Supporting Information

Tuning a structure of peptide nucleic acid (PNA) molecular beacon and DNA detection by the hybrid with quencher-modified DNA

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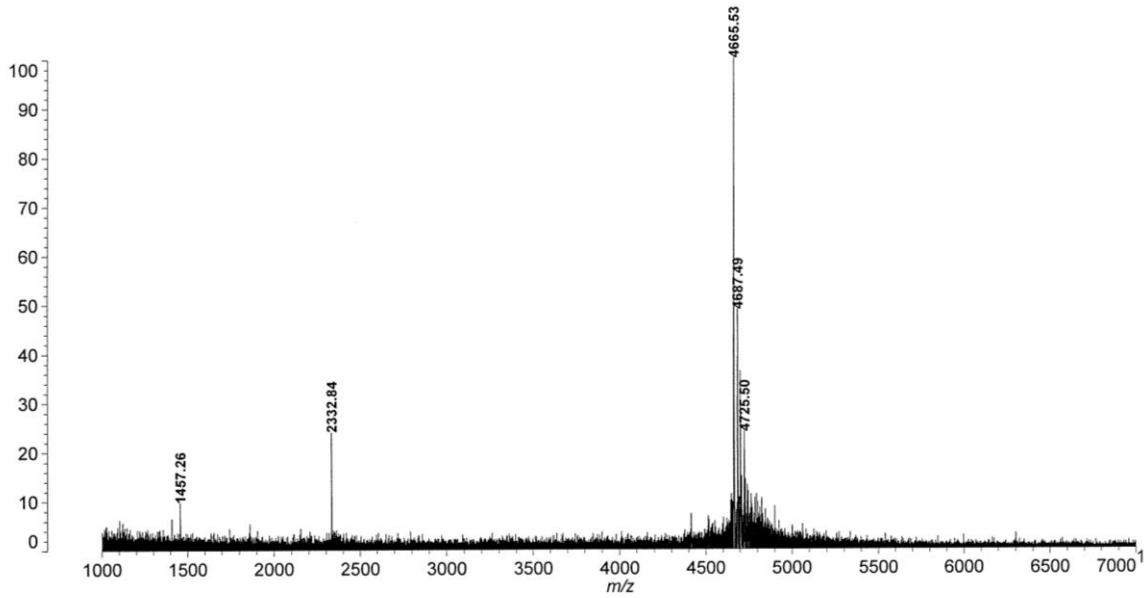

Figure S1. MALDI-TOF mass spectrum of **P1Q0**. An ⊙-CHCA was used as a matrix. calcd. $[M+H]^+$ =4663.08 and obsd. $[M+H]^+$ =4665.53.

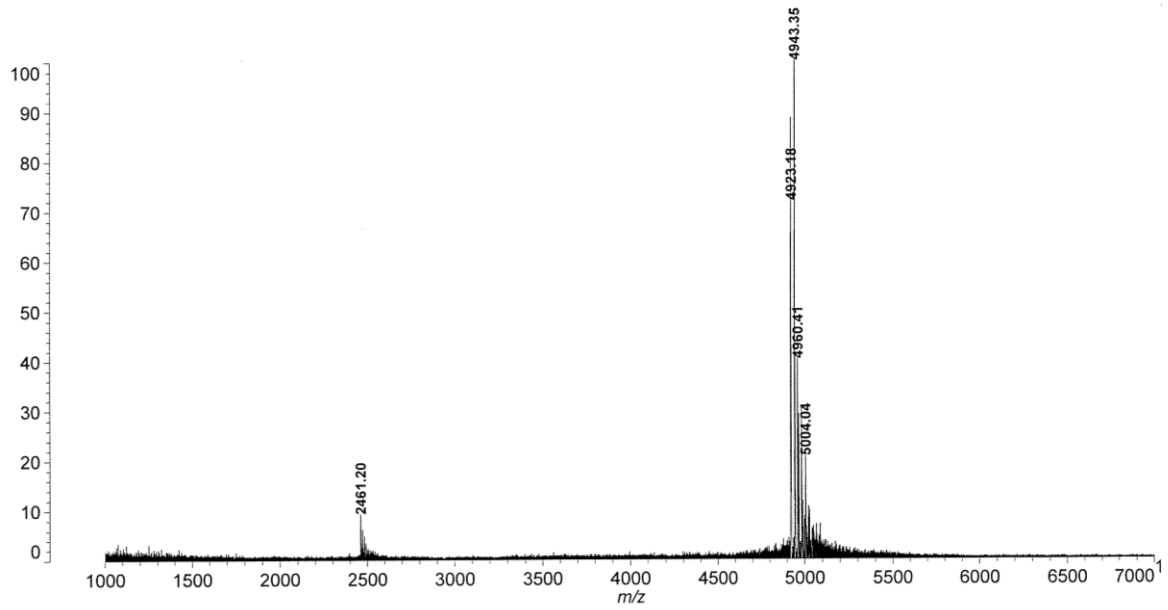

Figure S2. MALDI-TOF mass spectrum of **P2Q0**. An ⊙-CHCA was used as a matrix. calcd. $[M+H]^+$ =4920.22 and obsd. $[M+H]^+$ =4923.18.

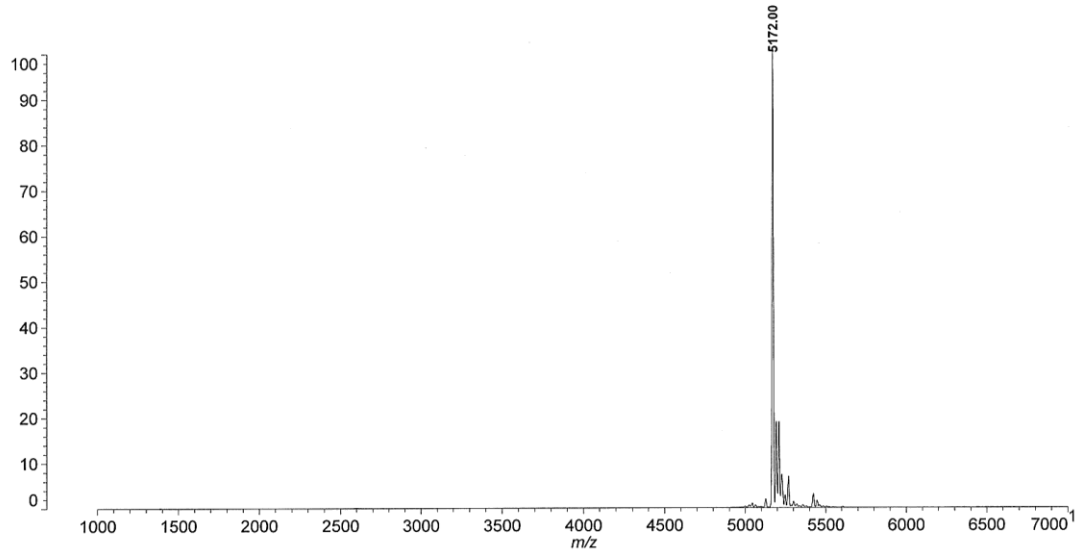

Figure S3. MALDI-TOF mass spectrum of **P3Q0**. An ⊙-CHCA was used as a matrix. calcd. $[M+H]^+$ = 5175.34 and obsd. $[M+H]^+$ = 5172.00.

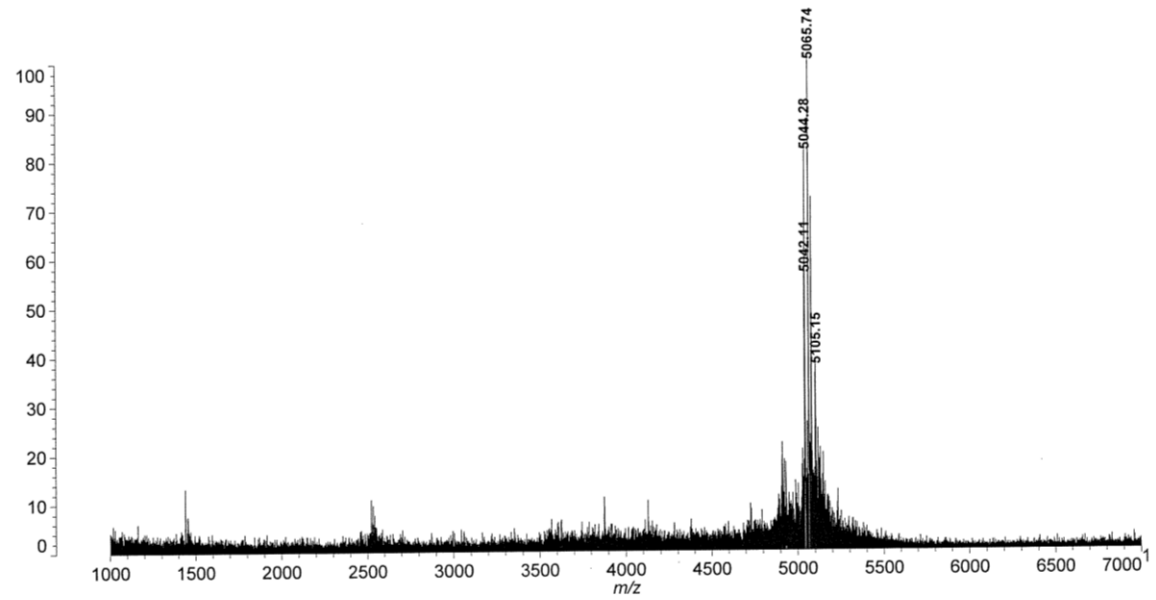

Figure S4. MALDI-TOF mass spectrum of **P1Q1**. An ◎-CHCA was used as a matrix. calcd. $[M+H]^+$ =5042.28 and obsd. $[M+H]^+$ = 5044.28.

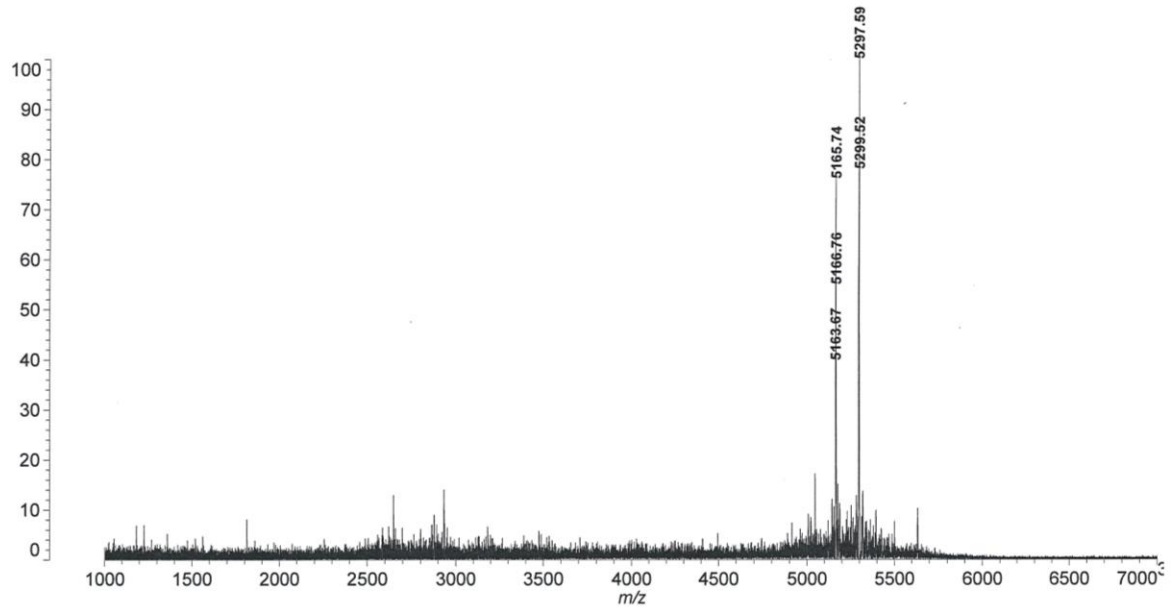

Figure S5. MALDI-TOF mass spectrum of **P2Q1**. An ◎-CHCA was used as a matrix. calcd. $[M+H]^+$ =5297.40 and obsd. $[M+H]^+$ =5297.59. The peak at 132 Da smaller than the purpose peak is the decomposition product of the Dabcyl group by the laser irradiated at the time of measurement. In other figures, the peaks at 132, 264 and/or 396 Da smaller than the purpose peak showing the decomposition product of the Dabcyl groups are also observed.

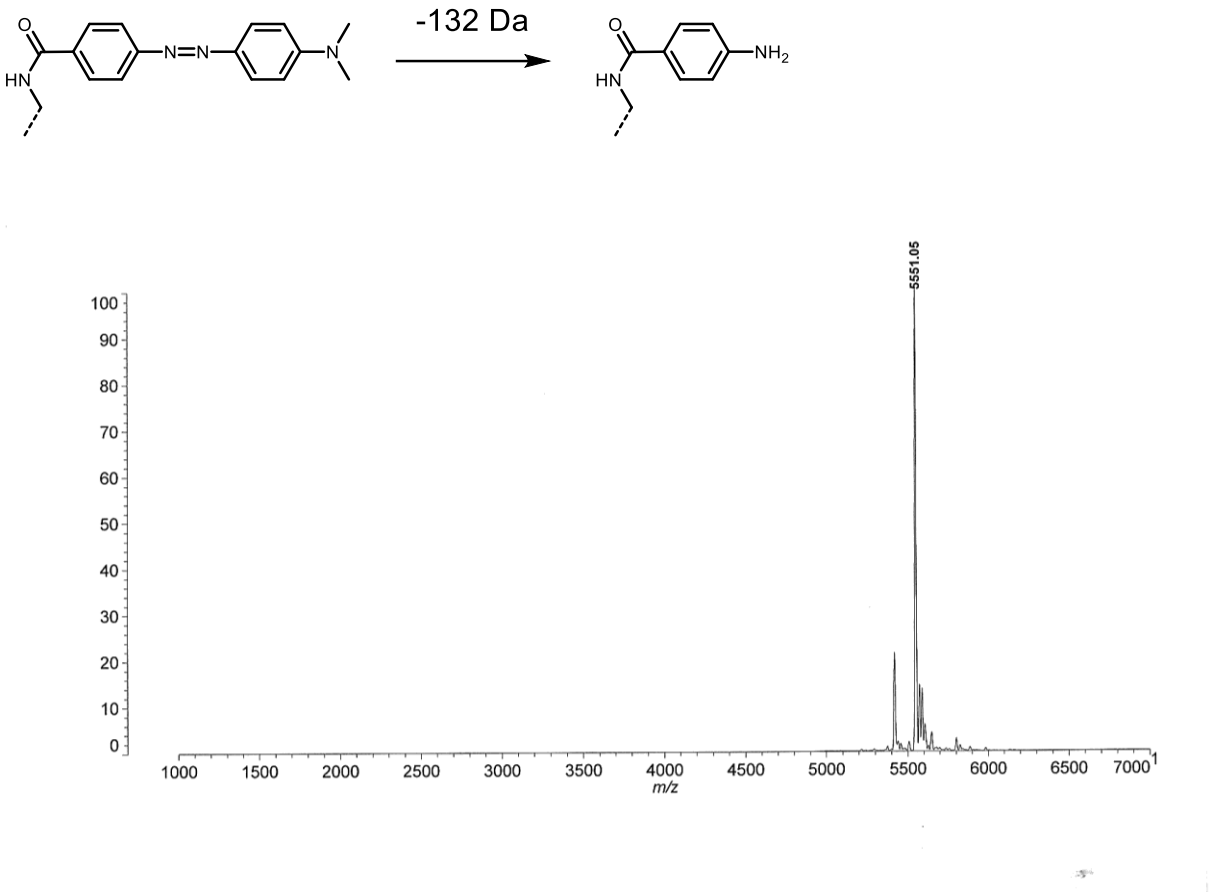

Figure S6. MALDI-TOF mass spectrum of **P3Q1**. An ⍵-CHCA was used as a matrix. calcd. $[M+H]^+$ = 5554.54 and obsd. $[M+H]^+$ =5551.05.

