Electronic Supplementary Information (ESI)

Pyrene-labeled pyrrolidinyl peptide nucleic acid as a hybridization-responsive DNA probe: Comparison between internal and terminal labeling

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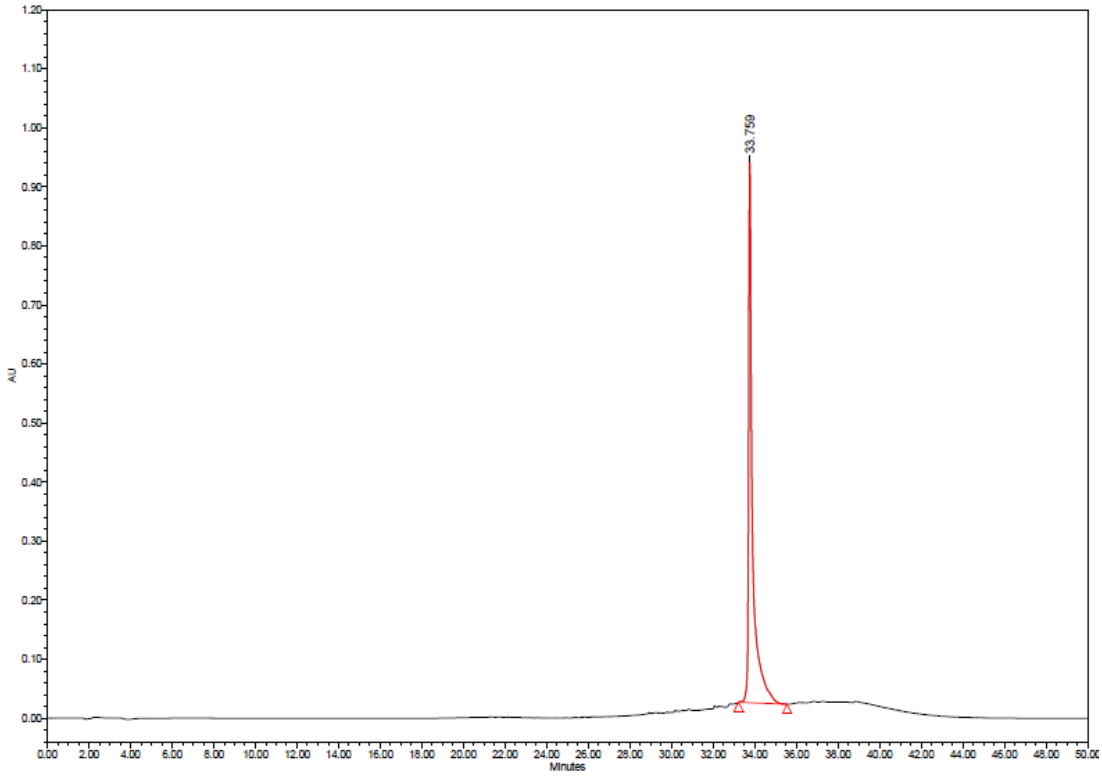
Content



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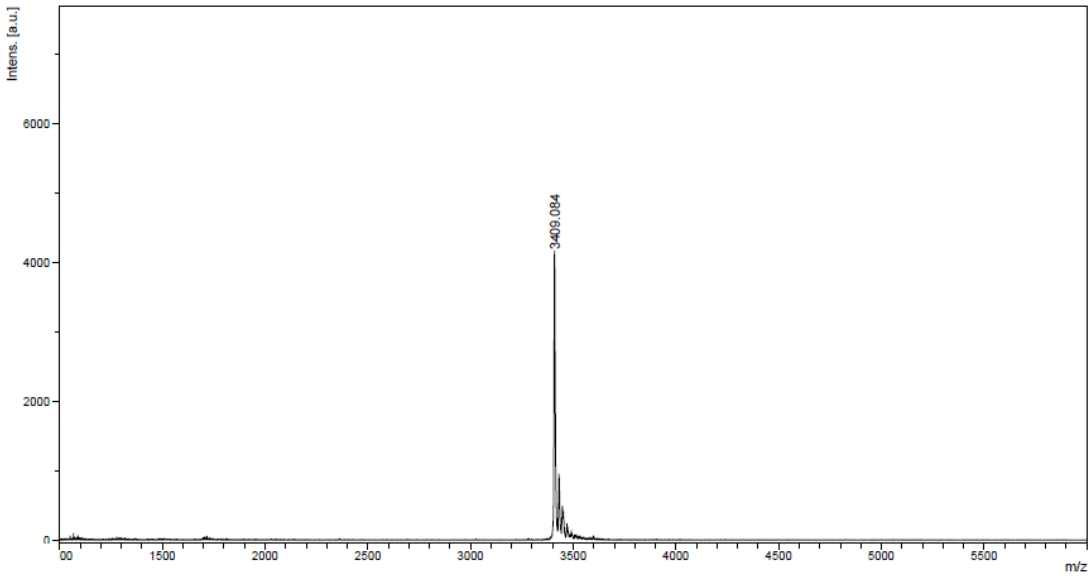
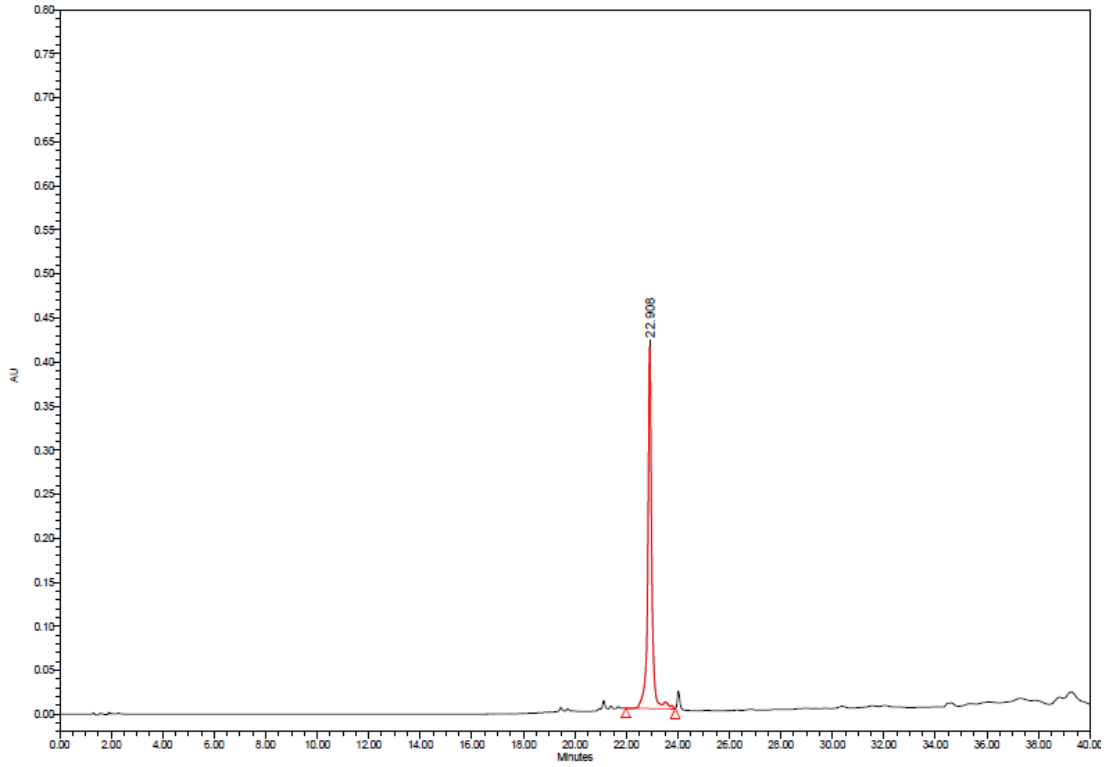


(b)

Fig. S1. Analytical HPLC chromatogram (a) and MALDI-TOF mass spectrum (b) of terminally PyBtr-labeled **T9** (calcd. for $[M+H]^+$: *m/z* = 3407.73).



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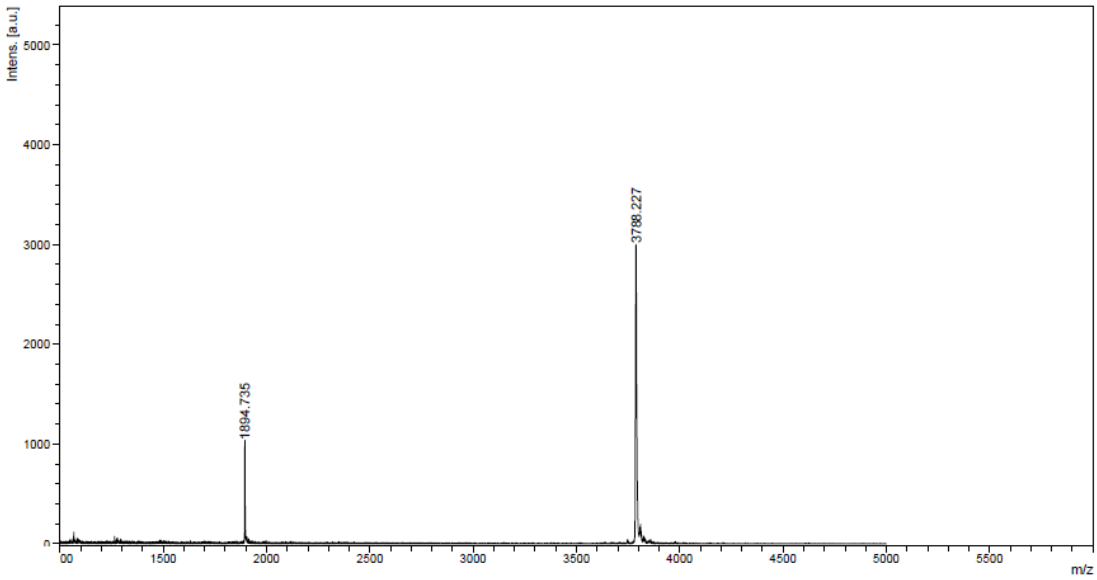
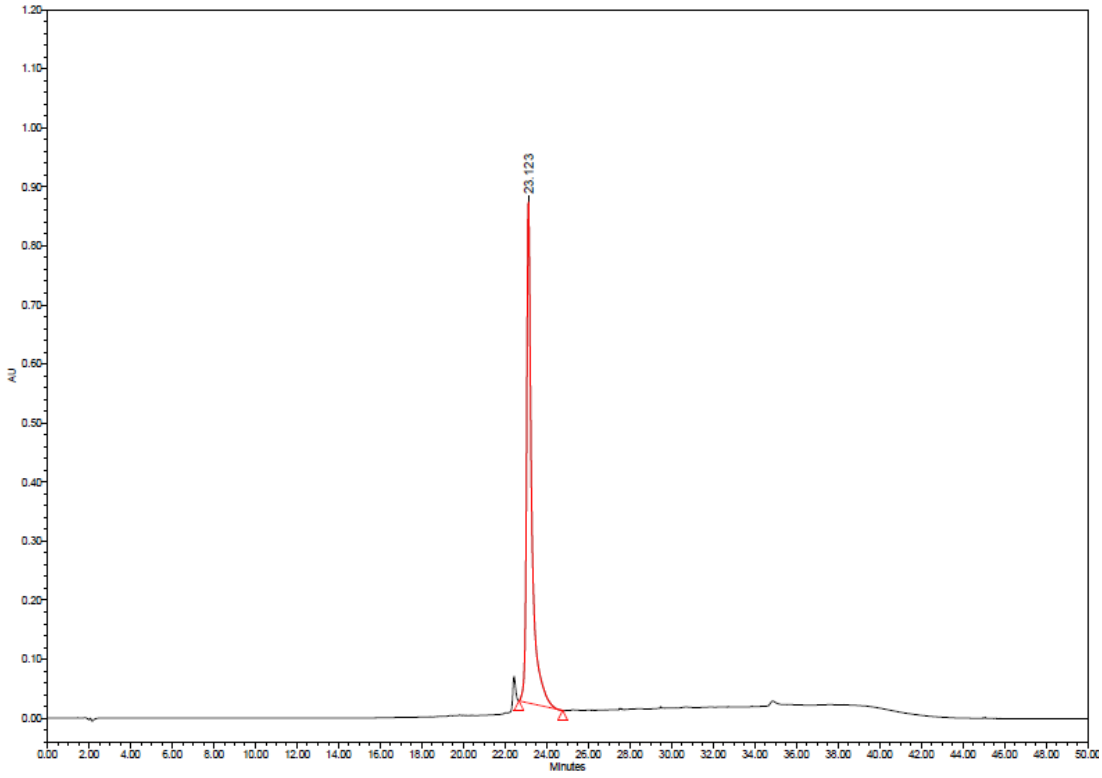


