Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information of

Assembly of plasmid DNA with Pyrene-amines cationic amphiphiles into nanoparticles and their Visible Lysosome Localization

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S1. General synthetic procedures of the **Py-amines** amphiphiles (**Py-1N**, **2N**, **3N, 4N**) and their molecular structure characterization by NMR, MS and IR spectrum

S2. Dynamic laser scattering analysis for the average particle sizes of the **Py-amines**/ pDNA complexes in distilled water at the N/P ratio of 20

S3. The DSC curves of the aqueous solution of **Py-amines** (1×10^{-2} M) amphiphiles. It could be seen that the phase transition temperature of water depended on the numbers of amino groups of **Py-amines,** indicated their different hydration capabilities

S4. Fluorescence images of **Py-amines** (**Py-1N**, **2N**, **3N** and **4N**)/pDNA (blue fluorescence) in COS-7 cell line under an N/P ratio of 30, Lysotracker-Red was used as a lysosomal specific labeling agent (red fluorescence)

S1. General synthetic procedures of the pyrene-amines compounds and their molecular structure characterization by NMR, MS and IR spectrums

General synthetic procedure for **Py-amines** cationic amphiphiles

1-aminopyrene (2.0 mmol), a N-Boc protected polyaminesamine (2.2 mmol), DCC/DMAP (0.5 g /0.1 g) were dissolved in 10 mL of dichloromethane, and the mixture was then stirred at ambient temperature for 24 h. After that, the produced DCU (dicyclohexyl urea) solids were removed by filtration and the filtrates were concentrated under reduced pressure, and then purified by flash column chromatography (EtOAC/Hexane=1/3 v/v) to achieve BOC-protected **Py-amines** precursors with isolated yield of 56~62%. Continuously, the above-synthesized BOC-protected Py-amines were deprotected in 10 mL mixture solution of dichloromethane and trifluoroacetic acid (5mL/5mL) for 3 h and the solvents were removed under reduced pressure, then cold diethyl ether 50 mL was added and stirred for another 30 min, and grey-white color solid products were collected and dried at 50 ℃ overnight to obtain the final products **Py-amines** with a yield of 75~78% . And their molecular structures were characterized by NMR, MS and IR.

Py-1N

^{1}H NMR (d_6-DMSO, δ in ppm) 3.0 (t, J = 7.7 Hz, 2H, CH_2), 3.2 (t, J = 7.1 Hz, 2H, CH_2),7.91 (s, 3H, -NH_3^+), 8.11- 8.37 (m, 9H, ArH)

^{13}C NMR (d_6-DMSO, δ in ppm) 31.09, 35.30, 114.87, 117.81, 120.34, 122.78, 123.07, 123.44, 124.22, 125.39, 126.01, 126.30, 127.22, 128.13, 128.94, 129.60, 129.81, 170.75

ESI-MS [M^+] (in m/z): 289.6

FTIR (in cm^{-1}) 3257.6, 3036.8, 1660.1, 1599.9, 1560.1, 1529.7, 1206.4, 1185.0, 1130.0, 839.3

Py-2N

^{1}H NMR (D_2O, δ in ppm) 3.0 (t, J = 7.4 Hz, 2H, $NHCOCH_2$), 3.2 (t, J = 7.0 Hz, 2H, CH_2N), 3.34-3.4 (m, 4H, NCH_2CH_2N), 7.56- 7.77 (m, 9H, ArH)

^{13}C NMR (D_2O, δ in ppm) 31.0, 35.1, 43.8, 44.1, 114.8, 117.7, 120.5, 120.5, 122.9, 123.4, 124.8, 125.2, 125.7, 126.5, 127.4, 128.0, 128.2, 129.2, 129.7, 171.1

ESI-MS [M^+] (in m/z): 332.2

FTIR (in cm^{-1}) 3256.7, 3038.8, 1672.3, 1602.0, 1562.6, 1525.4, 1197.9, 1128.9, 837.5