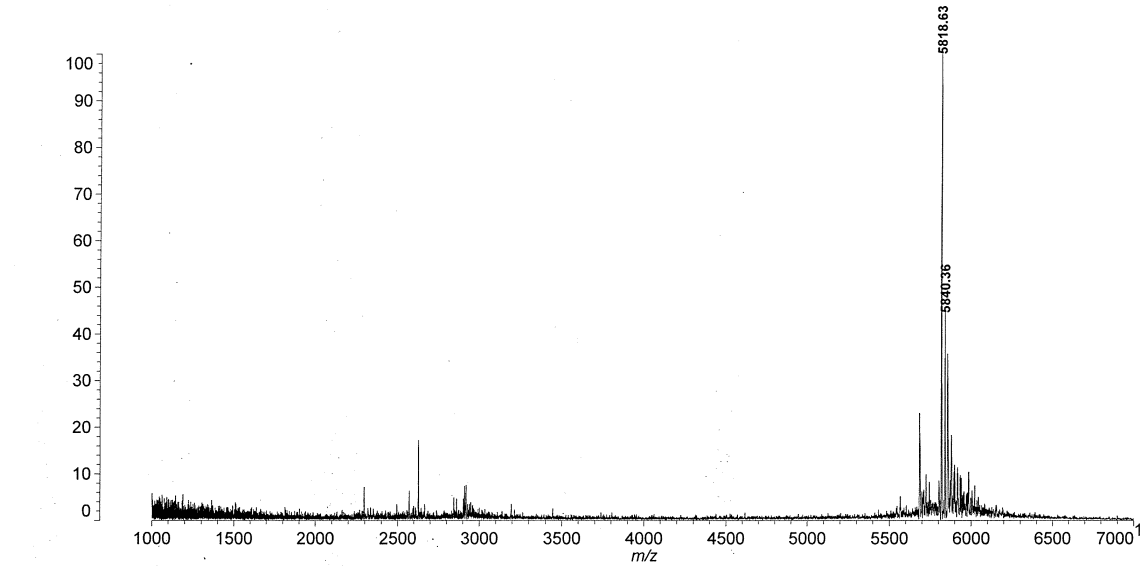

Figure S7. MALDI-TOF mass spectrum of **P4Q1**. An ◎-CHCA was used as a matrix. calcd. $[M+H]^+$ = 5815.16 and obsd. $[M+H]^+$ = 5818.63.

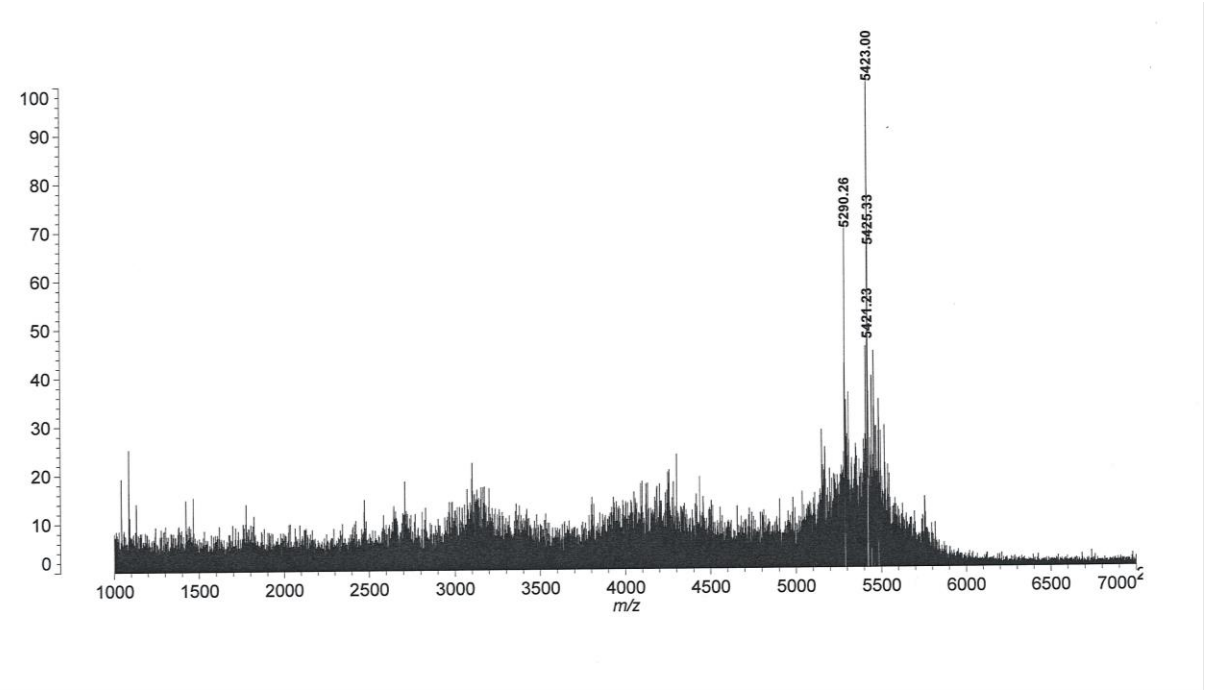

Figure S8. MALDI-TOF mass spectrum of **P1Q2**. An ◎-CHCA was used as a matrix. calcd. $[M+H]^+$ =5419.47 and obsd. $[M+H]^+$ = 5423.00.

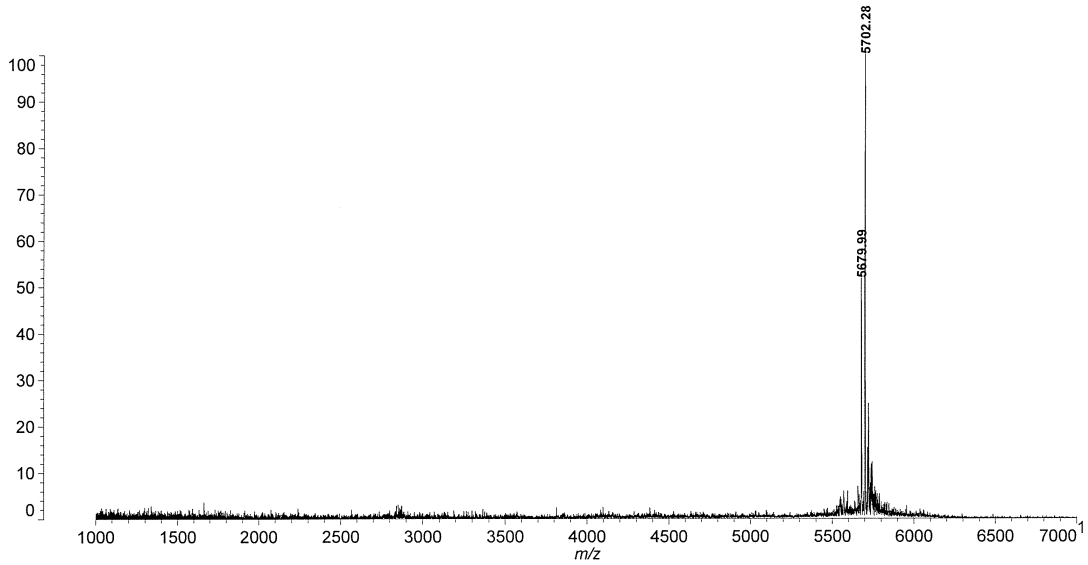

Figure S9. MALDI-TOF mass spectrum of **P2Q2**. An ⌾-CHCA was used as a matrix. calcd. $[M+H]^+$ =5676.60 and obsd. $[M+H]^+$ =5679.99.

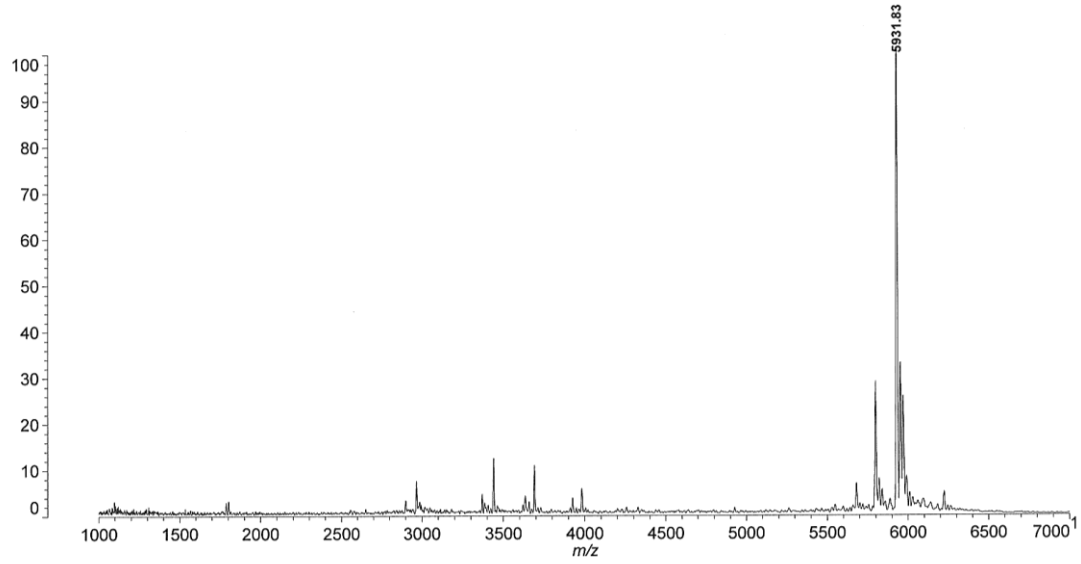

Figure S10. MALDI-TOF mass spectrum of **P3Q2**. An ⌾-CHCA was used as a matrix. calcd. $[M+H]^+$ =5933.74 and obsd. $[M+H]^+$ = 5931.83.

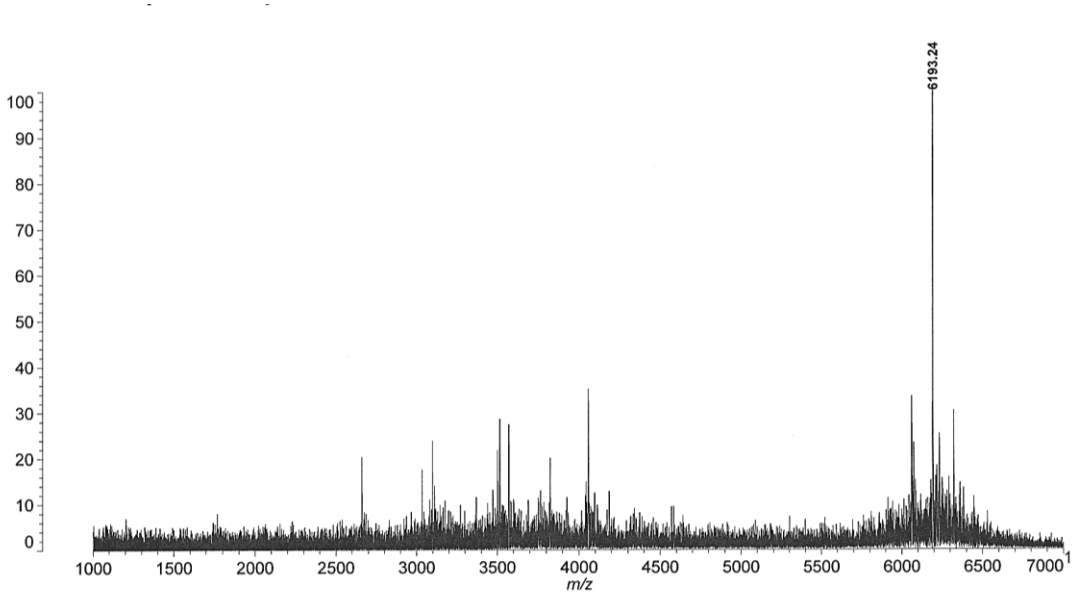

Figure S11. MALDI-TOF mass spectrum of **P4Q2**. An ⌾-CHCA was used as a matrix. calcd. $[M+H]^+$ = 6190.88 and obsd. $[M+H]^+$ = 6193.24.

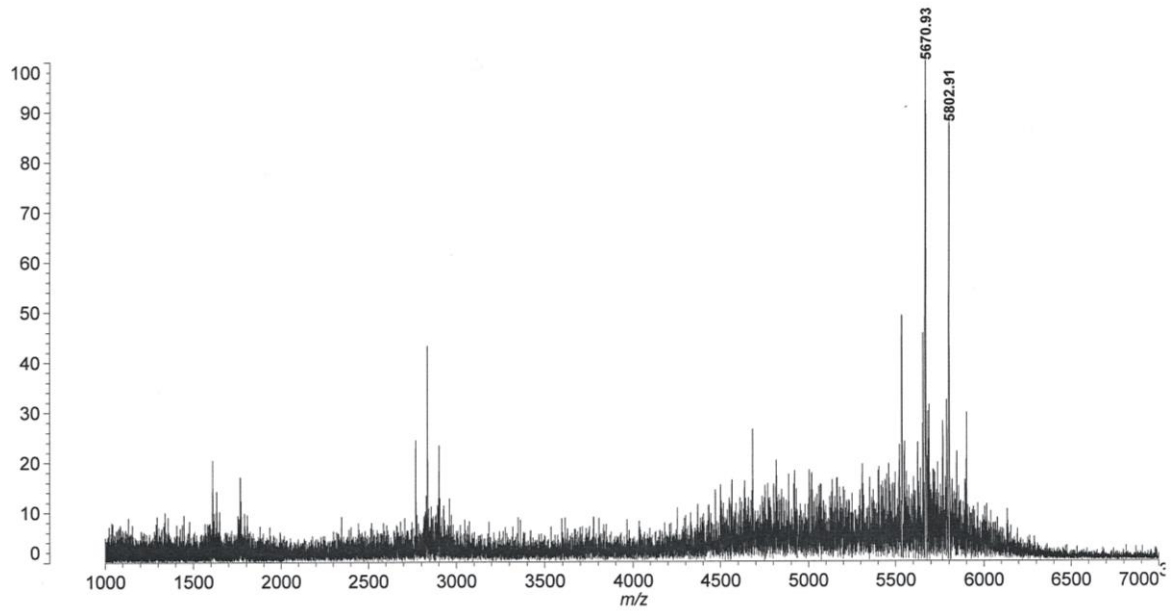

Figure S12. MALDI-TOF mass spectrum of **P1Q3**. An ⌾-CHCA was used as a matrix. calcd. $[M+H]^+$ =5798.67 and obsd. $[M+H]^+$ = 5802.91.