(b)

Fig. S2. Analytical HPLC chromatogram (a) and MALDI-TOF mass spectrum (b) of terminally PyBtr-labeled **M10** (calcd. for $[M+H]^+$: m/z = 3787.13).



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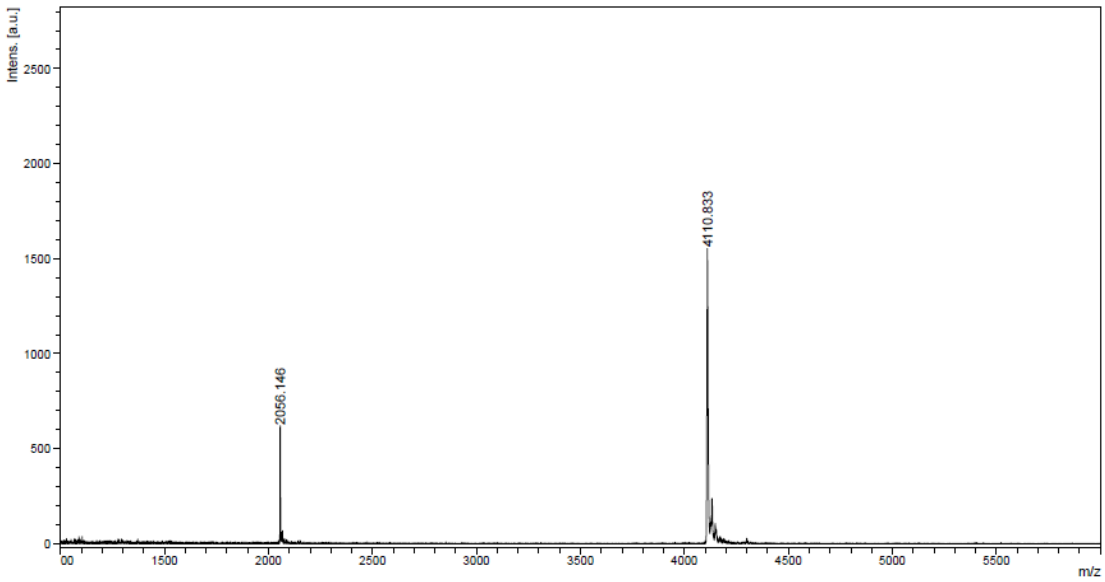
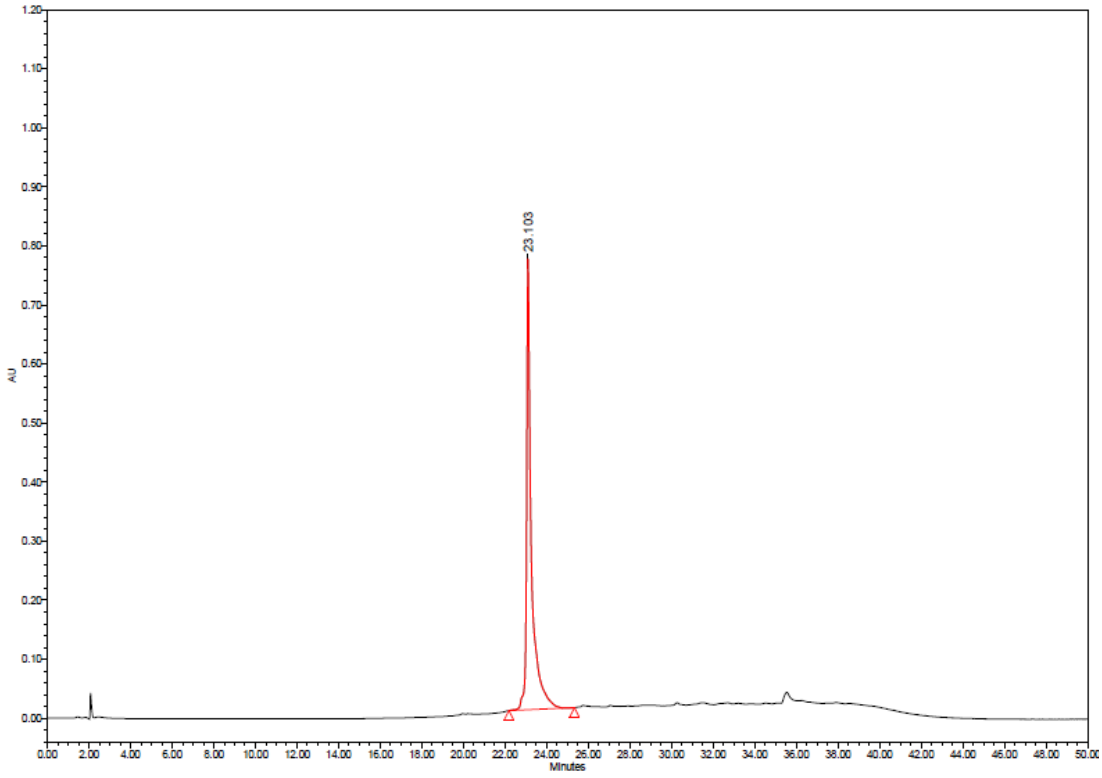


(b)

Fig. S3. Analytical HPLC chromatogram (a) and MALDI-TOF mass spectrum (b) of terminally PyBtr-labeled **M11** (calcd. for $[M+H]^+$: m/z = 4112.50).



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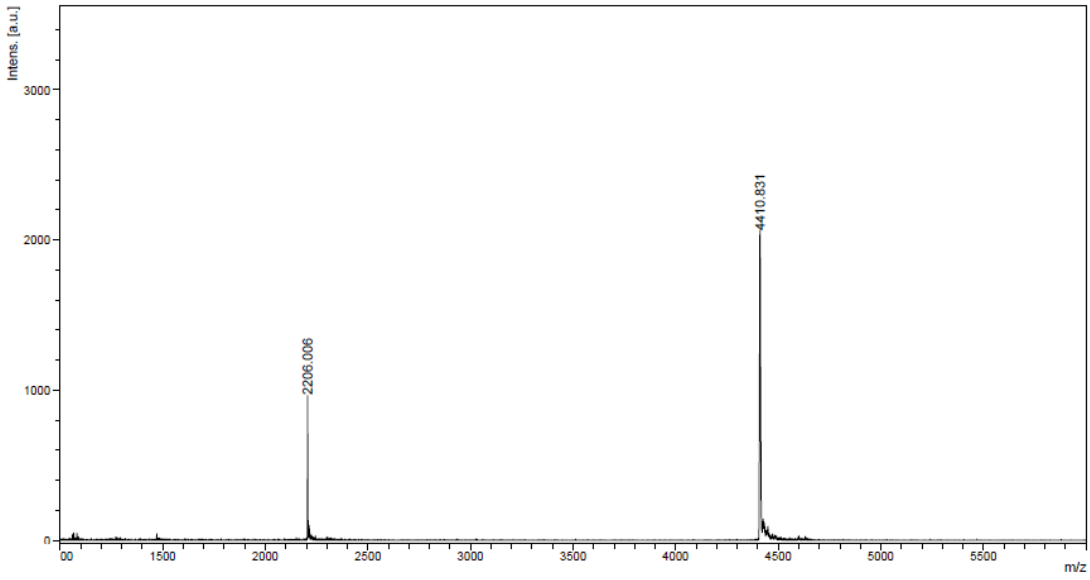