Py-3N

^{1}H NMR (D_2O, δ in ppm) 3.00 (m, 2H, $NHCOCH_2$), 3.14 (m, 2H, CH_2N), 3.16 (m, 2H, CH_2N), 3.34-3.4 (m, 6H, NCH_2CH_2N), 7.62-7.97 (m, 9H, ArH)

^{13}C NMR (D_2O, δ in ppm) 31.1, 35.2, 43.8, 44.1, 114.8, 117.7, 120.5, 120.5, 122.8, 123.3, 124.7, 125.1, 125.7, 126.5, 127.4, 128.0, 128.3, 129.2, 129.7, 170.9

ESI-MS [M^+] (in m/z): 375.2

FTIR (in cm^{-1}) 3259.8, 3031.2, 1671.4, 1601.6, 1558.1, 1526.3, 1199.7, 1130.4, 841.1

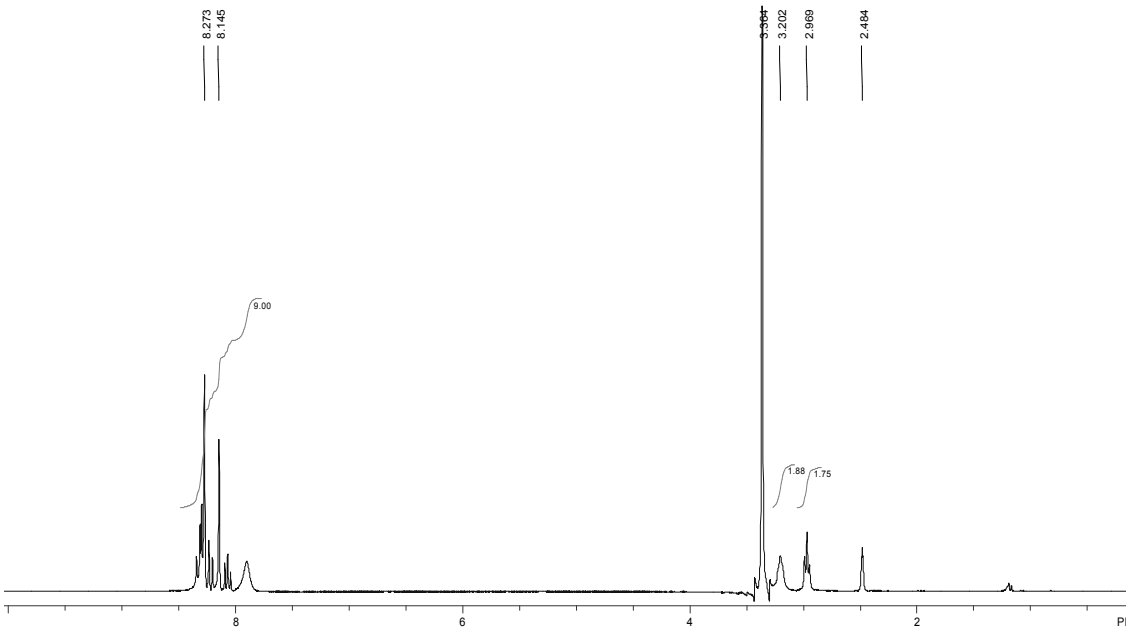
Py-4N

^{1}H NMR (D_2O, δ in ppm) 3.00 (m, 2H, $NHCOCH_2$), 3.14(m, 2H, CH_2N), 3.16 (m, 2H, CH_2N), 3.34-3.4(m, 10H, NCH_2CH_2N), 7.68-7.95(m, 9H, ArH)

