Supporting Information
for
EBNA1 specific luminescencesmall molecules for imaging and inhibition of latently EBV-infected tumor cells

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Experimental

1) Synthesis of JL**P**$_1$ and JLP$_2$

All chemicals used were of reagent-grade and were purchased from Sigma-Aldrich and used without further purification. All analytical-grade solvents were dried by standard procedures, distilled and deaerated before use. NMR spectra were recorded on a Bruker Ultrashield 400 Plus NMR spectrometer. The ^{1}H NMR chemical shifts were referenced to tetramethylsilane, TMS (d = 0.00). High-resolution mass spectra, reported as m/z, were obtained on a Bruker Autoflex MALDI-TOF mass spectrometer. The synthetic route of intermediates and LP_1, LP_2 were shown in the figures S1.

2: Yield: 96%; $^{1}HNMR$ ($CDCl_3$): δ 9.24 (d, J = 6.8 Hz, 2H), 7.87 (d, J = 6.4 Hz, 2H), 4.92 (m, 2H), 2.65 (s, 3H), 1.68 (t, J = 7.2 Hz, 3H); $^{13}CNMR$ ($CDCl_3$): δ 158.95, 143.67, 128.97, 56.46, 22.37, 17.14;

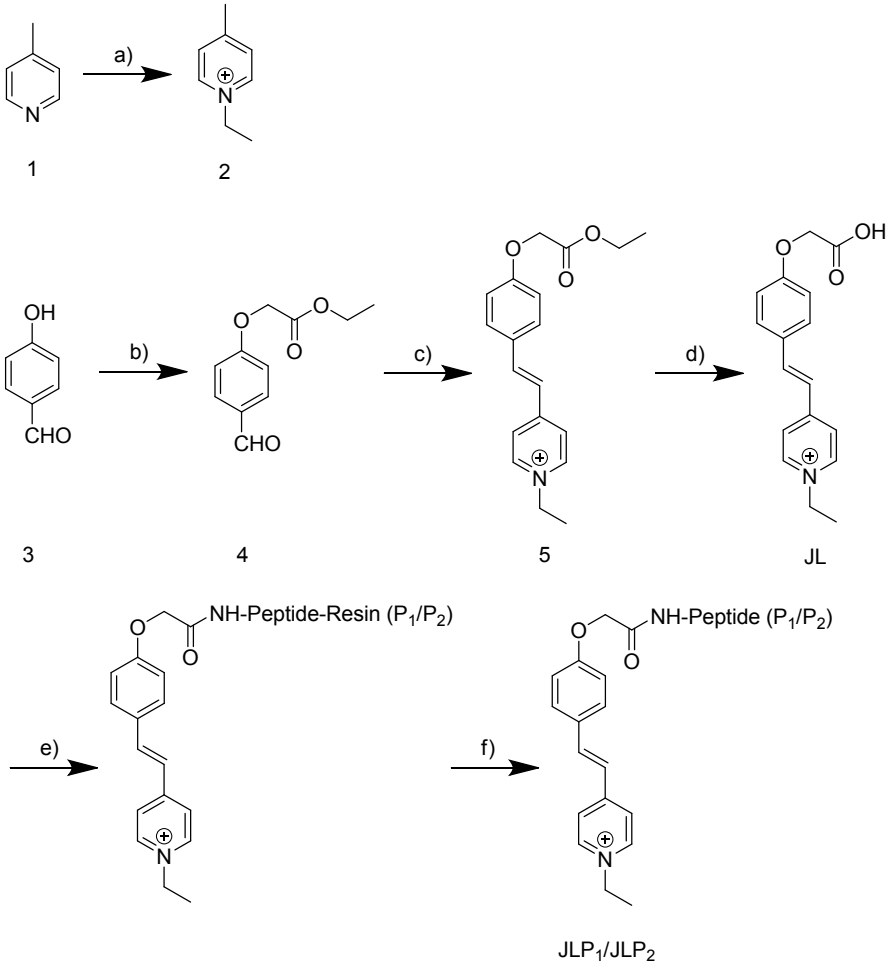
4: Yield: 90%; $^{1}HNMR$ ($CDCl_3$): δ 9.88 (s, 1H), 7.83 (d, J = 9.2 Hz, 2H), 6.99 (d, J = 8.4 Hz, 2H), 4.69 (s, 2H), 4.26 (m, 2H), 1.28 (t, J = 7.2 Hz, 3H); $^{13}CNMR$ ($CDCl_3$): δ 190.92, 168.24, 162.79, 132.15, 130.89, 115.06, 65.37, 61.86, 14.32;

5: Yield: 87%; $^{1}HNMR$ (MeOD): δ 8.76 (d, J = 6.8 Hz, 2H), 8.13 (d, J = 6.8 Hz, 2H), 7.90 (d, J = 16.4 Hz, 1H), 7.72 (d, J = 8.8 Hz, 2H), 7.30 (d, J = 16 Hz, 1H), 7.02 (d, J = 8.8 Hz, 2H); $^{13}CNMR$ (MeOD): δ 178.08, 169.09, 162.74, 153.48, 150.10, 139.55, 138.09, 133.09, 130.75, 124.84, 74.33, 70.40, 64.75, 25.81, 23.68; MALDI-TOF MS: calcd. For [M^+]: 312.16, found: 312.16;

