

Supporting Information

A bifunctional amino acid to study protein-protein interactions

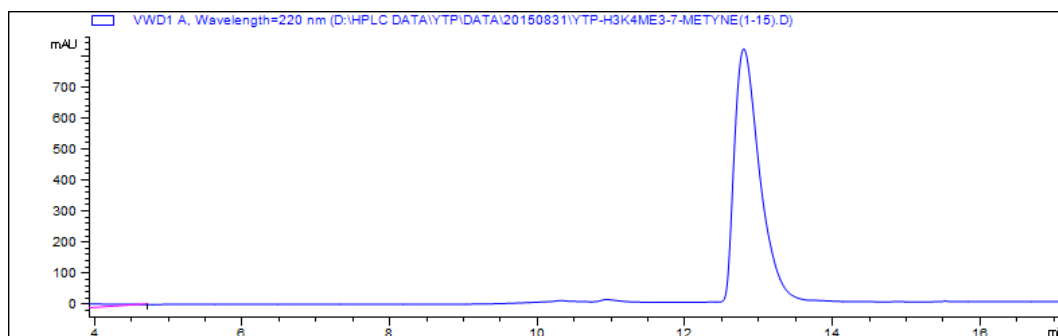
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YTP-H3K4me3Metyne(1-15) #858-871 RT: 13.52-13.71 AV: 14 NL: 6.65E7
 T: + c ESI Full ms [300.00-2000.00]

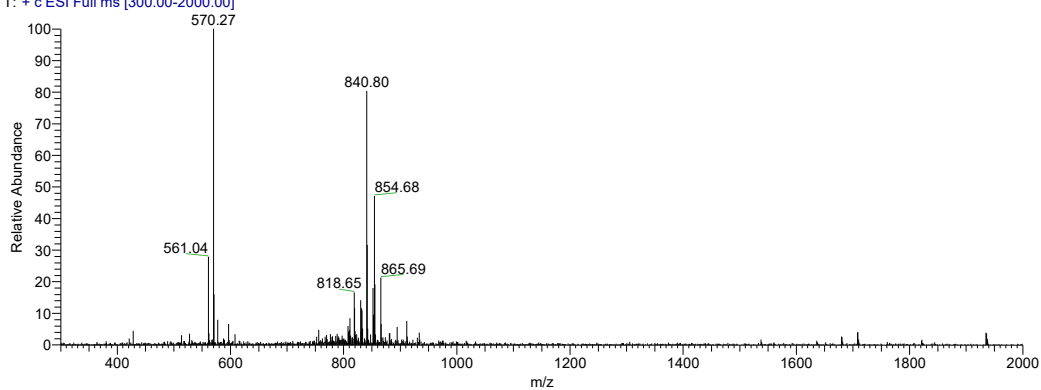
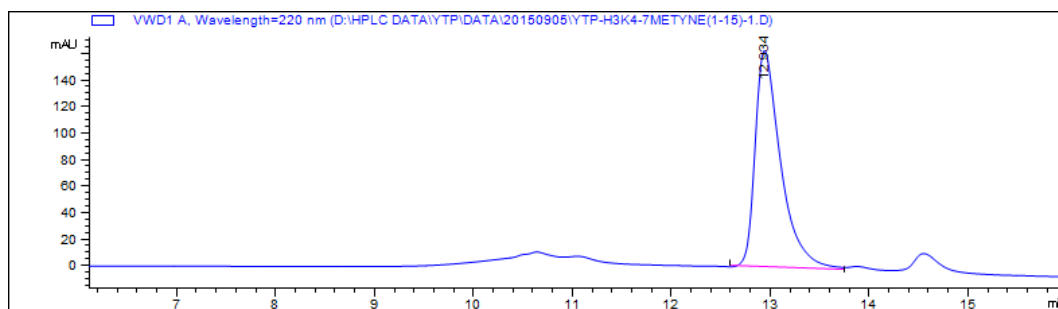


Fig. S2 LC–MS analysis of **probe 1**. m/z 854.68 ($M + 2H^+$), calculated m/z 854.50 ($M + 2H^+$); m/z 840.80 ($M - N_2 + 2H^+$), calculated m/z 840.50 ($M - N_2 + 2H^+$); m/z 570.27 ($M + 3H^+$), calculated m/z 570.00 ($M + 3H^+$); m/z 561.04 ($M - N_2 + 3H^+$), calculated m/z 560.67 ($M - N_2 + 3H^+$).