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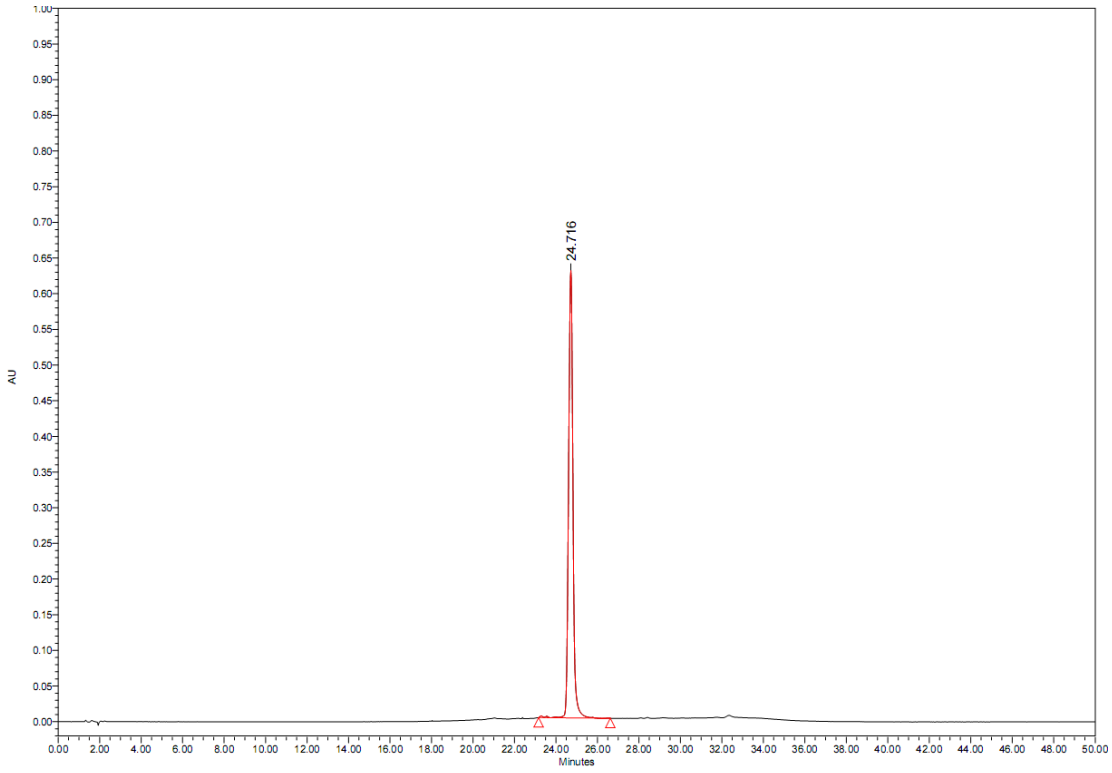
Fig. S4. Analytical HPLC chromatogram (a) and MALDI-TOF mass spectrum (b) of terminally PyBtr-labeled **M12** (calcd. for $[M+H]^+$: m/z = 4412.80).



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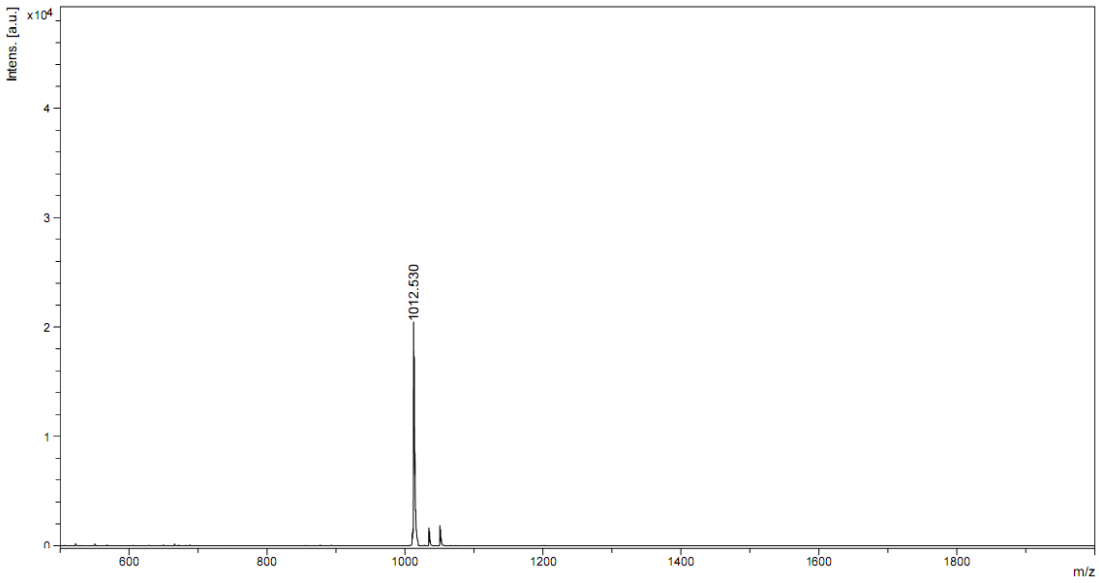
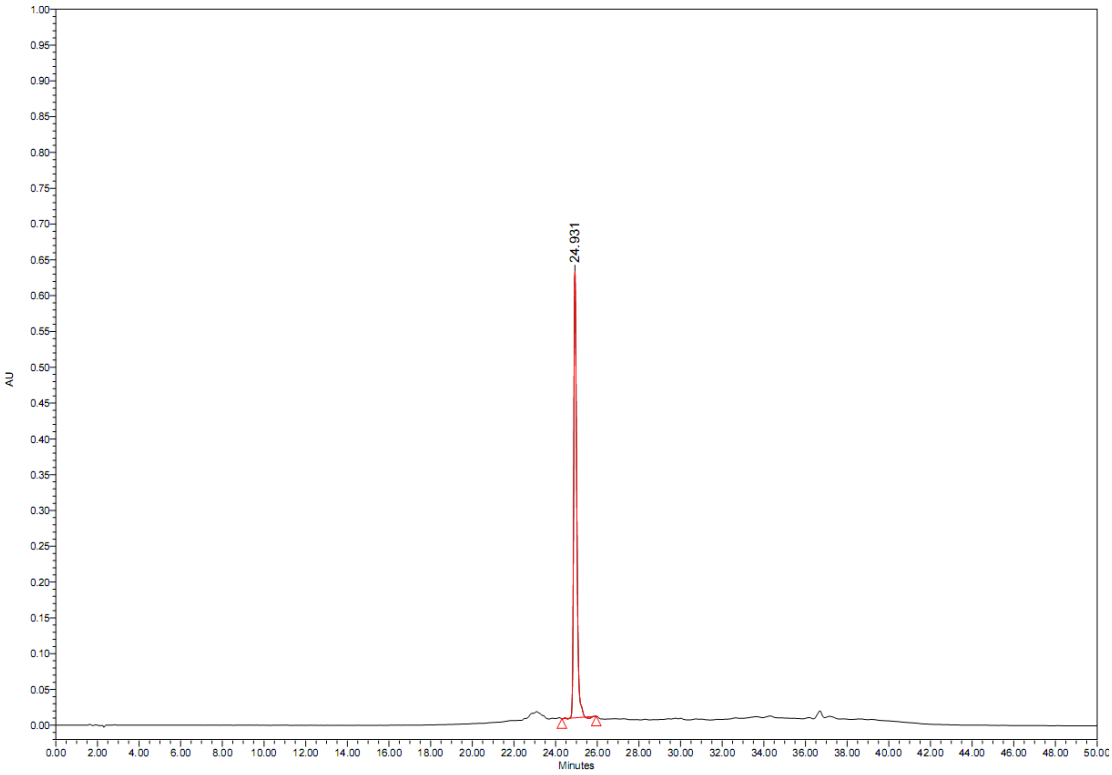


(b)

Fig. S5. Analytical HPLC chromatogram (a) and MALDI-TOF mass spectrum (b) of internally PyBtr-labeled **TT** (calcd. for $[M+H]^+$: m/z = 1013.20).



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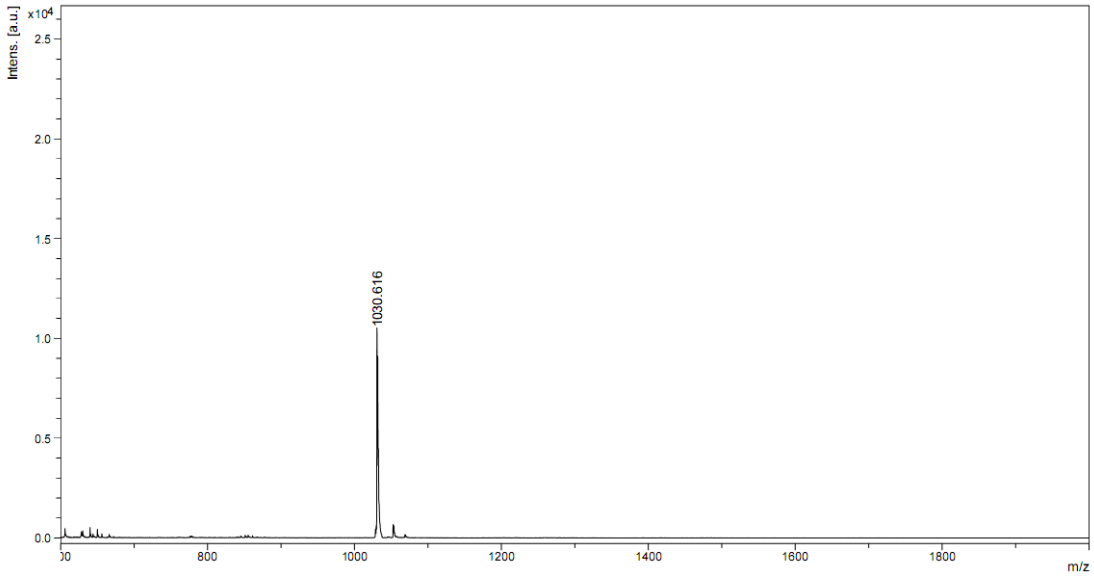

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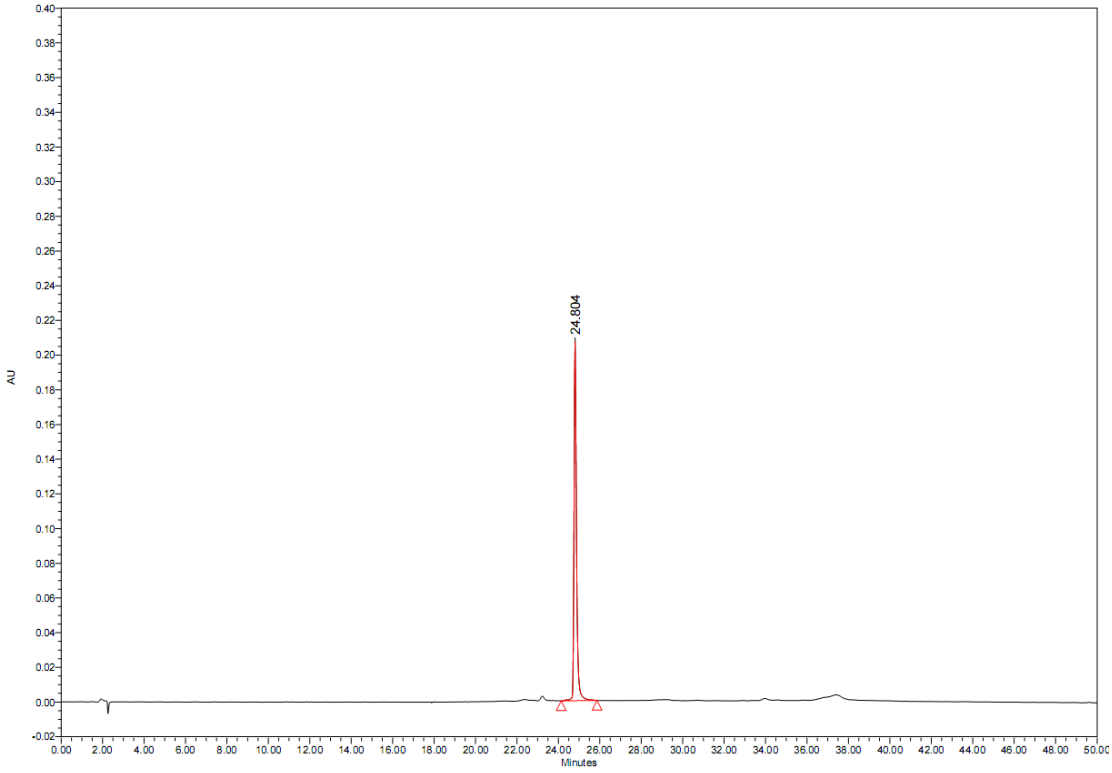
Fig. S6. Analytical HPLC chromatogram (a) and MALDI-TOF mass spectrum (b) of internally PyBtr-labeled **AA** (calcd. for $[M+H]^+$: m/z = 1031.23).



