

Supporting Information

Synthesis and Evaluation of a Glucose Attached Pyrene as a Fluorescent Molecular Probe in Sugar and Non-sugar Based Micro-heterogeneous Media

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India

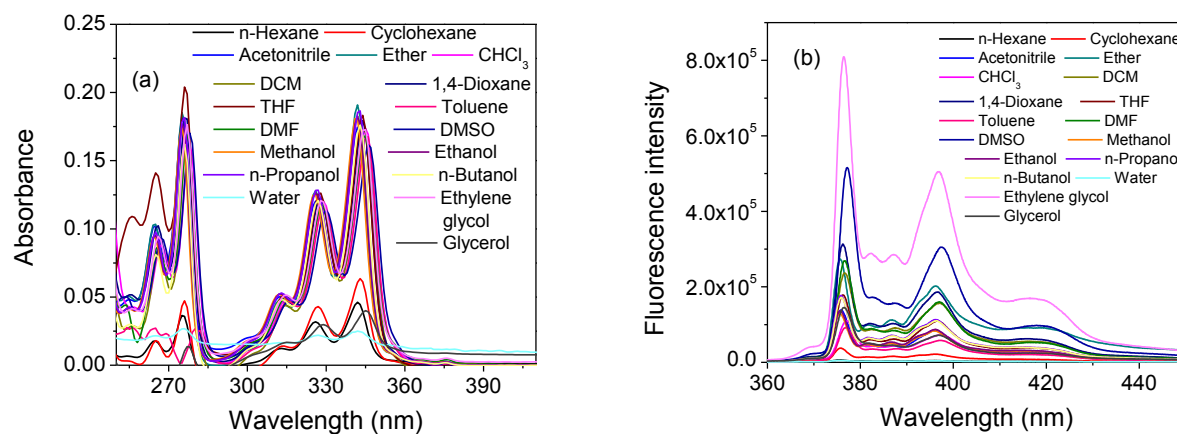


Figure S1: (a) Absorption spectra and (b) fluorescence spectra ($\lambda_{\text{ex}} = 340 \text{ nm}$) of pyd-glc at 4 μM in solvents of different polarity.

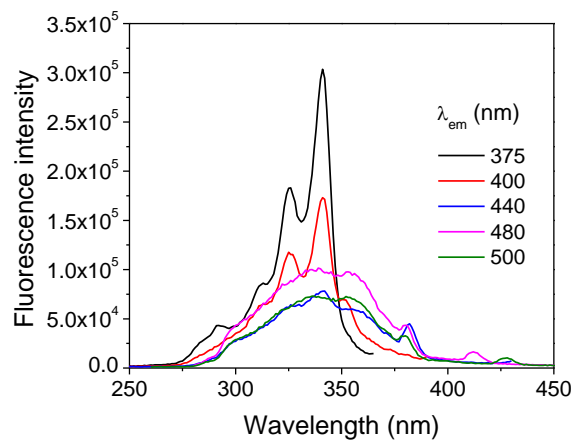


Figure S2: Fluorescence excitation spectra of pyd-glc (4 μM) in water with the variation of emission wavelength.

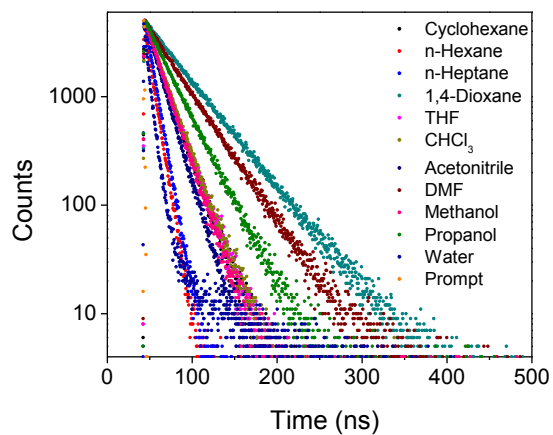
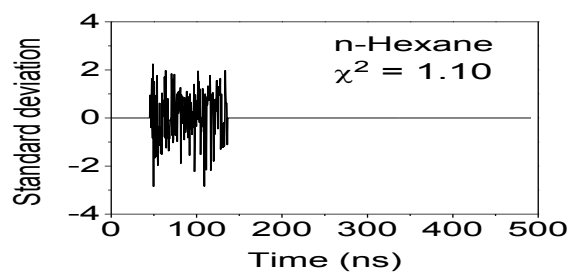
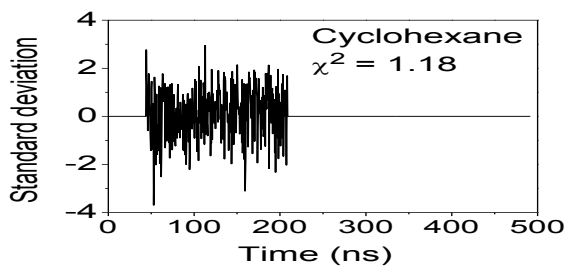


Figure S3: Fluorescence lifetime decay profiles of pyd-glc in different solvents, at $\lambda_{\text{ex}} = 340 \text{ nm}$, $\lambda_{\text{em}} = 375 \text{ nm}$.



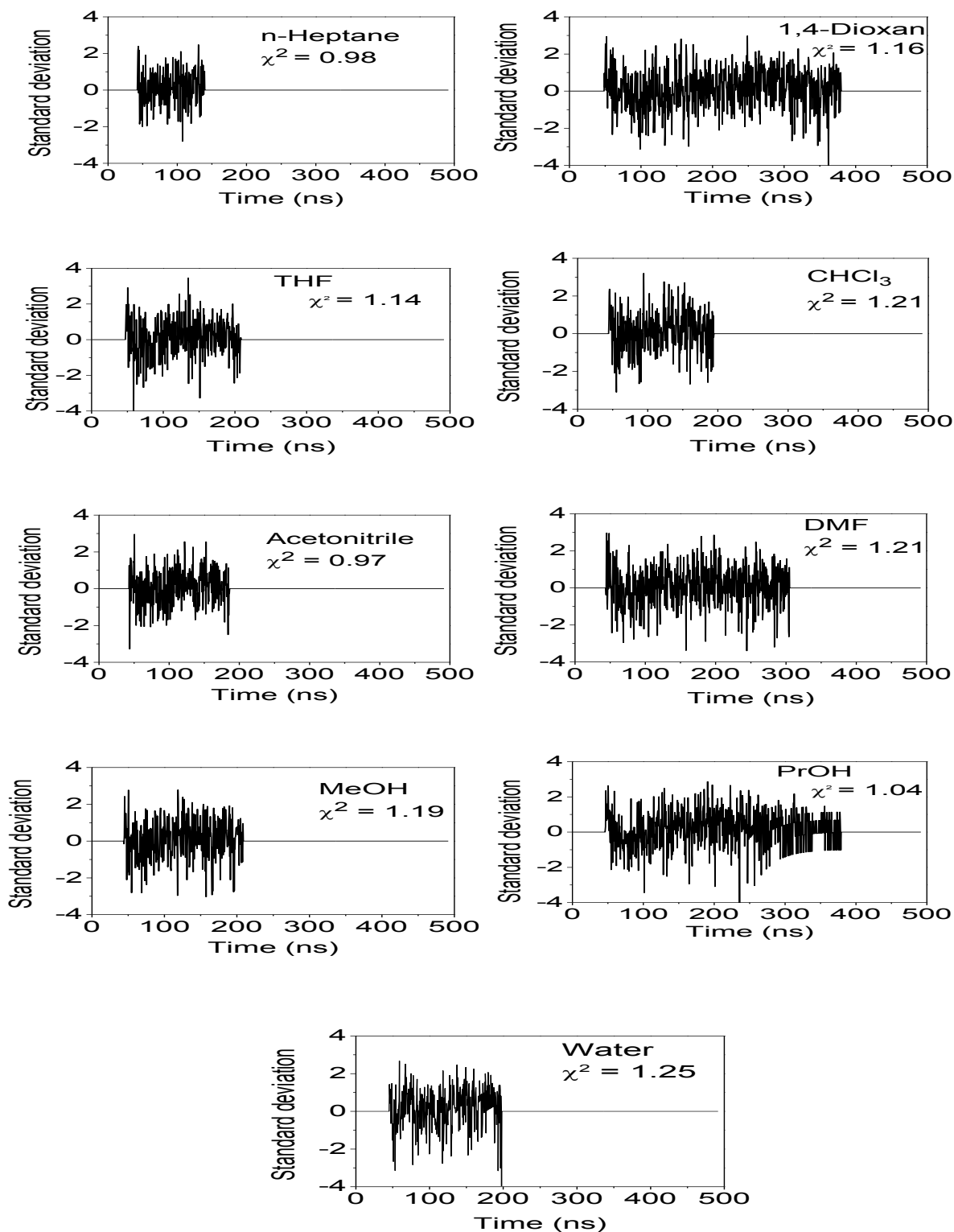


Figure S4: Residue distribution plots of pyd-glc in different solvents (corresponds to Table 1).