YTP-H3K4Metyne(1-15) #807-812 RT: 13.60-13.67 AV: 6 NL: 2.62E7
 T: + c ESI Full ms [300.00-2000.00]

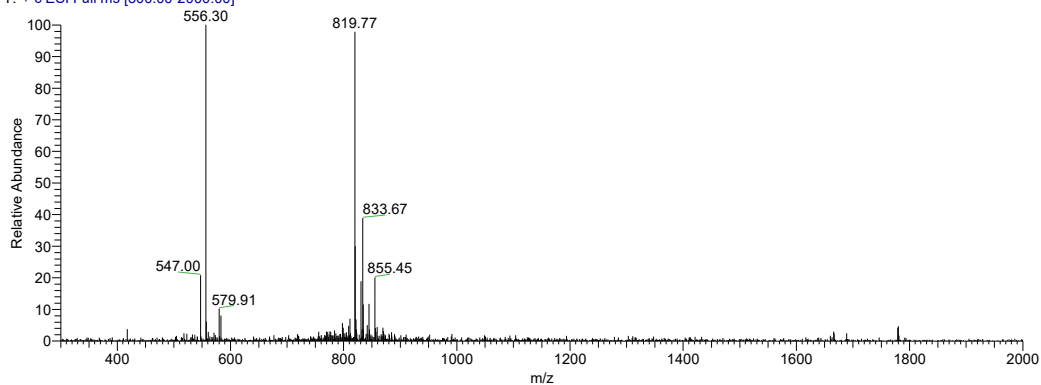
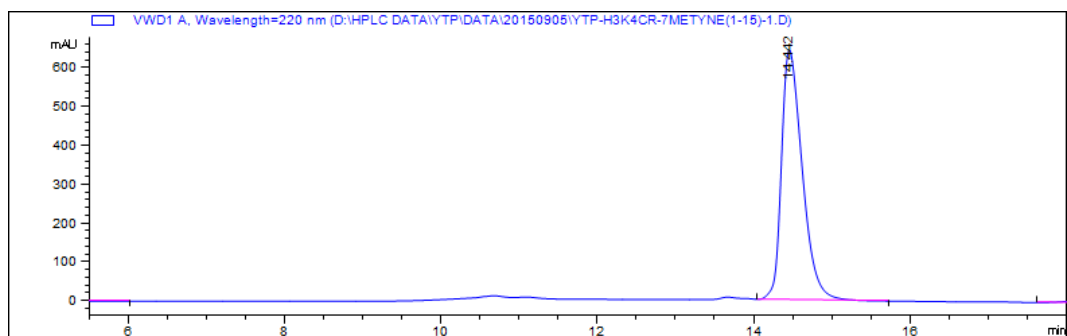


Fig. S3 LC–MS analysis of **probe 2**. m/z 855.45 ($M + 2Na^+$), calculated m/z 855.48 ($M + 2Na^+$); m/z 833.67 ($M + 2H^+$), calculated m/z 833.48 ($M + 2H^+$); m/z 819.77 ($M - N_2 + 2H^+$), calculated m/z 819.48 ($M - N_2 + 2H^+$); m/z 556.30 ($M + 3H^+$), calculated m/z 555.98 ($M + 3H^+$); m/z 547.00 ($M - N_2 + 3H^+$), calculated m/z 546.65 ($M - N_2 + 3H^+$).