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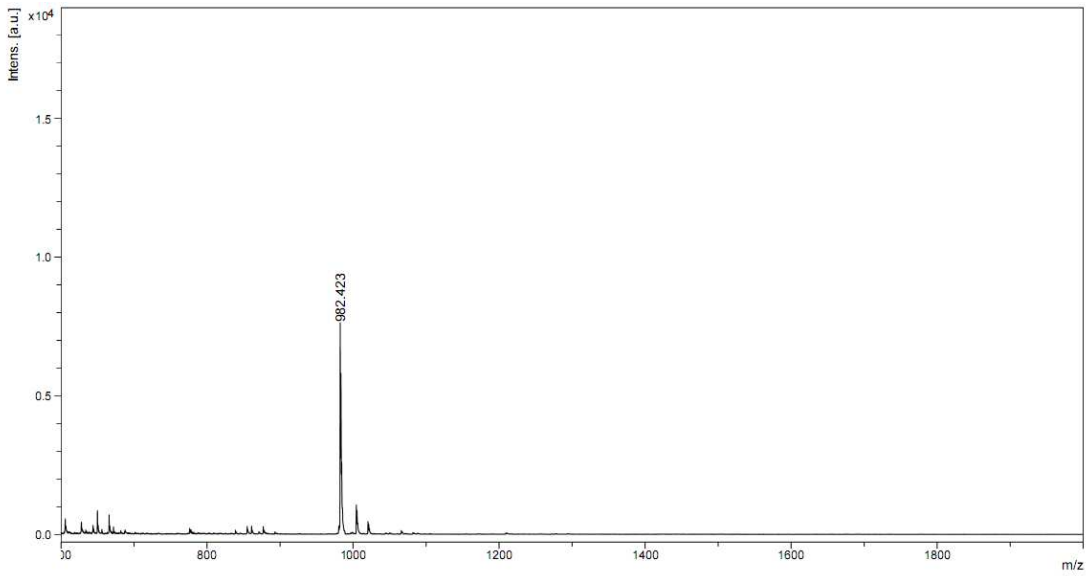
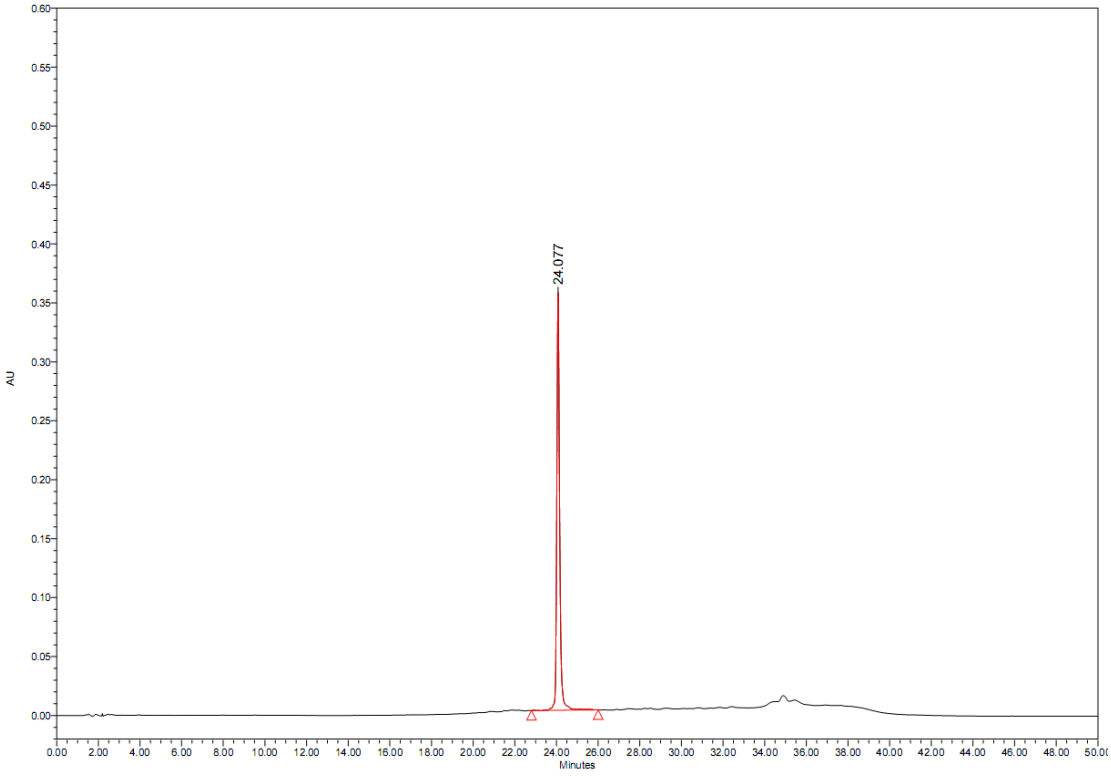


(b)

Fig. S7. Analytical HPLC chromatogram (a) and MALDI-TOF mass spectrum (b) of internally PyBtr-labeled **CC** (calcd. for $[M+H]^+$: m/z = 983.17).



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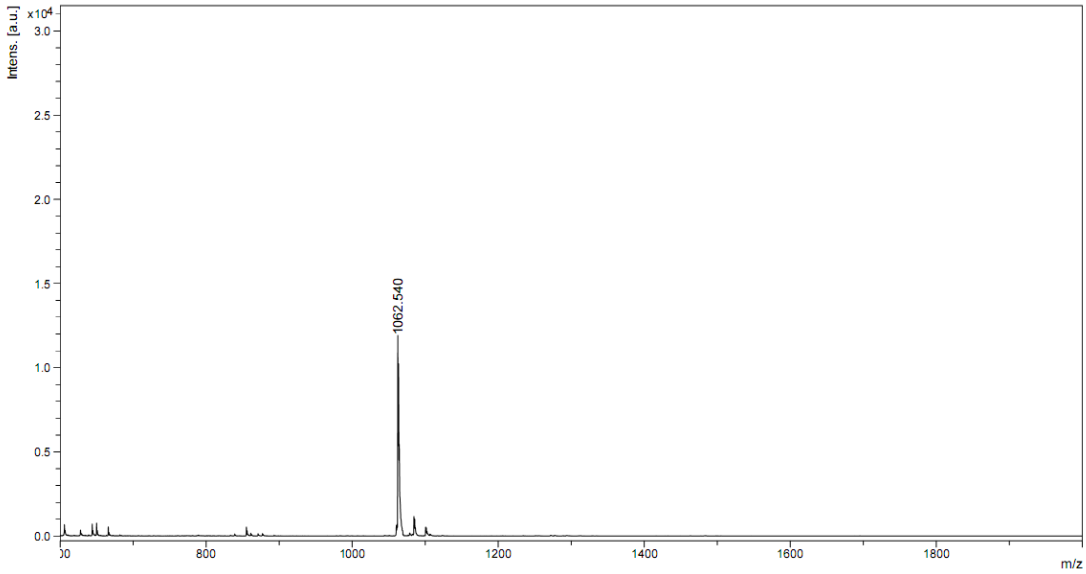
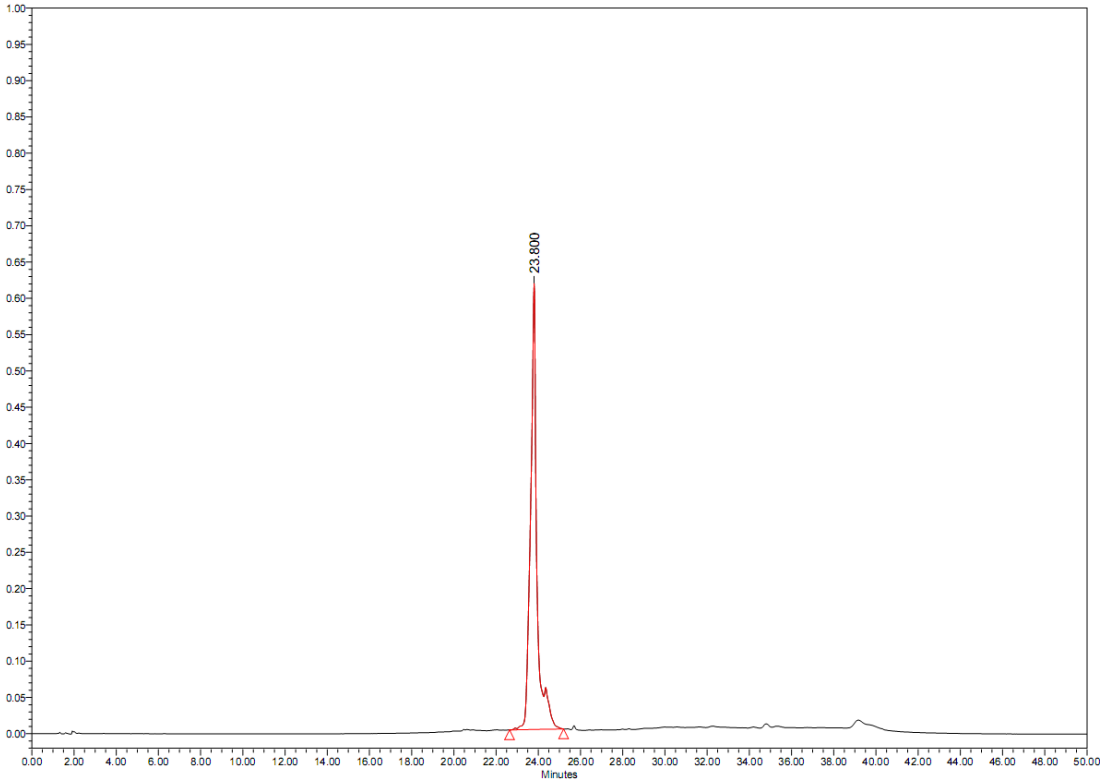


(b)

Fig. S8. Analytical HPLC chromatogram (a) and MALDI-TOF mass spectrum (b) of internally PyBtr-labeled **GG** (calcd. for $[M+H]^+$: m/z = 1063.22).