JL: Yield: 37%; $^{1}HNMR$ (dimethyl sulfoxide – d_6): δ 8.91 (d, J = 7.2 Hz, 2H), 8.18 (d, J = 6.8 Hz, 2H), 7.98 (d, J = 16.4 Hz, 1H), 7.71 (d, J = 8.8 Hz, 2H), 7.38 (d, J = 16.4 Hz, 1H), 7.04 (d, J = 8.8 Hz, 2H), 4.77 (s, 2H), 4.50 (m, 2H), 1.52 (t, J = 7.4 Hz, 3H); $^{13}CNMR$ (dimethyl sulfoxide – d_6): δ 169.92, 159.71, 153.15, 143.87, 140.59, 129.92, 128.25, 123.45, 121.01, 115.19, 55.14, 16.19; MALDI-TOF MS: calcd. For [M^+]: 284.13, found: 284.17;

JLP_1: MALDI-TOF MS: calcd. For [M^+]: 1073.46, found: 1074.92; Elemental Analysis: Calculated C = 66.78, H = 6.64, N = 10.10; Found = C = 66.18, H = 6.32, N = 10.01.

JLP_2: MALDI-TOF MS: calcd. For [M^+]: 970.45, found: 971.44; Calculated C = 63.72, H = 6.47, N = 10.43; Found C = 63.66, H = 6.44, N = 10.31.



a) CH_3CH_2I, ACN, 90℃, 4h;

b) $BrCH_2COOCH_2CH_3$, K_2CO_3, ACN, reflux, overnight;

c) 2, Piperidine, EtOH, 90℃, 6h;

d) 0.4 mol/L NaOH, dioxane, rt, 4h;

e) Peptide-Resin, PyBOP, DIPEA, DMF, rt, overnight;

f) TFA/DCM, rt, 3h.