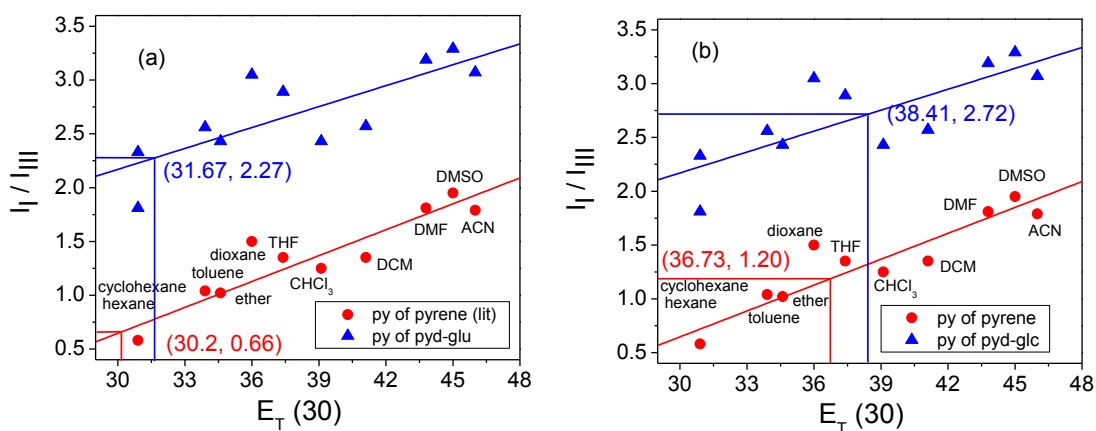
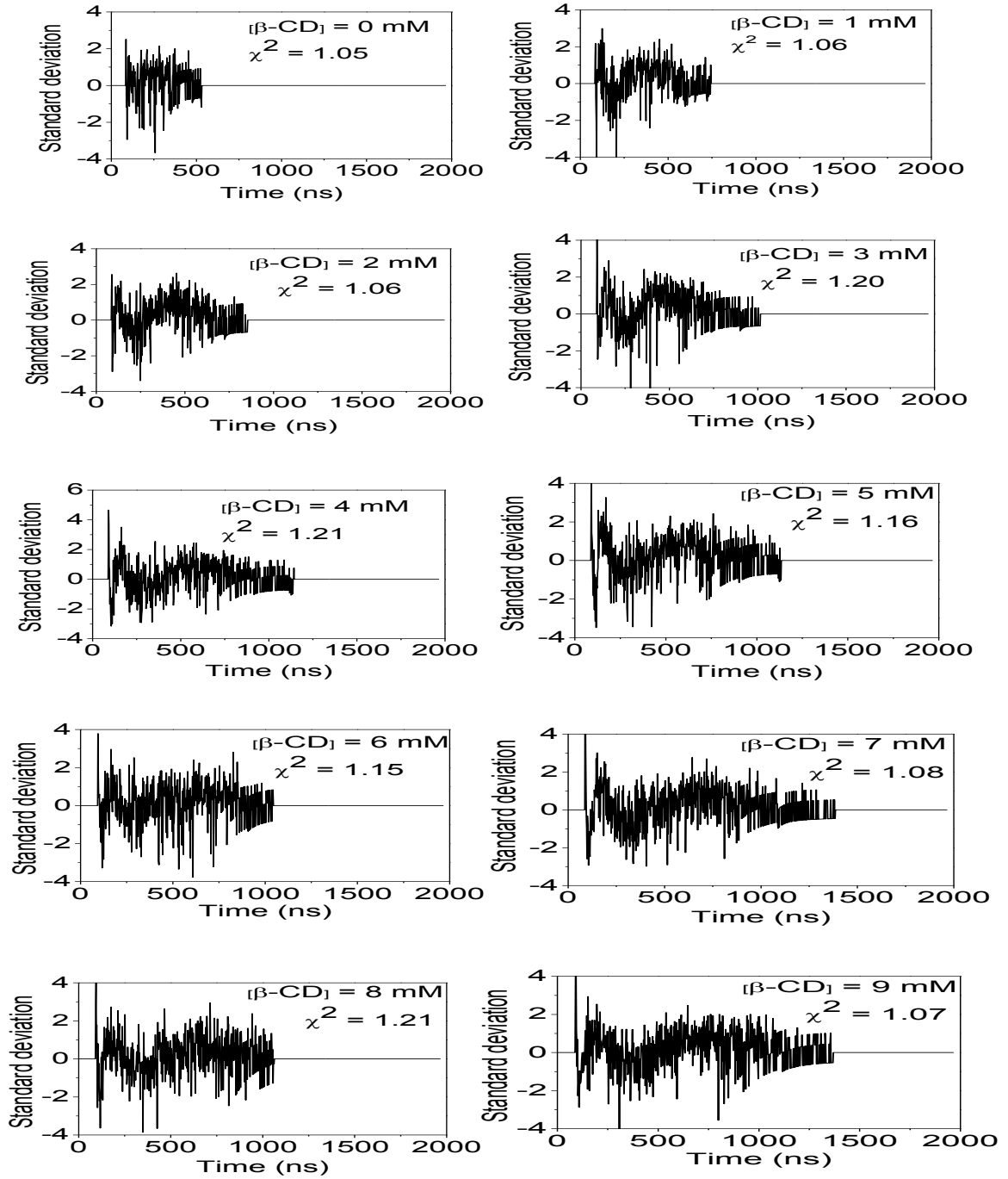


Figure S5: Determination of the medium polarity from py value using $E_T(30)$ scale for (a) β -CD and (d) tween 20 media.

Table S1: Fluorescence lifetime data of pyd-glc ($\lambda_{ex} = 340$ nm, $\lambda_{em} = 375$ nm) in β -CD media.

[β -CD] (mM)	τ_1 (β_1)	τ_2 (β_2)	τ_{aveg} (ns)	χ^2
0	6.23 (0.98)	50.58 (0.02)	7.12	1.05
1	6.61 (0.93)	59.76 (0.07)	10.33	1.06
2	8.36 (0.91)	68.49 (0.09)	13.77	1.06
3	13.61 (0.77)	81.71 (0.23)	29.27	1.20
4	20.02 (0.74)	105.43 (0.26)	42.23	1.21
5	20.82 (0.72)	104.59 (0.28)	44.28	1.16
6	29.47 (0.70)	118.04 (0.30)	56.04	1.15
7	23.87 (0.75)	123.22 (0.25)	48.71	1.08
8	29.61 (0.72)	128.79 (0.28)	57.38	1.21
9	29.82 (0.70)	133.81 (0.30)	61.02	1.07
10	30.09 (0.65)	138.88 (0.35)	68.17	1.09
12	33.88 (0.64)	150.41 (0.36)	75.83	1.12
14	34.13 (0.63)	155.50 (0.37)	79.04	1.11
16	36.92 (0.66)	163.08 (0.34)	79.81	1.08