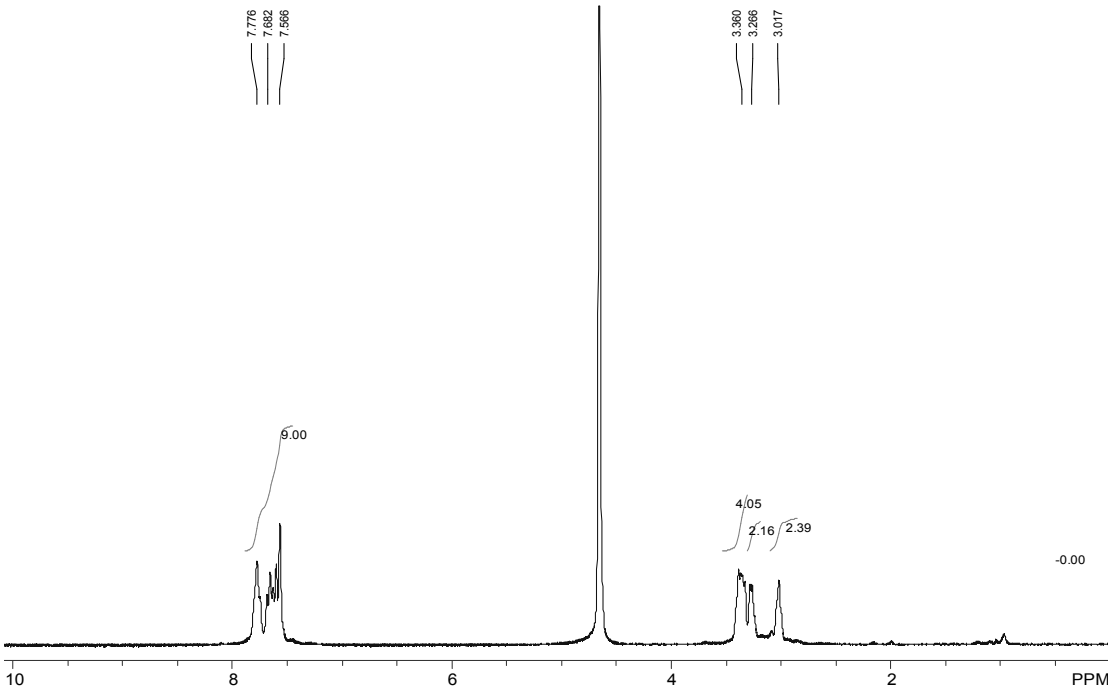
^{13}C NMR (D_2O, δ in ppm) 44.5, 43.4, 43.1, 44.5, 114.9, 117.7, 120.7, 120.9, 123.0, 123.3, 123.9, 124.9, 125.5, 126.2, 126.5, 127.9, 128.3, 129.7, 129.9, 130.2, 171.5.