Figure S1. The synthetic routes of JL and JLP_1/JLP_2

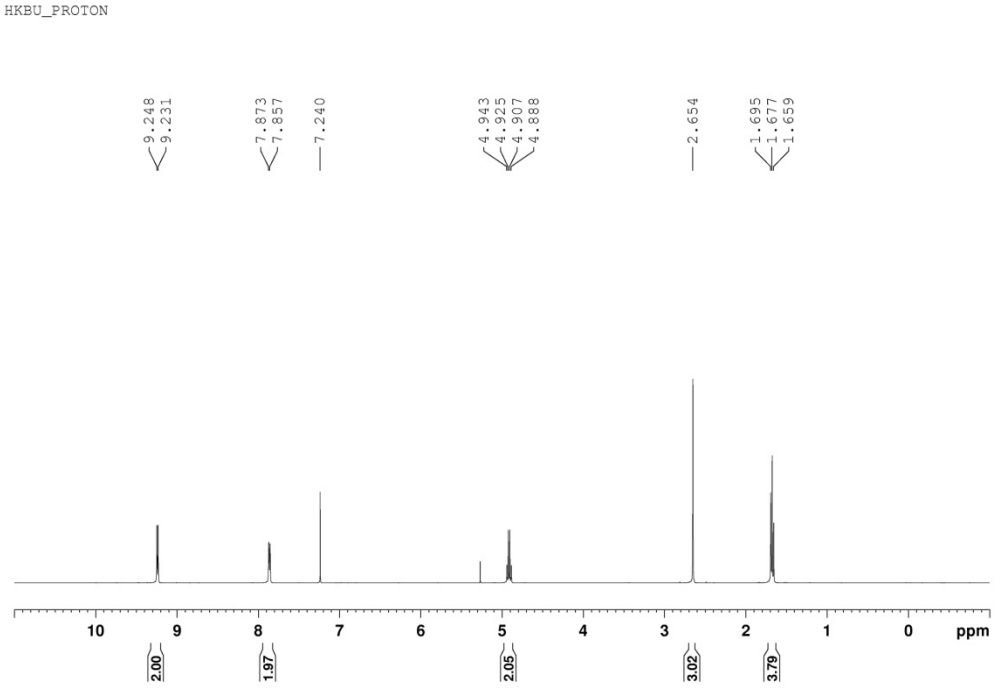


Figure S2. 400 MHz-^{1}H-NMR ($CDCl_3$) spectrum of intermediate **2**

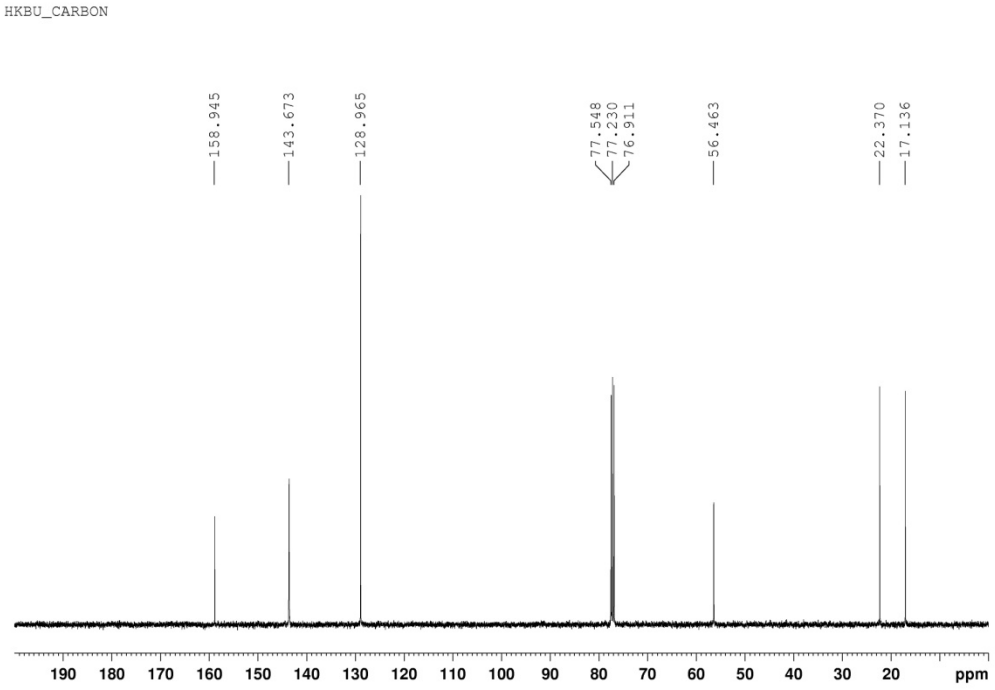


Figure S3. 400 MHz-^{13}C-NMR ($CDCl_3$) spectrum of intermediate **2**