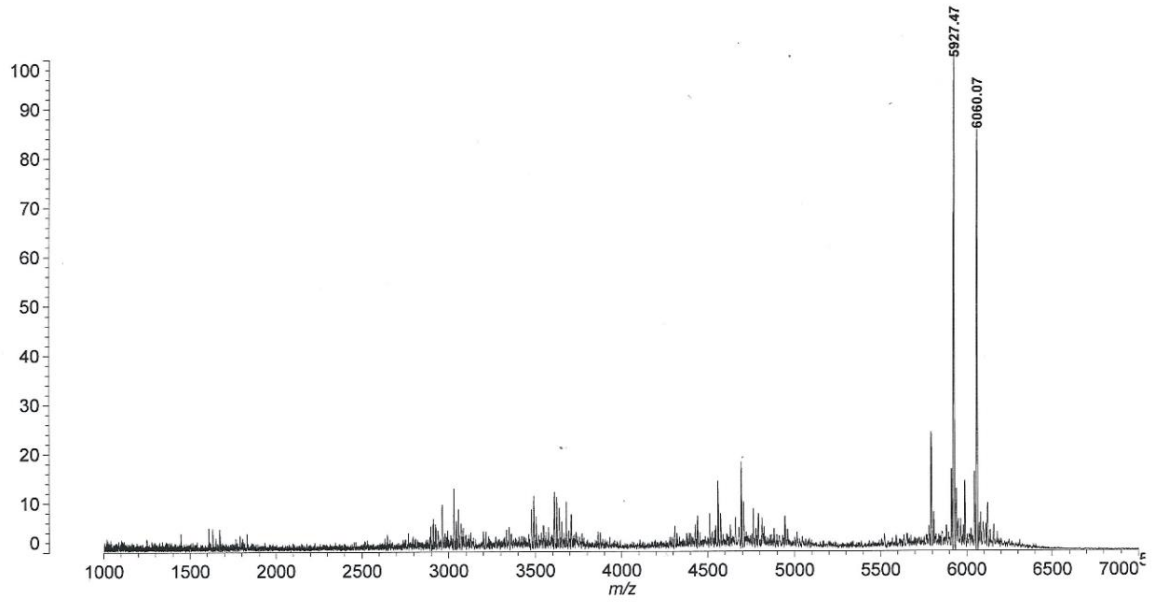

Figure S13. MALDI-TOF mass spectrum of **P2Q3**. An ⌾-CHCA was used as a matrix. calcd. $[M+H]^+$ =6055.81 and obsd. $[M+H]^+$ = 6060.07.

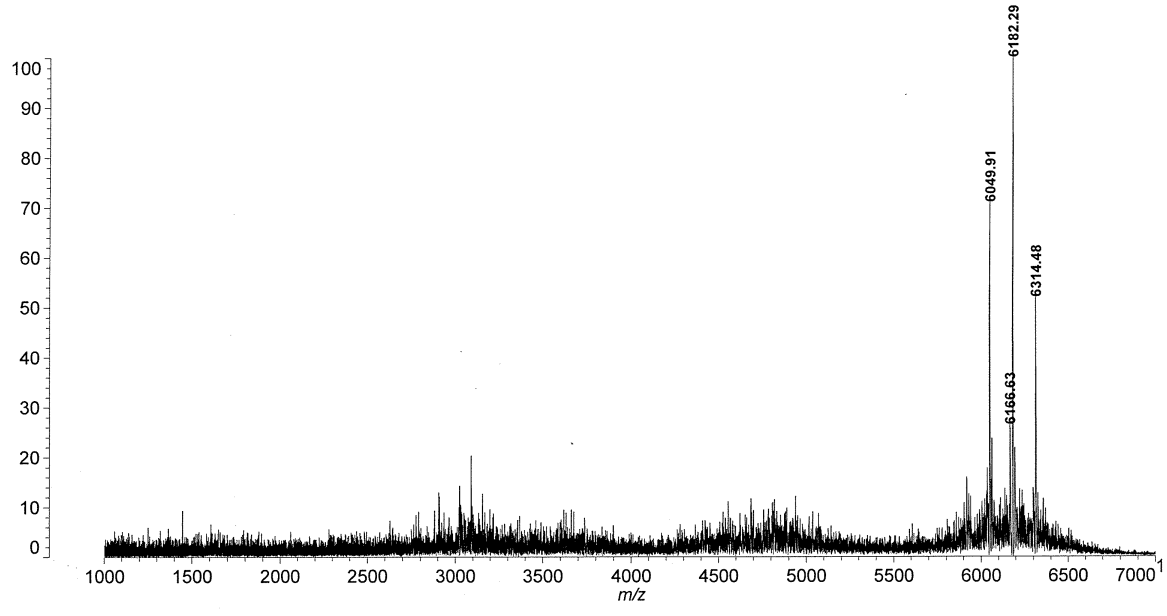

Figure S14. MALDI-TOF mass spectrum of **P3Q3**. An ⌾-CHCA was used as a matrix. calcd. $[M+H]^+$ =6312.94 and obsd. $[M+H]^+$ = 6314.48.

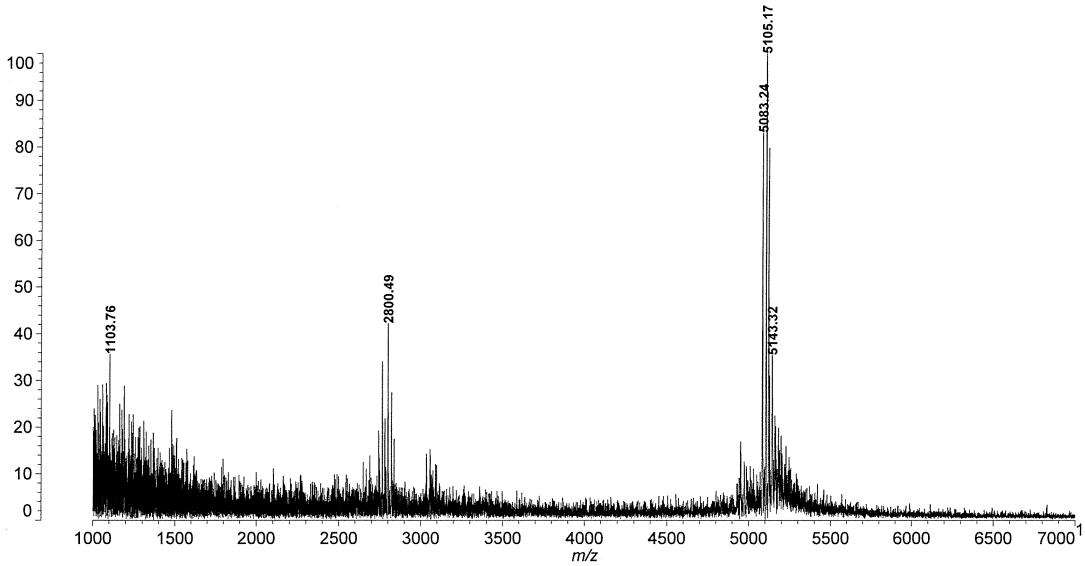

Figure S15. MALDI-TOF mass spectrum of **P1Q1(T790M)**. An ⌾-CHCA was used as a matrix. calcd. $[M+H]^+$ = 5080.30 and obsd. $[M+H]^+$ = 5083.24.

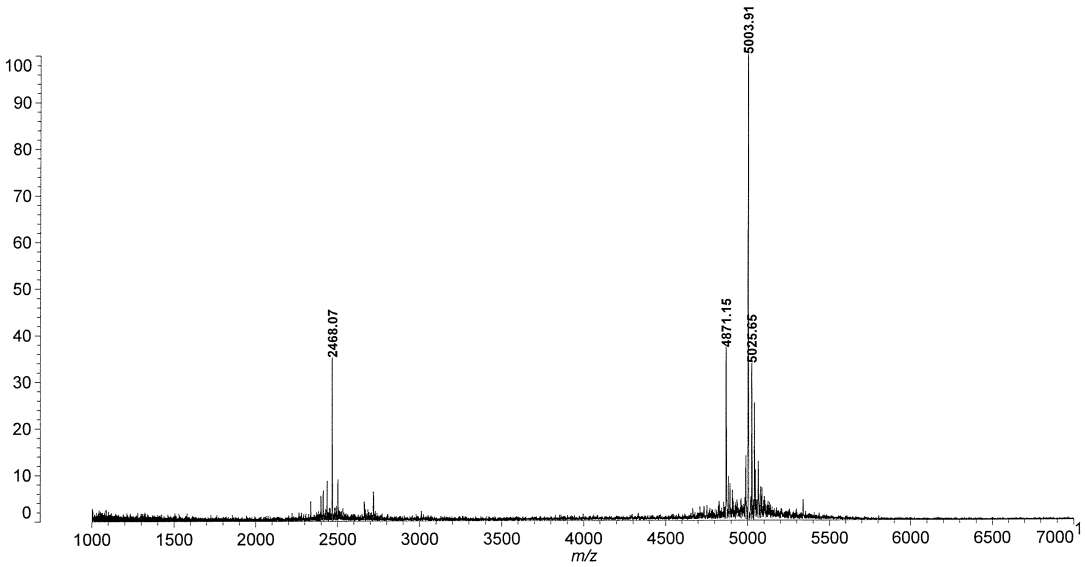

Figure S16. MALDI-TOF mass spectrum of **P1Q1(L858R)**. An ⌾-CHCA was used as a matrix. calcd. $[M+H]^+$ = 5001.24 and obsd. $[M+H]^+$ = 5003.91.

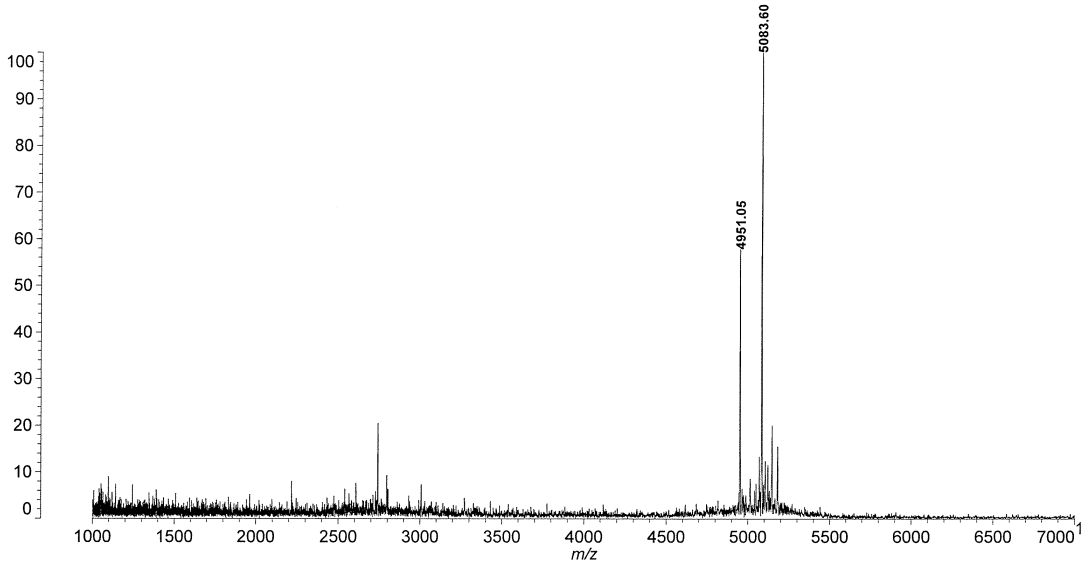

Figure S17. MALDI-TOF mass spectrum of **P1Q1(exon19del)**. An ⌾-CHCA was used as a matrix. calcd. $[M+H]^+$ = 5082.24 and obsd. $[M+H]^+$ = 5083.60.

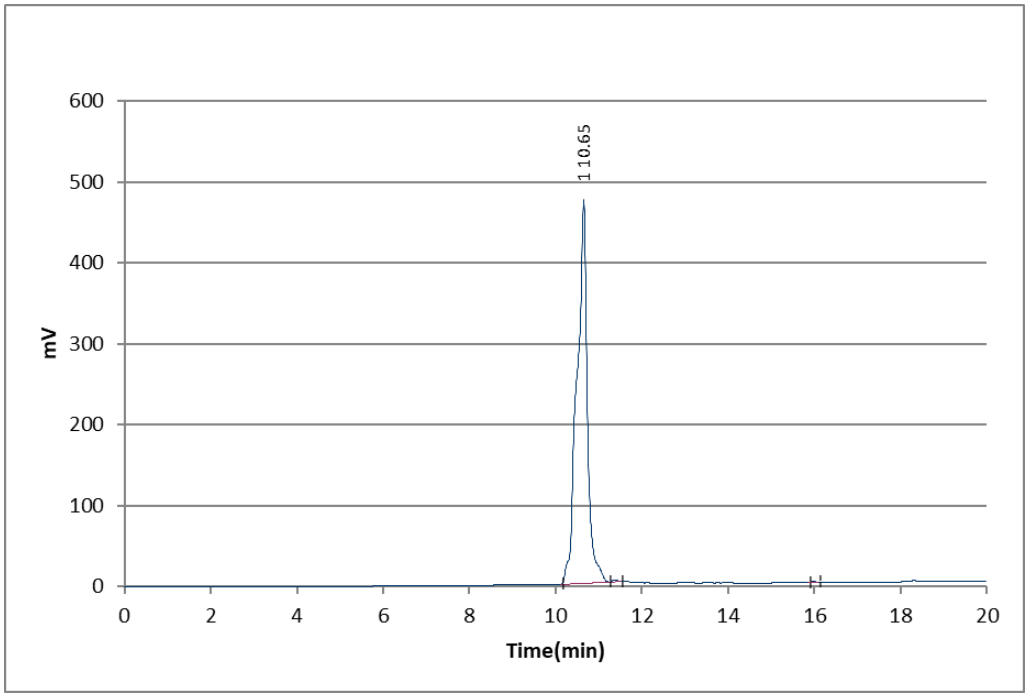

Figure S18. RP-HPLC chart of **P1Q0**. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 260 nm with a gradient of 0-100% for 20 min.

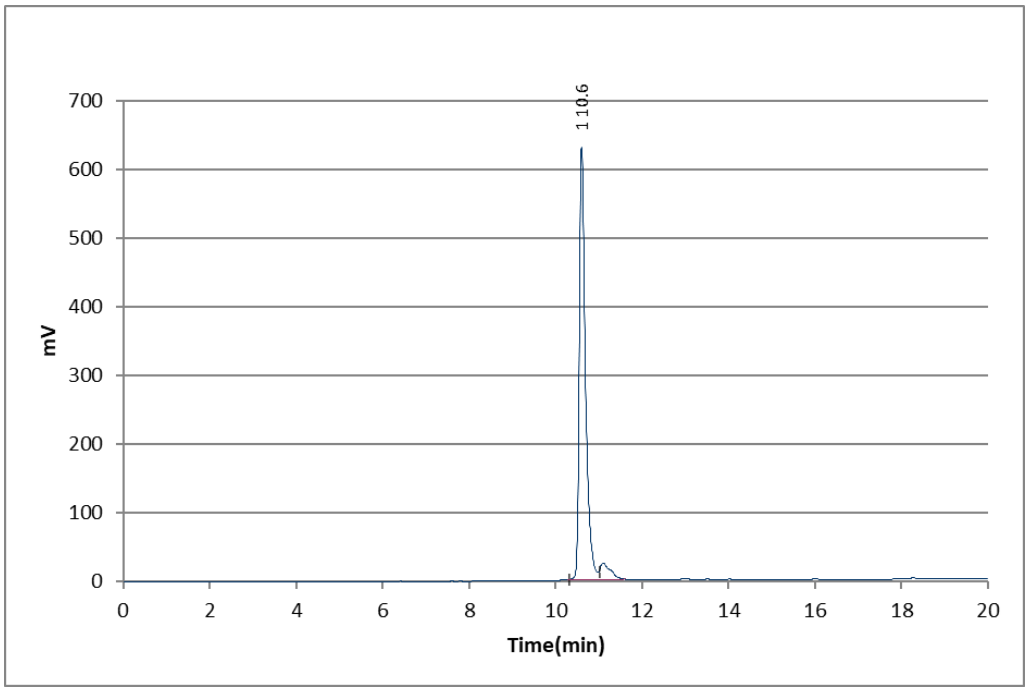

Figure S19. RP-HPLC chart of **P2Q0**. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 260 nm with a gradient of 0-100% for 20 min.

