# Supplementary Materials: Hydrogen–Deuterium Exchange Mass Spectrometry Reveals a Novel Binding Region of a Neutralizing Fully Human Monoclonal Antibody to Anthrax Protective Antigen

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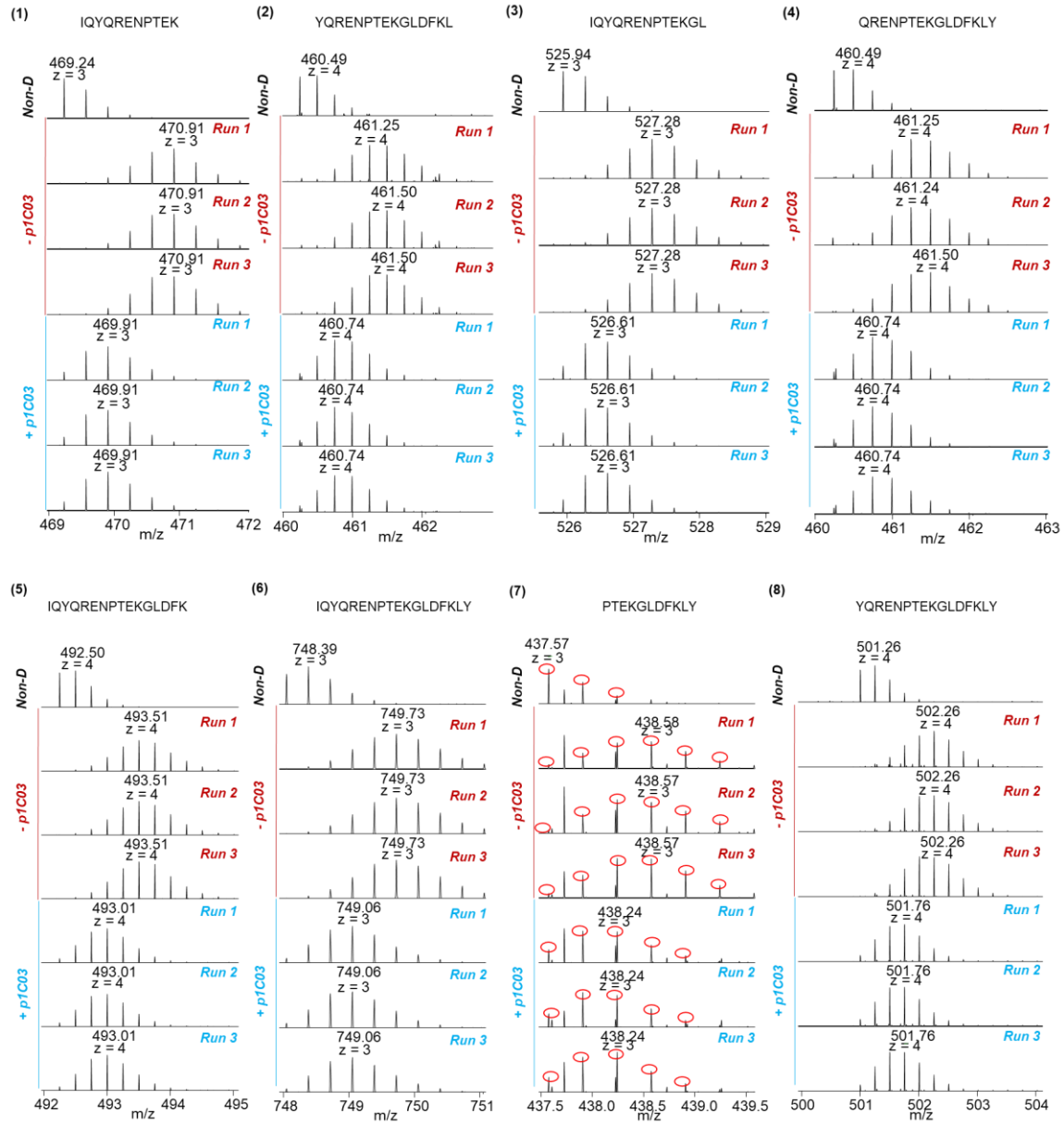
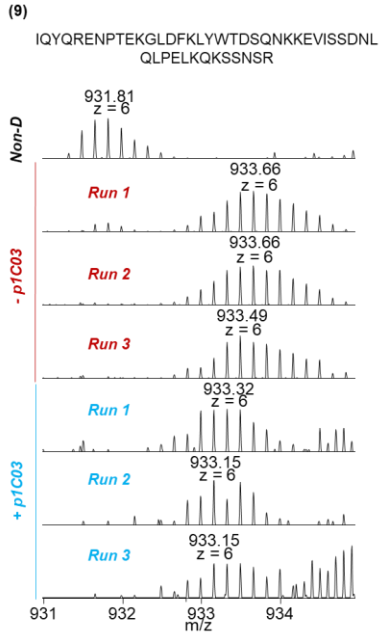
**(A)**