ytp-H3K4Cr-7Metyne(1-15)-1 #902 RT: 14.94 AV: 1 NL: 7.34E7
 T: + c ESI Full ms [300.00-2000.00]

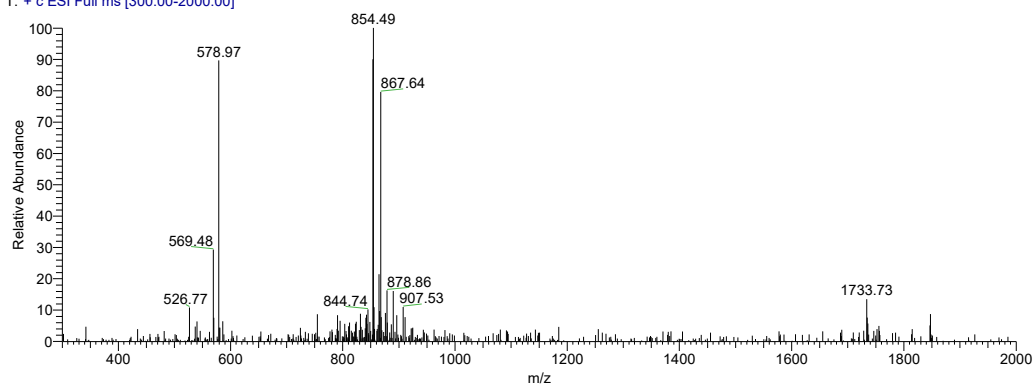
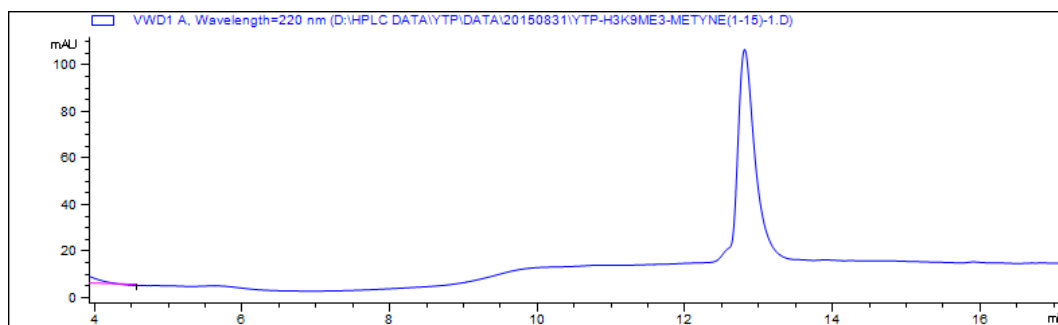


Fig. S4 LC–MS analysis of **probe 3**. m/z 1733.73 ($M + 1H^+$), calculated m/z 1733.98 ($M + 1H^+$); m/z 867.64 ($M + 2H^+$), calculated m/z 867.49 ($M + 2H^+$); m/z 854.49 ($M - N_2 + 2H^+$), calculated m/z 853.49 ($M - N_2 + 2H^+$); m/z 578.97 ($M + 3H^+$), calculated m/z 578.60 ($M + 3H^+$).



ytp-h3k9me3-Metyne(1-15) #782-796 RT: 13.00-13.21 AV: 15 NL: 3.30E7
 T: + c ESI Full ms [300.00-2000.00]