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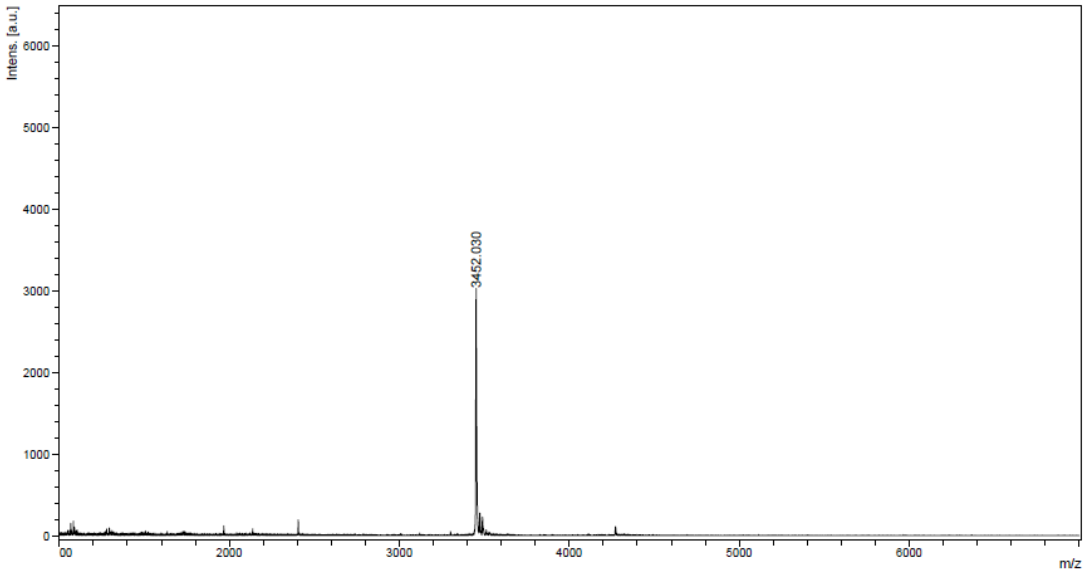

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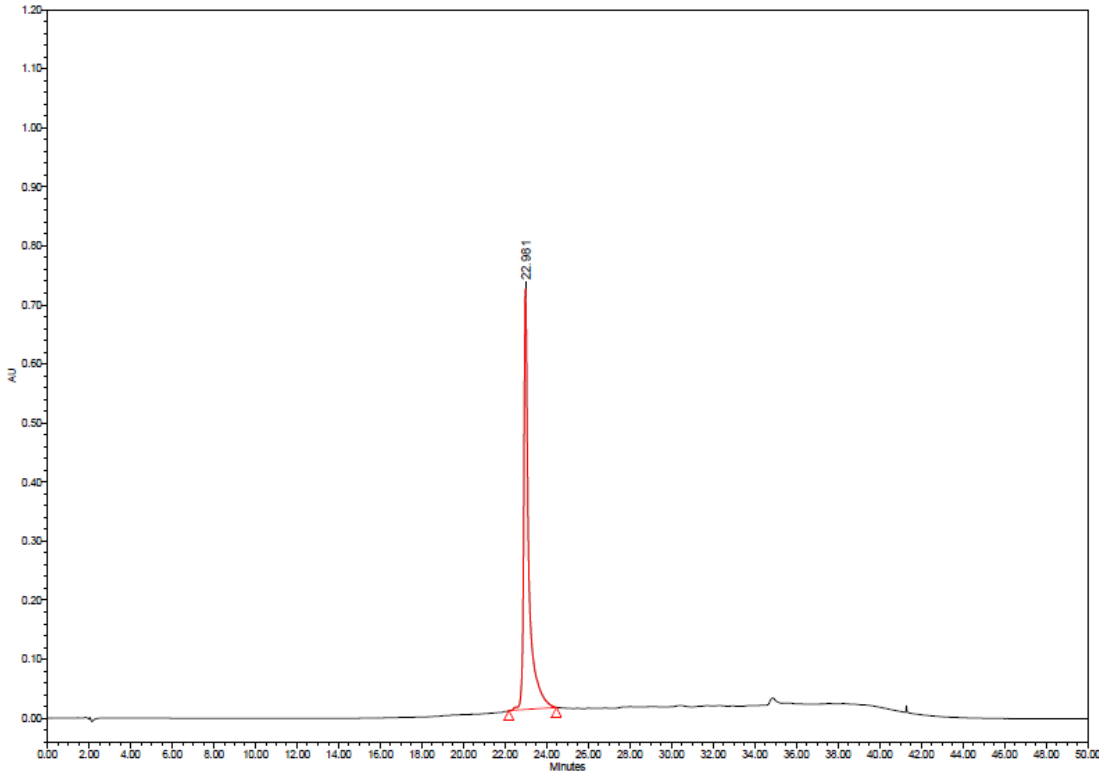
Fig. S9. Analytical HPLC chromatogram (a) and MALDI-TOF mass spectrum (b) of internally PyBtr-labeled **T9_TT** (calcd. for $[M+H]^+$: *m/z* = 3450.75).



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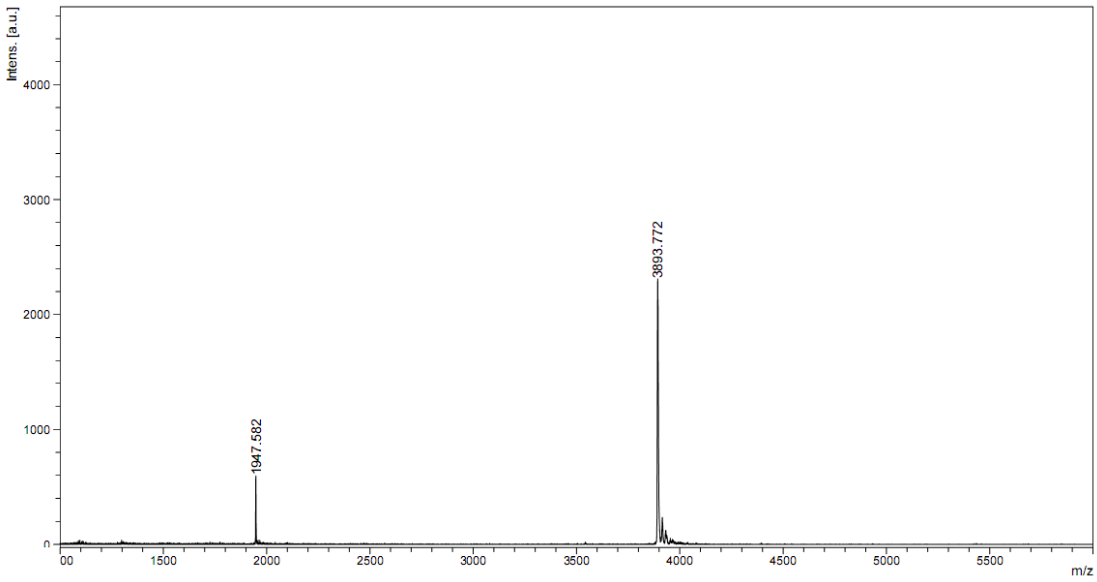
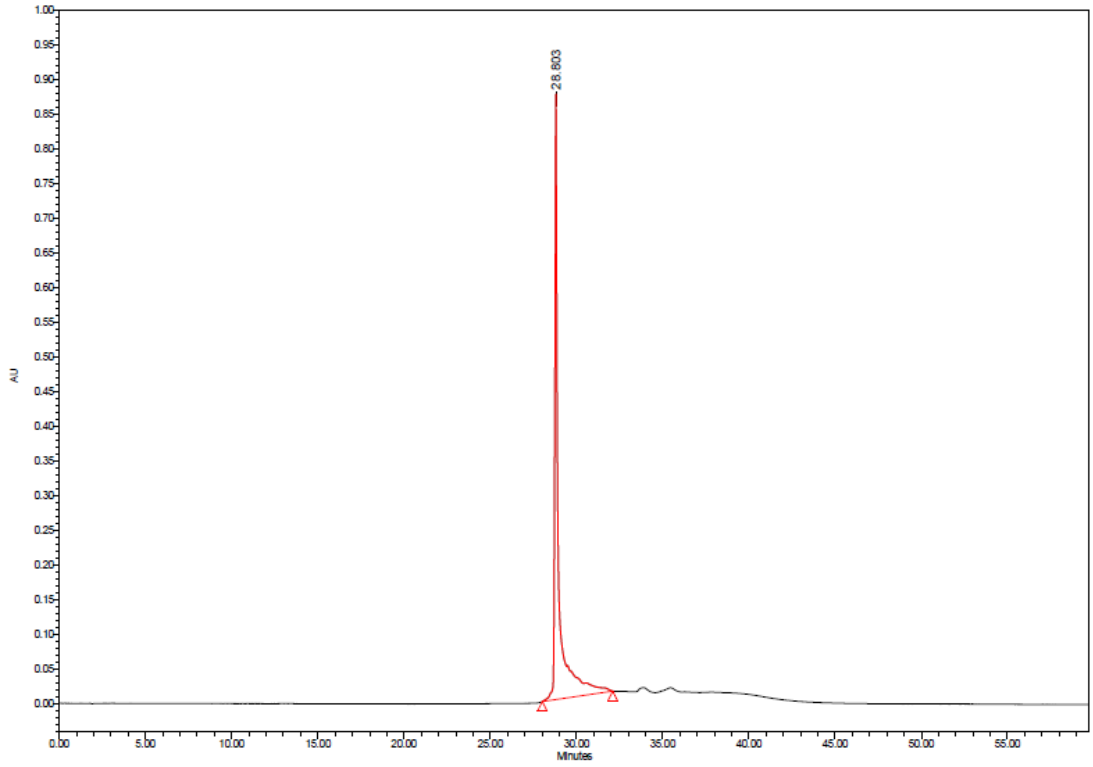


(b)

Fig. S10. Analytical HPLC chromatogram (a) and MALDI-TOF mass spectrum (b) of internally PyBtr-labeled **M10_AT** (calcd. for $[M+H]^+$: *m/z* = 3892.21).