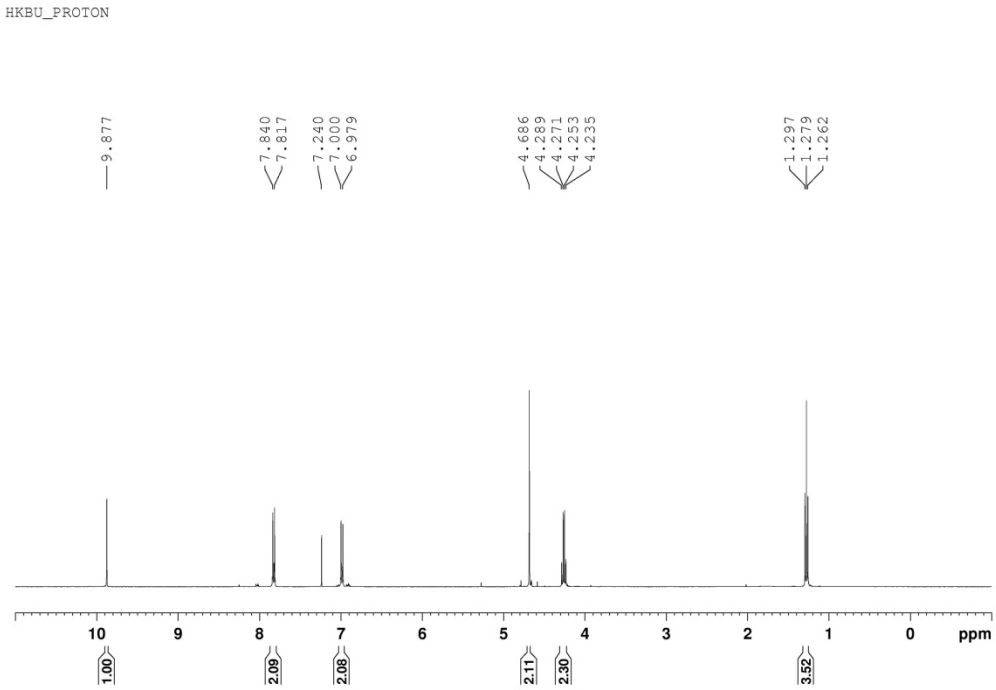


Figure S4. 400 MHz-^{1}H-NMR ($CDCl_3$) spectrum of intermediate **4**

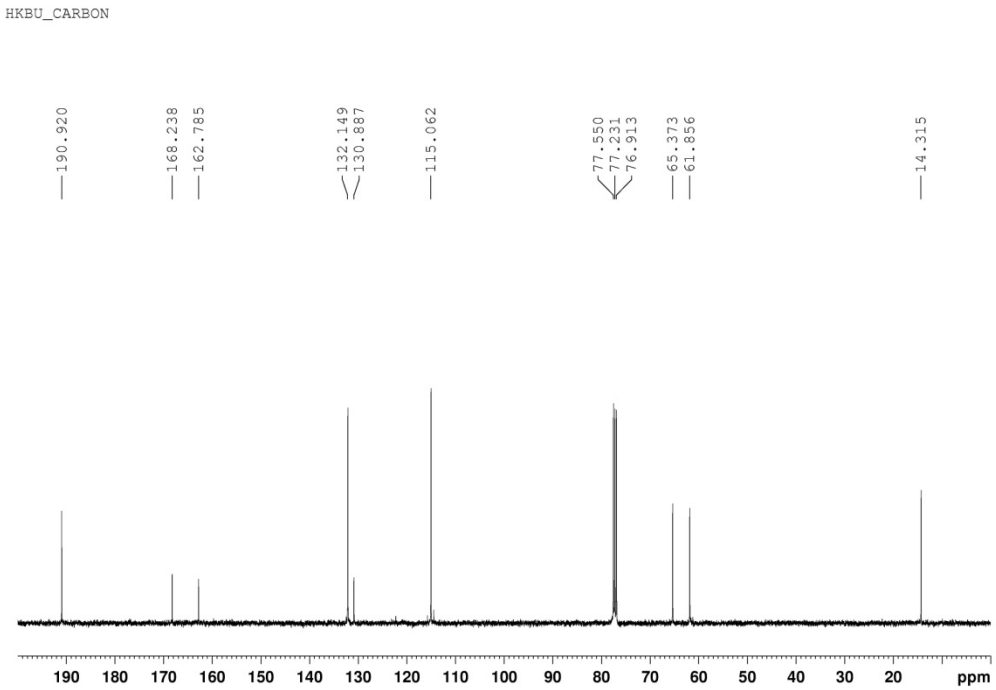


Figure S5. 400 MHz-^{13}C-NMR ($CDCl_3$) spectrum of intermediate **4**

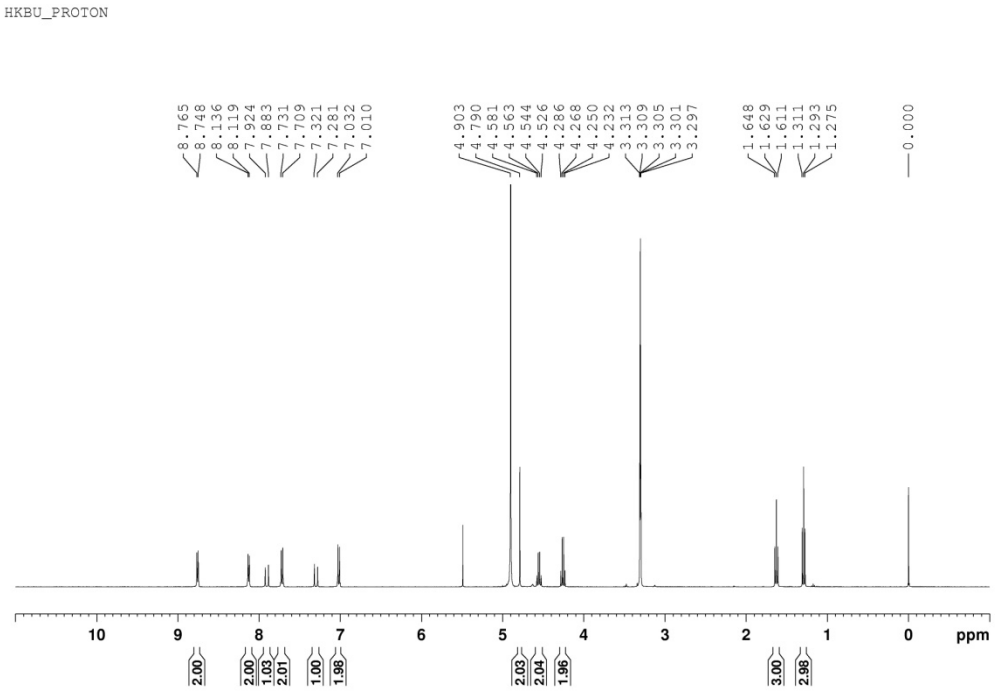