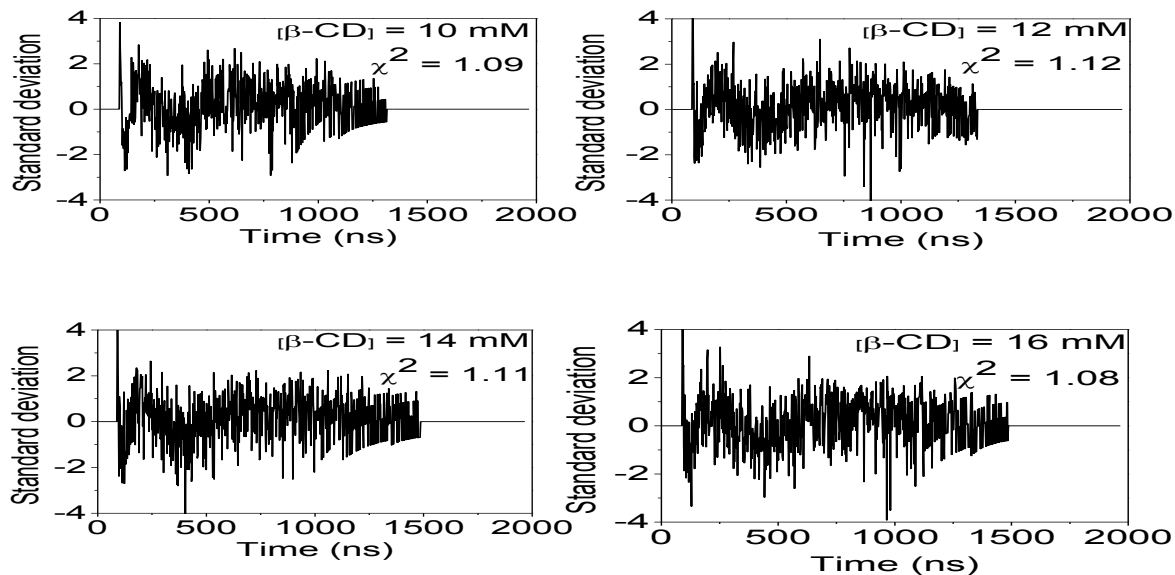
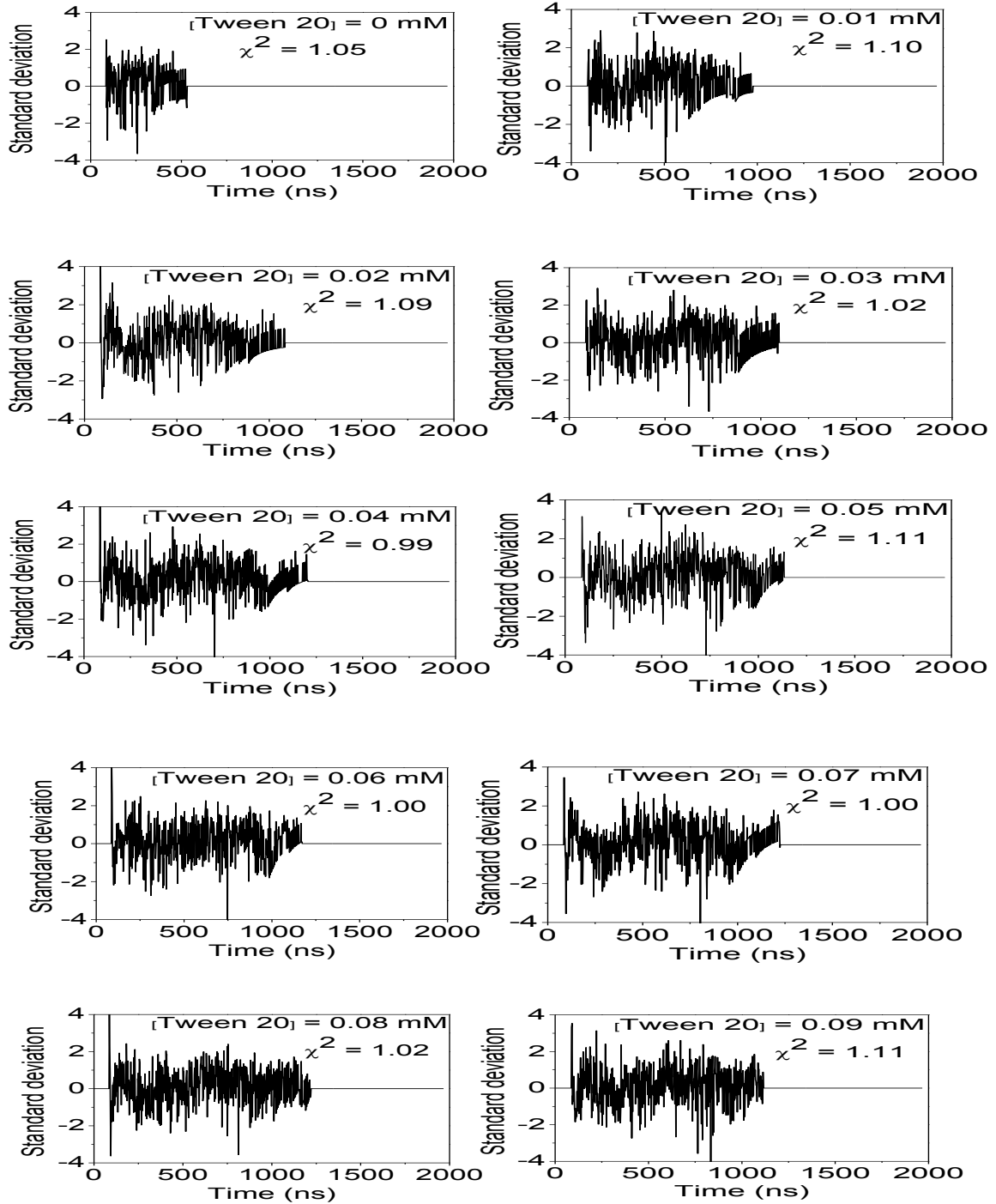


Figure S6: Residue distribution plots of pyd-glc in β -CD (corresponds to Table S1).

Table S2: Fluorescence lifetime data of pyd-glc ($\lambda_{\text{ex}} = 340 \text{ nm}$, $\lambda_{\text{em}} = 375 \text{ nm}$) in tween-20 media.

[Tween-20] (mM)	τ_1 (β_1)	τ_2 (β_2)	τ_{aveg} (ns)	χ^2
0	6.23 (0.98)	50.58 (0.02)	7.12	1.05
0.01	14.88 (0.71)	91.85 (0.29)	37.20	1.10
0.02	17.68 (0.59)	107.60 (0.41)	54.55	1.09
0.03	22.19 (0.55)	112.13 (0.45)	62.66	1.02
0.04	18.05 (0.46)	114.20 (0.54)	69.97	0.99
0.05	30.58 (0.37)	119.94 (0.63)	86.88	1.11
0.06	31.43 (0.38)	120.45 (0.62)	86.62	1.00
0.07	15.25 (0.38)	115.88 (0.62)	77.64	1.00
0.08	21.09 (0.39)	120.05 (0.61)	81.46	1.02
0.09	33.41 (0.28)	122.46 (0.72)	97.53	1.11
0.10	33.57 (0.30)	125.60 (0.70)	97.99	0.99
0.13	29.11 (0.26)	123.51 (0.74)	98.97	1.11
0.15	33.51 (0.22)	124.72 (0.78)	104.65	1.19
0.17	45.03 (0.22)	129.12 (0.78)	110.62	1.13