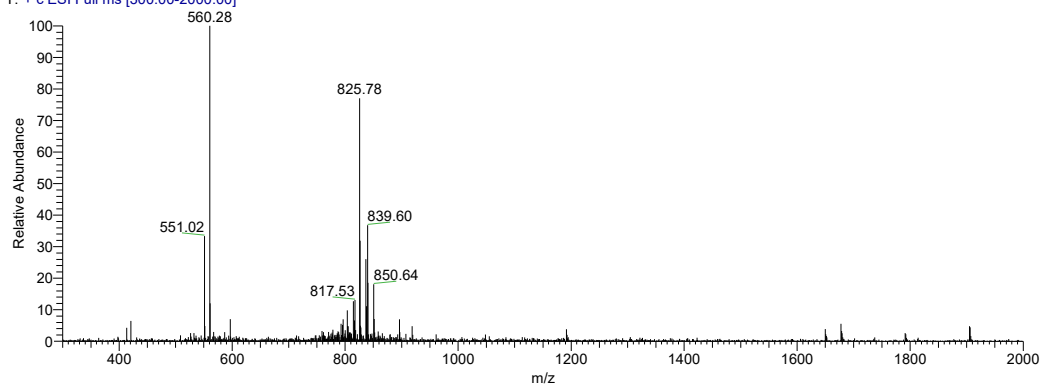
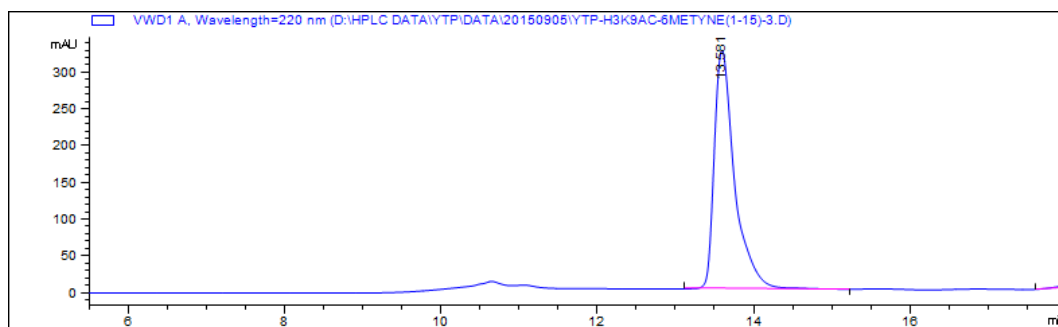


Fig. S5 LC–MS analysis of **probe 4**. m/z 839.60 ($M + 2H^+$), calculated m/z 839.50 ($M + 2H^+$); m/z 825.78 ($M - N_2 + 2H^+$), calculated m/z 825.50 ($M - N_2 + 2H^+$); m/z 560.28 ($M + 3H^+$), calculated m/z 560.00 ($M + 3H^+$); m/z 551.02 ($M - N_2 + 3H^+$), calculated m/z 550.67 ($M - N_2 + 3H^+$).



YTP-H3K9ac-Metyne(1-15) #849-862 RT: 14.26-14.46 AV: 14 NL: 3.87E7
 T: + c ESI Full ms [300.00-2000.00]