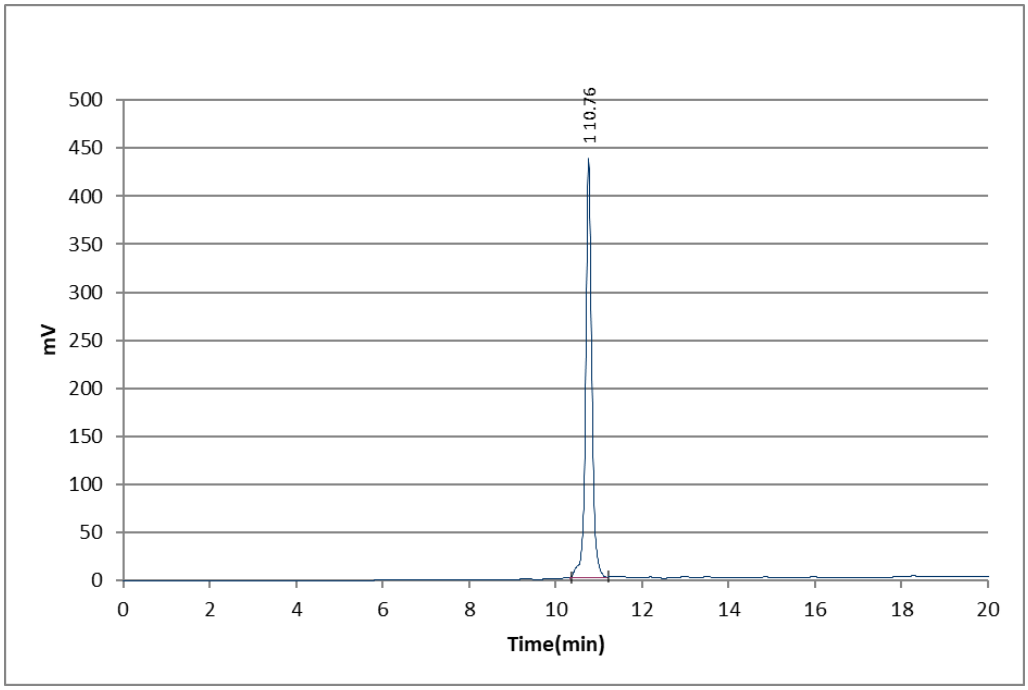

Figure S20. RP-HPLC chart of **P3Q0**. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 260 nm with a gradient of 0-100% for 20 min.

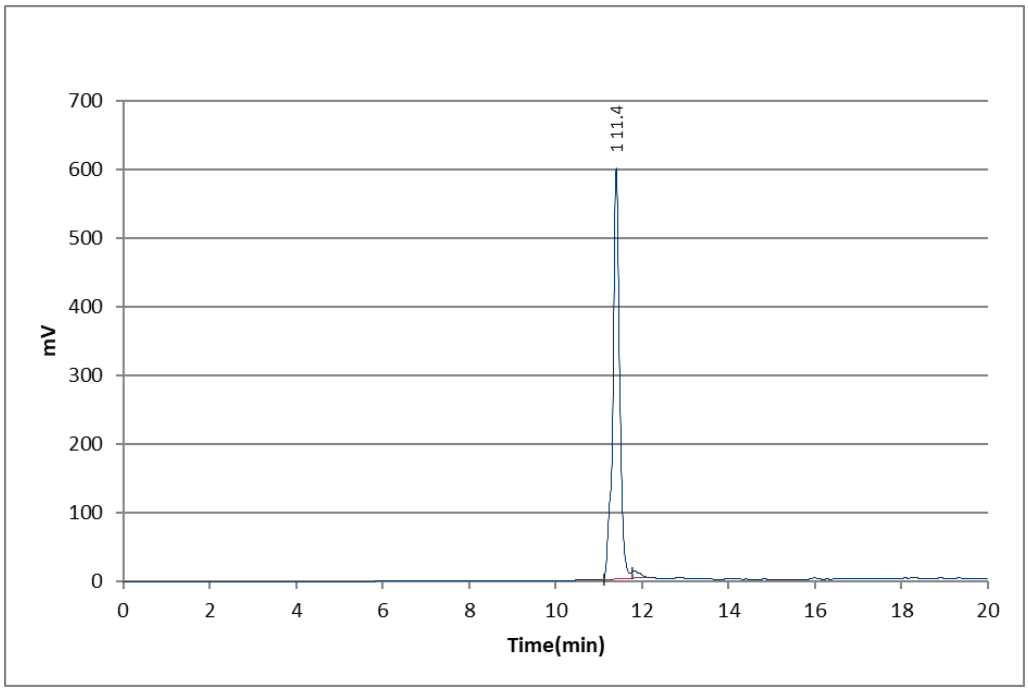

Figure S21. RP-HPLC chart of **P1Q1**. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 260 nm with a gradient of 0-100% for 20 min.

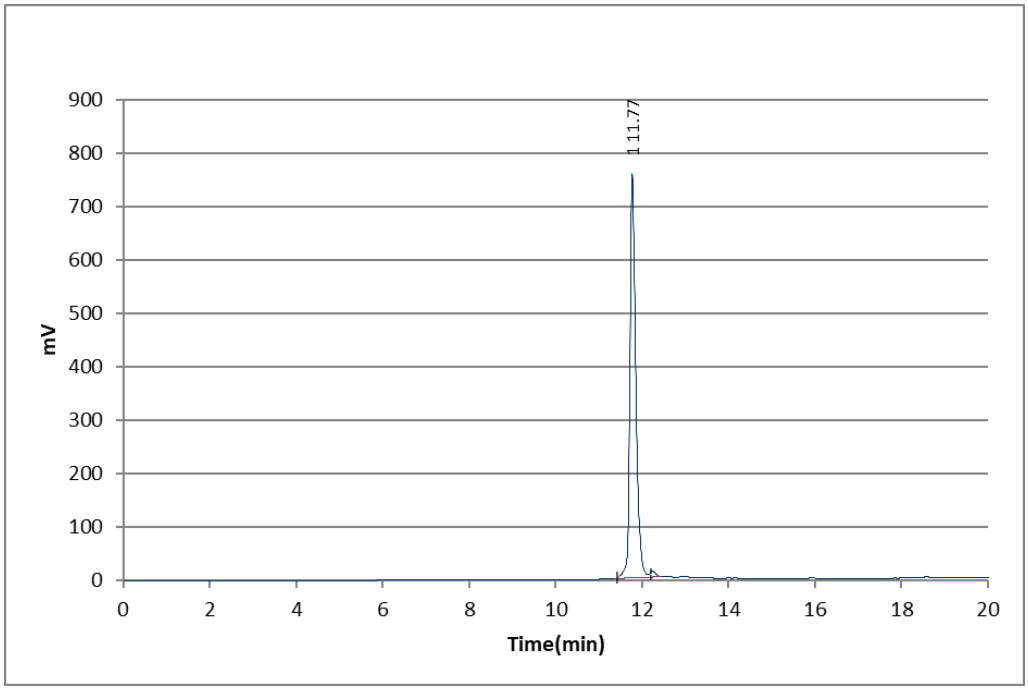

Figure S22. RP-HPLC chart of **P2Q1**. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 260 nm with a gradient of 0-100% for 20 min.

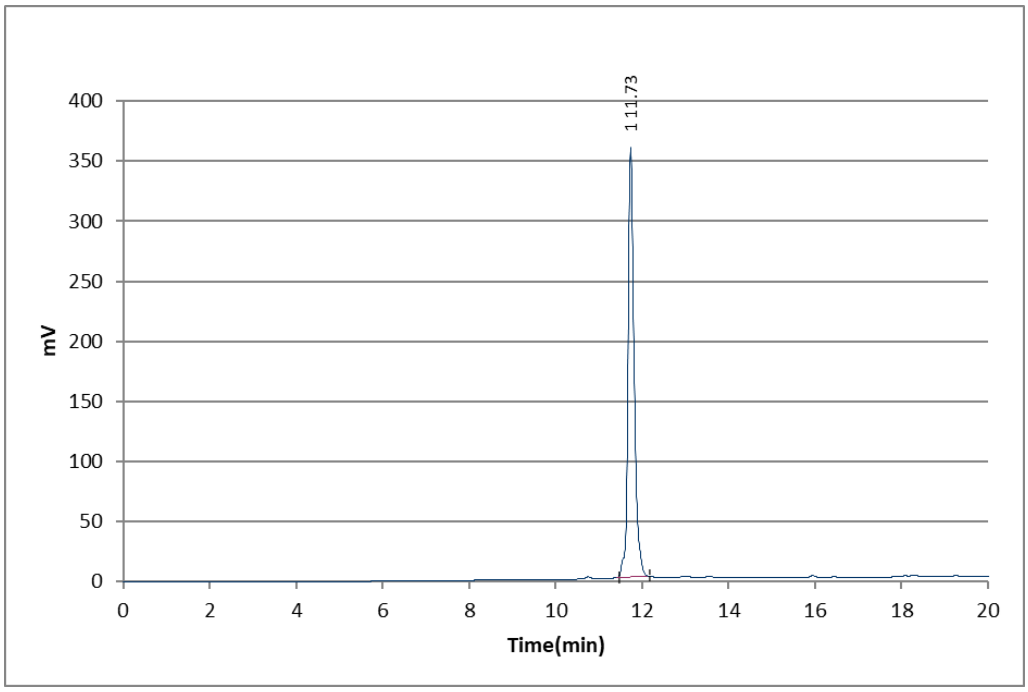

Figure S23. RP-HPLC chart of **P3Q1**. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 260 nm with a gradient of 0-100% for 20 min.

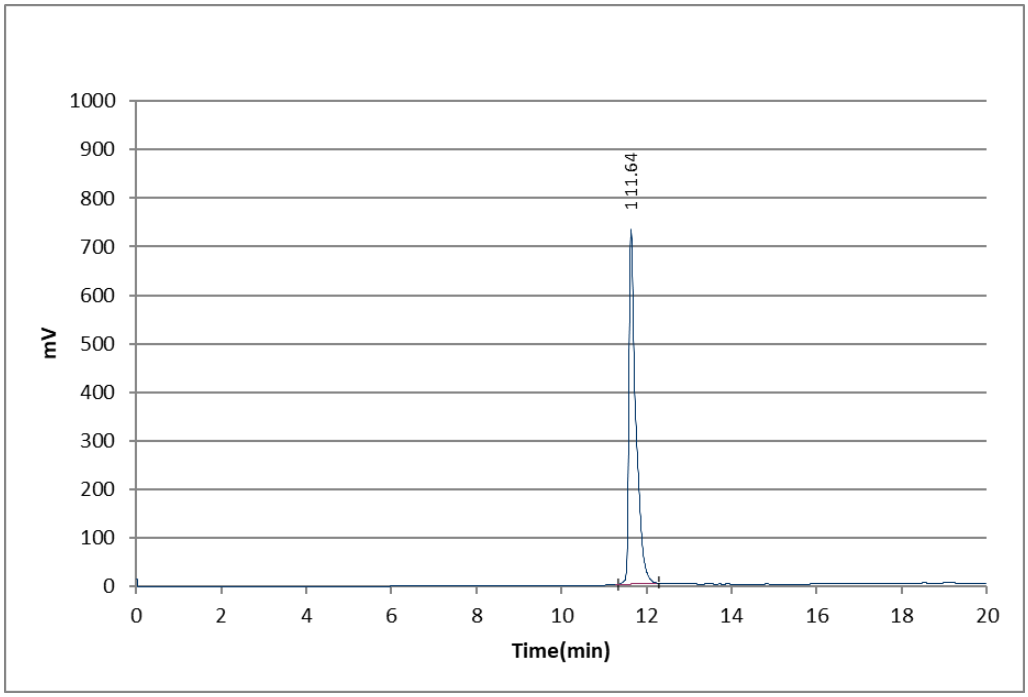

Figure S24. RP-HPLC chart of **P4Q1**. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 260 nm with a gradient of 0-100% for 20 min.

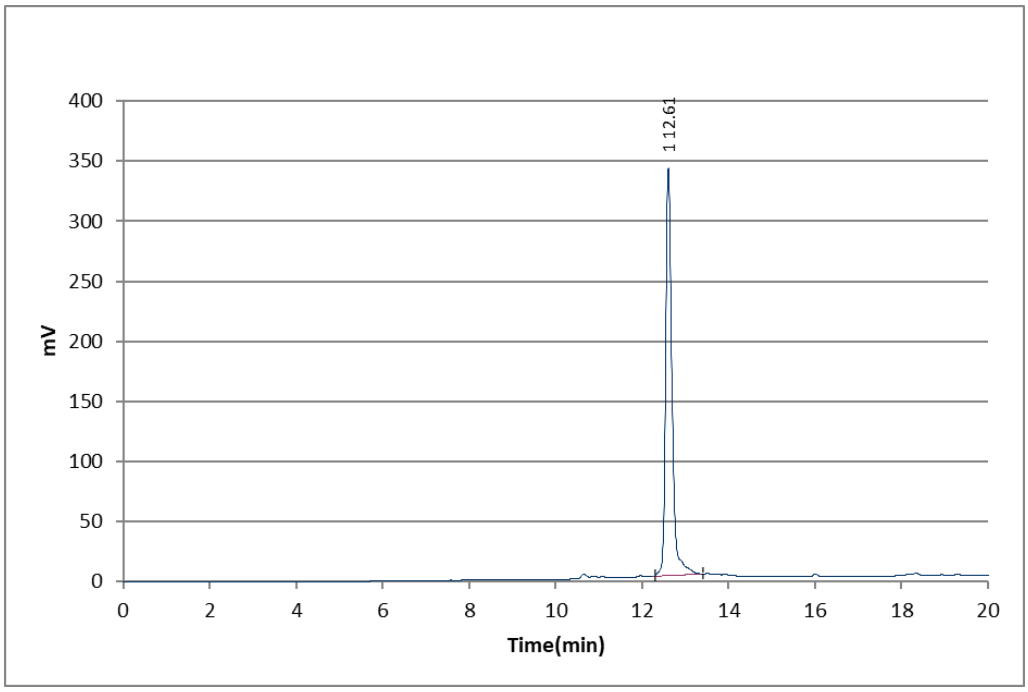

Figure S25. RP-HPLC chart of **P1Q2**. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 260 nm with a gradient of 0-100% for 20 min.

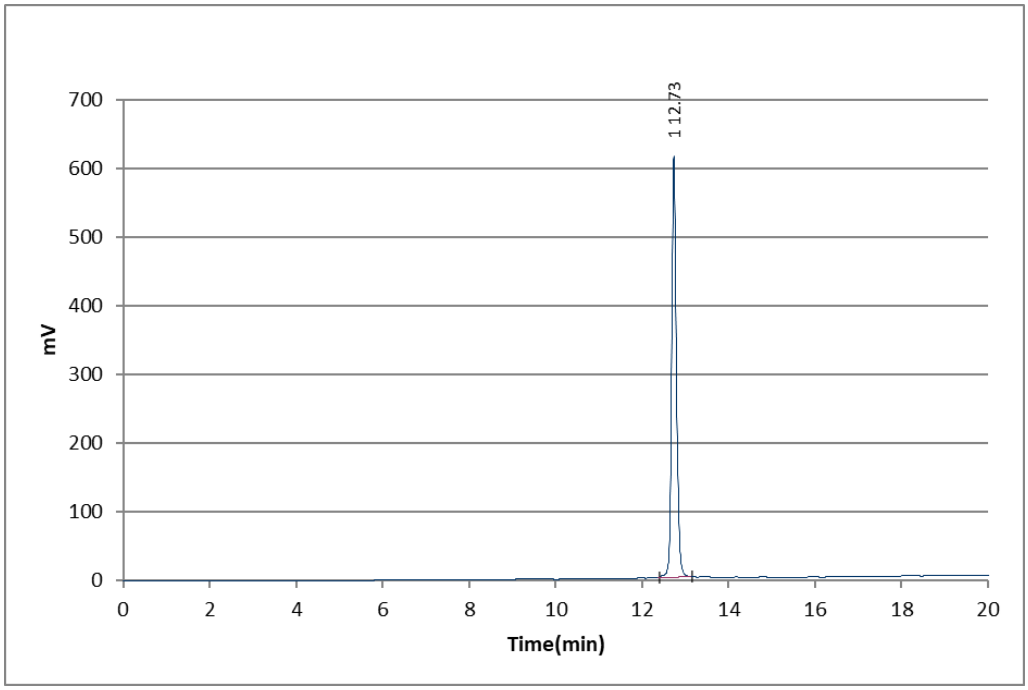

Figure S26. RP-HPLC chart of **P2Q2**. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 260 nm with a gradient of 0-100% for 20 min.