**(B)**

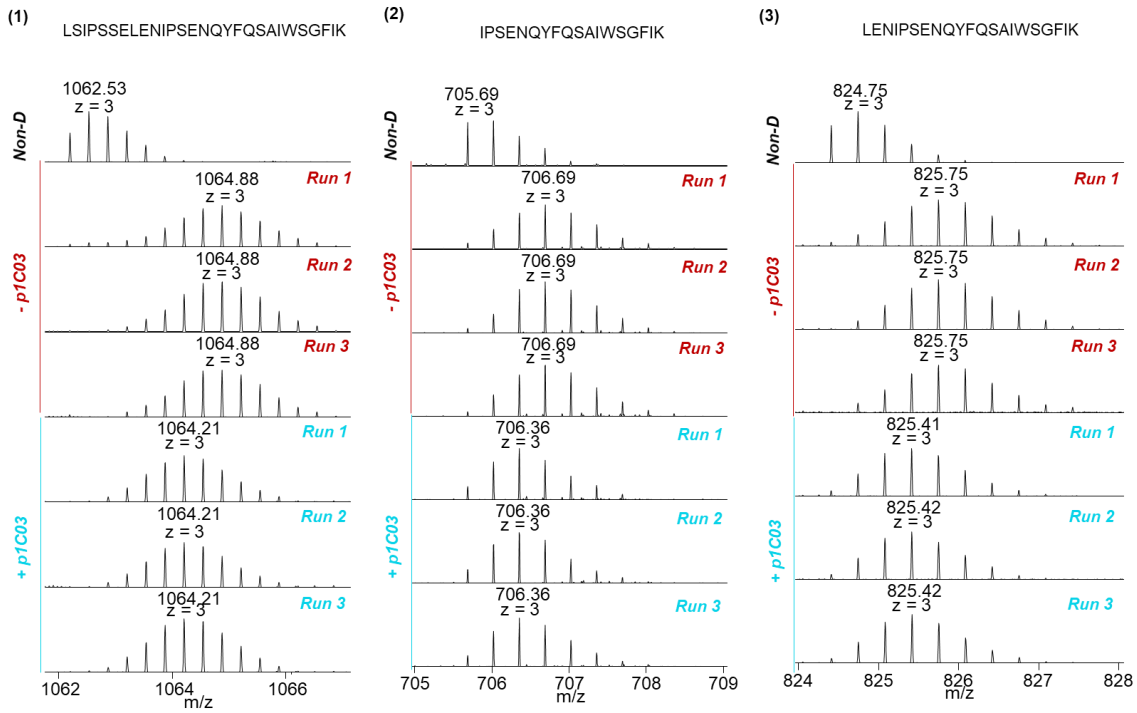
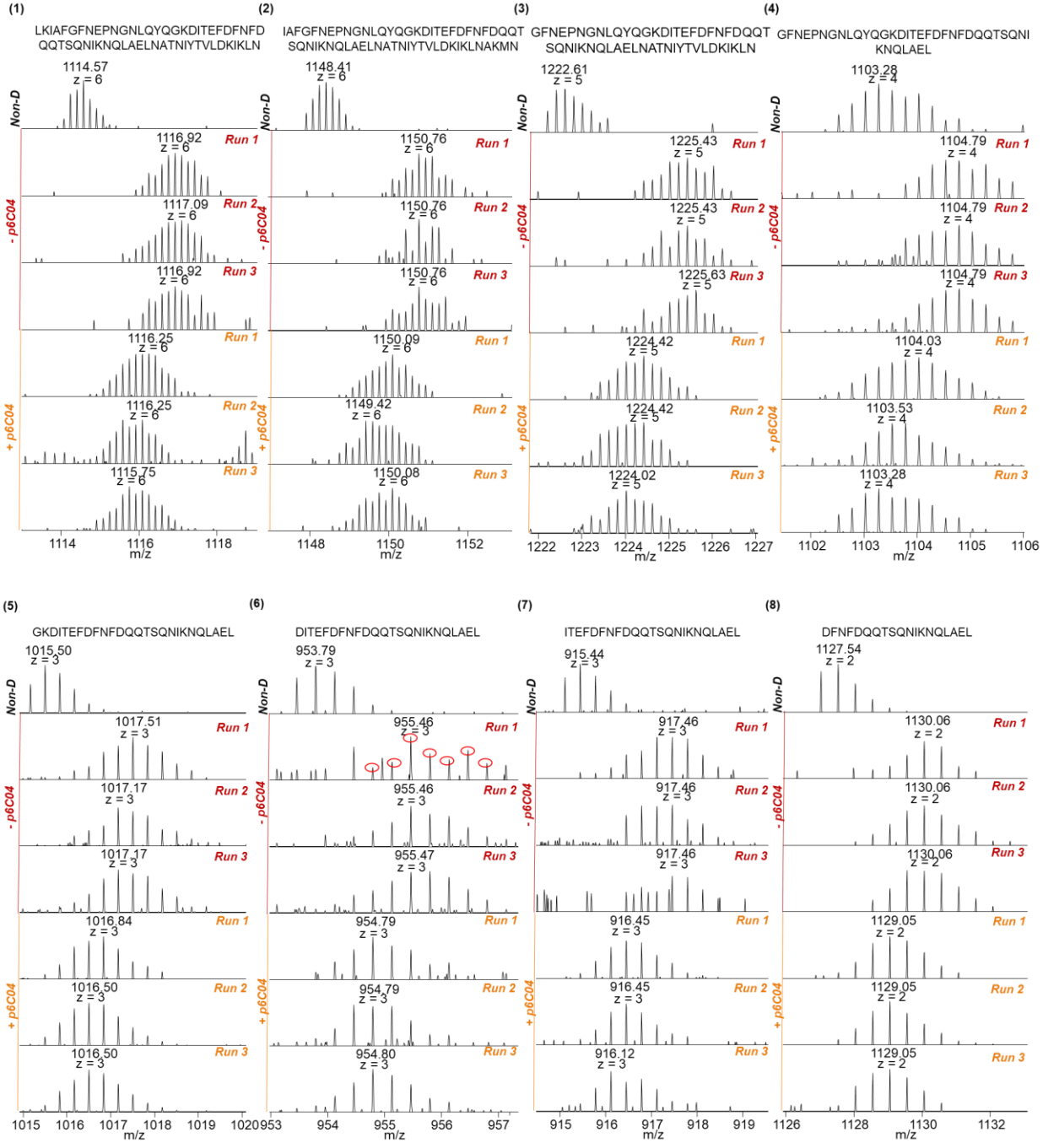



**Figure S1.** MS spectra of 12 identified peptides for p1C03 binding.(**A**) MS spectra of 9 identified peptides in primary epitope. (**B**) MS spectra of 3 identified peptides in secondary epitope. Red ovals highlight the correct peak distribution for peptide 7.