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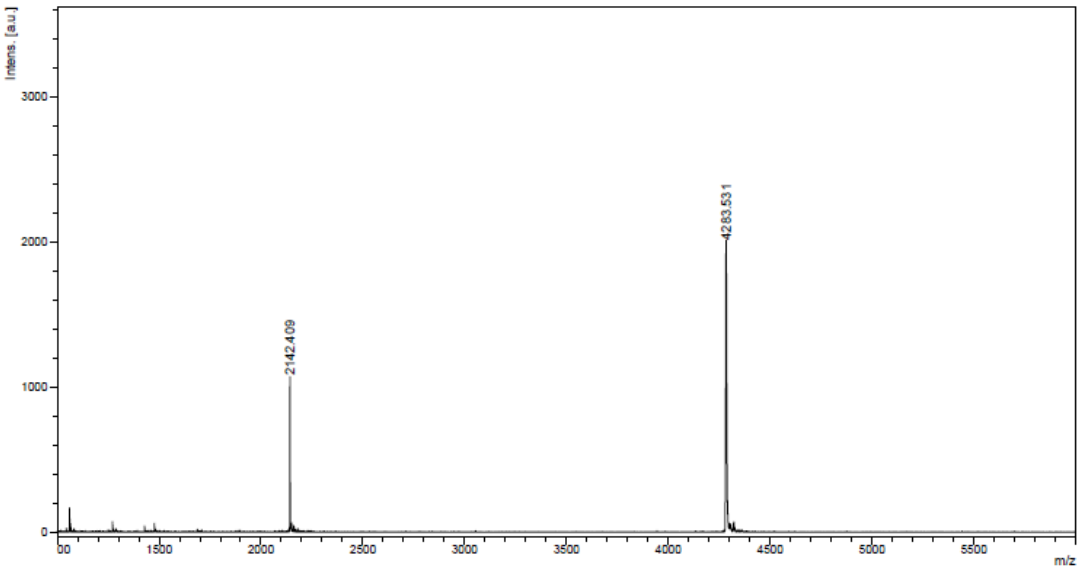

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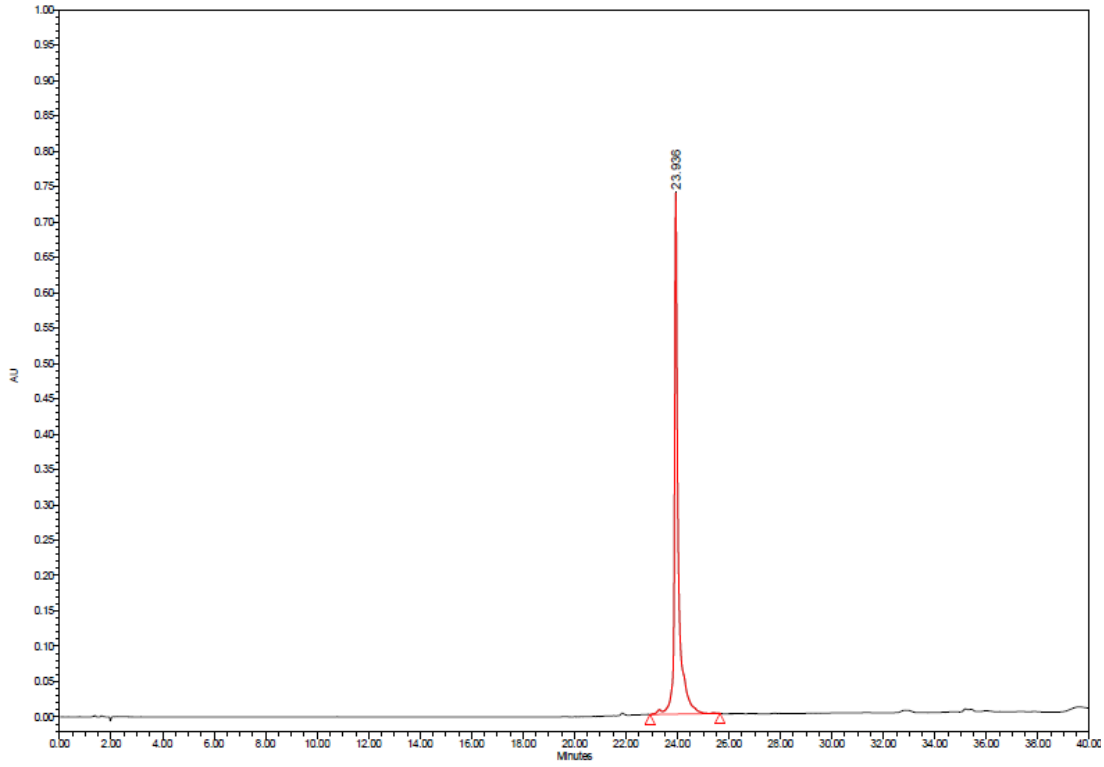
Fig. S11. Analytical HPLC chromatogram (a) and MALDI-TOF mass spectrum (b) of internally PyBtr-labeled **M11_TT** (calcd. for $[M+H]^+$: m/z = 4283.69).



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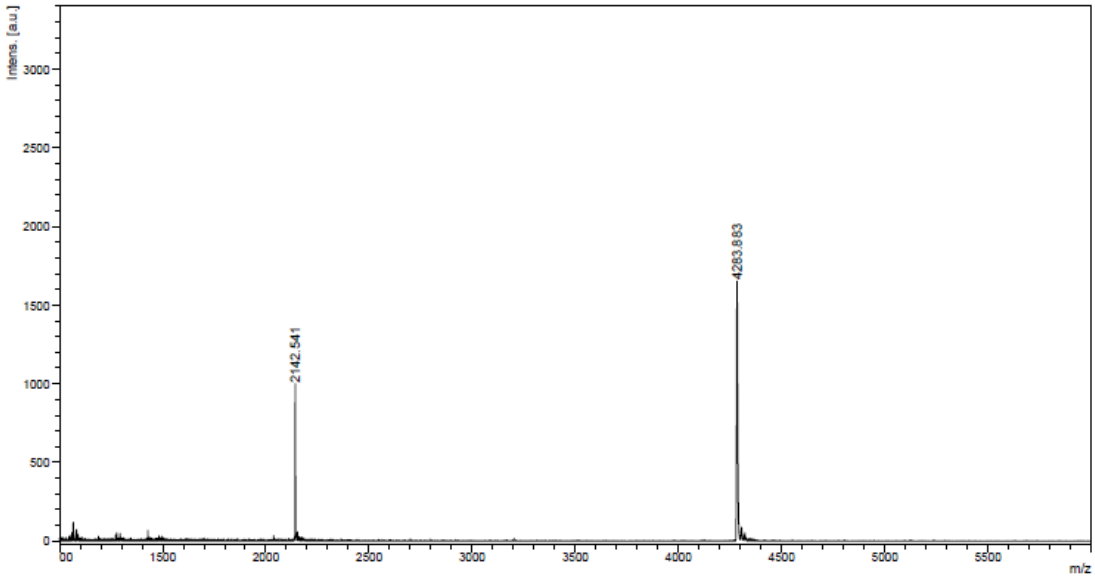
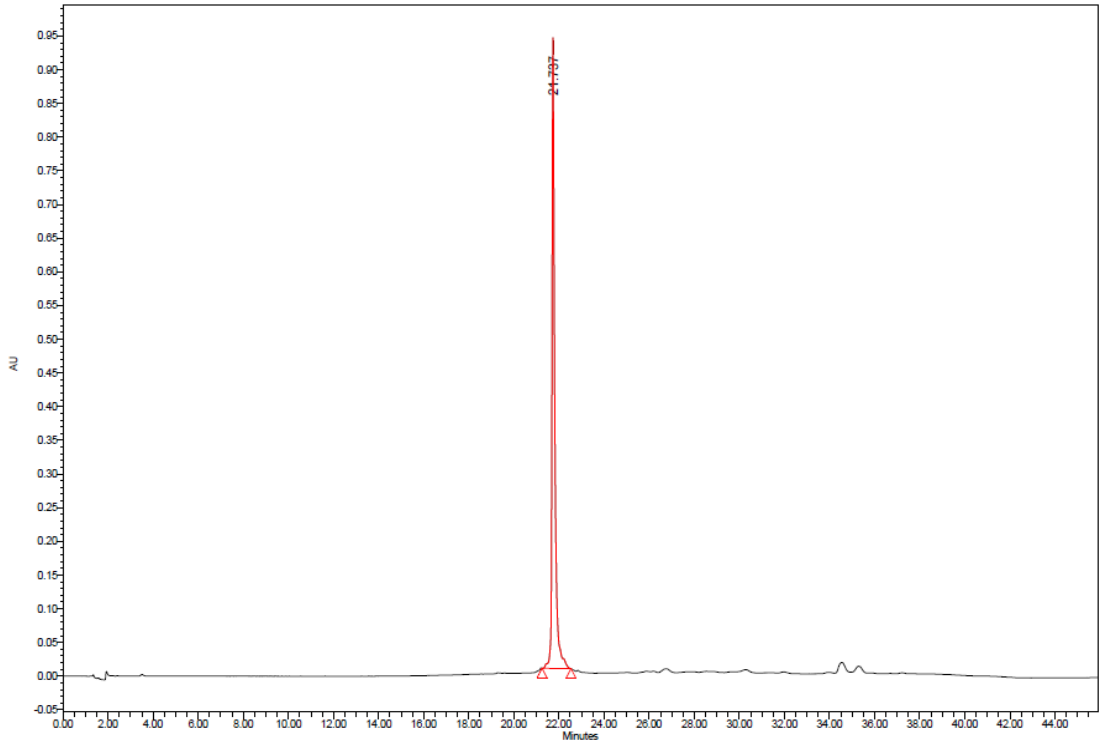


(b)

Fig. S12. Analytical HPLC chromatogram (a) and MALDI-TOF mass spectrum (b) of internally PyBtr-labeled **M11_TC** (calcd. for $[M+H]^+$: *m/z* = 4283.69).