Figure S6. 400 MHz-^{1}H-NMR (MeOD) spectrum of intermediate **5**

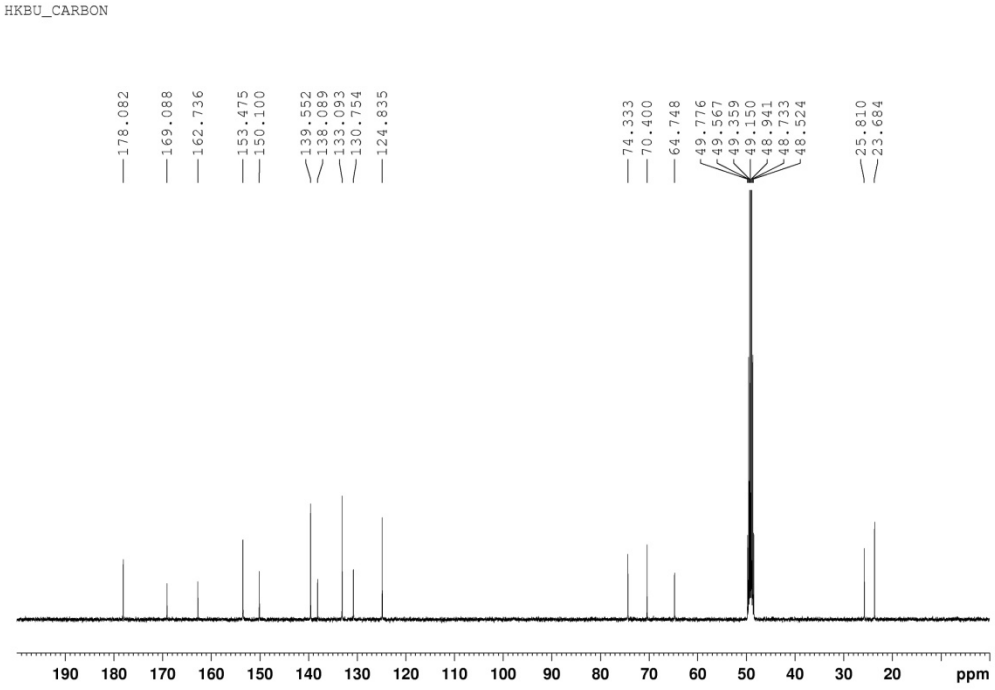


Figure S7. 400 MHz-^{13}C-NMR (MeOD) spectrum of intermediate **5**

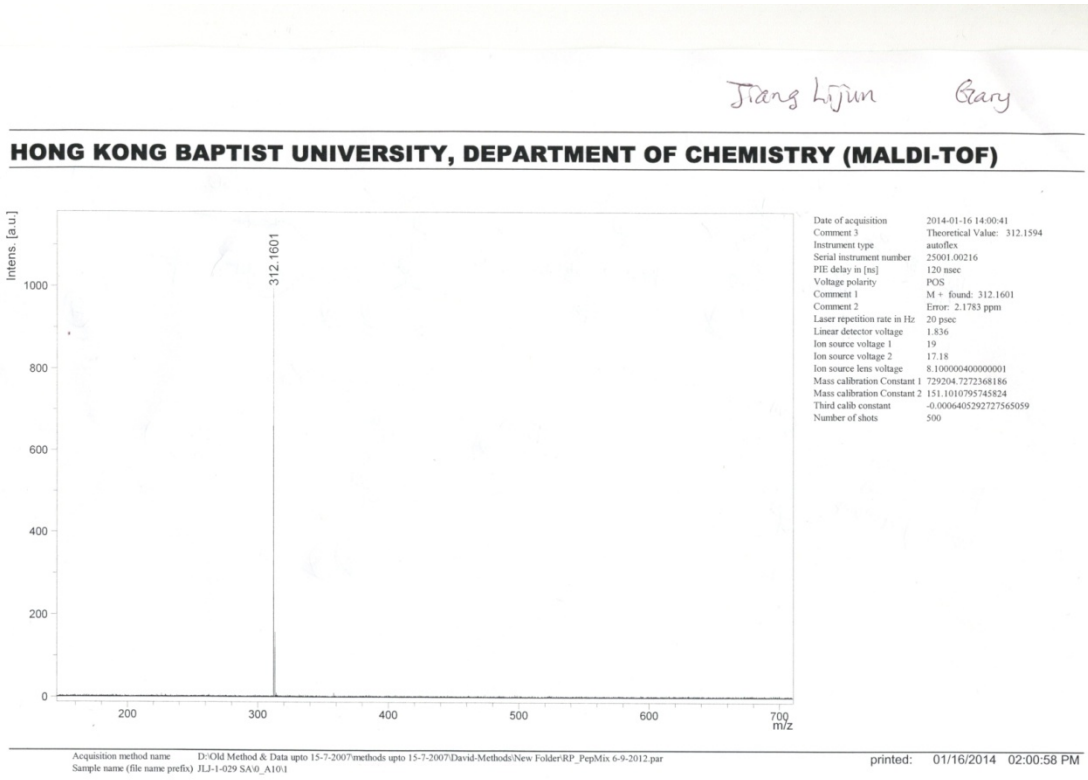