(1)
LKIAFGFNEPNGNLQYQGKDITEFDFNFD
QQTSQNIKNQLAELNATNIYTVLDKIKLN
(2)
IAFGFNEPNGNLQYQGKDITEFDFNFDQQT
SQNIKNQLAELNATNIYTVLDKIKLNAKMN
(3)
GFNEPNGNLQYQGKDITEFDFNFDQQT
SQNIKNQLAELNATNIYTVLDKIKLN
(4)
GFNEPNGNLQYQGKDITEFDFNFDQQTSQNI
KNQLAEL
(5)
GKDITEFDFNFDQQTSQNIKNQLAEL
(6)
DITEFDFNFDQQTSQNIKNQLAEL
(7)
ITEFDFNFDQQTSQNIKNQLAEL
(8)
DFNFDQQTSQNIKNQLAEL
Non-D
- p6C04
+ p6C04
Run 1
Run 2
Run 3
m/z

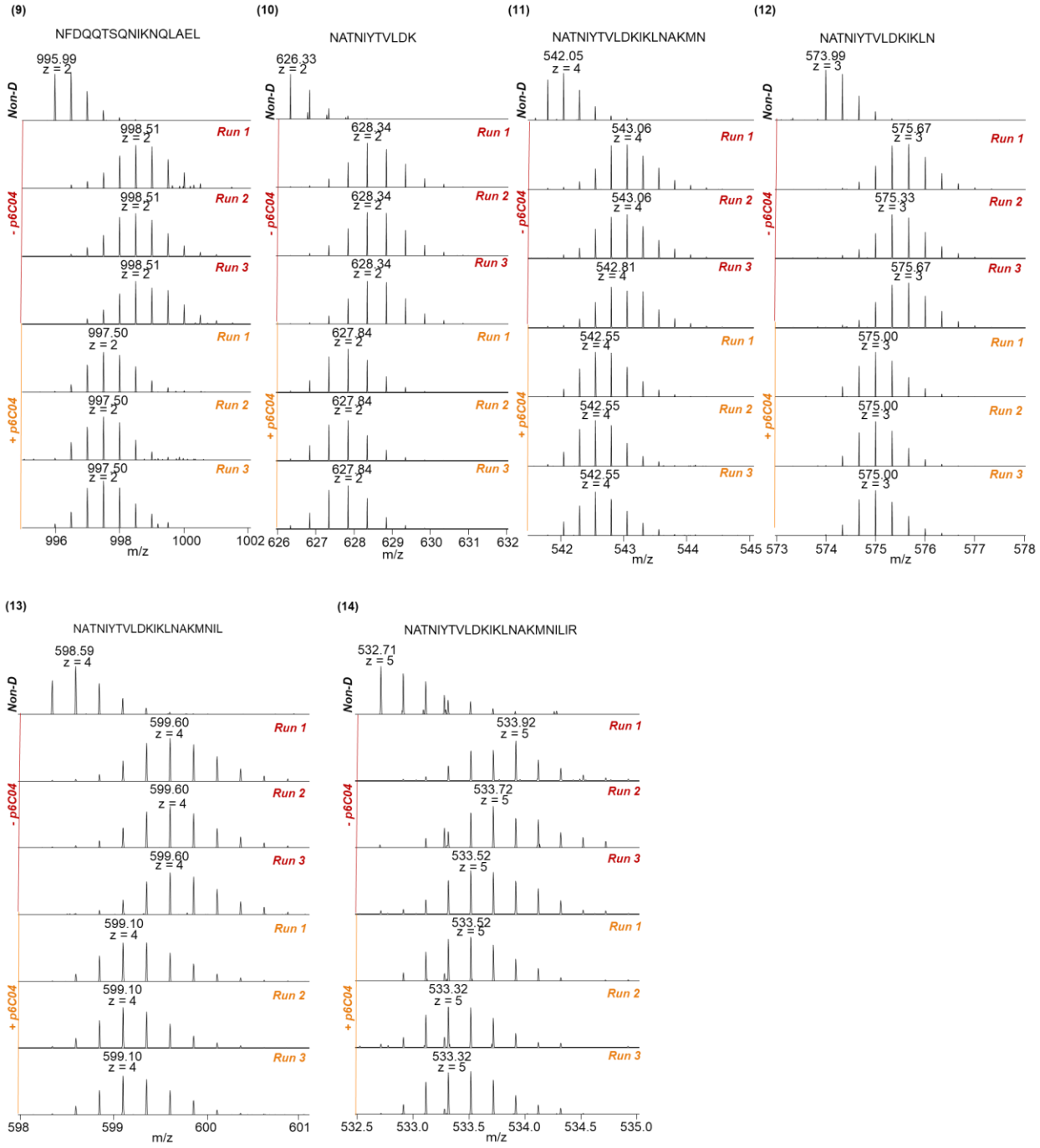
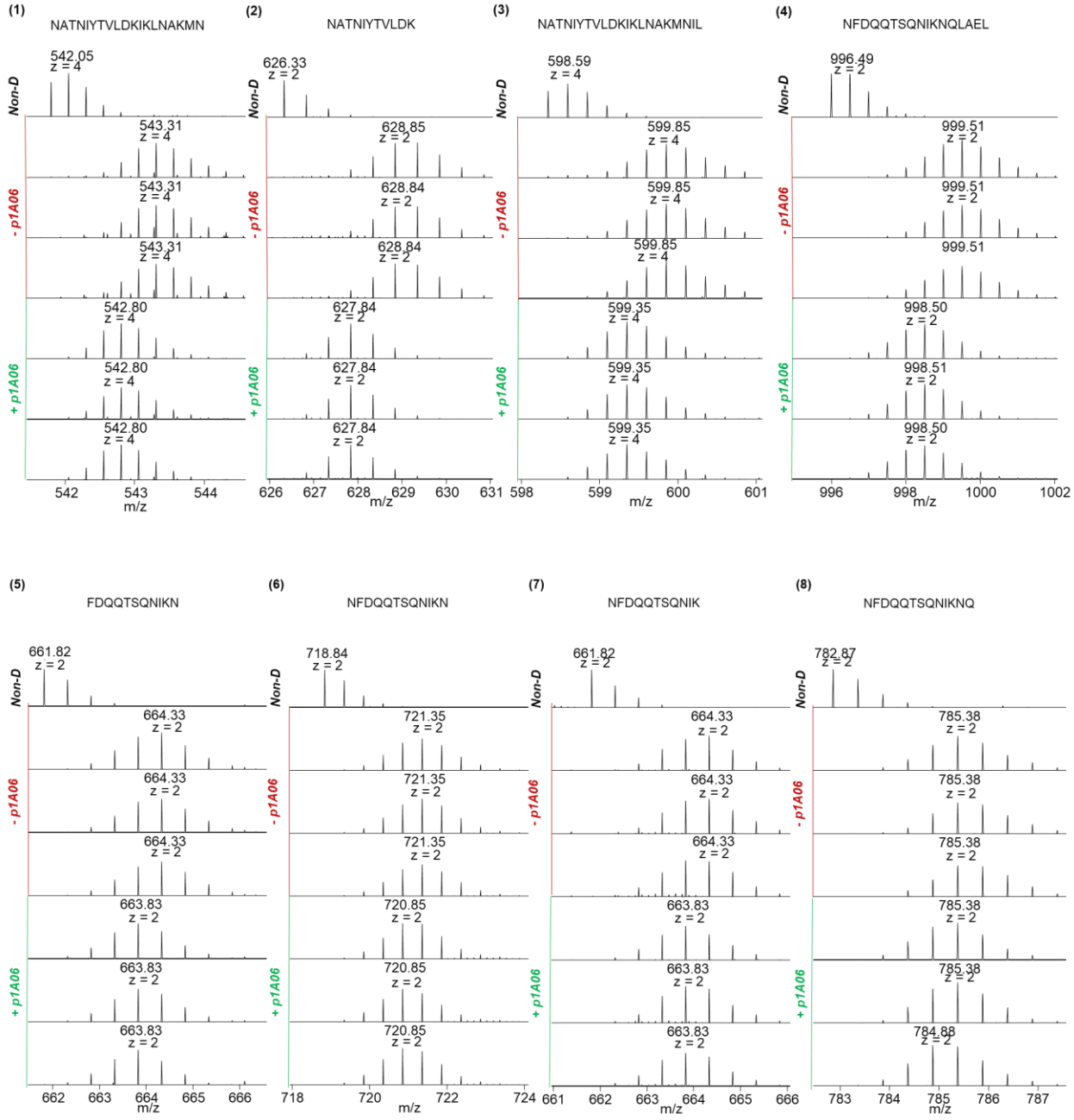