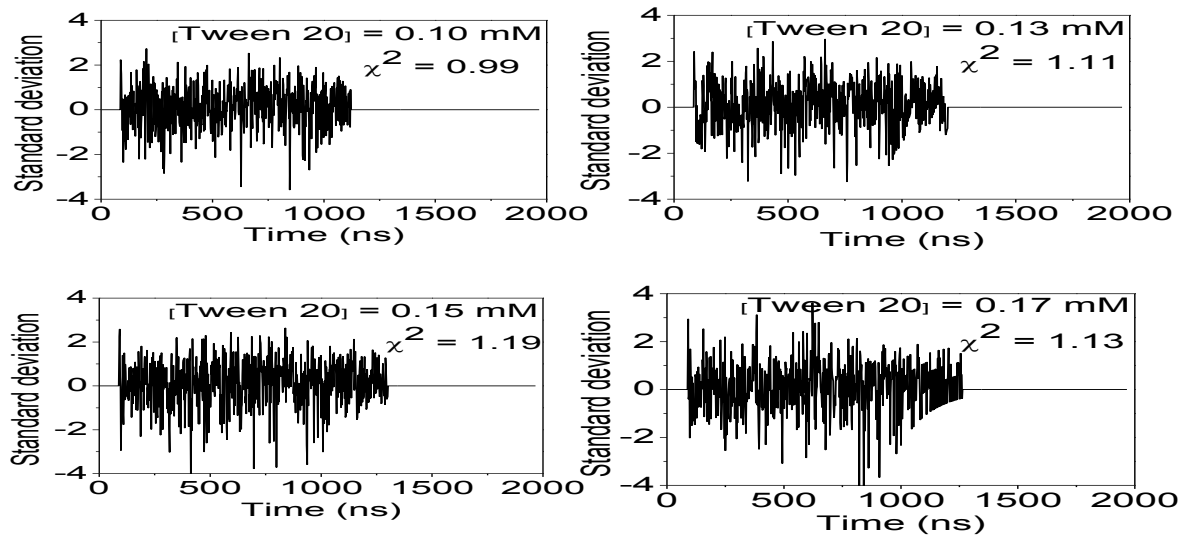


Figure S7: Residue distribution plots of pyd-glc in tween 20 (corresponds to Table S2).

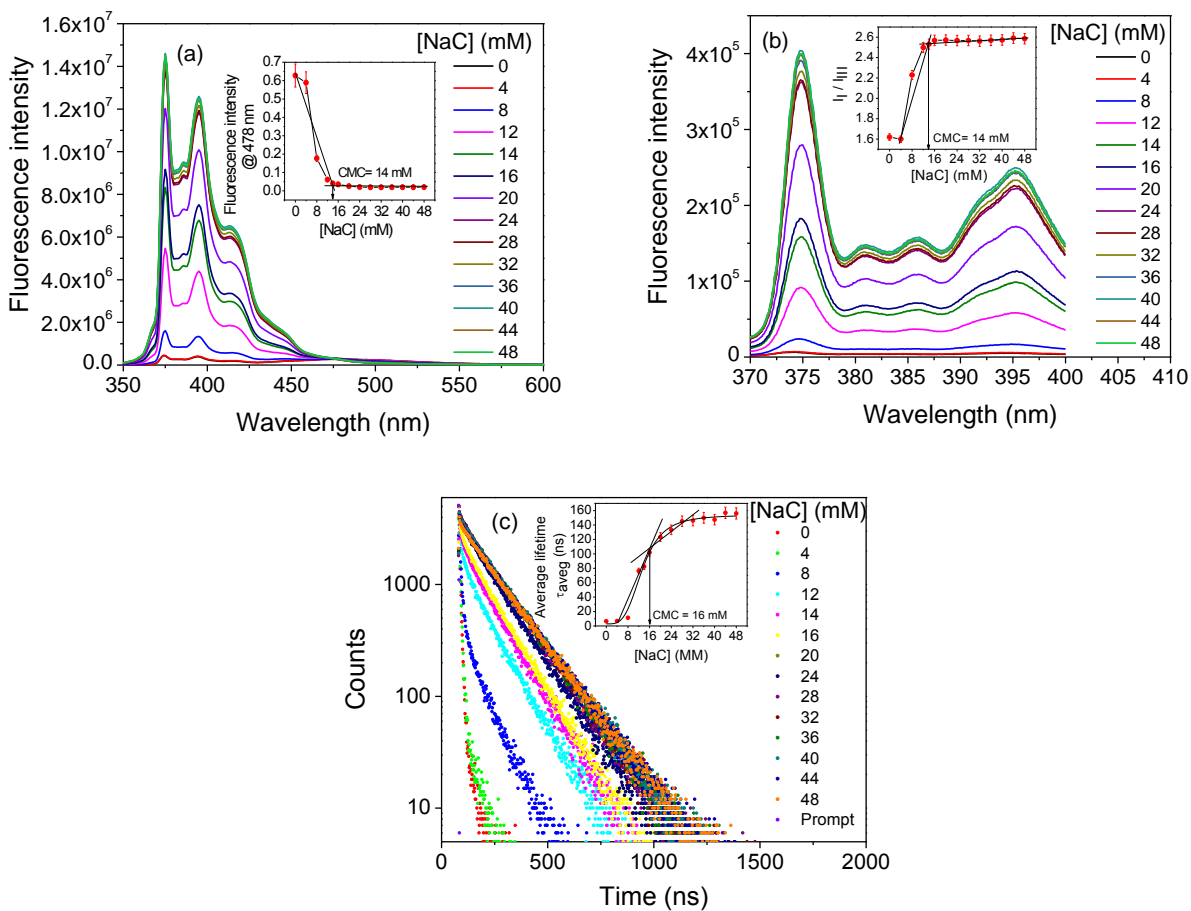


Figure S8: (a) Fluorescence spectra of pyd-glc (4 μM) with increasing concentration of NaC, inset shows decrease of excimer fluorescence intensity, (b) fluorescence spectra of pyd-glc (4 μM) with increasing concentration of NaC under high resolution, inset shows variation of I_I / I_{III} value; here $\lambda_{\text{ex}} = 340 \text{ nm}$ and (c) fluorescence lifetime decay profiles of pyd-glc in NaC media, at $\lambda_{\text{ex}} = 340 \text{ nm}$, $\lambda_{\text{em}} = 375 \text{ nm}$.