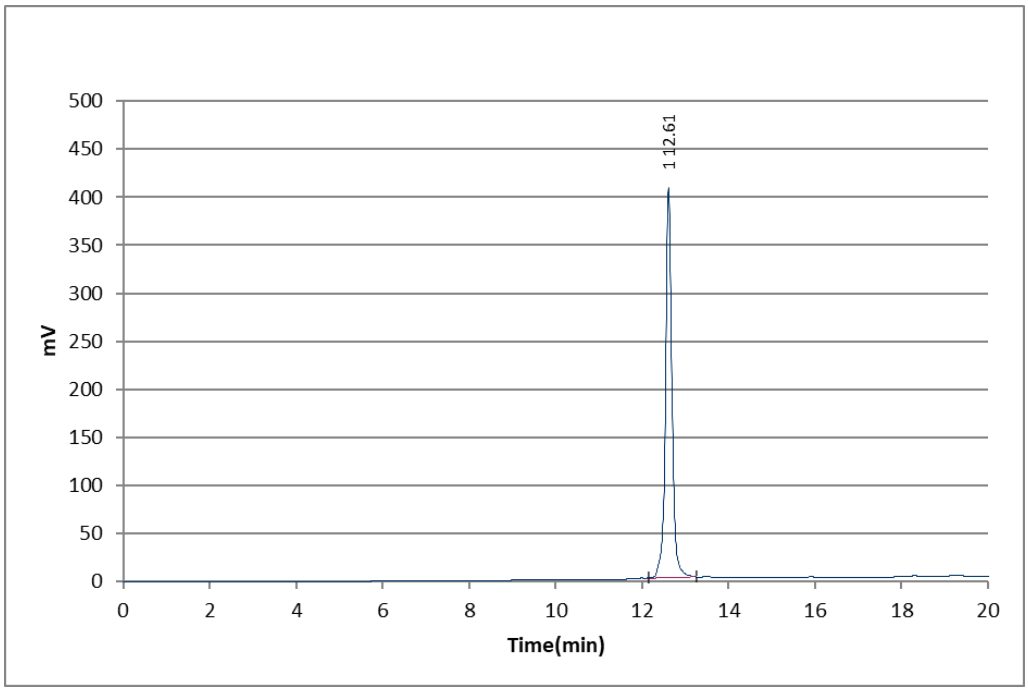

Figure S27. RP-HPLC chart of **P3Q2**. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 260 nm with a gradient of 0-100% for 20 min.

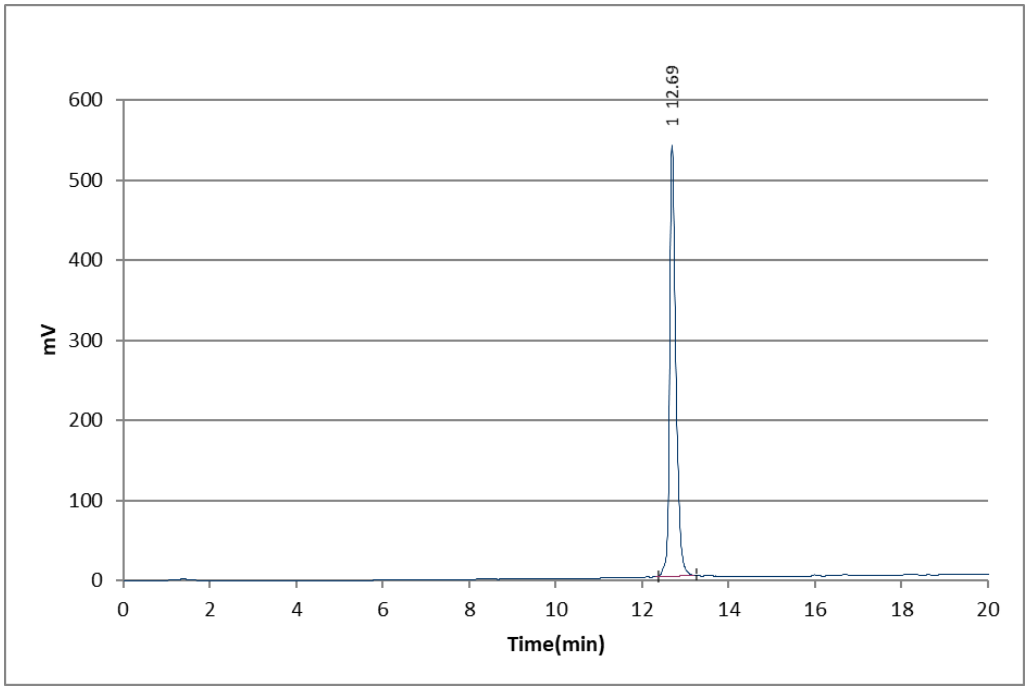

Figure S28. RP-HPLC chart of **P4Q2**. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 260 nm with a gradient of 0-100% for 20 min.

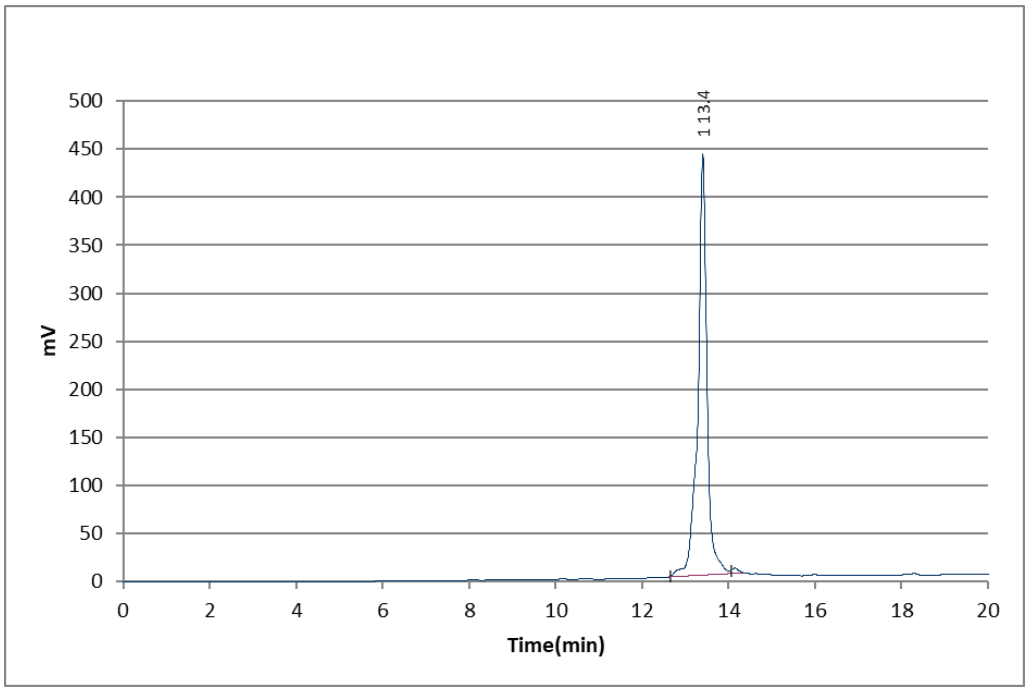

Figure S29. RP-HPLC chart of **P1Q3**. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 260 nm with a gradient of 0-100% for 20 min.

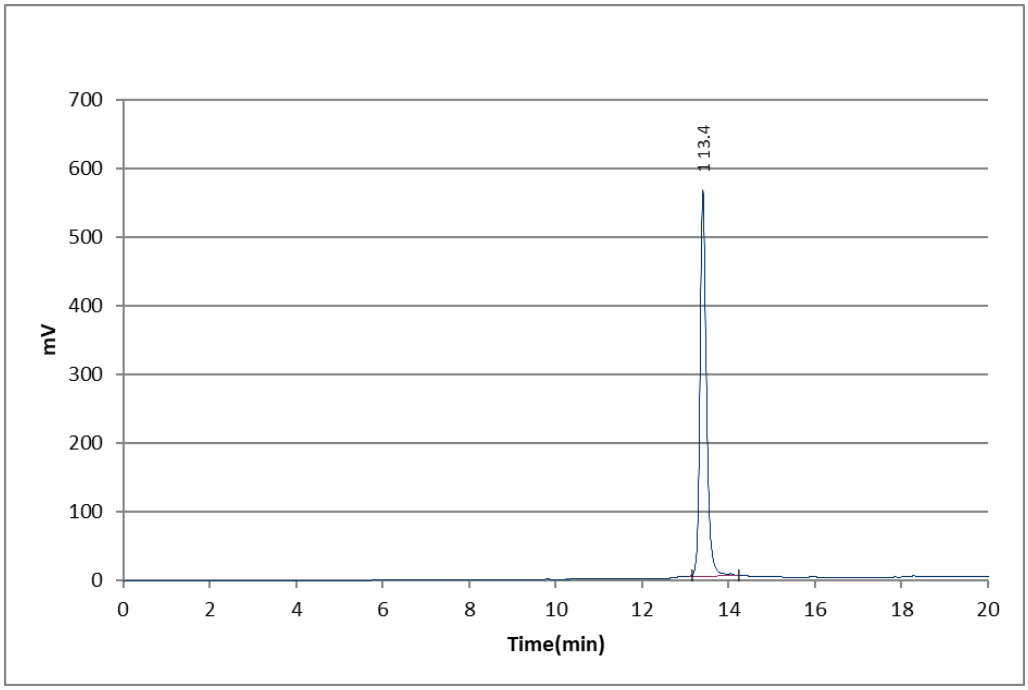

Figure S30. RP-HPLC chart of **P2Q3**. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 260 nm with a gradient of 0-100% for 20 min.

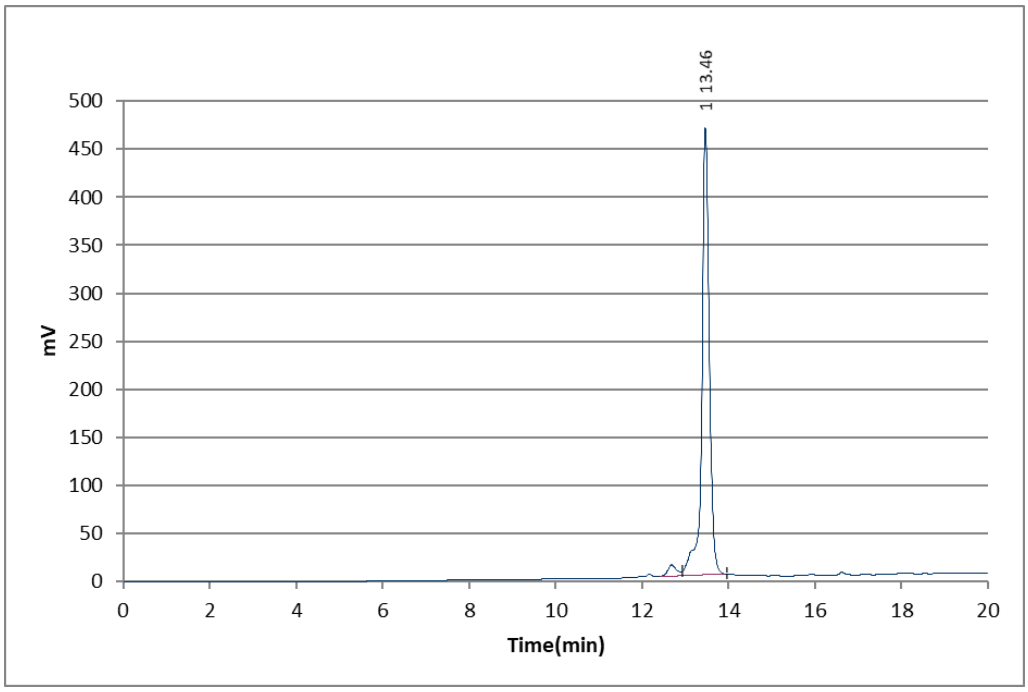

Figure S31. RP-HPLC chart of **P3Q3**. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 260 nm with a gradient of 0-100% for 20 min.

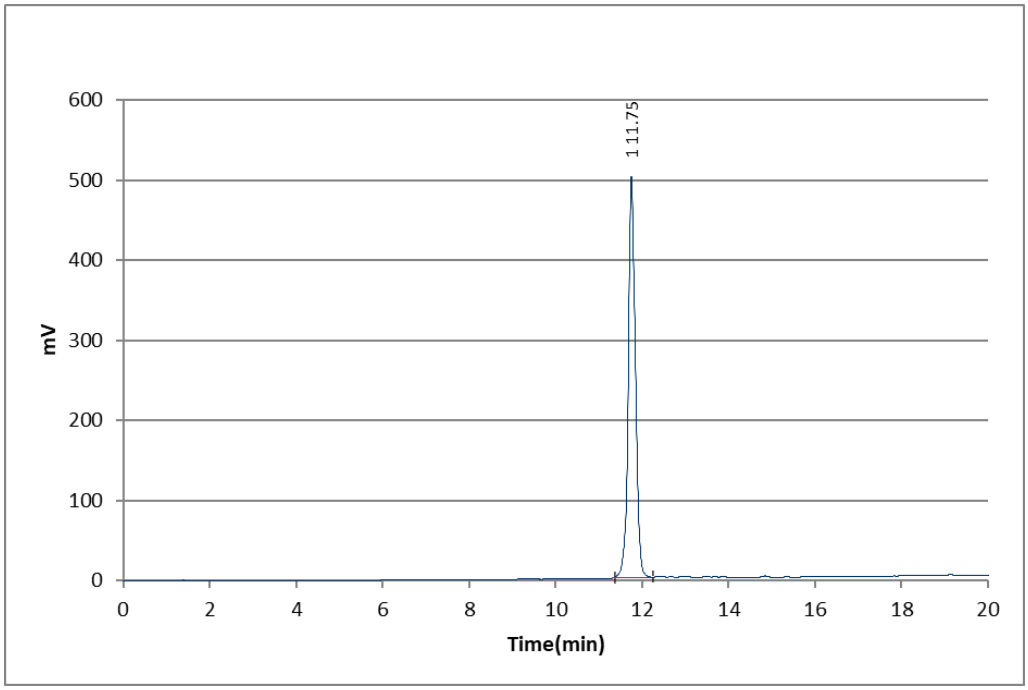

Figure S32. RP-HPLC chart of **P1Q1(T790M)**. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 260 nm with a gradient of 0-100% for 20 min.