**Figure S2.** MS spectra of 14 identified peptides in primary epitope for p6C04 binding.


(1)
NATNIYTVLDKIKLNAKMN
542.05 z = 4
543.31 z = 4
543.31 z = 4
543.31 z = 4
542.80 z = 4
542.80 z = 4
542.80 z = 4
Non-D
- p1A06
+ p1A06
542 543 544
m/z
(2)
NATNIYTVLDK
626.33 z = 2
628.85 z = 2
628.84 z = 2
628.84 z = 2
627.84 z = 2
627.84 z = 2
627.84 z = 2
626 627 628 629 630 631
m/z
(3)
NATNIYTVLDKIKLNAKMNIL
598.59 z = 4
599.85 z = 4
599.85 z = 4
599.85 z = 4
599.35 z = 4
599.35 z = 4
599.35 z = 4
598 599 600 601
m/z
(4)
NFDQQTSQNIKNQLAEL
996.49 z = 2
999.51 z = 2
999.51 z = 2
999.51
998.50 z = 2
998.51 z = 2
998.50 z = 2
996 998 1000 1002
m/z
(5)
FDQQTSQNIKN
661.82 z = 2
664.33 z = 2
664.33 z = 2
664.33 z = 2
663.83 z = 2
663.83 z = 2
663.83 z = 2
662 663 664 665 666
m/z
(6)
NFDQQTSQNIKN
718.84 z = 2
721.35 z = 2
721.35 z = 2
721.35 z = 2
720.85 z = 2
720.85 z = 2
720.85 z = 2
718 720 722 724
m/z
(7)
NFDQQTSQNIK
661.82 z = 2
664.33 z = 2
664.33 z = 2
664.33 z = 2
663.83 z = 2
663.83 z = 2
663.83 z = 2
661 662 663 664 665 666
m/z
(8)
NFDQQTSQNIKNQ
782.87 z = 2
785.38 z = 2
785.38 z = 2
785.38 z = 2
785.38 z = 2
785.38 z = 2
784.88 z = 2
783 784 785 786 787
m/z

