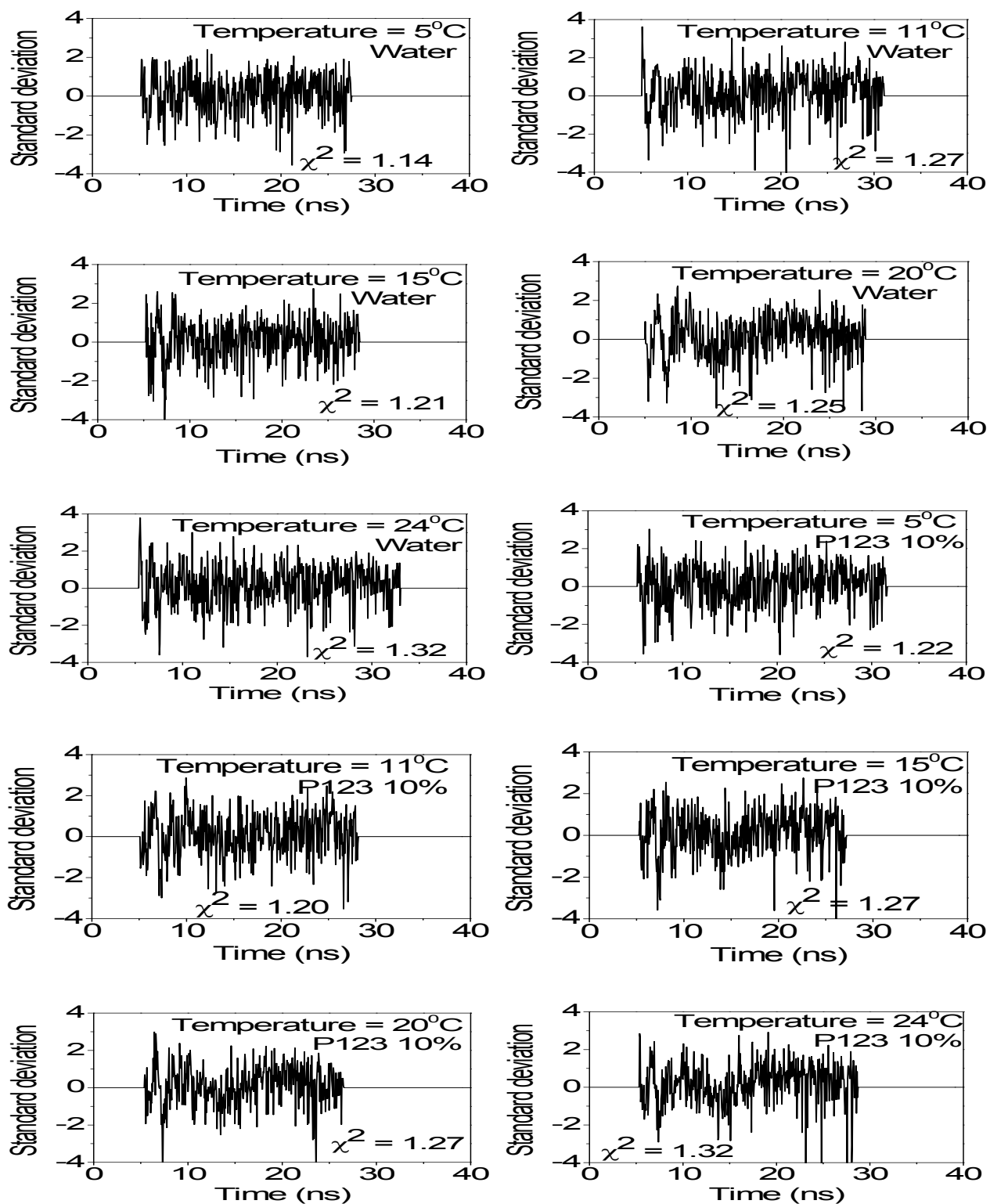


Figure S7: Residue distribution plots of pyd-lact in water and 10% P123 with temperature (corresponds to Table S4).