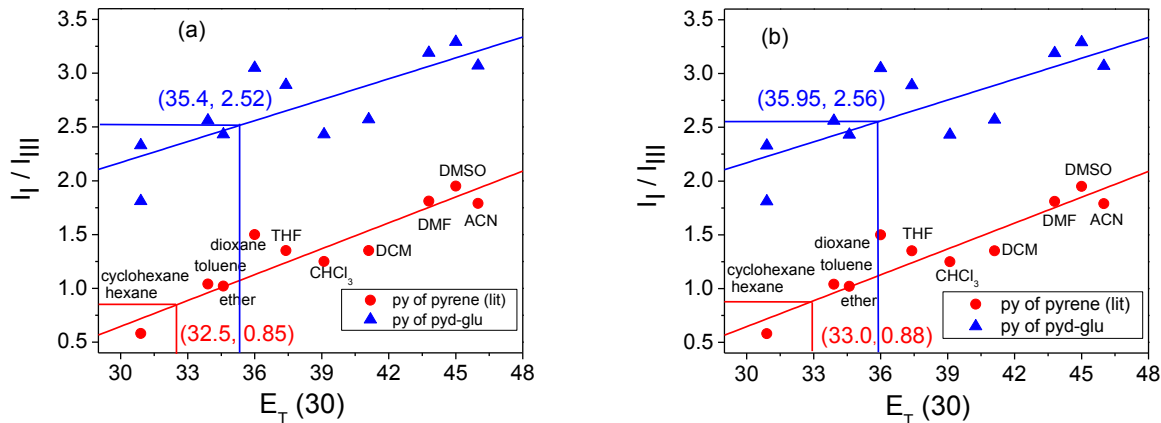


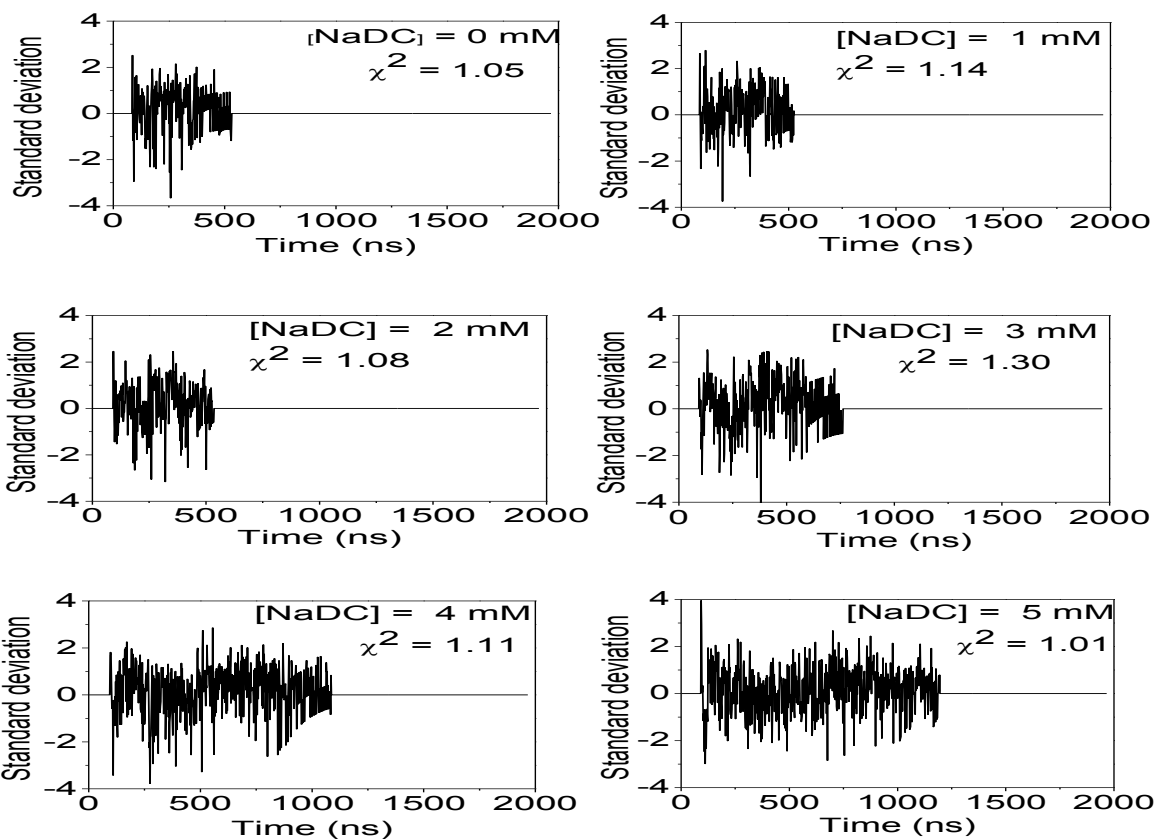
Figure S9: Determination of the medium polarity from py value using E_T (30) scale for (a) NaDC and (b) NaC media.

Table S3: Fluorescence lifetime data of pyd-glc ($\lambda_{\text{ex}} = 340 \text{ nm}$, $\lambda_{\text{em}} = 375 \text{ nm}$) in NaDC.

[NaDC] (mM)	τ_1 (β_1)	τ_2 (β_2)	τ_{aveg} (ns)	χ^2
0	6.23 (0.98)	50.58 (0.02)	7.12	1.05
1	6.28 (0.99)	48.65 (0.01)	6.70	1.14
2	8.55 (0.99)	66.75 (0.01)	9.13	1.08
3	10.72 (0.75)	85.42 (0.25)	29.39	1.30
4	24.44 (0.57)	123.15 (0.43)	66.89	1.11
5	31.62 (0.38)	141.50 (0.62)	99.75	1.01
6	28.77 (0.24)	143.78 (0.76)	116.18	1.14
7	24.34 (0.21)	145.14 (0.79)	119.77	1.34
8	33.62 (0.23)	149.40 (0.77)	122.77	1.01
10	73.14 (0.26)	164.14 (0.74)	140.48	1.09
12	74.03 (0.20)	163.83 (0.80)	145.87	1.13
14	63.49 (0.16)	164.11 (0.84)	148.01	1.08
16	61.90 (0.14)	165.40 (0.86)	150.91	1.04
18	93.89 (0.22)	172.65 (0.78)	155.32	1.17

Table S4: Fluorescence lifetime data of pyd-glc ($\lambda_{\text{ex}} = 340 \text{ nm}$, $\lambda_{\text{em}} = 375 \text{ nm}$) in NaC.

[NaC] (mM)	τ_1 (β_1)	τ_2 (β_2)	τ_{aveg} (ns)	χ^2
0	6.23 (0.98)	50.58 (0.02)	7.12	1.05
4	6.35 (0.99)	47.62 (0.01)	6.76	1.07
8	8.89 (0.97)	91.16 (0.03)	11.36	1.14
12	19.27 (0.44)	121.06 (0.56)	76.27	1.12
14	26.27 (0.46)	130.17 (0.54)	82.38	1.13
16	23.72 (0.29)	133.70 (0.71)	101.81	1.02
20	44.15 (0.23)	147.85 (0.77)	123.99	1.08
24	74.75 (0.24)	151.85 (0.76)	133.35	1.03
28	81.34 (0.19)	160.30 (0.81)	145.30	1.14
32	37.00 (0.11)	159.60 (0.89)	146.11	1.13
36	50.52 (0.11)	162.22 (0.89)	149.93	1.13
40	51.39 (0.16)	165.72 (0.84)	147.43	1.03
44	79.21 (0.14)	169.55 (0.86)	156.90	1.24
48	79.65 (0.17)	171.67 (0.83)	156.03	1.28