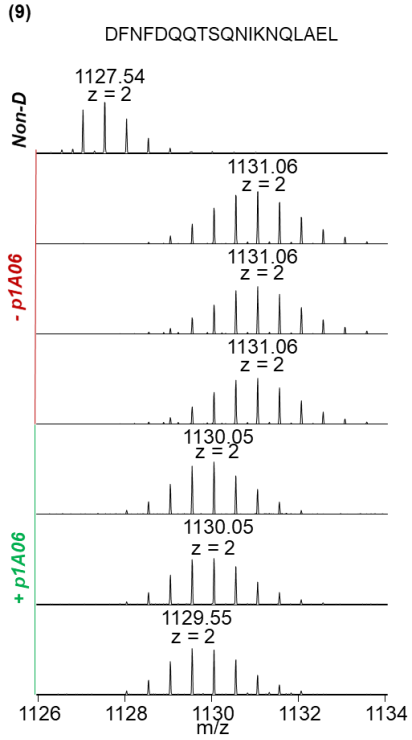
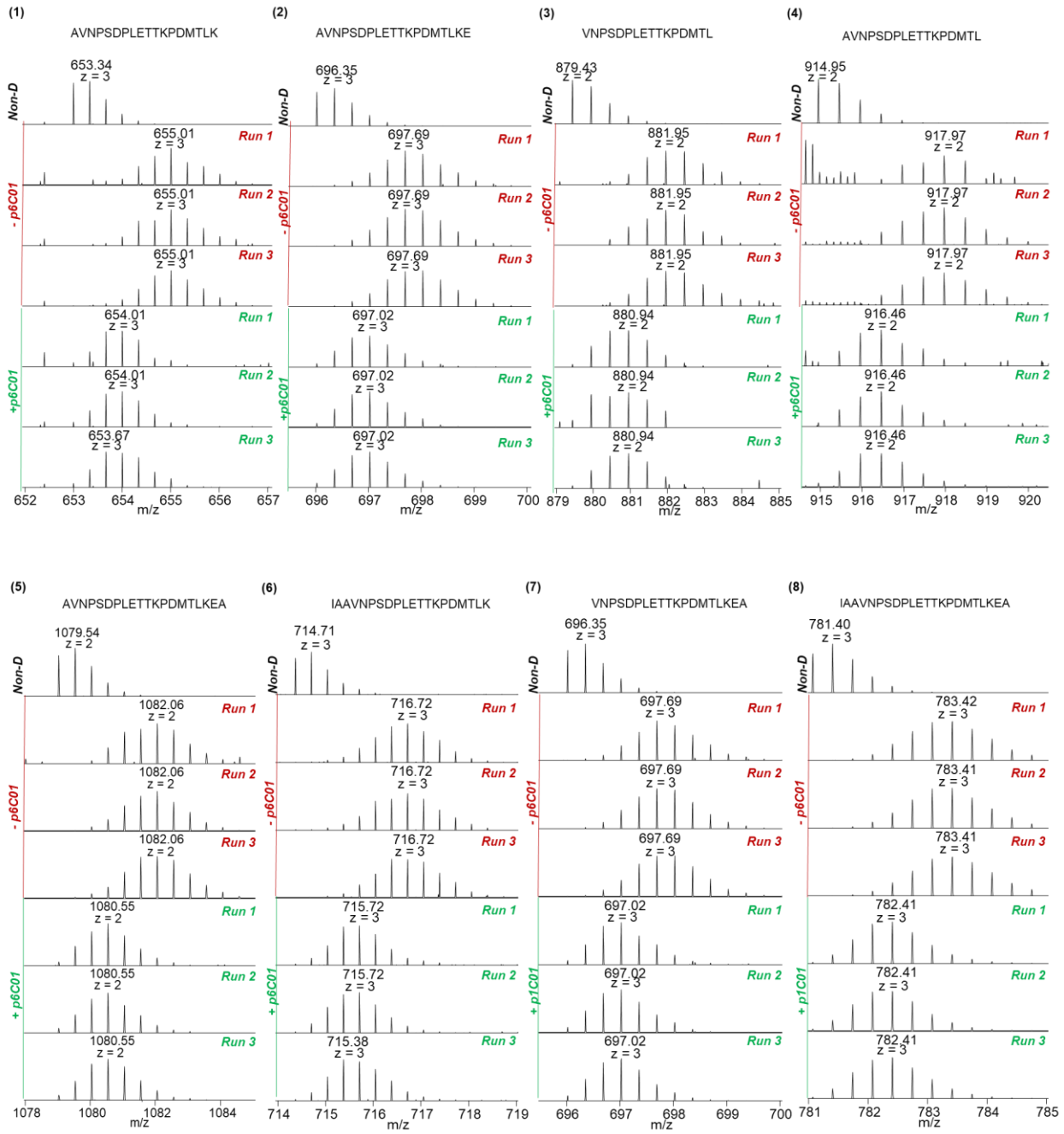
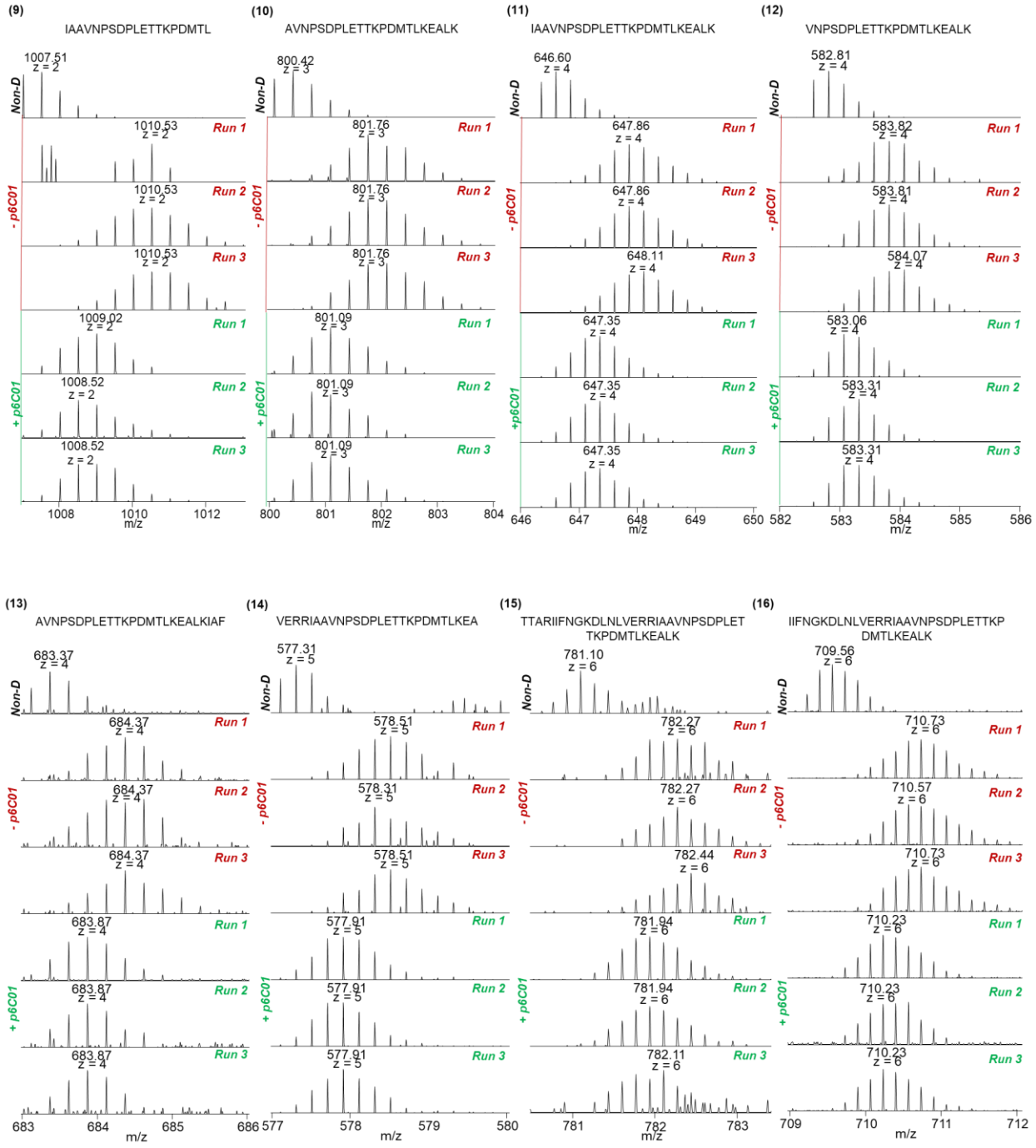