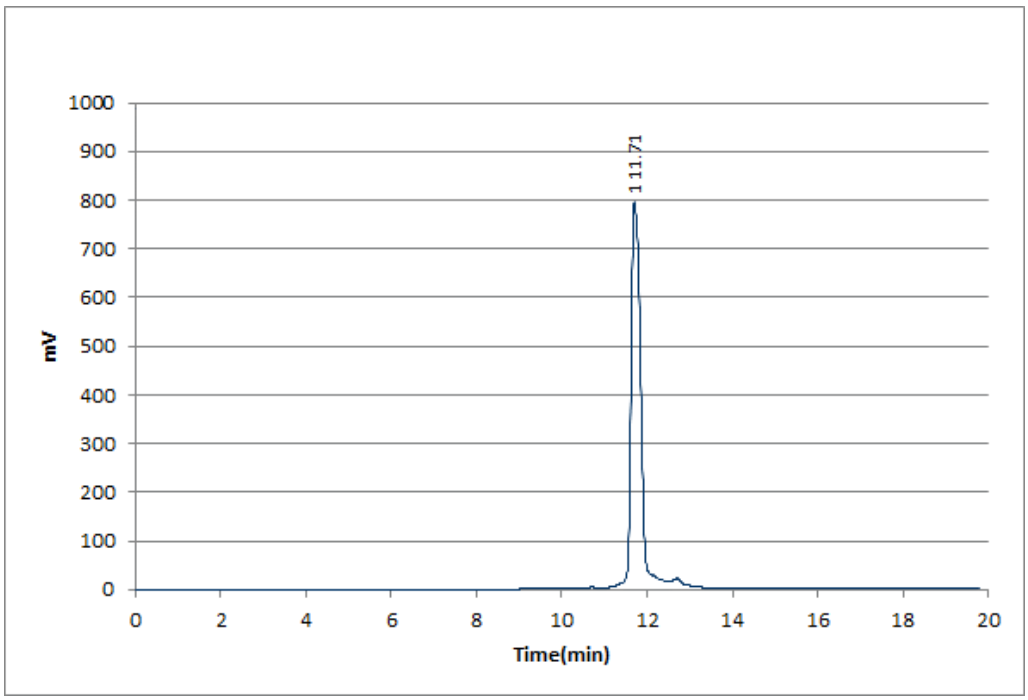

Figure S33. RP-HPLC chart of **P1Q1(L858R)**. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 260 nm with a gradient of 0-100% for 20 min.

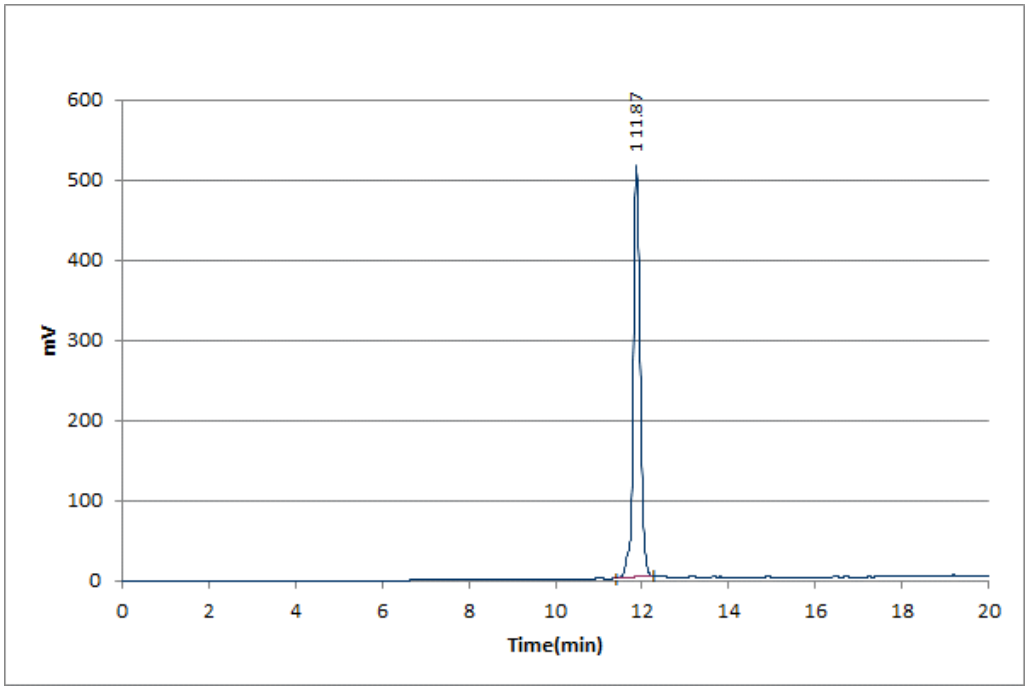

Figure S34. RP-HPLC chart of **P1Q1(exon19del)**. Buffer A. 0.1% TFA in water; buffer B, acetonitrile and monitoring at 260 nm with a gradient of 0-100% for 20 min.

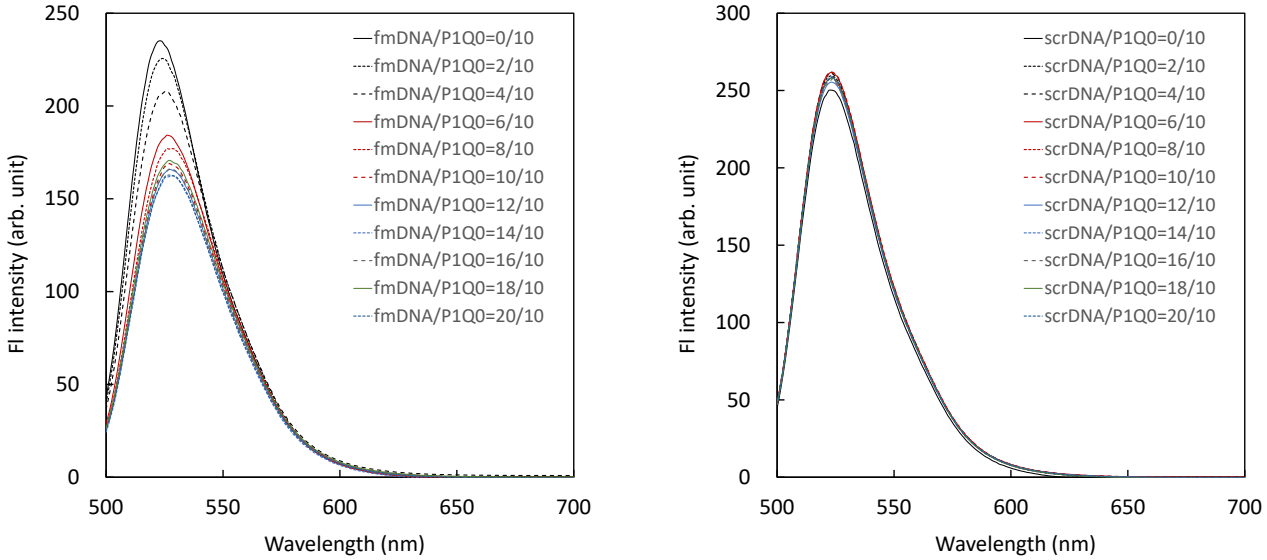

Figure S35. Fluorescence spectra of **P1Q0** (500 nM constant) with various concentration of fmDNA (TCTGCTGGGT) (left), and with scrDNA (CGTGGTTCTG) (right) in PBS (100 mM, pH 7.0) at 495 nm excitation.

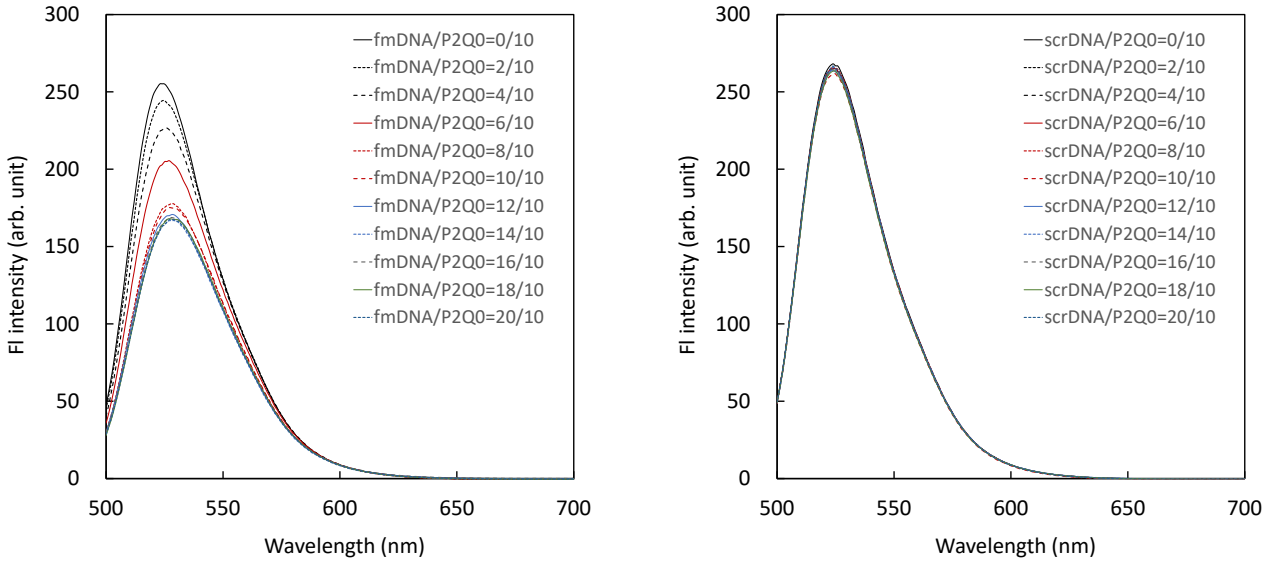

Figure S36. Fluorescence spectra of **P2Q0** (500 nM constant) with various concentration of fmDNA (left), and with scrDNA (right) in PBS (100 mM, pH 7.0) at 495 nm excitation.

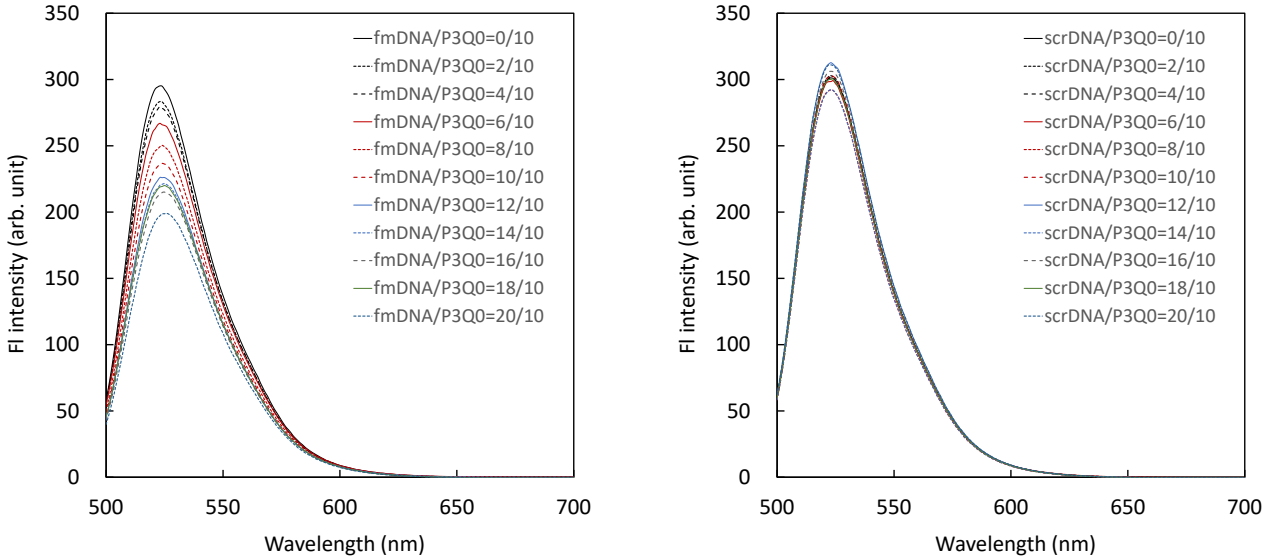

Figure S37. Fluorescence spectra of **P3Q0** (500 nM constant) with various concentration of fmDNA (left), and with scrDNA (right) in PBS (100 mM, pH 7.0) at 495 nm excitation.

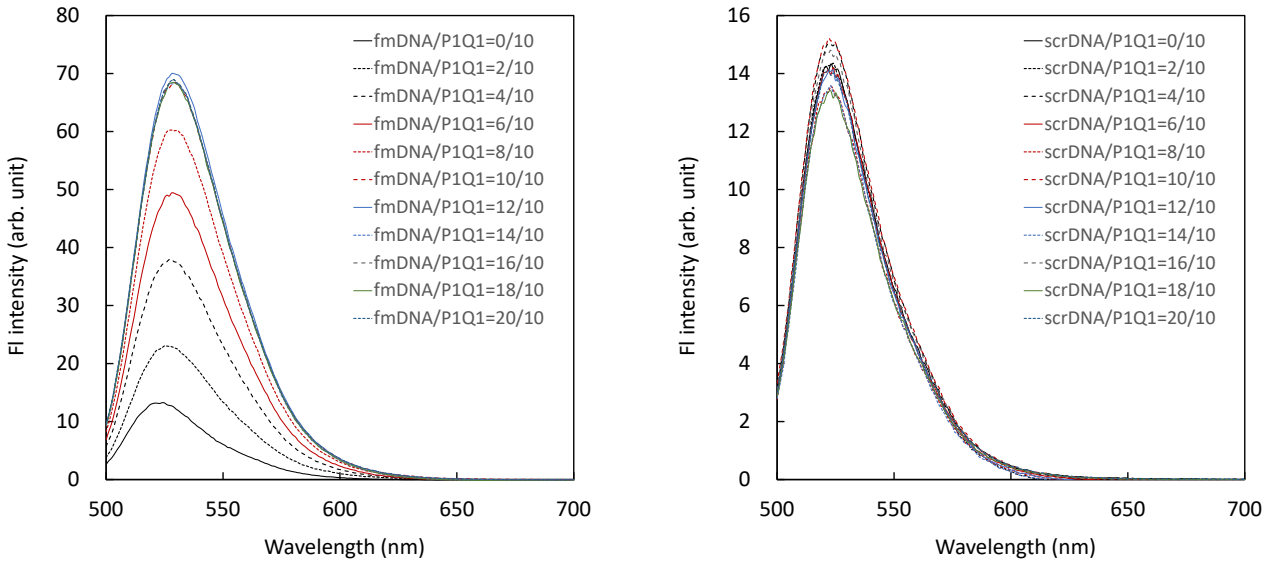

Figure S38. Fluorescence spectra of **P1Q1** (500 nM constant) with various concentration of fmDNA (left), and with scrDNA (right) in PBS (100 mM, pH 7.0) at 495 nm excitation.

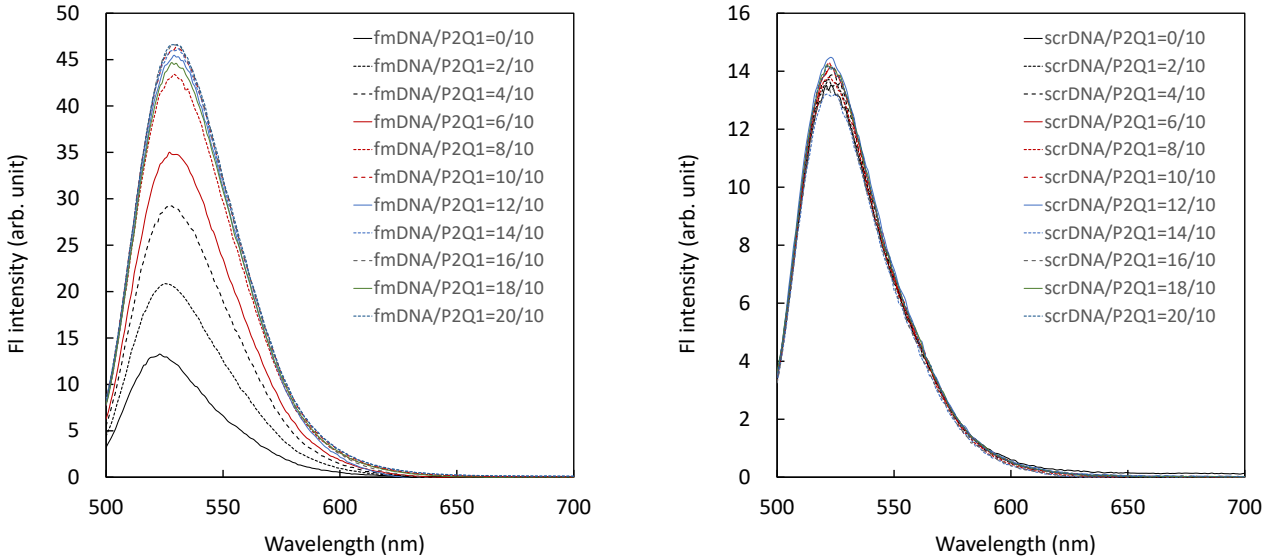

Figure S39. Fluorescence spectra of **P2Q1** (500 nM constant) with various concentration of fmDNA (left), and with scrDNA (right) in PBS (100 mM, pH 7.0) at 495 nm excitation.