ESI-MS [M^+] (in m/z) 418.2

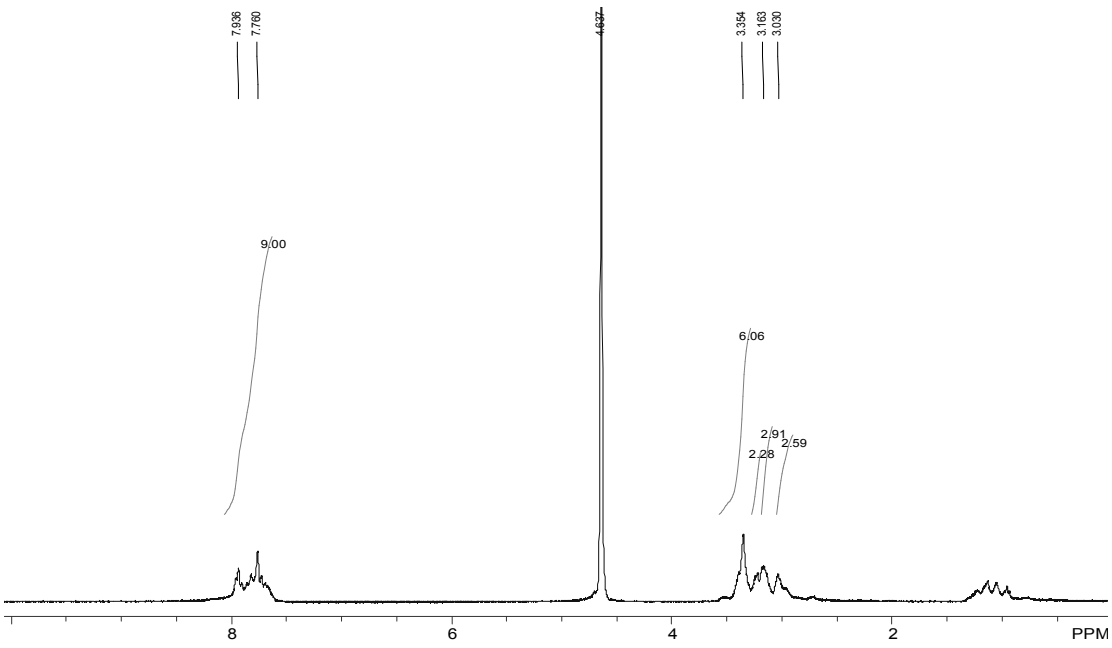
FTIR (in cm^{-1}) 3258.8, 3022.8, 1661.8,1602.7, 1557.7, 1526.1, 1201.6, 1180.5, 1128.4, 842.3