UNIV. OF MADRAS

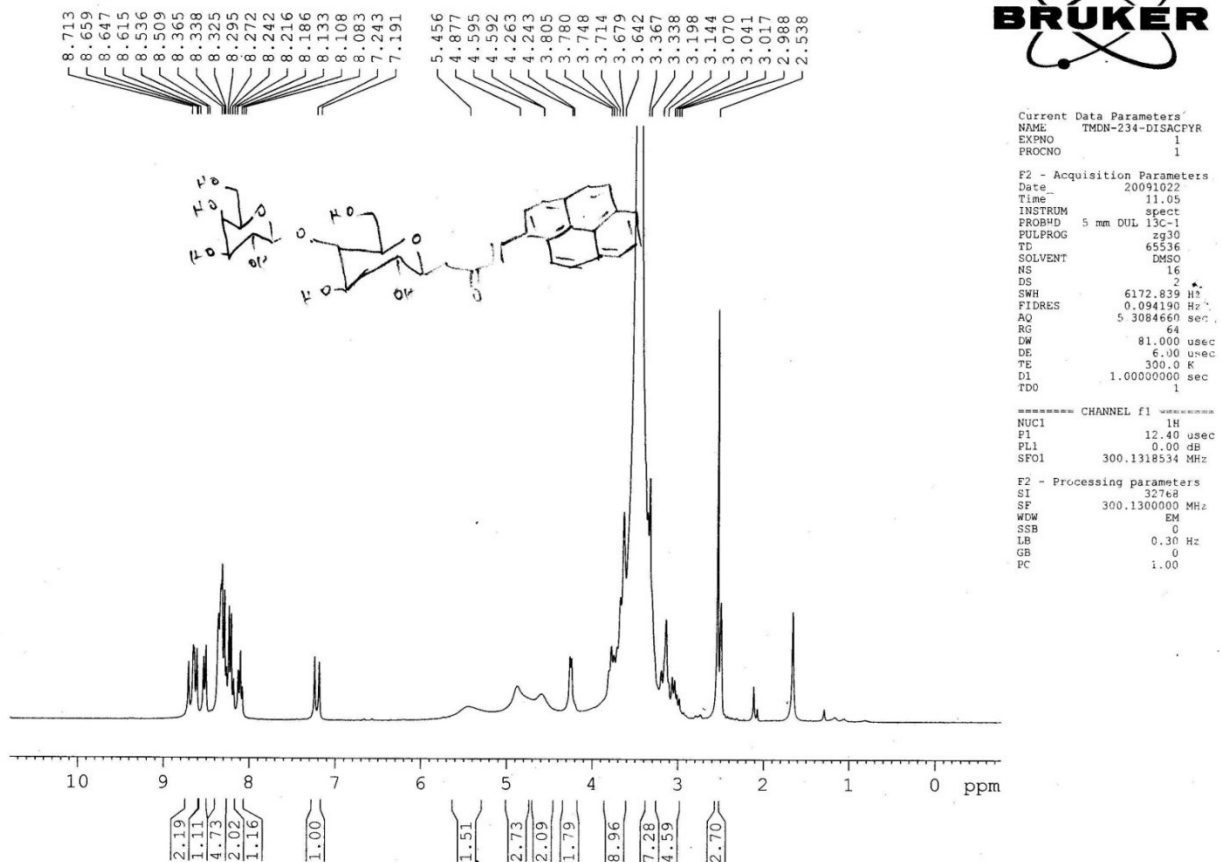


Figure S8: ¹H NMR spectrum of pyd-lact.