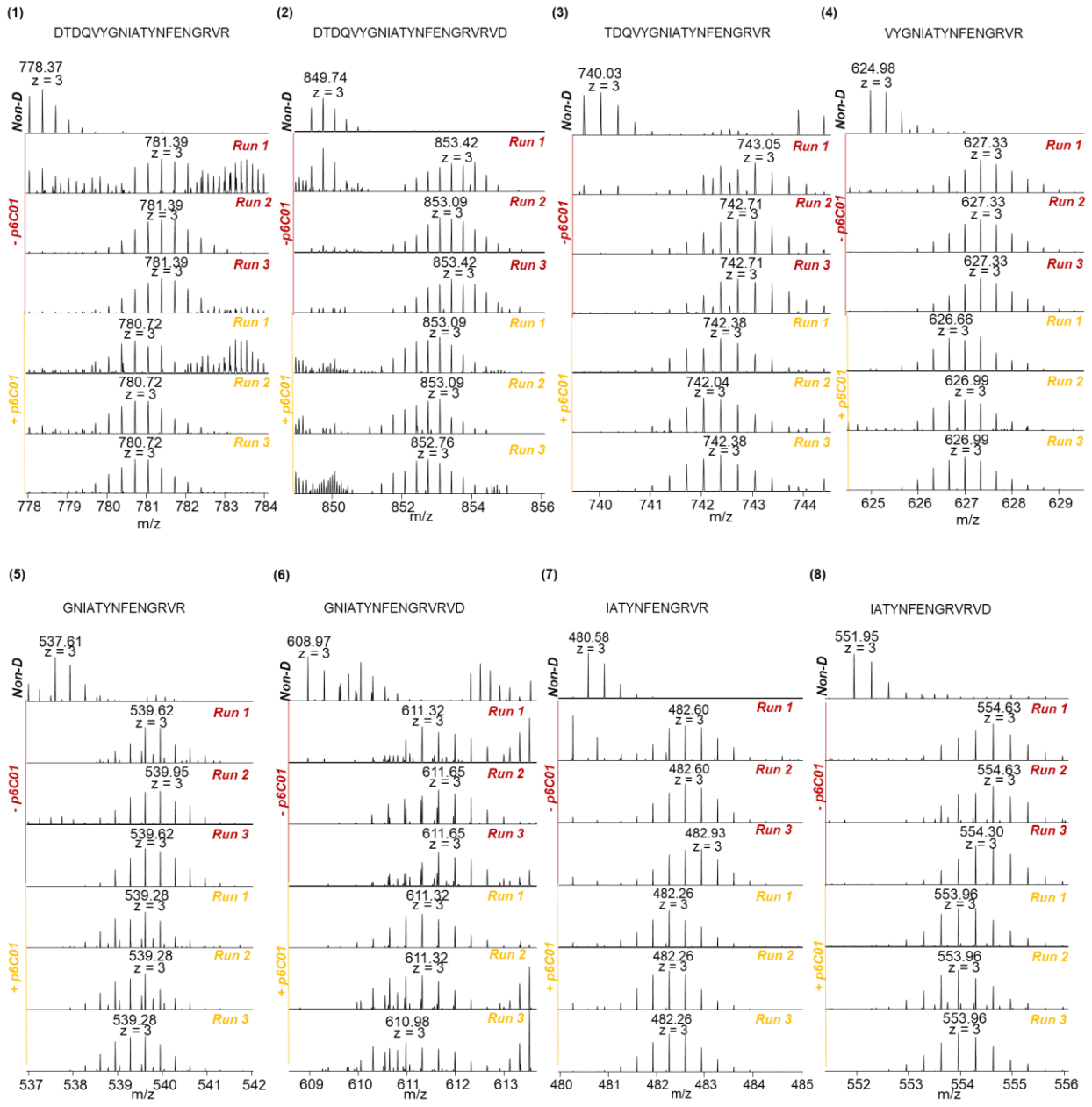

**Figure S3.** MS spectra of 9 identified peptides in primary epitope for p1A06 binding.

**(A)**


(1)
AVNPSDPLETTKPDMTLK
653.34 z = 3
655.01 z = 3
654.01 z = 3
653.67 z = 3
(2)
AVNPSDPLETTKPDMTLKE
696.35 z = 3
697.69 z = 3
697.02 z = 3
(3)
VNPSDPLETTKPDMTL
879.43 z = 2
881.95 z = 2
880.94 z = 2
(4)
AVNPSDPLETTKPDMTL
914.95 z = 2
917.97 z = 2
916.46 z = 2
(5)
AVNPSDPLETTKPDMTLKEA
1079.54 z = 2
1082.06 z = 2
1080.55 z = 2
(6)
IAAVNPSDPLETTKPDMTLK
714.71 z = 3
716.72 z = 3
715.72 z = 3
715.38 z = 3
(7)
VNPSDPLETTKPDMTLKEA
696.35 z = 3
697.69 z = 3
697.02 z = 3
(8)
IAAVNPSDPLETTKPDMTLKEA
781.40 z = 3
783.42 z = 3
783.41 z = 3
782.41 z = 3
Non-D
- p6C01
+p6C01
+ p1C01
Run 1
Run 2
Run 3
m/z


(9)
IAAVNPSDPLETTKPDMTL
(10)
AVNPSDPLETTKPDMTLKEALK
(11)
IAAVNPSDPLETTKPDMTLKEALK
(12)
VNPSDPLETTKPDMTLKEALK
(13)
AVNPSDPLETTKPDMTLKEALKIAF
(14)
VERRIAAVNPSDPLETTKPDMTLKEA
(15)
TTARIIFNGKDLNLVERRIAAVNPSDPLET
TKPDMTLKEALK
(16)
IIFNGKDLNLVERRIAAVNPSDPLETTKP
DMTLKEALK
Non-D
- p6C01
+ p6C01
Run 1
Run 2
Run 3
m/z

**(B)**


(1)
DTDQVYGNIATYNFENGRVR
778.37
z = 3
781.39
z = 3
780.72
z = 3
(2)
DTDQVYGNIATYNFENGRVRVD
849.74
z = 3
853.42
z = 3
853.09
z = 3
852.76
z = 3
(3)
TDQVYGNIATYNFENGRVR
740.03
z = 3
743.05
z = 3
742.71
z = 3
742.38
z = 3
742.04
z = 3
(4)
VYGNIATYNFENGRVR
624.98
z = 3
627.33
z = 3
626.66
z = 3
626.99
z = 3
(5)
GNIATYNFENGRVR
537.61
z = 3
539.62
z = 3
539.95
z = 3
539.28
z = 3
(6)
GNIATYNFENGRVRVD
608.97
z = 3
611.32
z = 3
611.65
z = 3
610.98
z = 3
(7)
IATYNFENGRVR
480.58
z = 3
482.60
z = 3
482.93
z = 3
482.26
z = 3
(8)
IATYNFENGRVRVD
551.95
z = 3
554.63
z = 3
554.30
z = 3
553.96
z = 3
Non-D
- p6C01
+ p6C01
Run 1
Run 2
Run 3
m/z