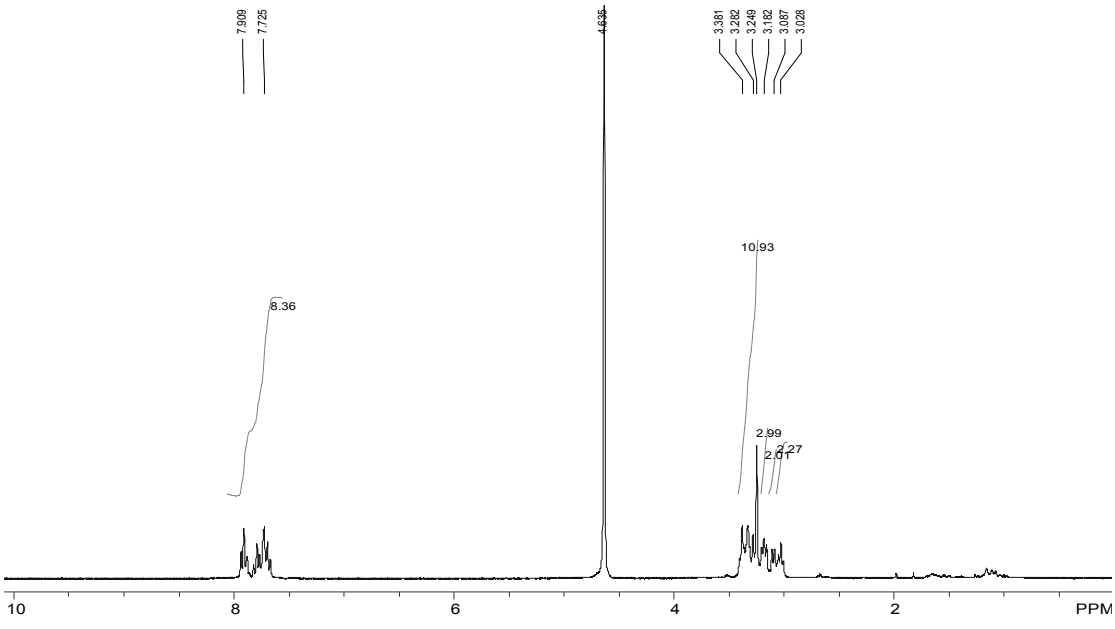
^{1}H NMR of **Py-1N** in d_6-DMSO



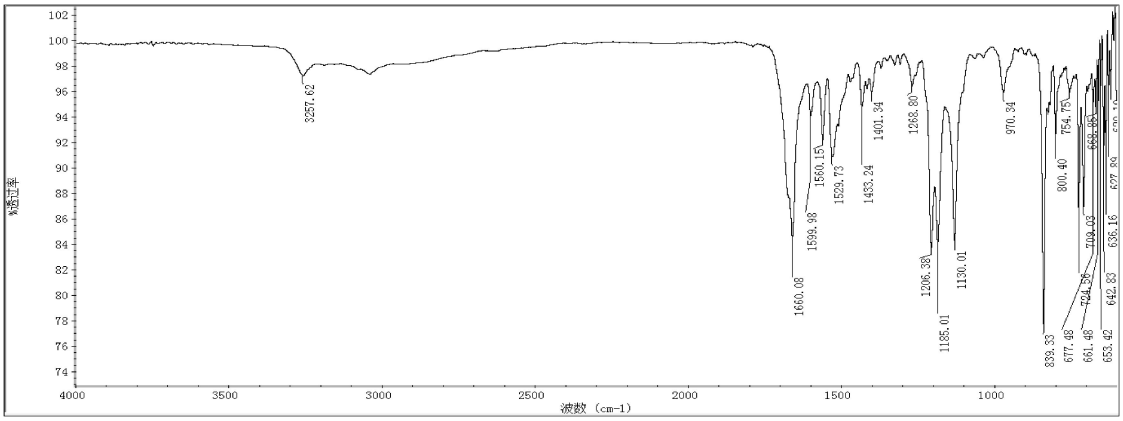
^{1}H NMR of **Py-2N** in D_2O