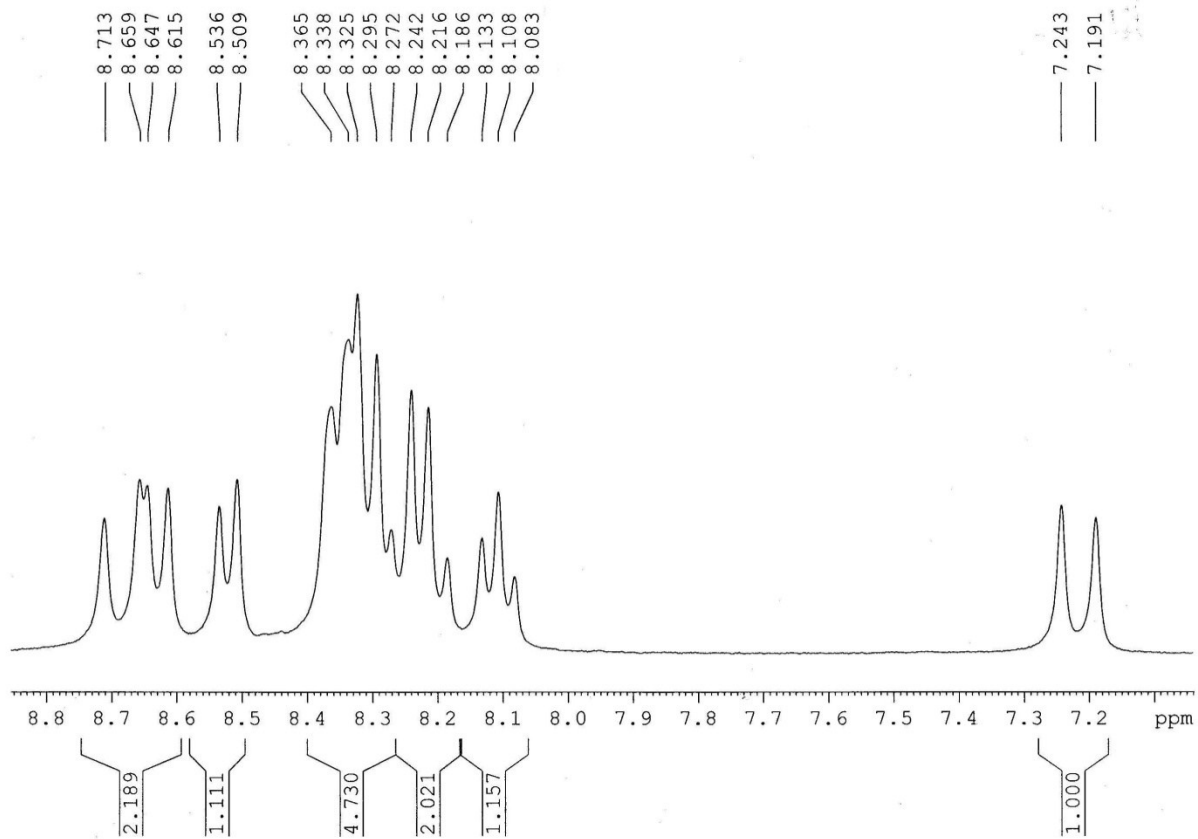


Figure S9: ^1H NMR expansion spectrum of pyd-lact.

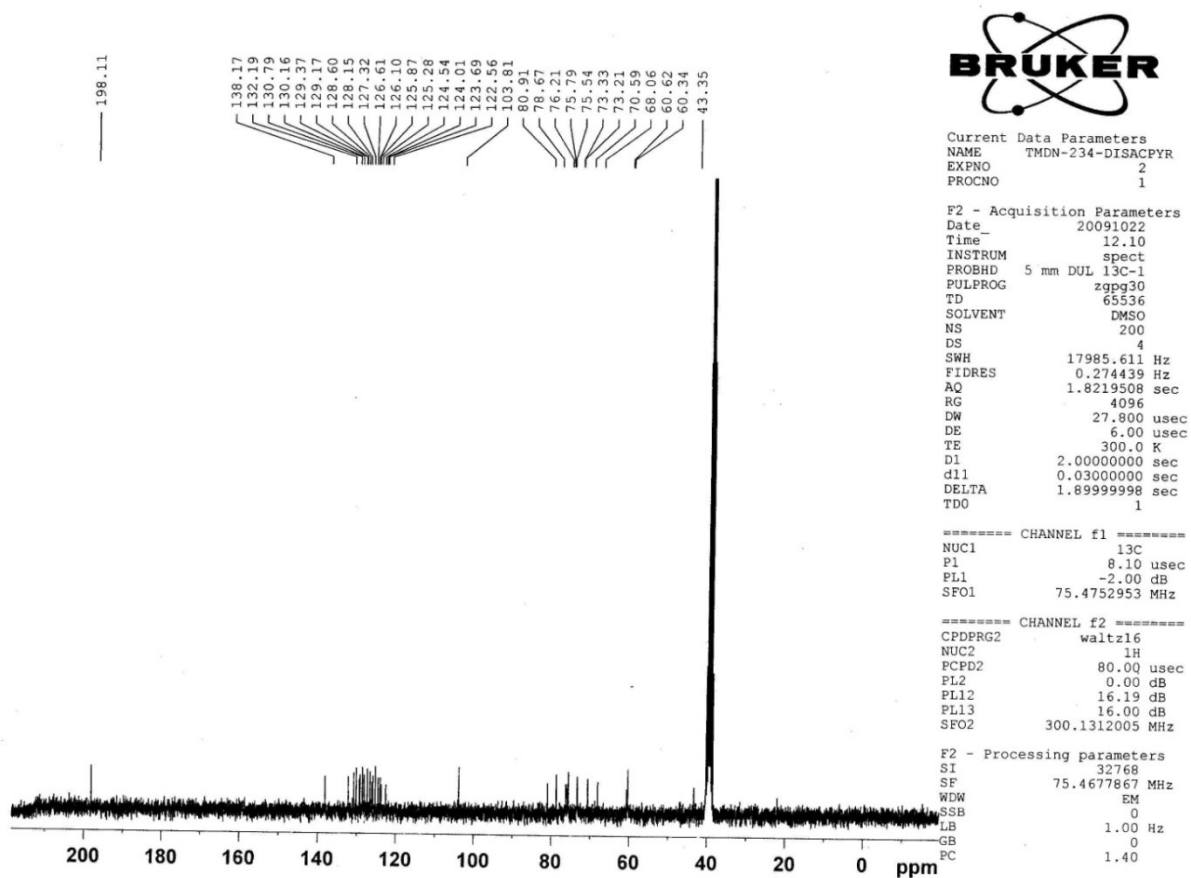


Figure S10: ¹³C NMR spectrum of pyd-lact.