Figure S8. MALDI-TOF spectrum of intermediate **5**

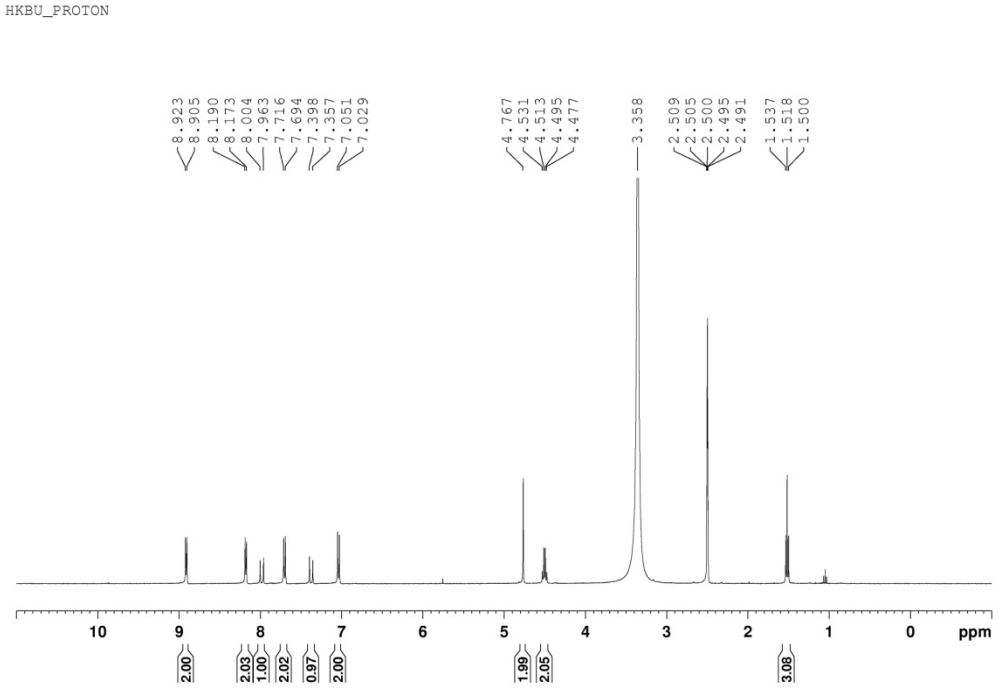


Figure S9. 400 MHz-^{1}H-NMR (dimethyl sulfoxide-d_6) spectrum of **JL**

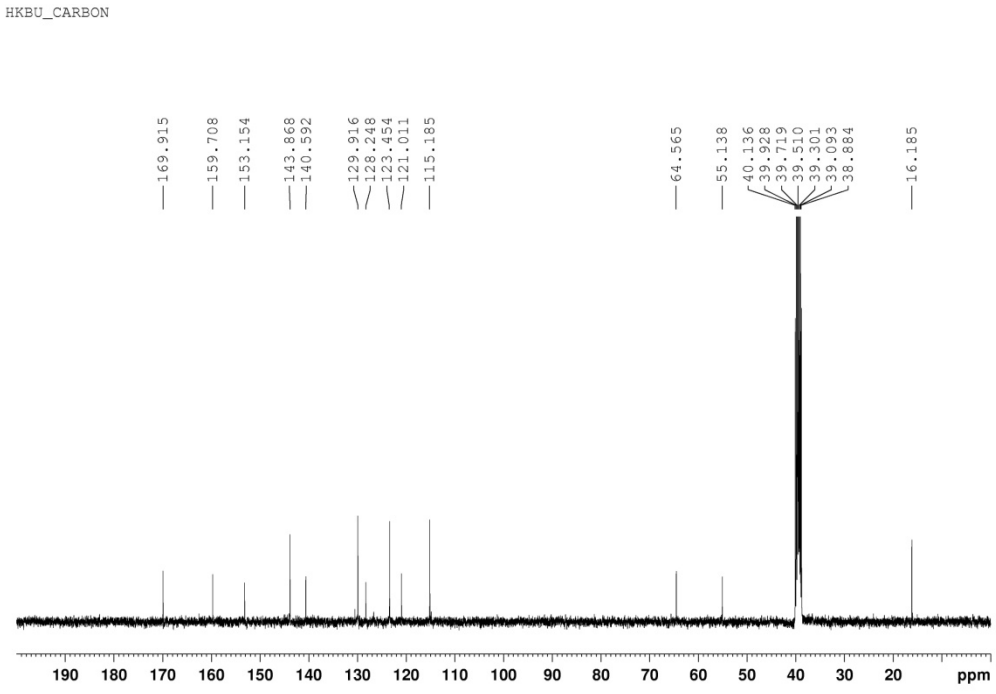


Figure S10. 400 MHz-^{13}C-NMR (dimethyl sulfoxide-d_6) spectrum of **JL**