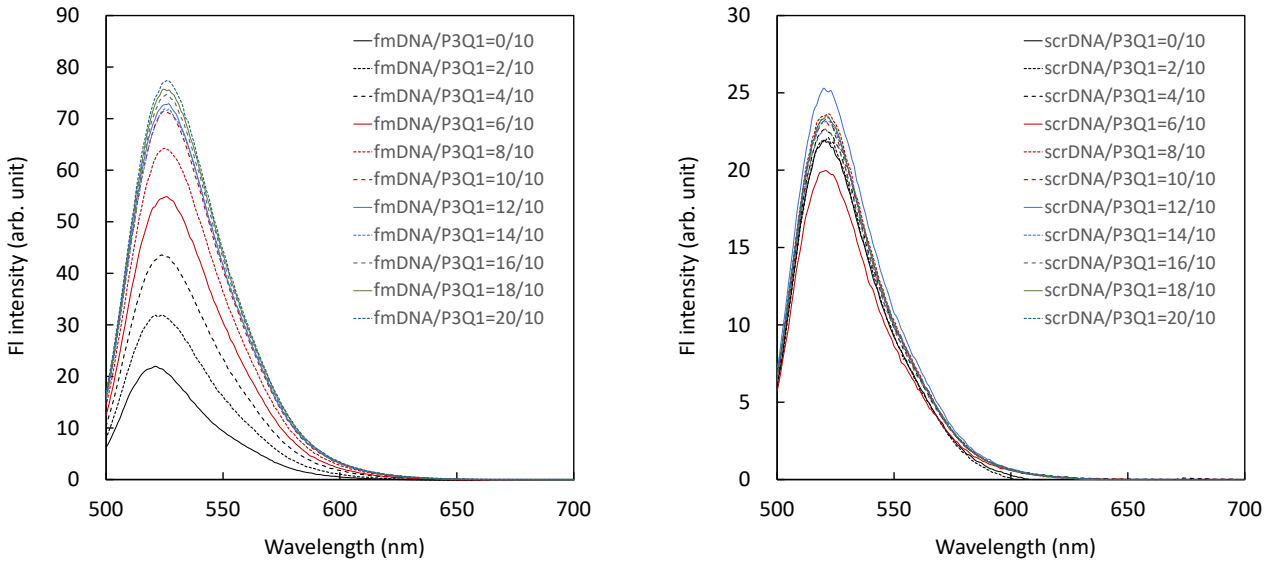

Figure S40. Fluorescence spectra of P3Q1 (500 nM constant) with various concentration of fmDNA (left), and with scrDNA (right) in PBS (100 mM, pH 7.0) at 495 nm excitation.

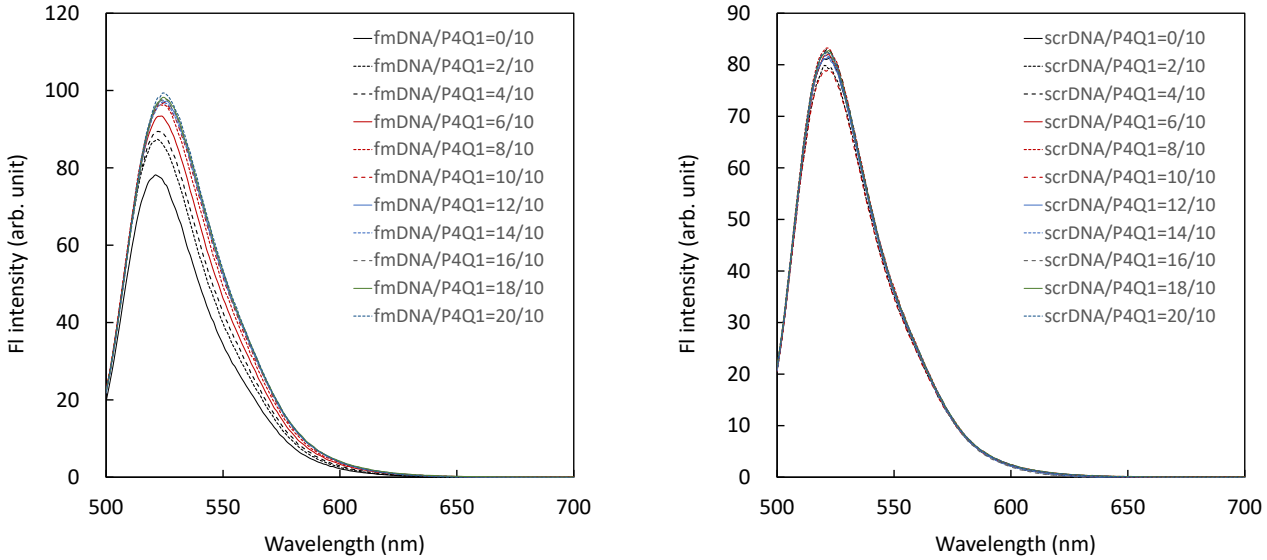

Figure S41. Fluorescence spectra of **P4Q1** (500 nM constant) with various concentration of fmDNA (left), and with scrDNA (right) in PBS (100 mM, pH 7.0) at 495 nm excitation.

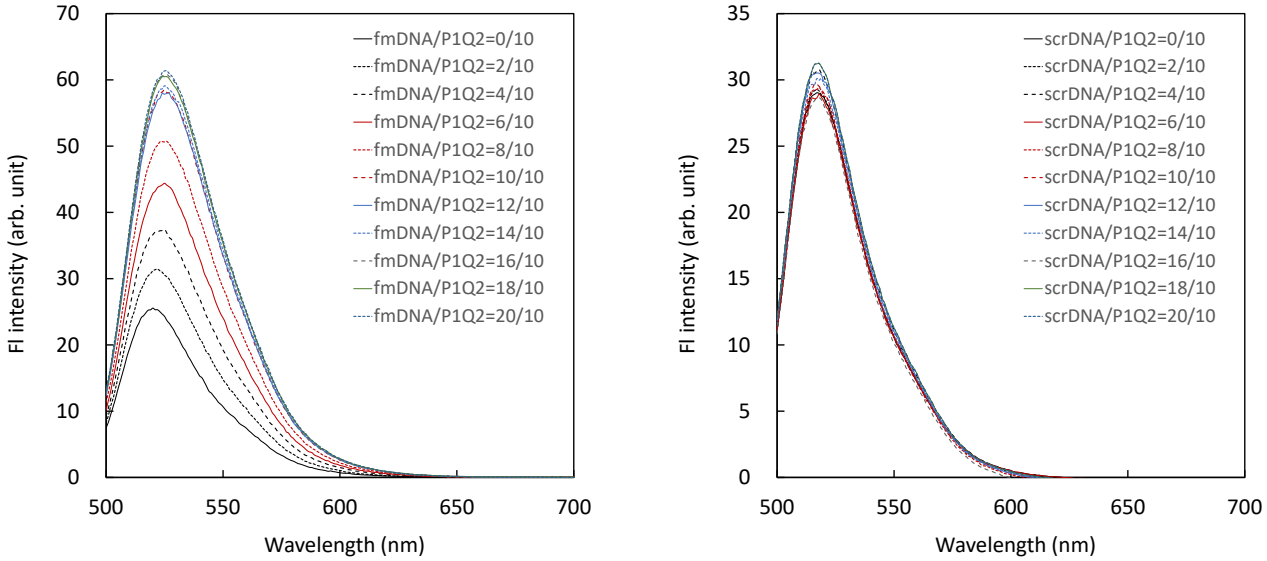

Figure S42. Fluorescence spectra of **P1Q2** (500 nM constant) with various concentration of fmDNA (left), and with scrDNA (right) in PBS (100 mM, pH 7.0) at 495 nm excitation.

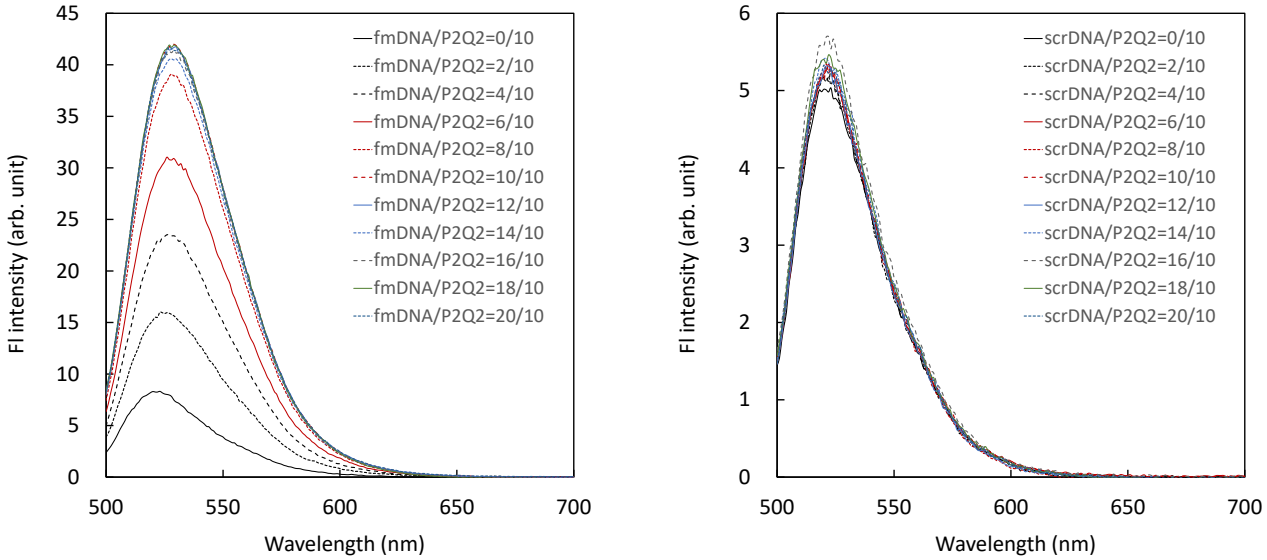

Figure S43. Fluorescence spectra of **P2Q2** (500 nM constant) with various concentration of fmDNA (left), and with scrDNA (right) in PBS (100 mM, pH 7.0) at 495 nm excitation.

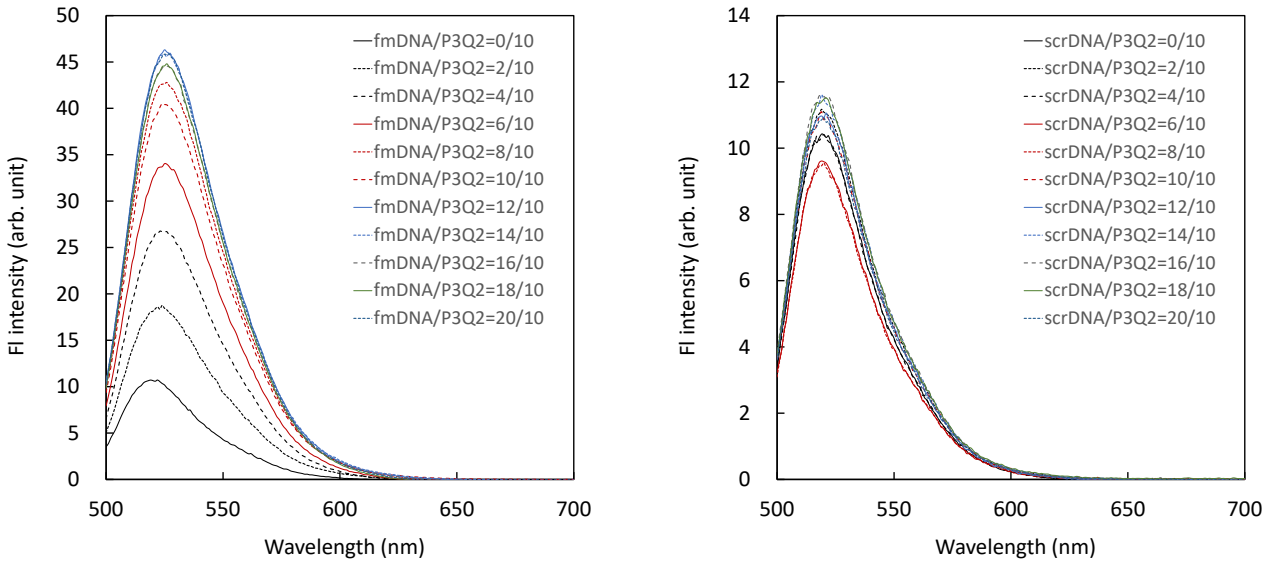

Figure S44. Fluorescence spectra of P3Q2 (500 nM constant) with various concentration of fmDNA (left), and with scrDNA (right) in PBS (100 mM, pH 7.0) at 495 nm excitation.

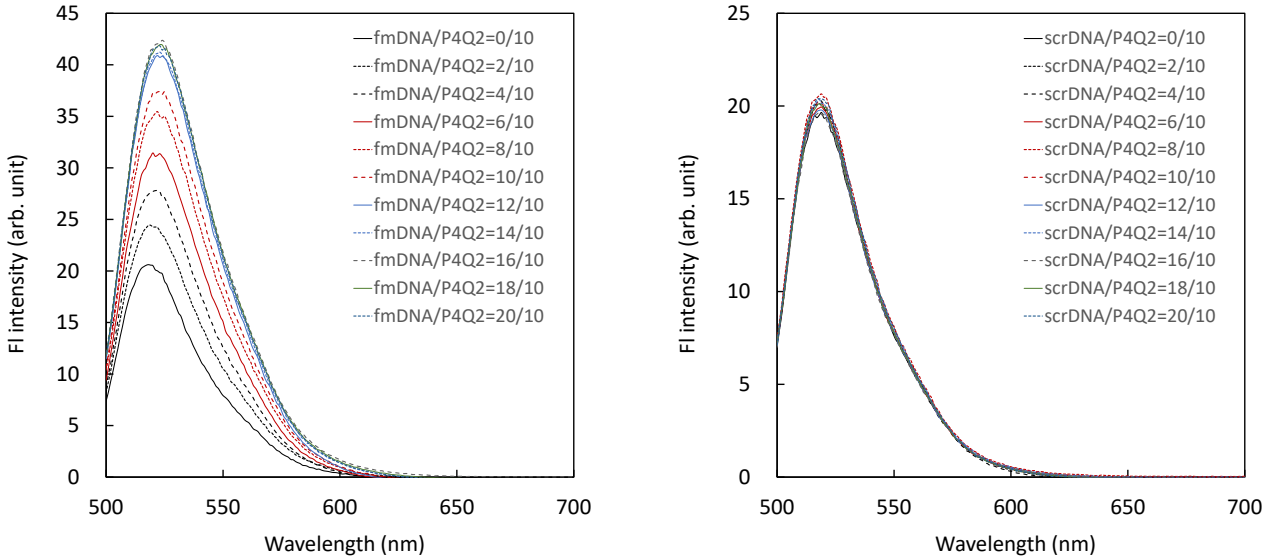

Figure S45. Fluorescence spectra of **P4Q2** (500 nM constant) with various concentration of fmDNA (left), and with scrDNA (right) in PBS (100 mM, pH 7.0) at 495 nm excitation.