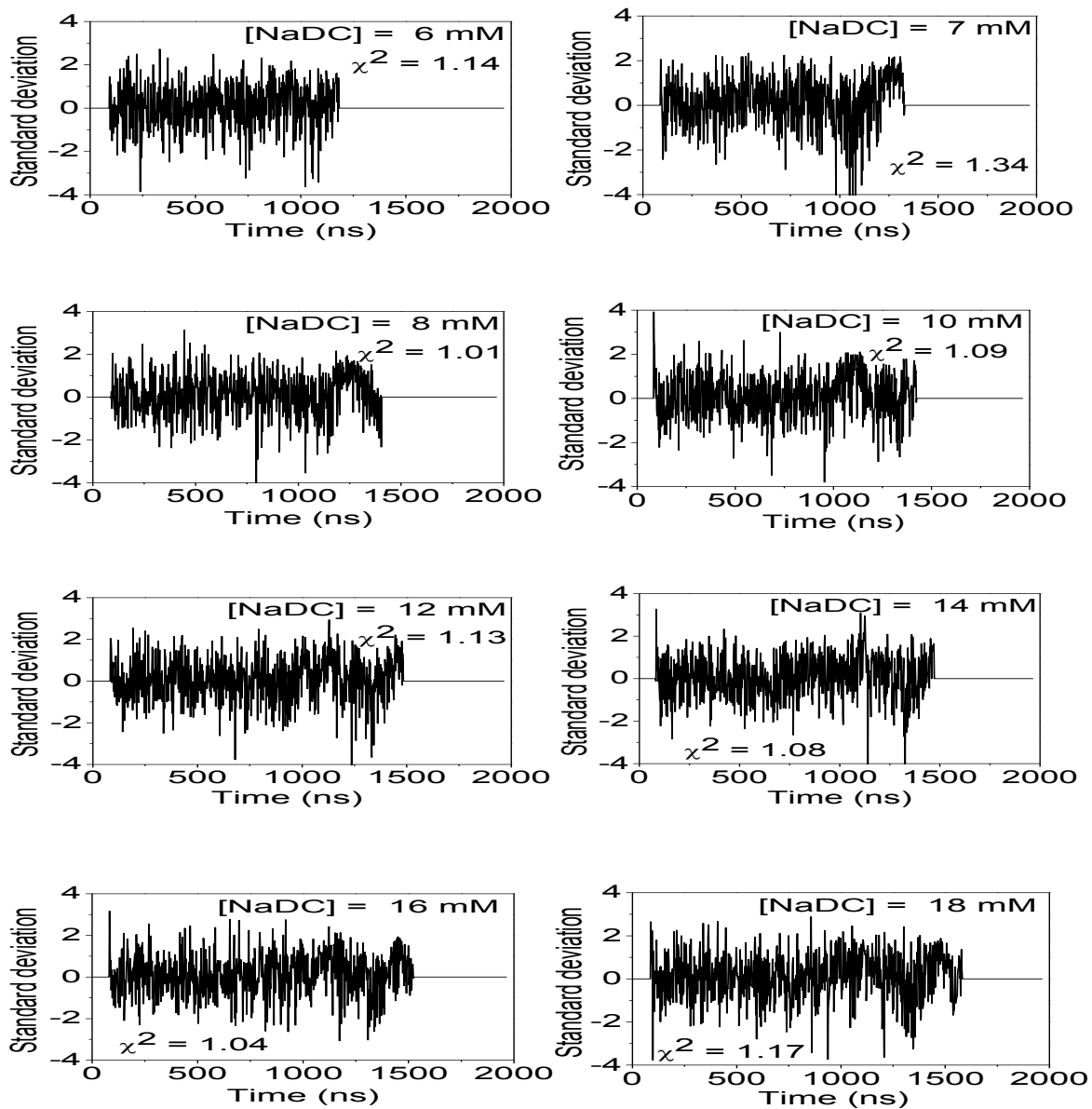
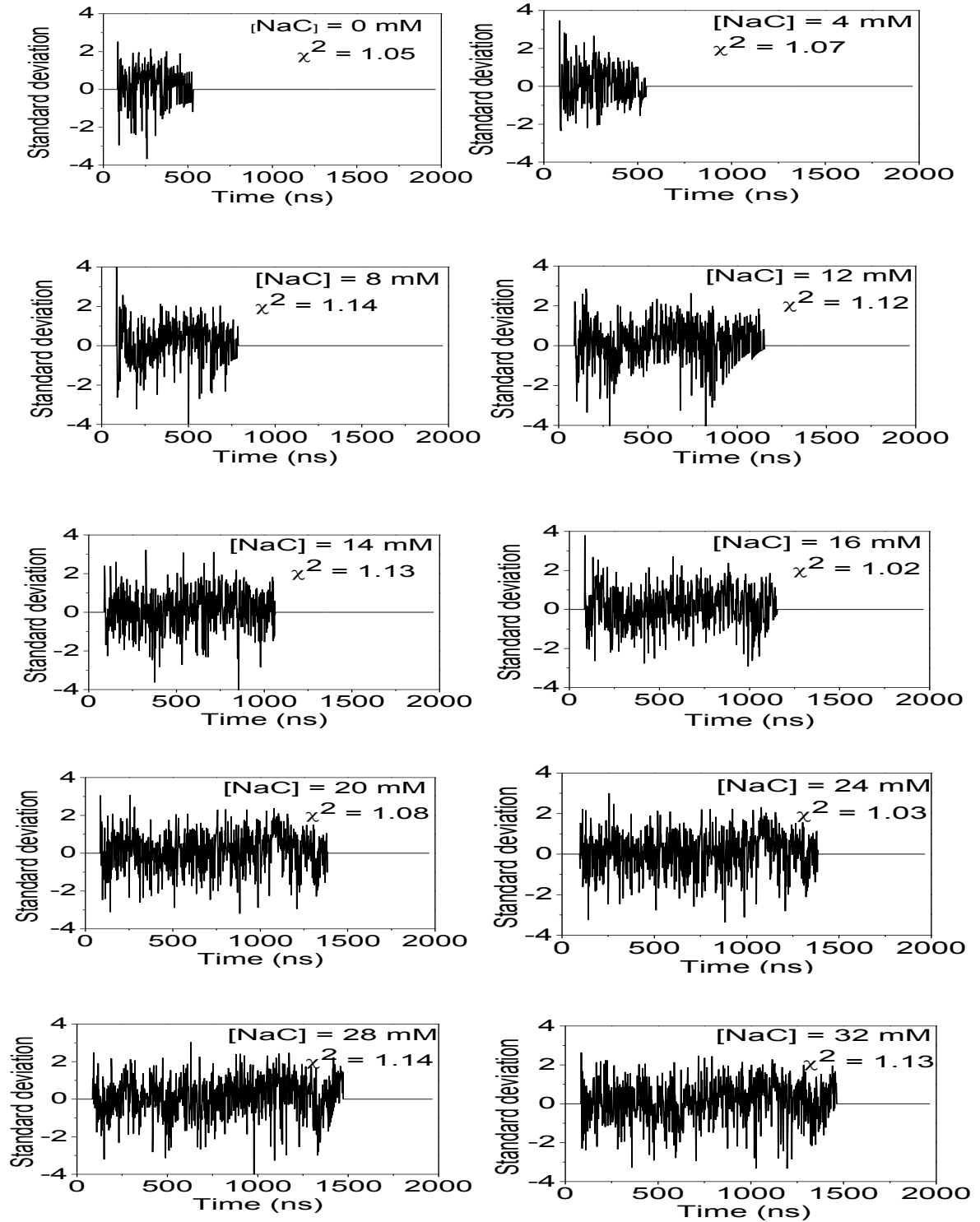


Figure S10: Residue distribution plots of pyd-glc in and NaDC (corresponds to Table S3).



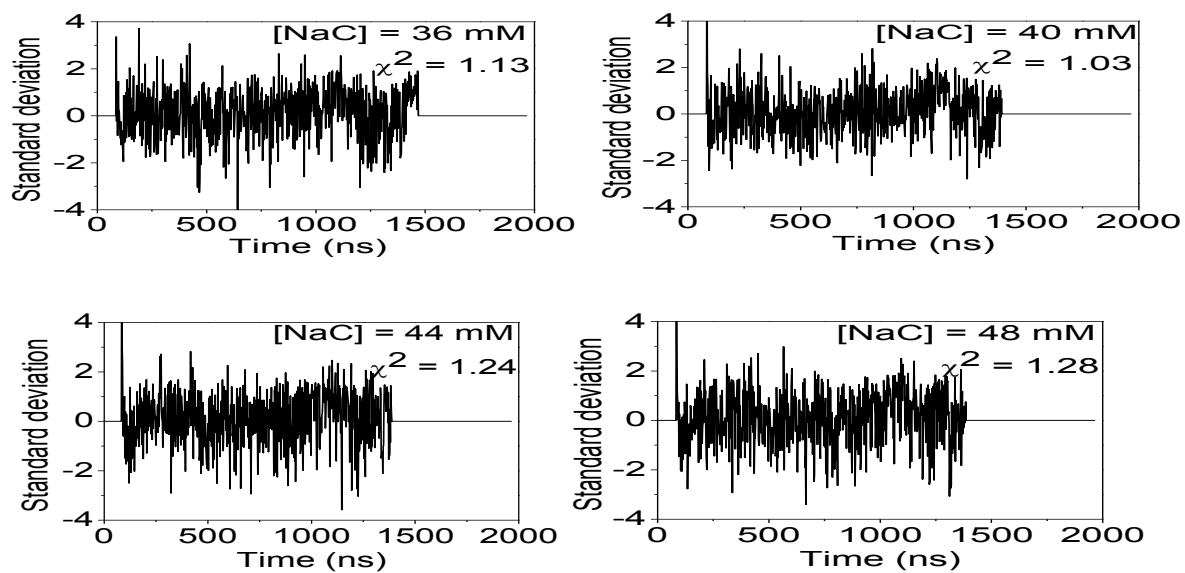


Figure S11: Residue distribution plots of pyd-glc in NaC (corresponds to Table S4).