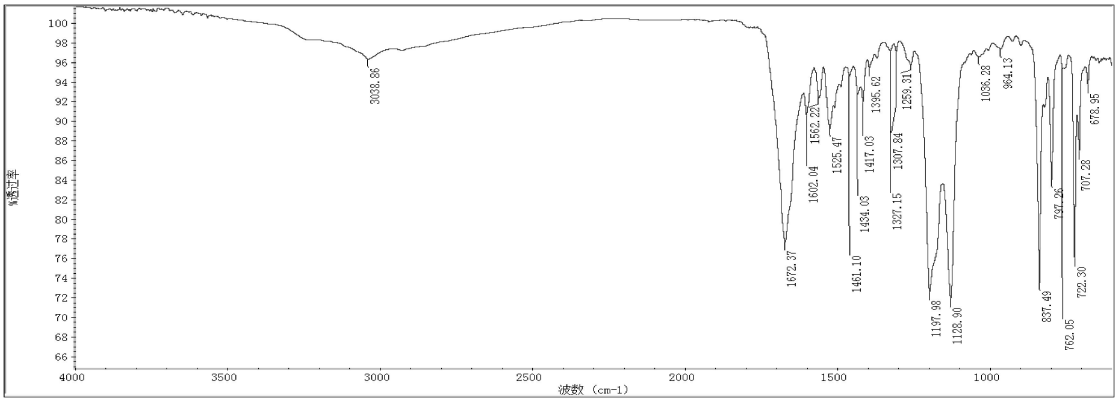
^{1}H NMR of **Py-3N** in D_2O



^{1}H NMR of **Py-4N** in D_2O



FTIR of **Py-1N**



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