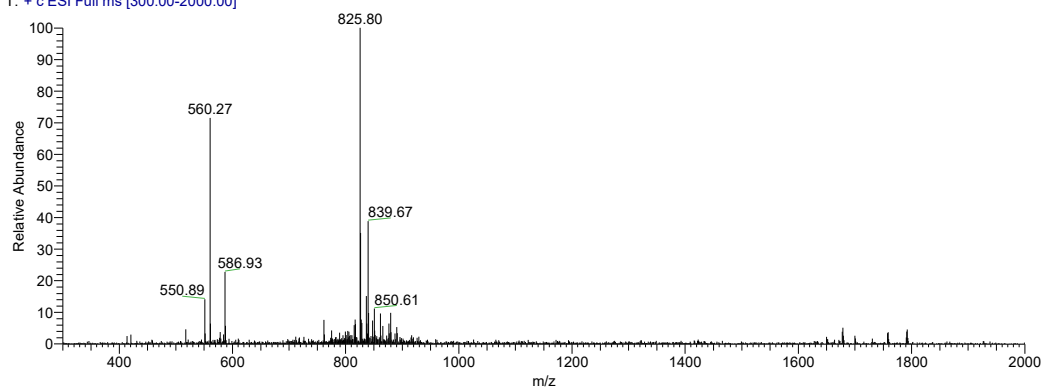
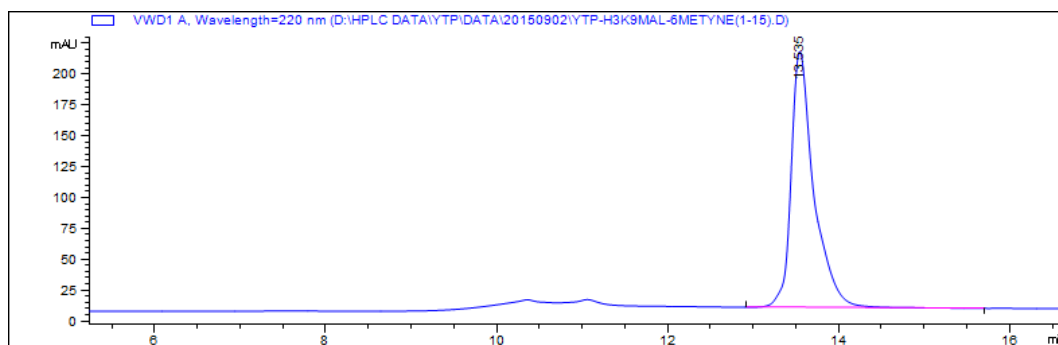


Fig. S6 LC–MS analysis of **probe 5**. m/z 839.67 ($M + 2H^+$), calculated m/z 839.48 ($M + 2H^+$); m/z 825.80 ($M - N_2 + 2H^+$), calculated m/z 825.48 ($M - N_2 + 2H^+$); m/z 560.27 ($M + 3H^+$), calculated m/z 559.98 ($M + 3H^+$); m/z 550.89 ($M - N_2 + 3H^+$), calculated m/z 550.65 ($M - N_2 + 3H^+$).



ytp-h3k9mal-6-Metyne(1-15) #841-848 RT: 14.05-14.15 AV: 8 NL: 1.02E8
T: + c ESI Full ms [300.00-2000.00]

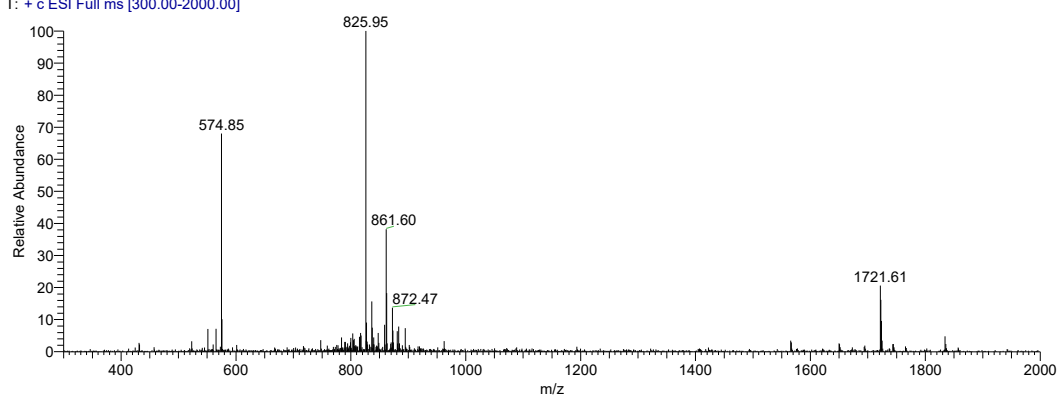
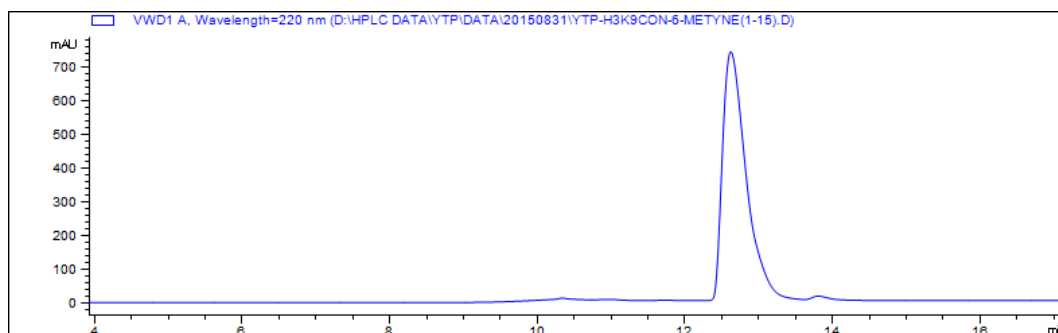