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 PROCNO 1

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 TD 65536
 SOLVENT CDC13
 NS 17
 DS 2
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 FIDRES 0.094190 Hz
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 RG 287.4
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

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 P1 13.15 usec
 PL1 0.00 dB
 SF01 300.1318534 MHz

F2 - Processing parameters
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 SF 300.1300070 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

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8.194
8.178
8.161
8.152
8.125
8.110
8.094
8.084
8.021
7.993
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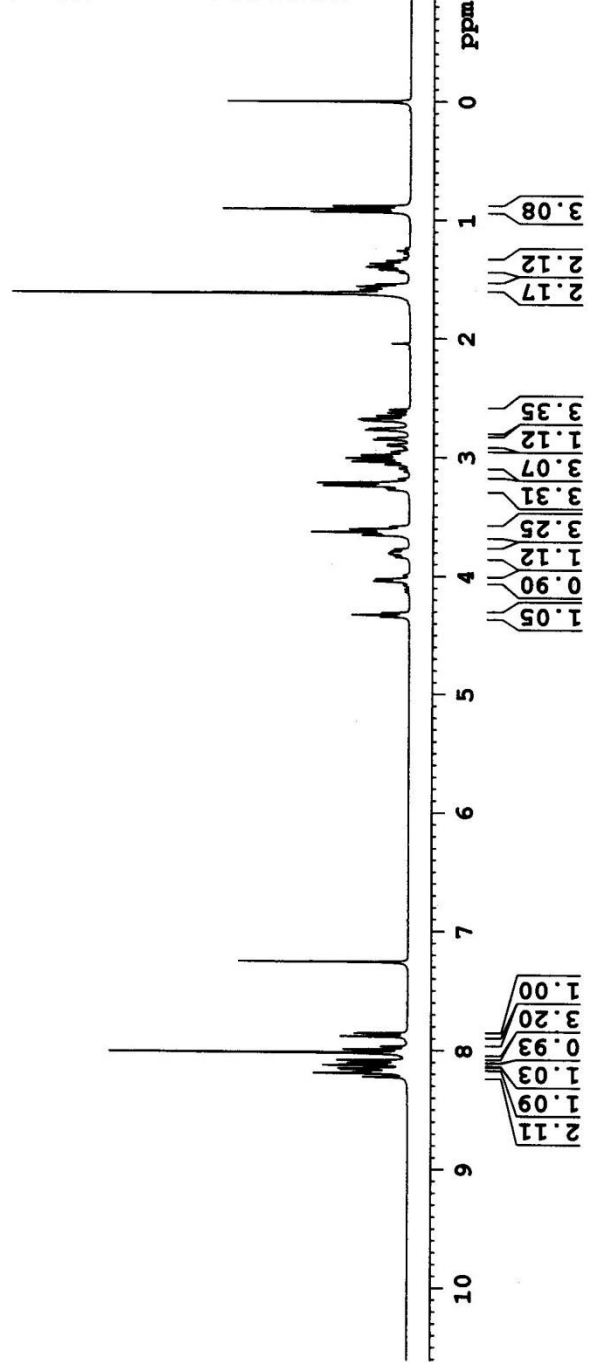
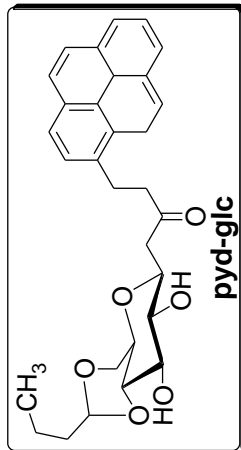


Figure S12: ¹H NMR spectrum (300 MHz, CDCl₃) of compound, pyd-glc.



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 PROCNO 1

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 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 1448.2
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.89999998 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 9.30 usec
 PL1 0.00 dB
 SFO1 75.4752953 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PLI2 15.68 dB
 PLI3 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
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 WDW EM
 SSB 0
 LB 0
 GB 0
 PC 1.40

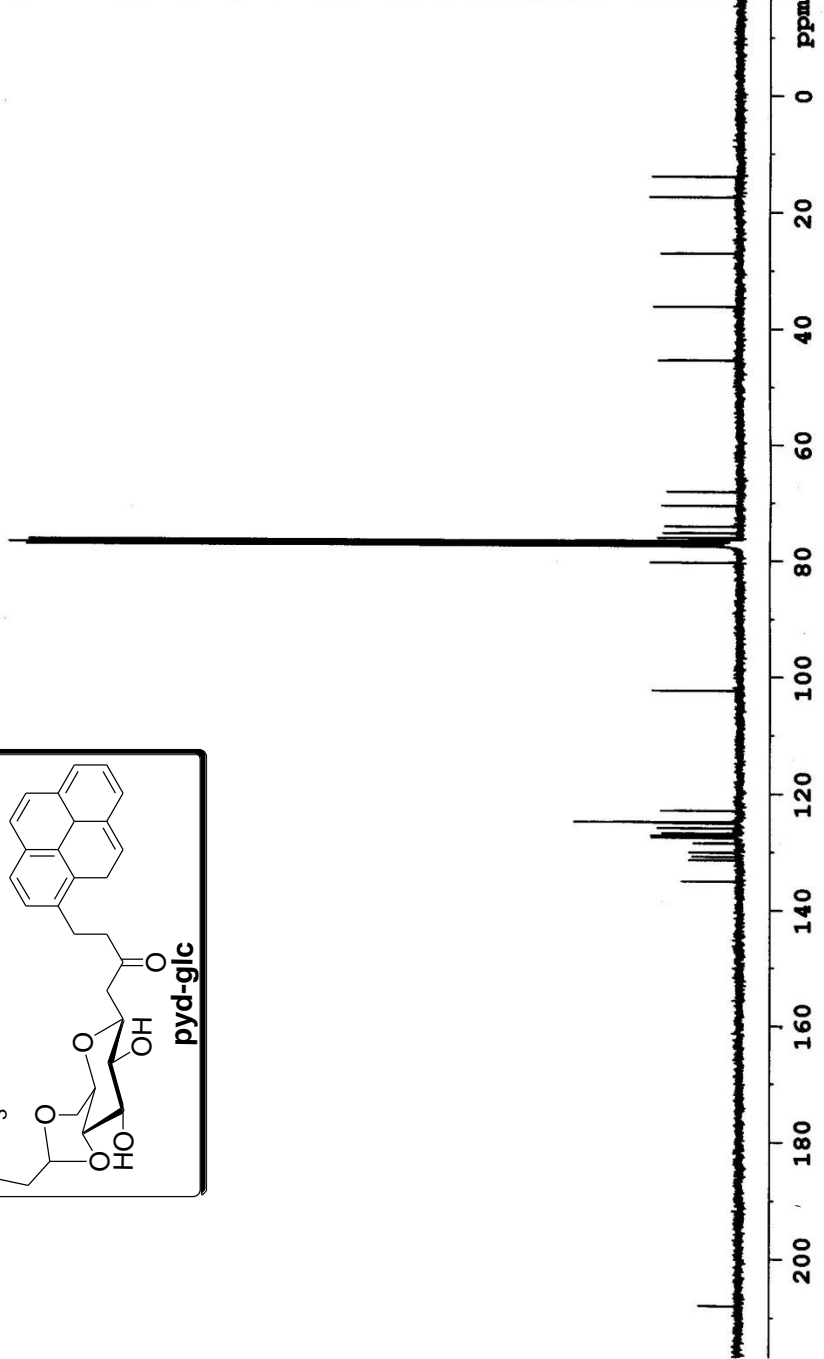
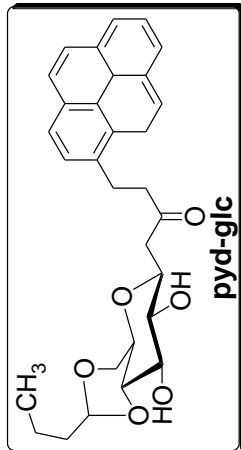
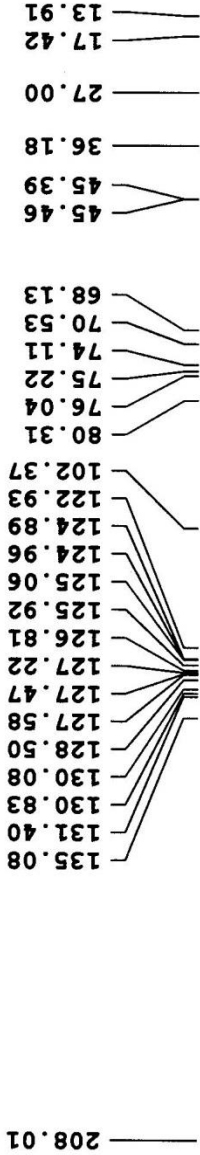


Figure S13: ¹³C NMR spectrum (75 MHz, CDCl₃) of compound, pyd-glc.