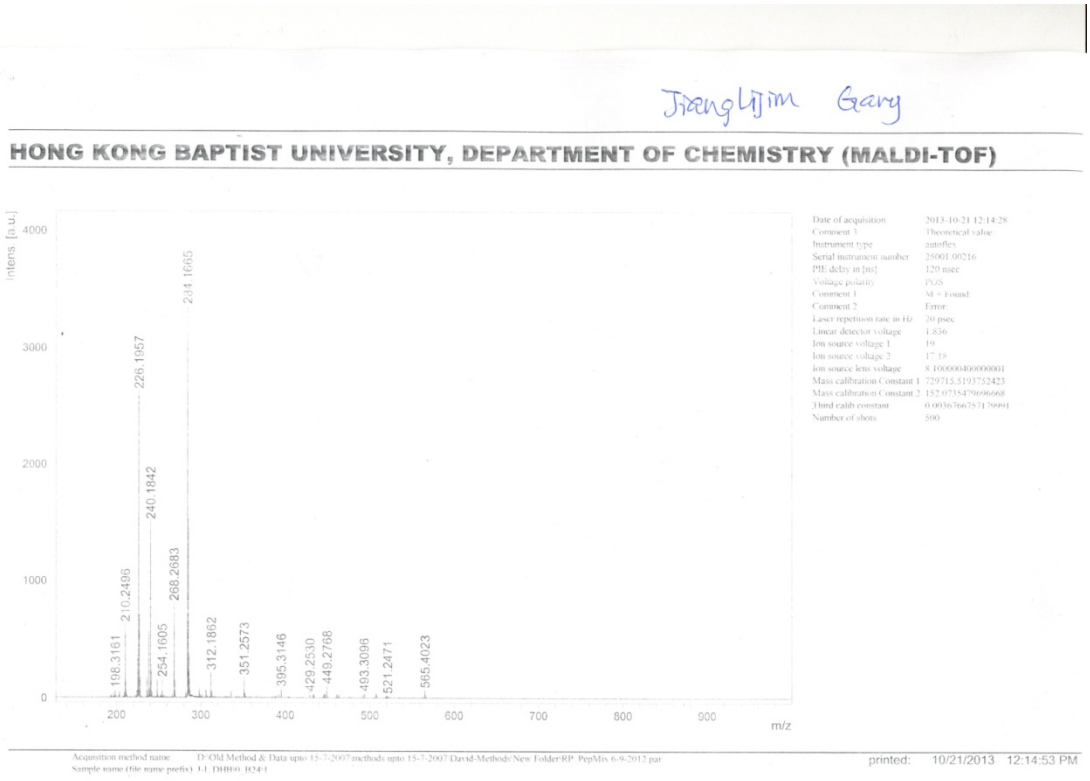


Figure S11. MALDI-TOF spectrum of **JL**

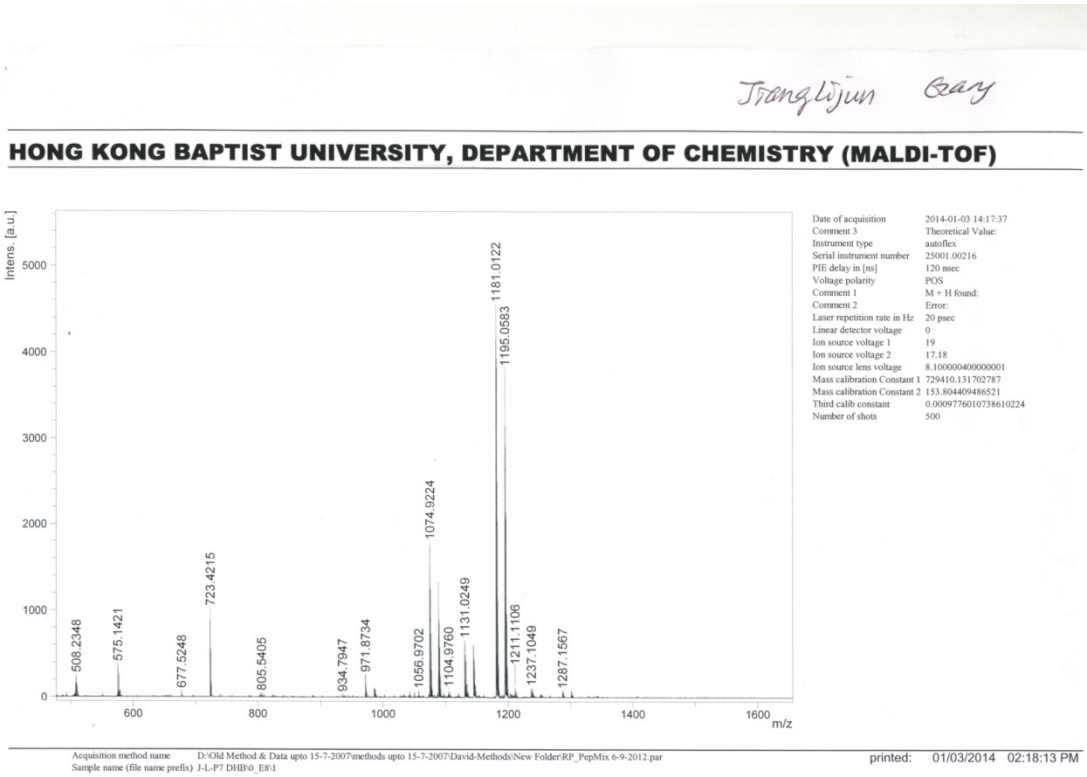


Figure S12. MALDI-TOF spectrum of **JLP_1**

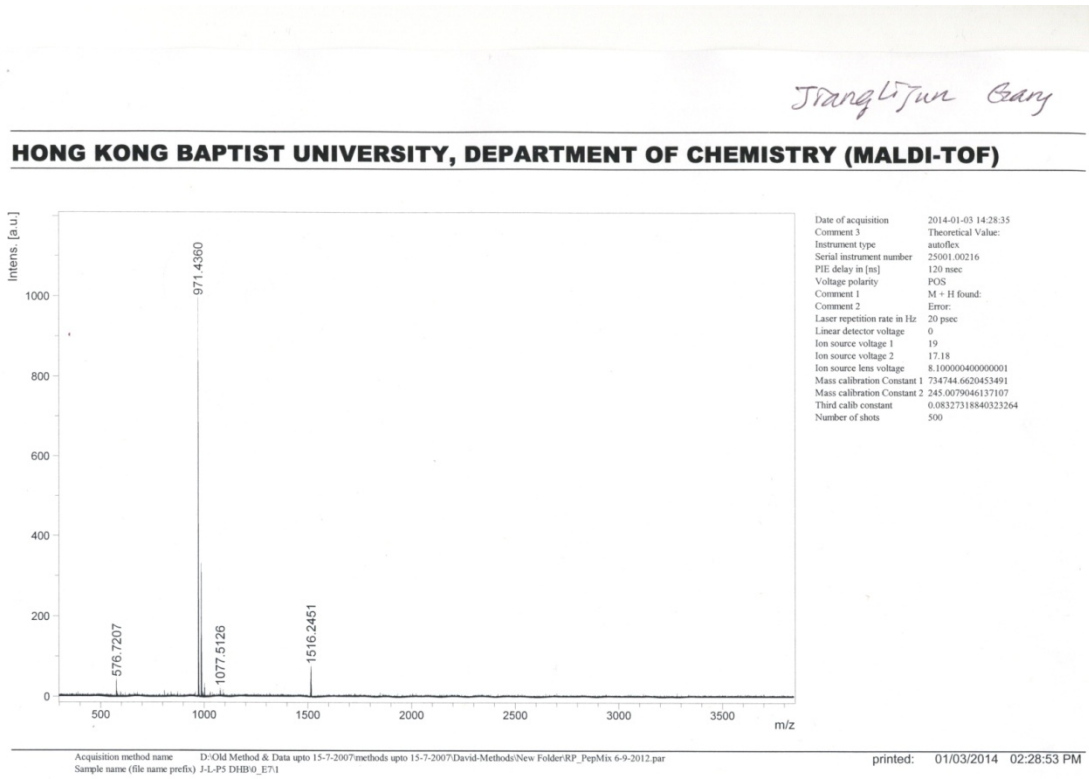


Figure S13. MALDI-TOF spectrum of **JLP_2**