Fig. S7 LC–MS analysis of **probe 6**. m/z 1721.61 ($M + 1H^+$), calculated m/z 1721.94 ($M + 1H^+$); m/z 861.60 ($M + 2H^+$), calculated m/z 861.47 ($M + 2H^+$); m/z 825.95 ($M - N_2 - CO_2 + 2H^+$), calculated m/z 825.47 ($M - N_2 - CO_2 + 2H^+$); m/z 574.85 ($M + 3H^+$), calculated m/z 574.65 ($M + 3H^+$).



H3K9Metyne(1-15) #108-111 RT: 2.57-2.63 AV: 4 NL: 3.69E8
T: + c ESI Full ms [300.00-2000.00]

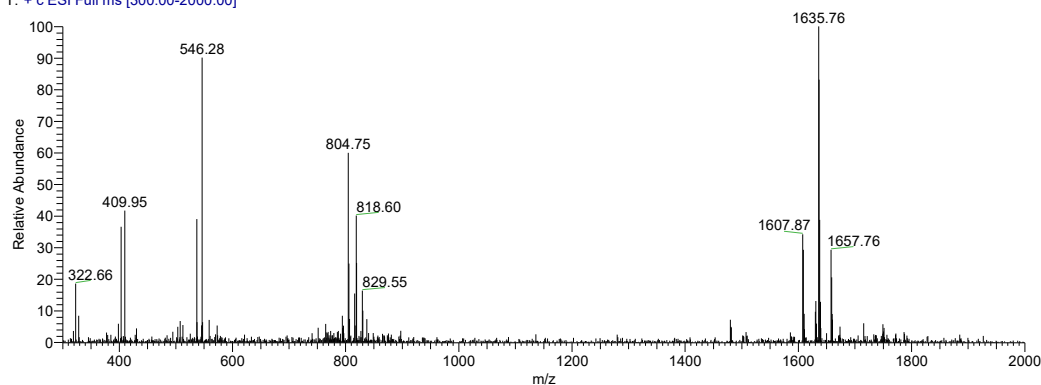


Fig. S8 LC–MS analysis of **probe 7**. m/z 1657.76 ($M + Na^+$), calculated m/z 1657.94 ($M + Na^+$); m/z 1635.76 ($M + 1H^+$), calculated m/z 1635.94 ($M + 1H^+$); m/z 1607.87 ($M - N_2 + 1H^+$), calculated m/z 1607.94 ($M - N_2 + 1H^+$); m/z 818.60 ($M + 2H^+$), calculated m/z 818.47 ($M + 2H^+$); m/z 804.75 ($M - N_2 + 2H^+$), calculated m/z 804.47 ($M - N_2 + 2H^+$); m/z 546.28 ($M + 3H^+$), calculated m/z 545.98 ($M + 3H^+$); m/z 409.95 ($M + 4H^+$), calculated m/z 409.74 ($M + 4H^+$).

The synthesis of H3K4me0 and H3K4me3 peptides have been reported previously.²