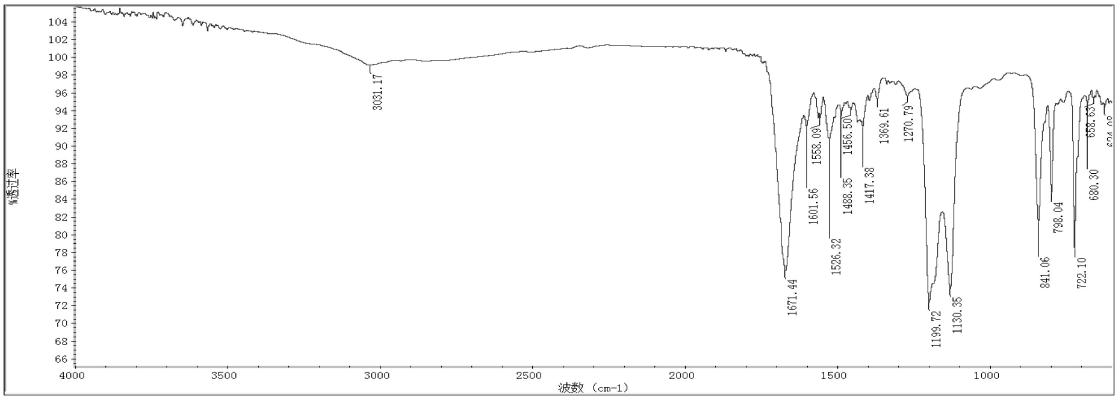

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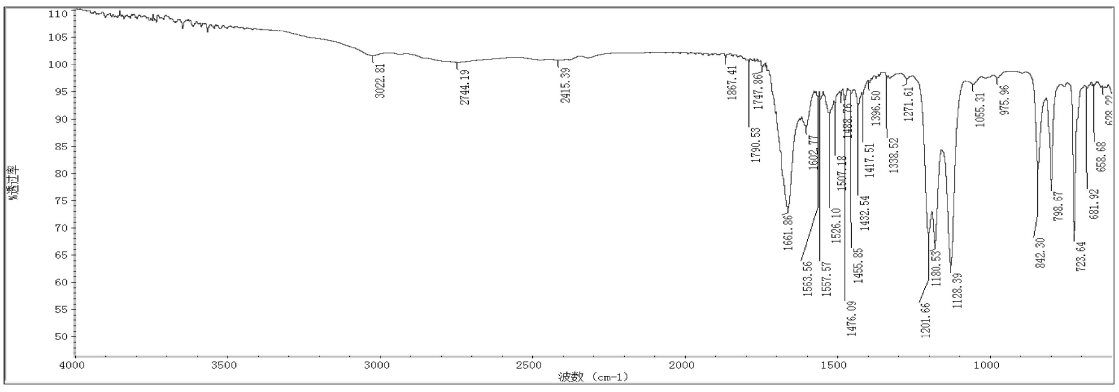
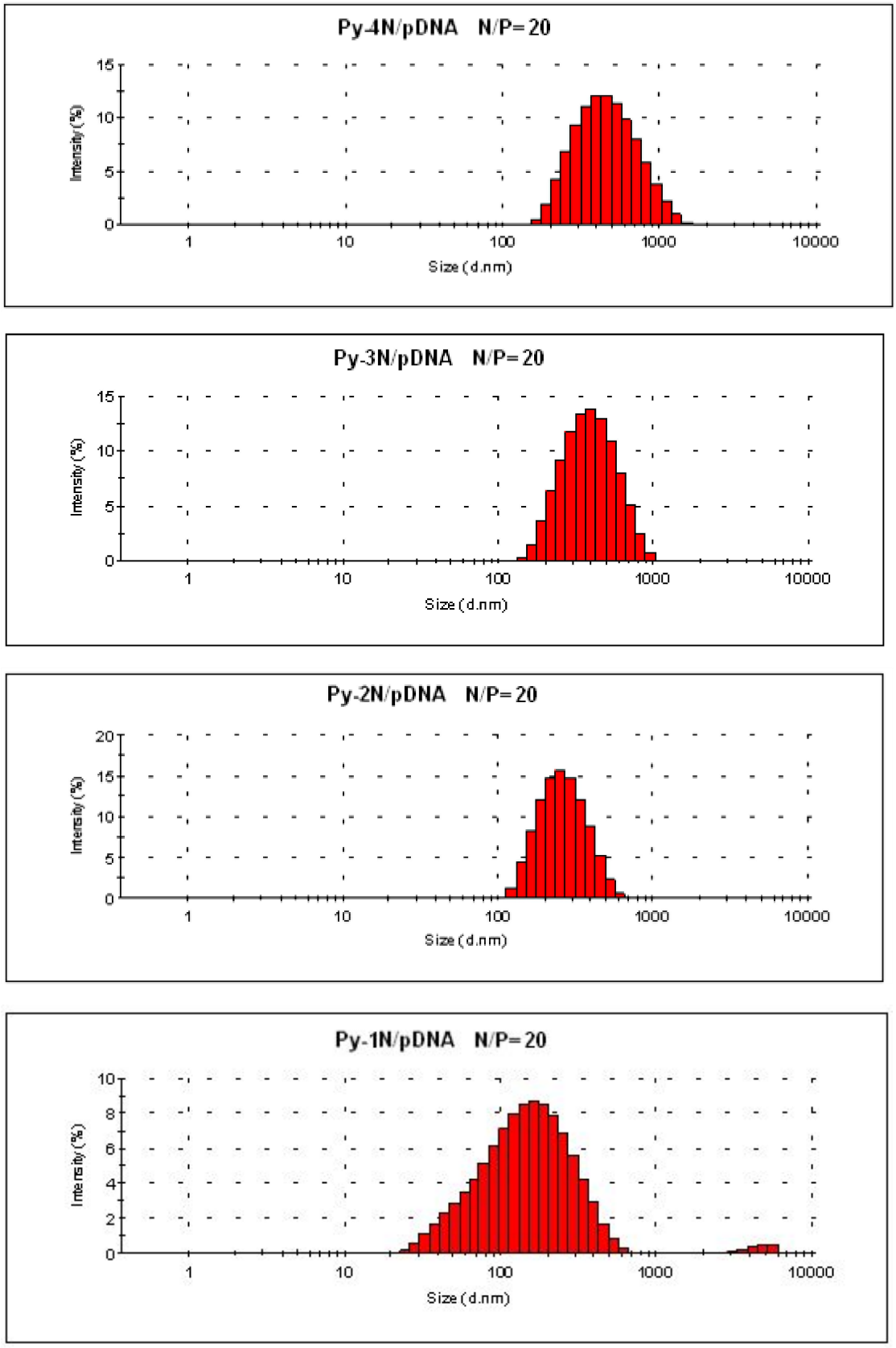