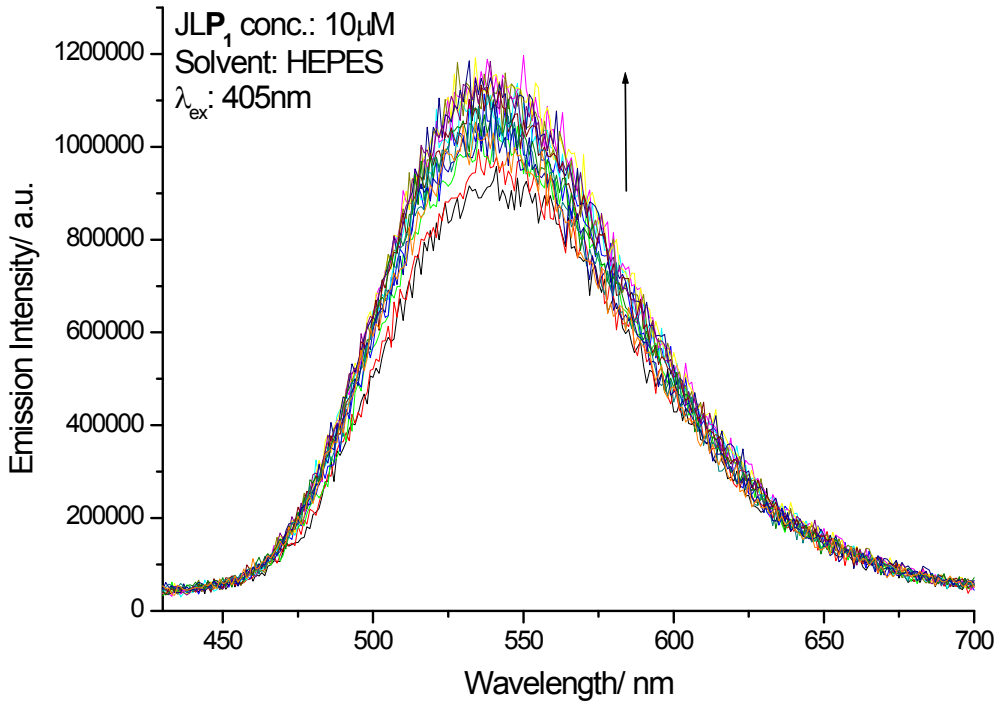


Figure S14. The emission titration of JL**P**$_1$ upon the addition of the 200 nM EBNA1.

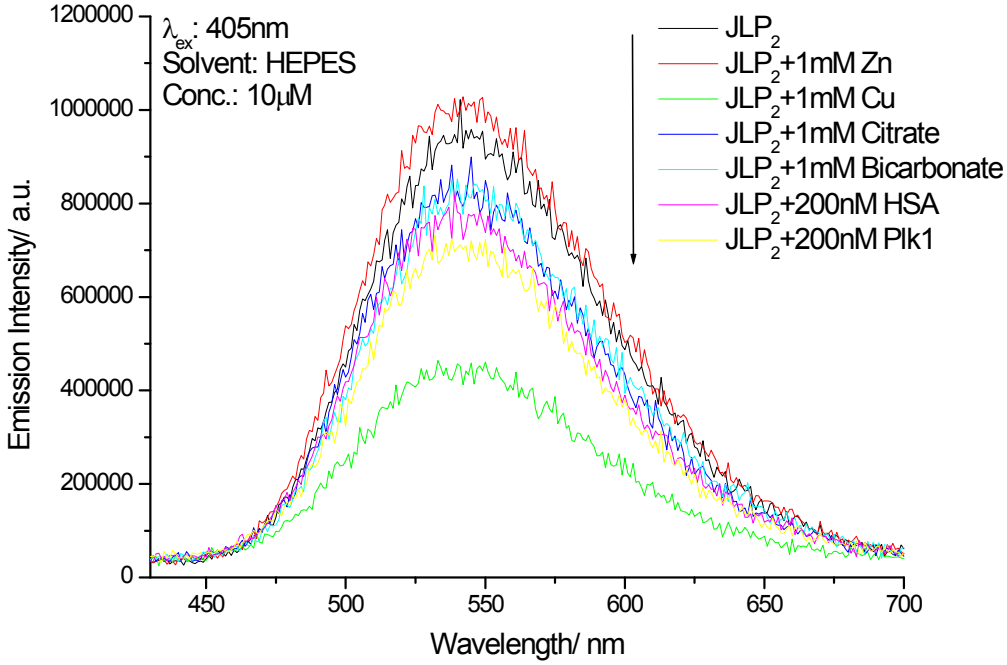


Figure S15. The emission spectra of JL**P**$_2$ upon the addition of the various protein and small molecules.