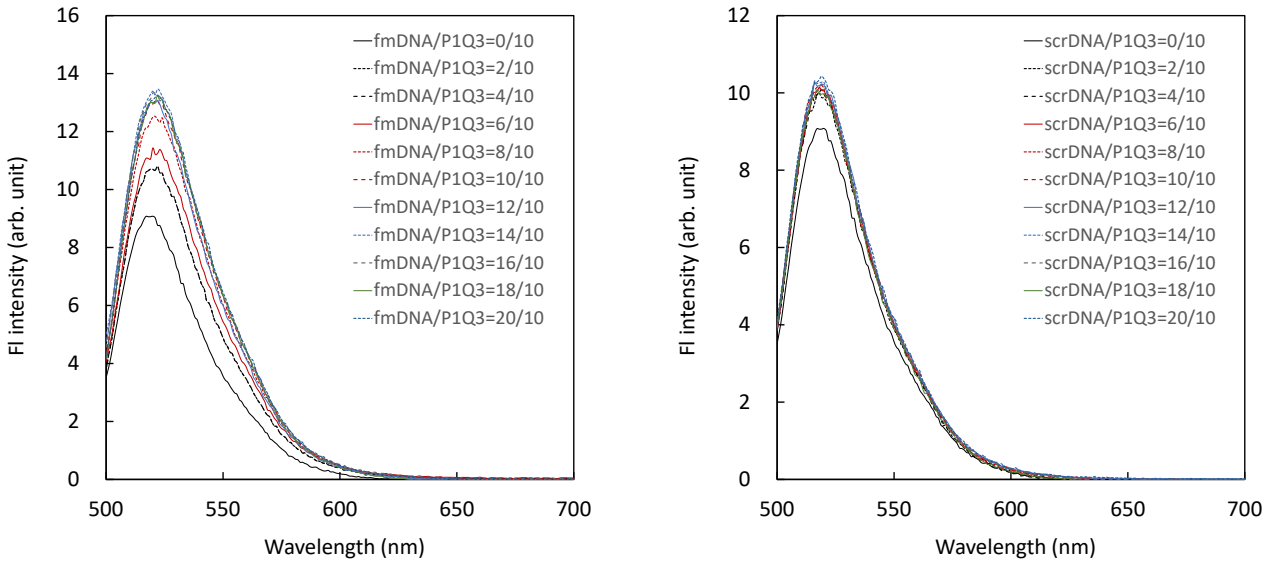

Figure S46. Fluorescence spectra of **P1Q3** (500 nM constant) with various concentration of fmDNA (left), and with scrDNA (right) in PBS (100 mM, pH 7.0) at 495 nm excitation.

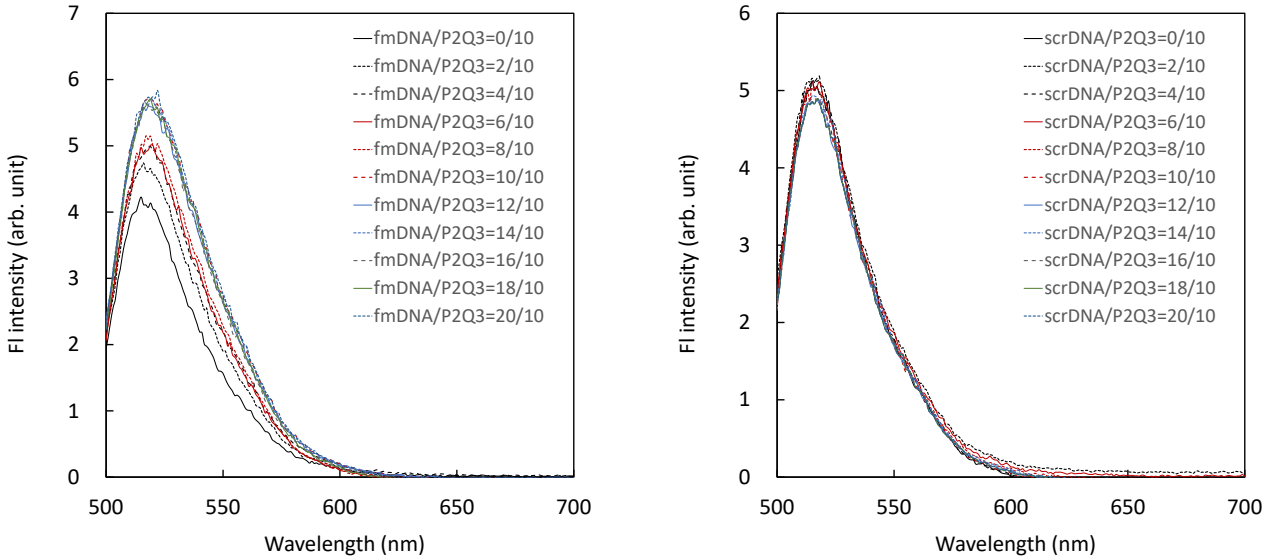

Figure S47. Fluorescence spectra of **P2Q3** (500 nM constant) with various concentration of fmDNA (left), and with scrDNA (right) in PBS (100 mM, pH 7.0) at 495 nm excitation.

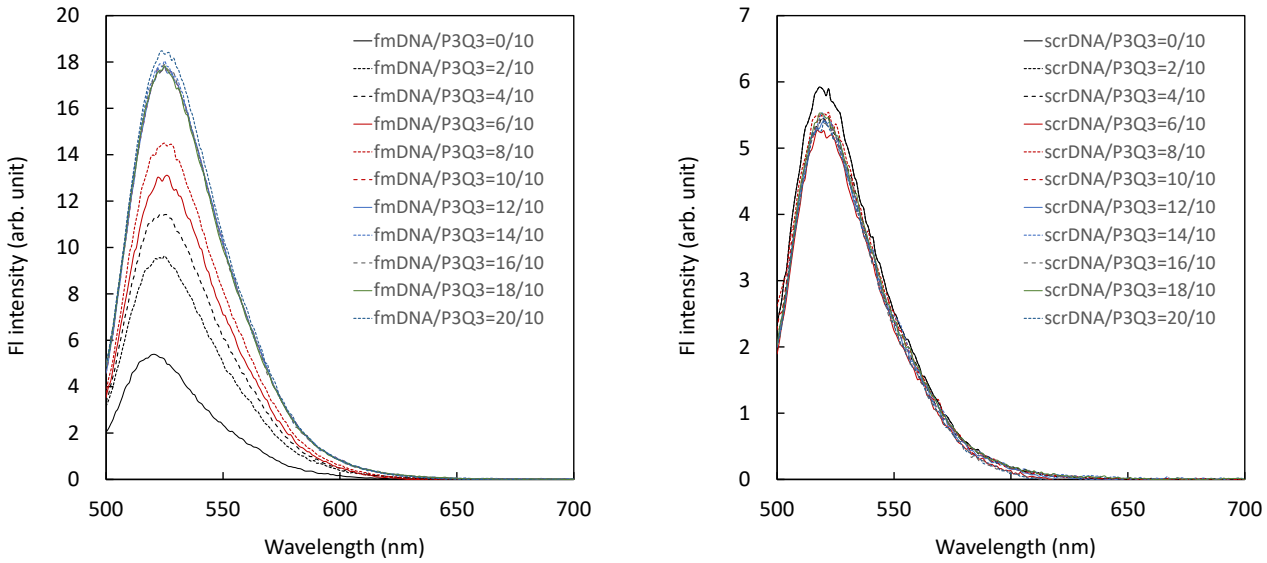

Figure S48. Fluorescence spectra of **P3Q3** (500 nM constant) with various concentration of fmDNA (left), and with scrDNA (right) in PBS (100 mM, pH 7.0) at 495 nm excitation.

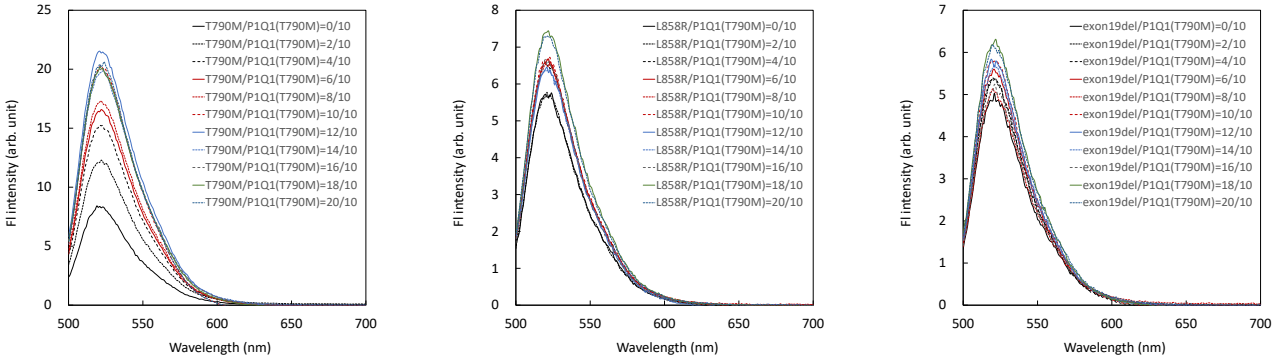

Figure S49. Fluorescence spectra of **P1Q1(T790M)** (500 nM constant) with various concentration of T790M (left), with L858R (center), and with exon19del (right) in PBS (100 mM, pH 7.0) at 495 nm excitation.

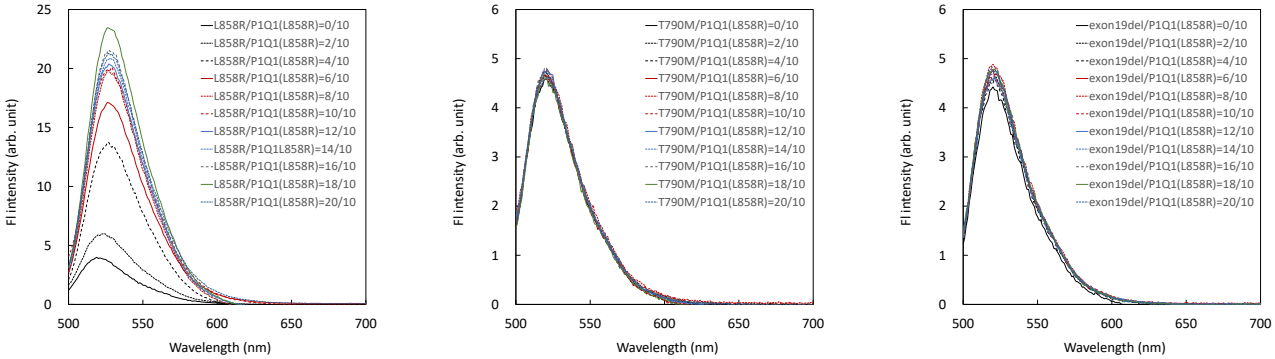

Figure S50. Fluorescence spectra of **P1Q1(L858R)** (500 nM constant) with various concentration of L858R (left), with T790M (center), and with exon19del (right) in PBS (100 mM, pH 7.0) at 495 nm excitation.

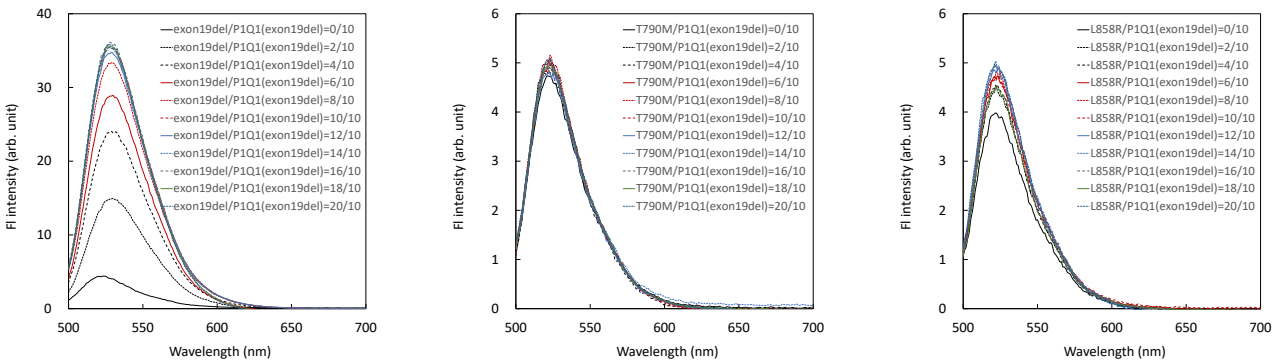

Figure S51. Fluorescence spectra of **P1Q1(exon19del)** (500 nM constant) with various concentration of exon19del (left), with T790M (center), and with L858R (right) in PBS (100 mM, pH 7.0) at 495 nm excitation.

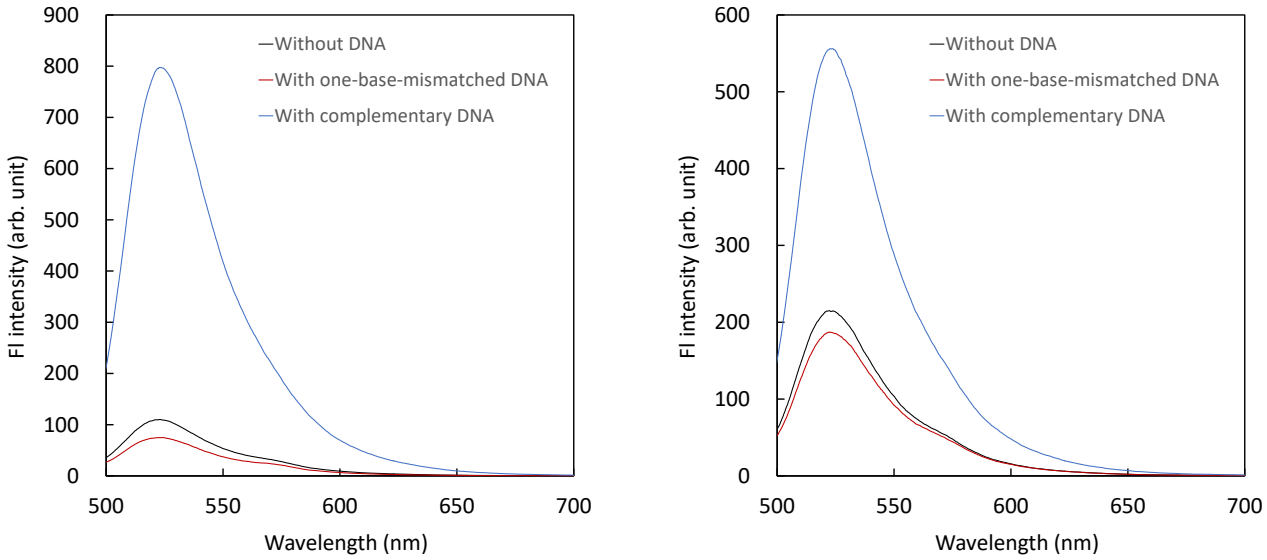

Figure S52. Fluorescence spectra of **P1Q1(T790M)/Q-DNA** (left) and **P1Q1(T790M)** (right) with equimolar complementary DNA (blue line), one-base mismatched DNA (red line) and without DNA (black line).