FTIR of **Py-4N**



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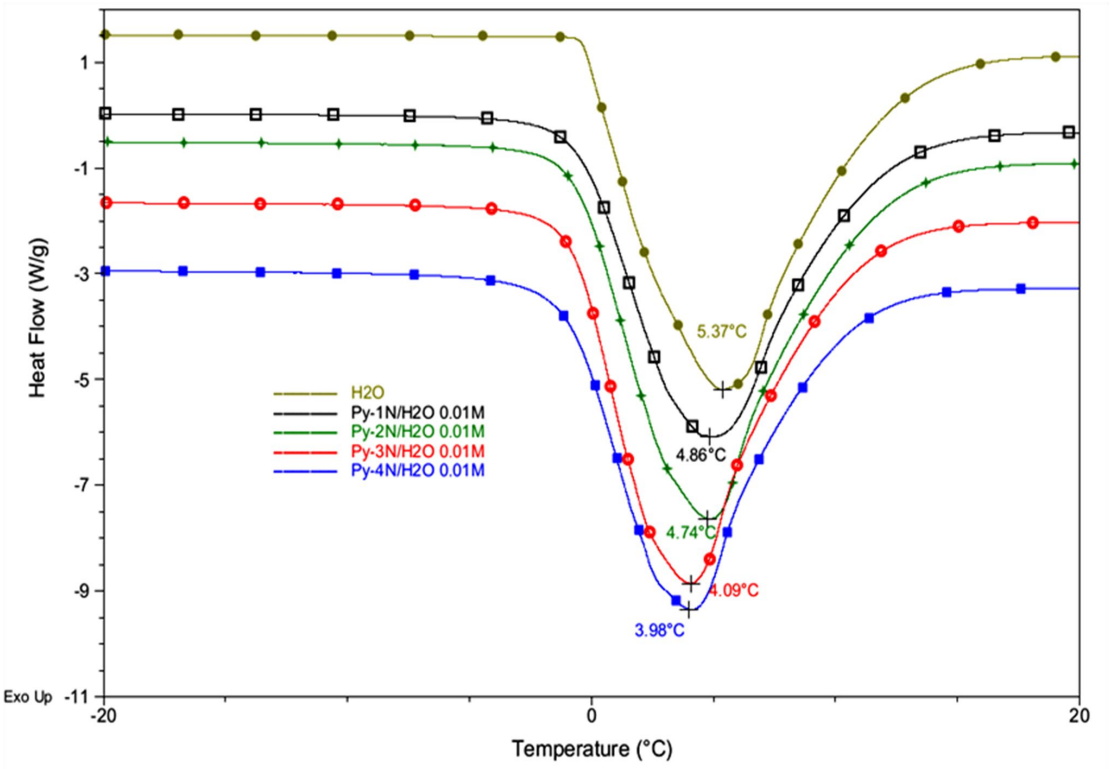

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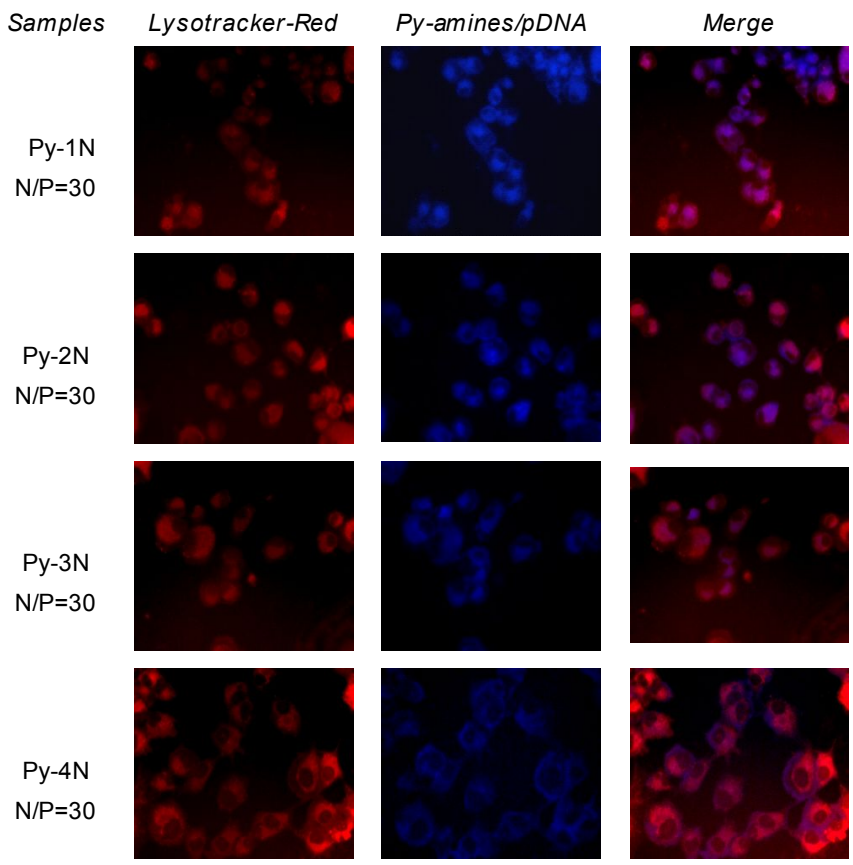

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