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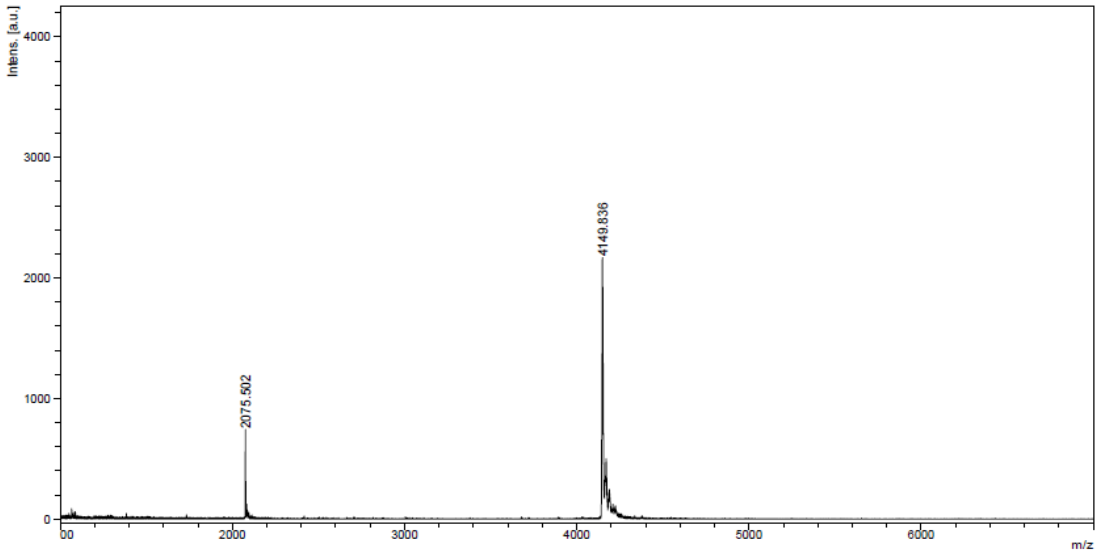
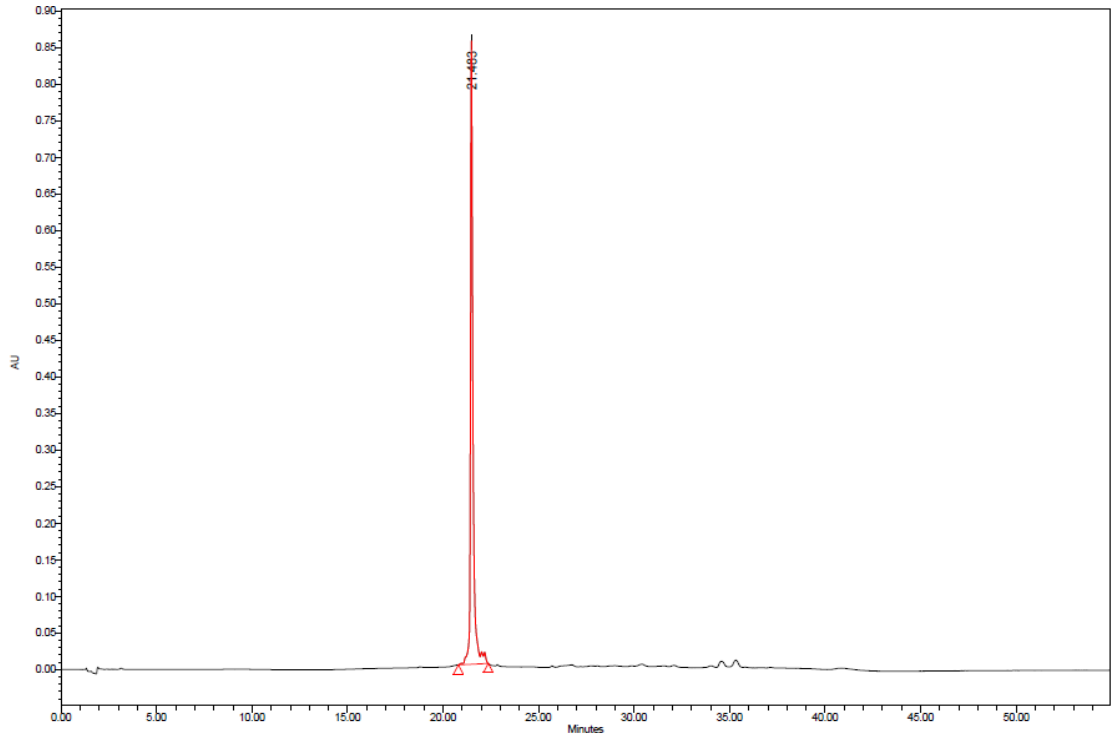


(b)

Fig. S13. Analytical HPLC chromatogram (a) and MALDI-TOF mass spectrum (b) of internally PyBtl-labeled **M11_AAAA** (calcd. for $[M+H]^+$: m/z = 4150.45).



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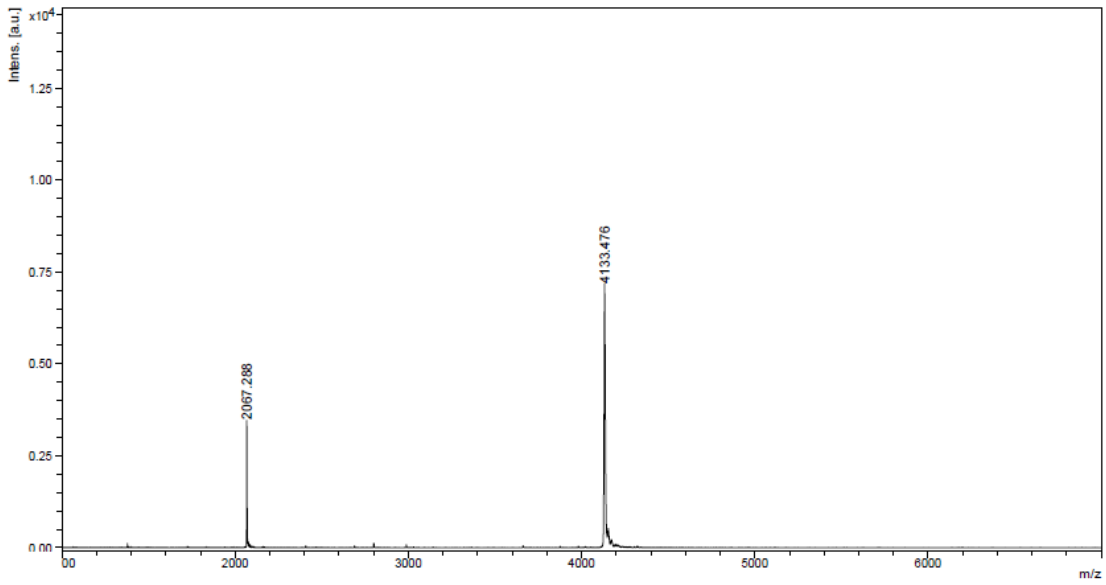
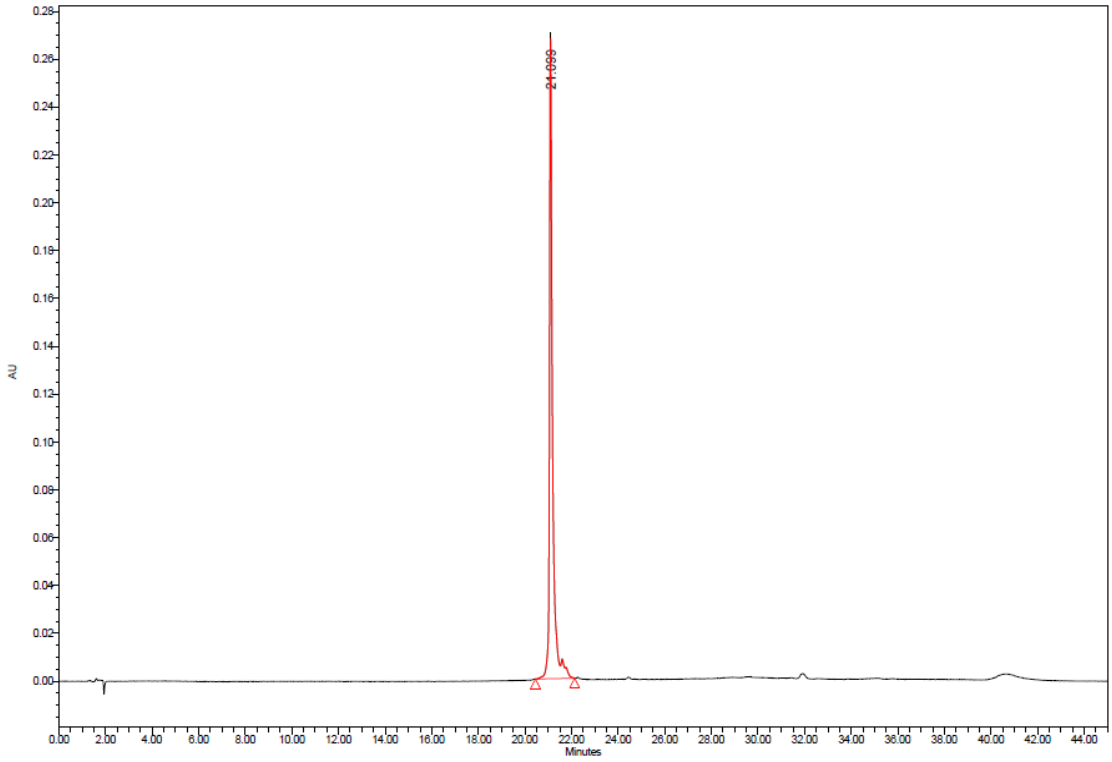


(b)

Fig. S14. Analytical HPLC chromatogram (a) and MALDI-TOF mass spectrum (b) of internally PyBtl-labeled **M11_ATTA** (calcd. for $[M+H]^+$: m/z = 4132.42).