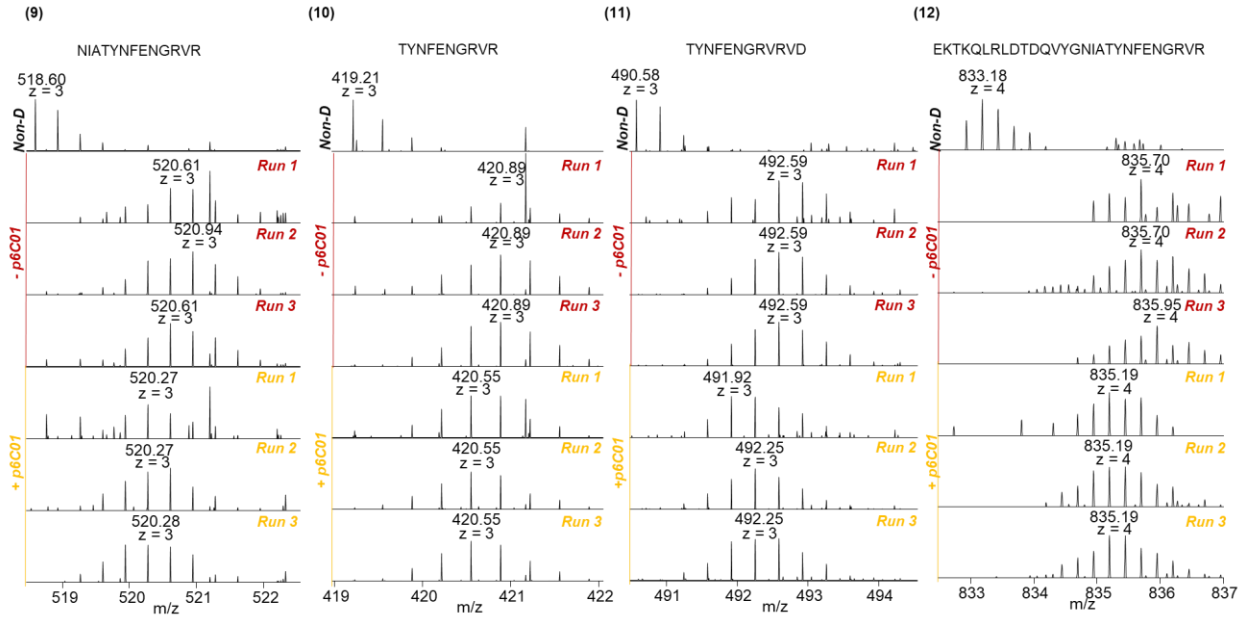



**Figure S4.** MS spectra of 28 identified peptides for p6C01 binding.(**A**) MS spectra of 16 identified peptides in primary epitope. (**B**) MS spectra of 12 identified peptides in secondary epitope.

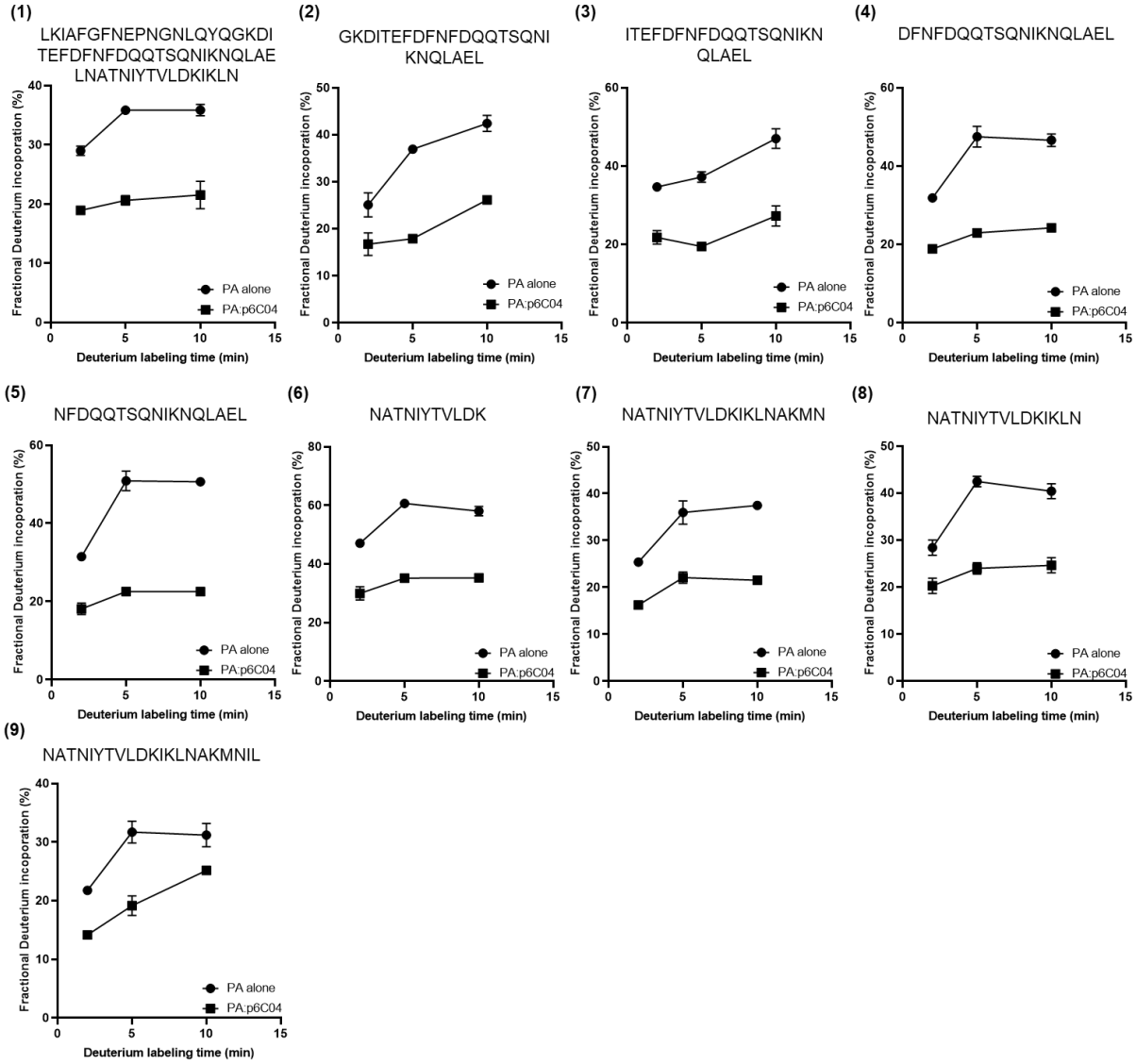



**Figure S5.** HDX time-course study for PA upon p6C04 binding. Relative fractional deuterium incorporation for 9 peptides in binding region were compared in the absence (Free PA) and presence of p6C04 (PA:p6C04) under 2 minutes, 5 minutes, and 10 minutes deuterium labeling conditions. Experiments were performed in triplicate.