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 PROCNO 1

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 SOLVENT CDCl3
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 DS 4
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 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 16384
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 CNST2 145.000000
 D1 2.0000000 sec
 d2 0.00344828 sec
 d12 0.0002000 sec
 DELTA 0.00001184 sec
 TDO 1

==== CHANNEL f1 =====
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 P1 9.30 usec
 P2 18.60 usec
 PL1 0.00 dB
 SF01 75.4752953 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P3 13.15 usec
 P4 26.30 usec
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

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 127.47
 127.24
 126.82
 125.93
 125.06
 124.89
 122.94
 102.37
 80.29
 76.02
 75.20
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 45.47
 45.38
 36.18
 27.00
 17.43
 13.93

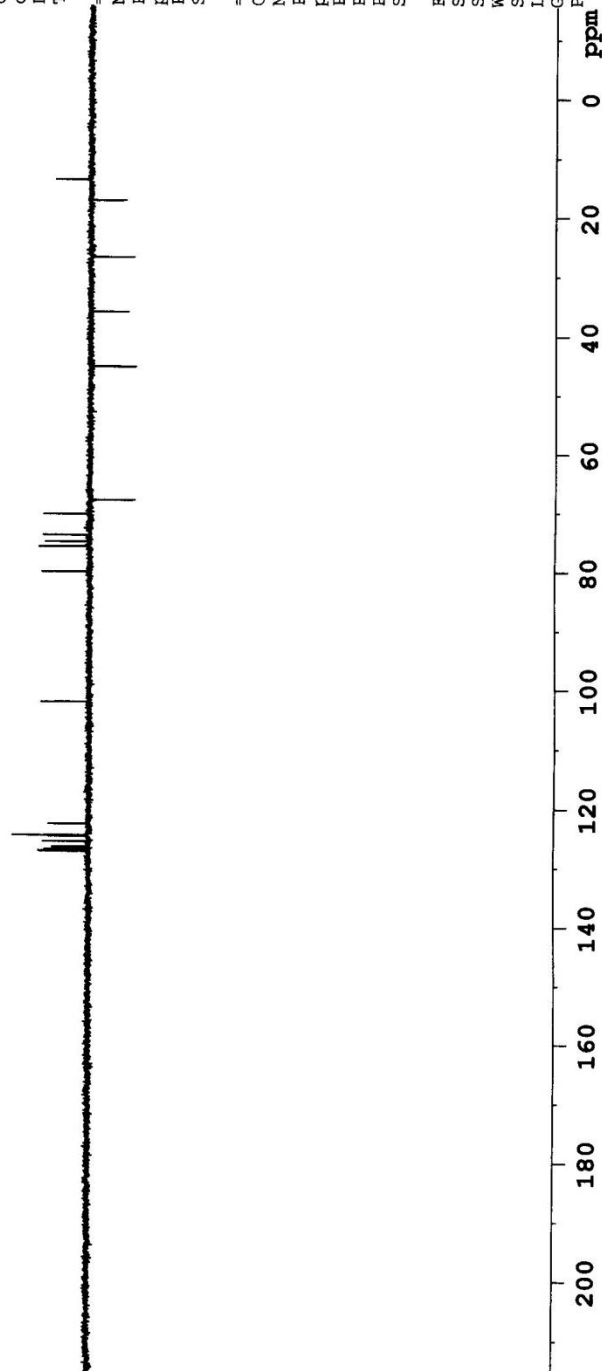
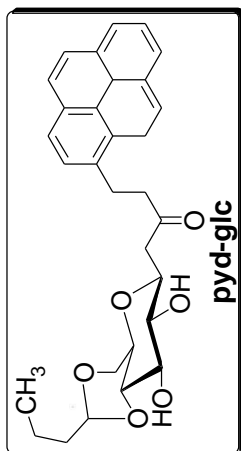


Figure S14: DEPT-135 spectrum (75 MHz, CDCl₃) of compound, pyd-glc.

QTOF MICRO

DEPARTMENT OF CHEMISTRY IITM

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10-Sep-2013 13:27:54
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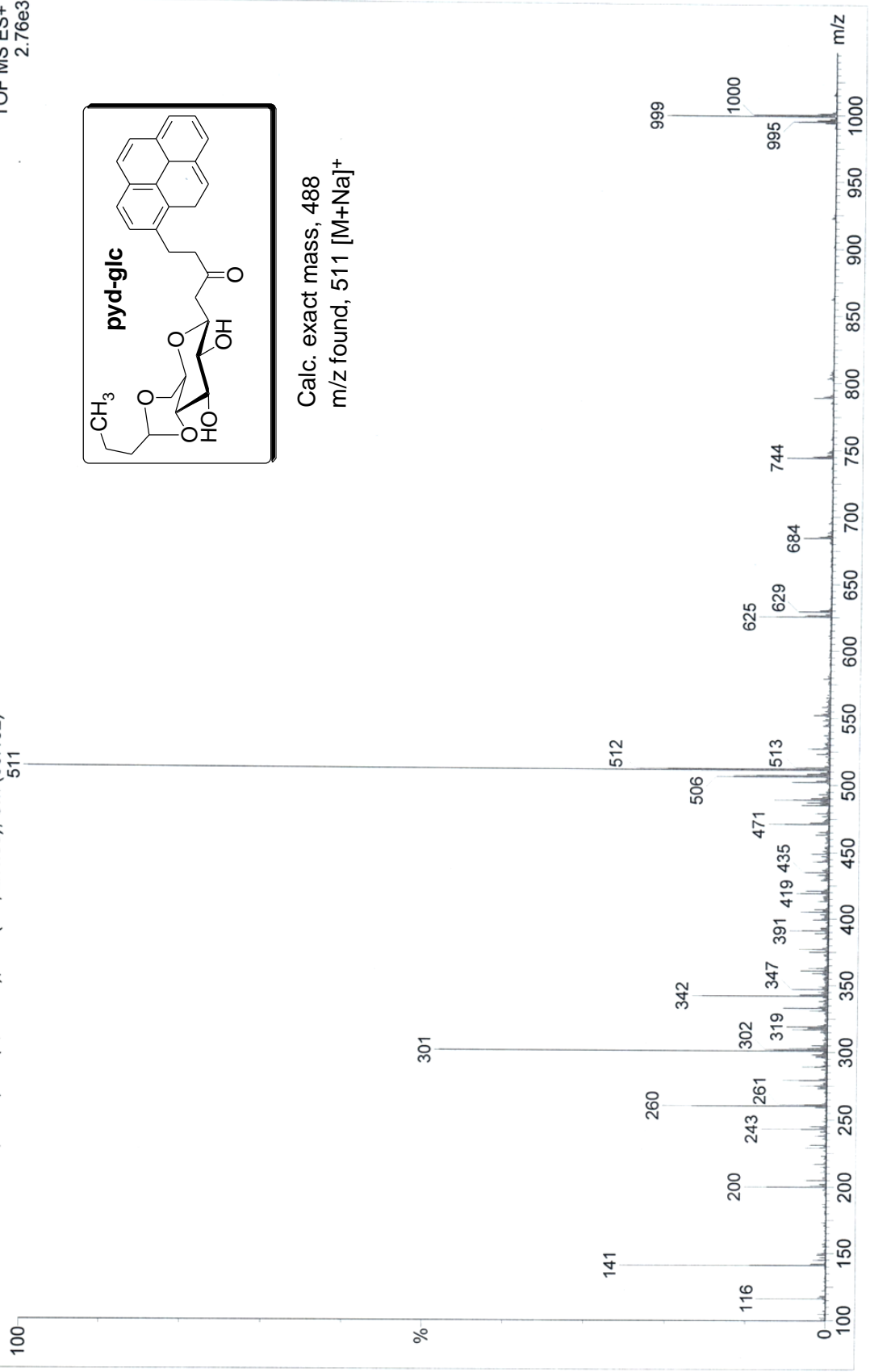


Figure S15: Mass spectrum of compound, pyd-glc.