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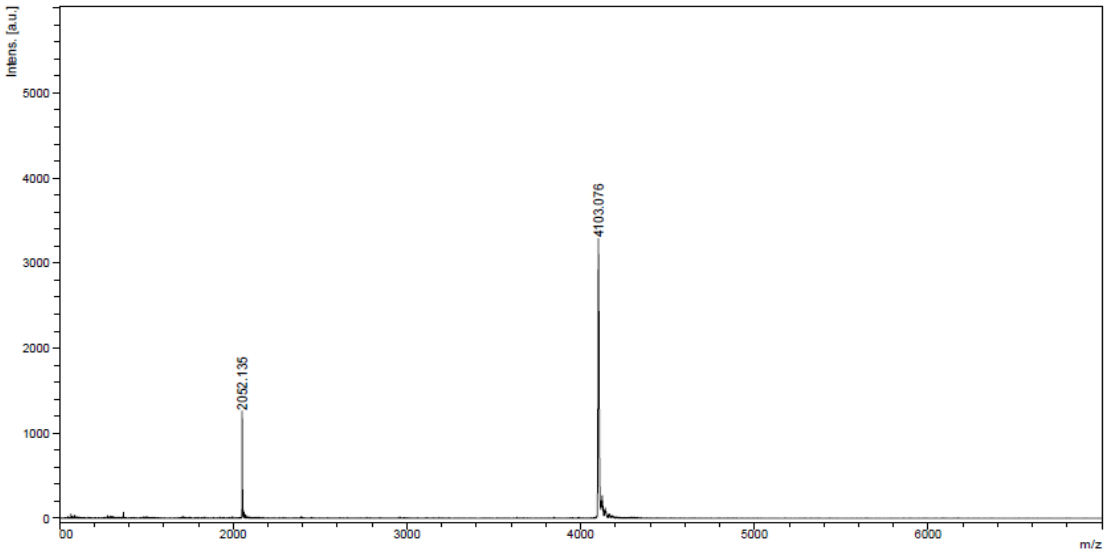
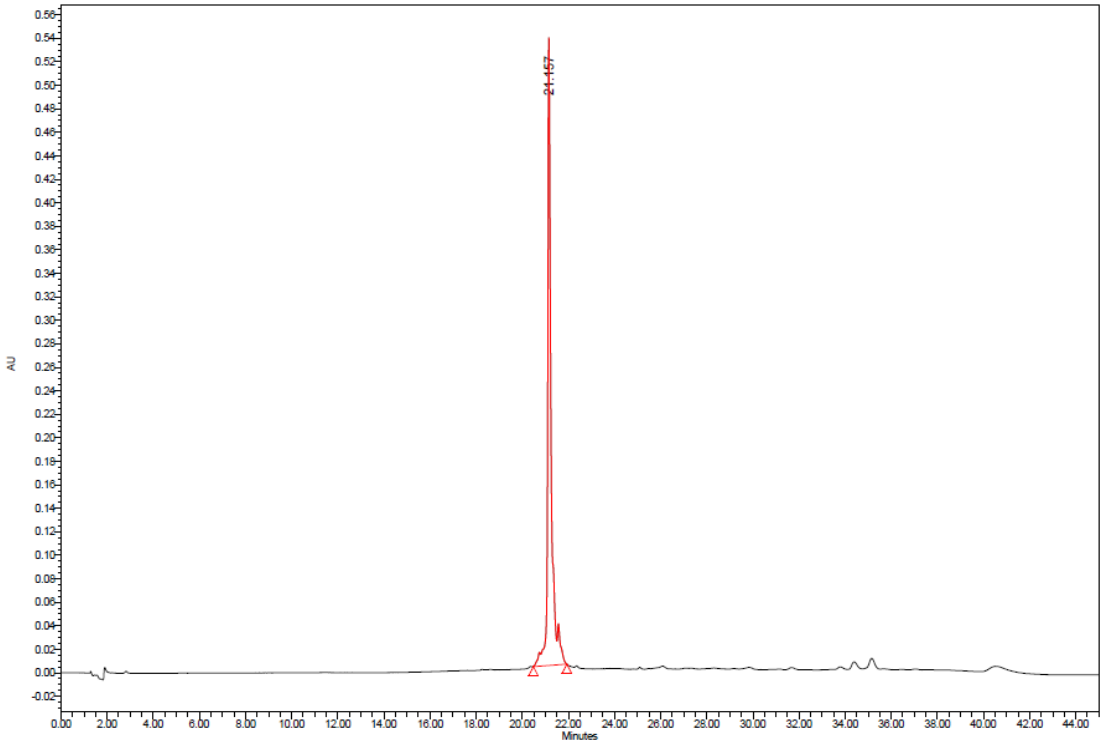


(b)

Fig. S15. Analytical HPLC chromatogram (a) and MALDI-TOF mass spectrum (b) of internally PyBtl-labeled **M11_ACCA** (calcd. for $[M+H]^+$: m/z = 4102.40).



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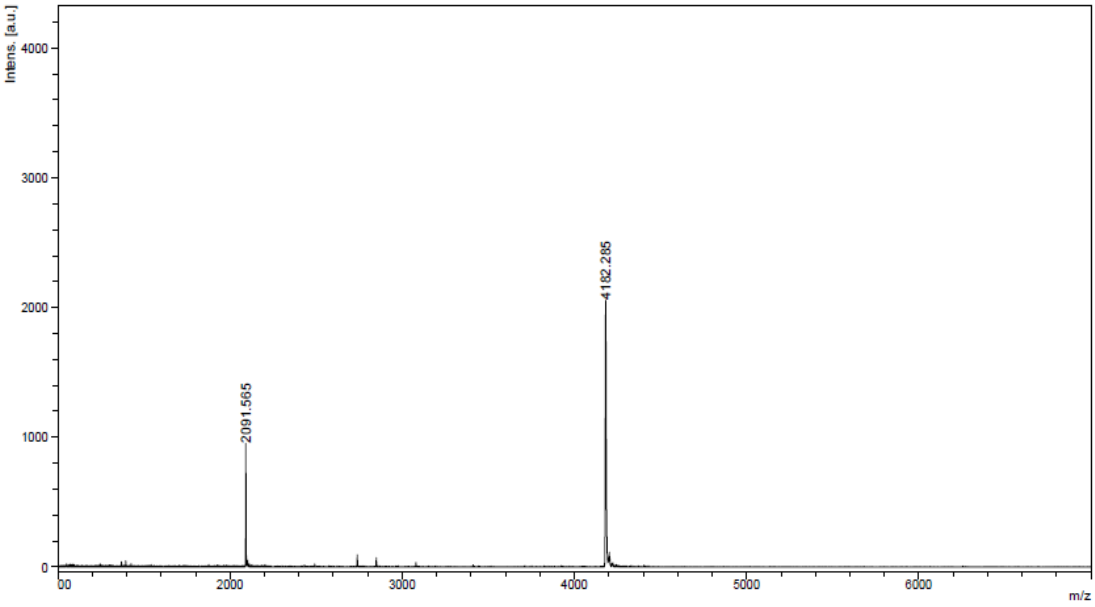
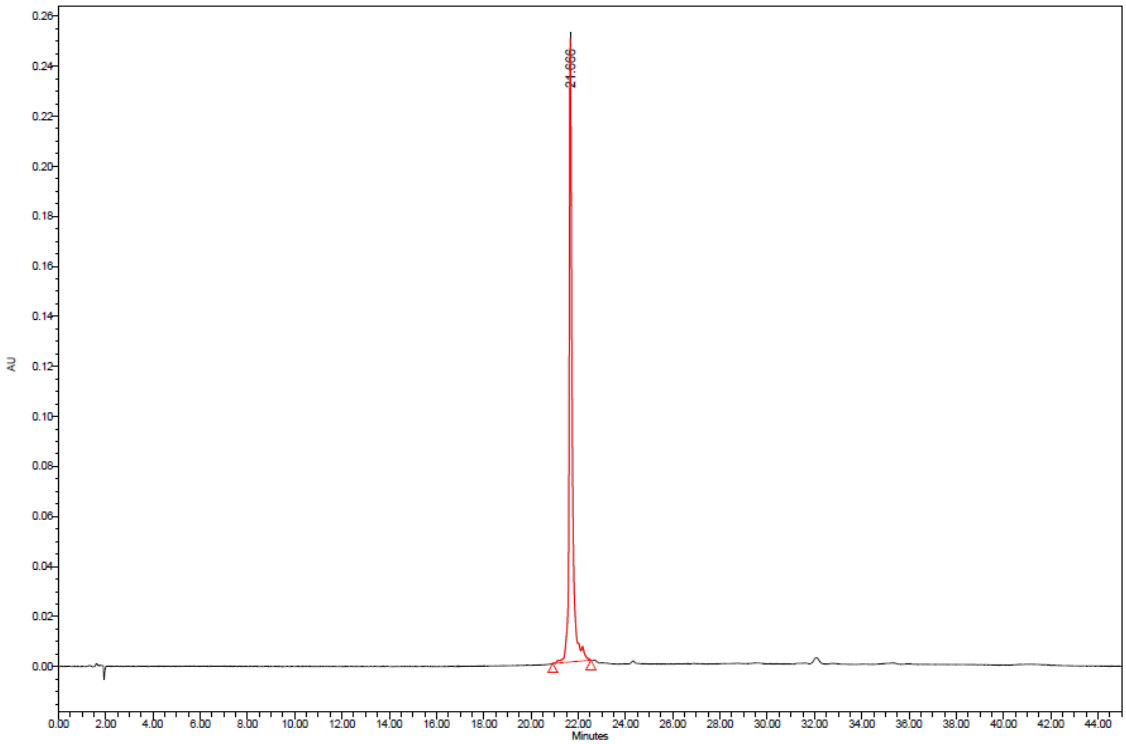


(b)

Fig. S16. Analytical HPLC chromatogram (a) and MALDI-TOF mass spectrum (b) of internally PyBtl-labeled **M11_AGGA** (calcd. for $[M+H]^+$: m/z = 4182.45).



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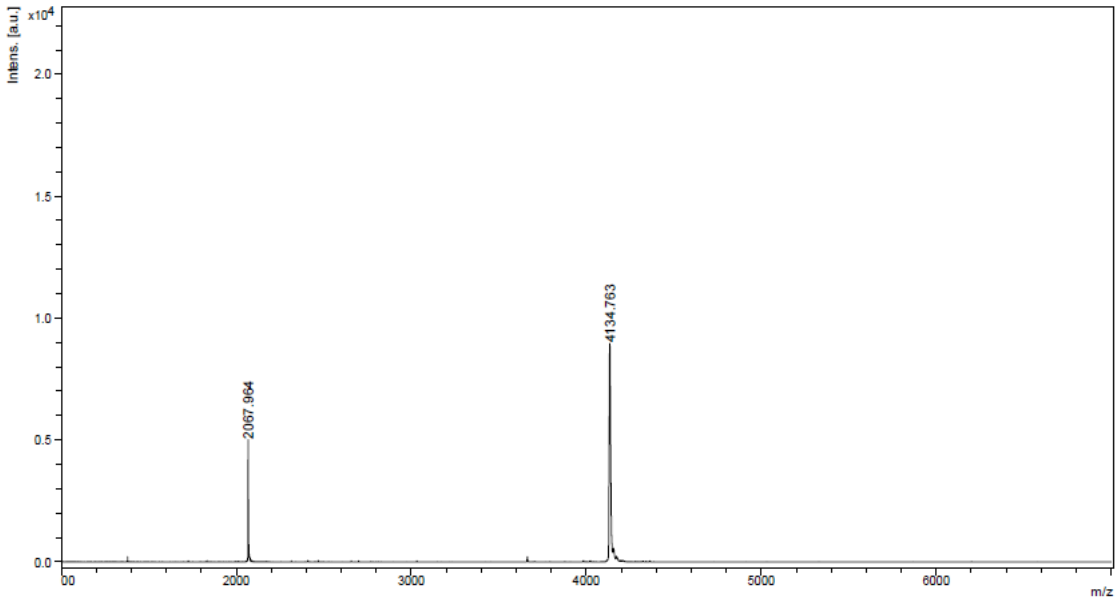
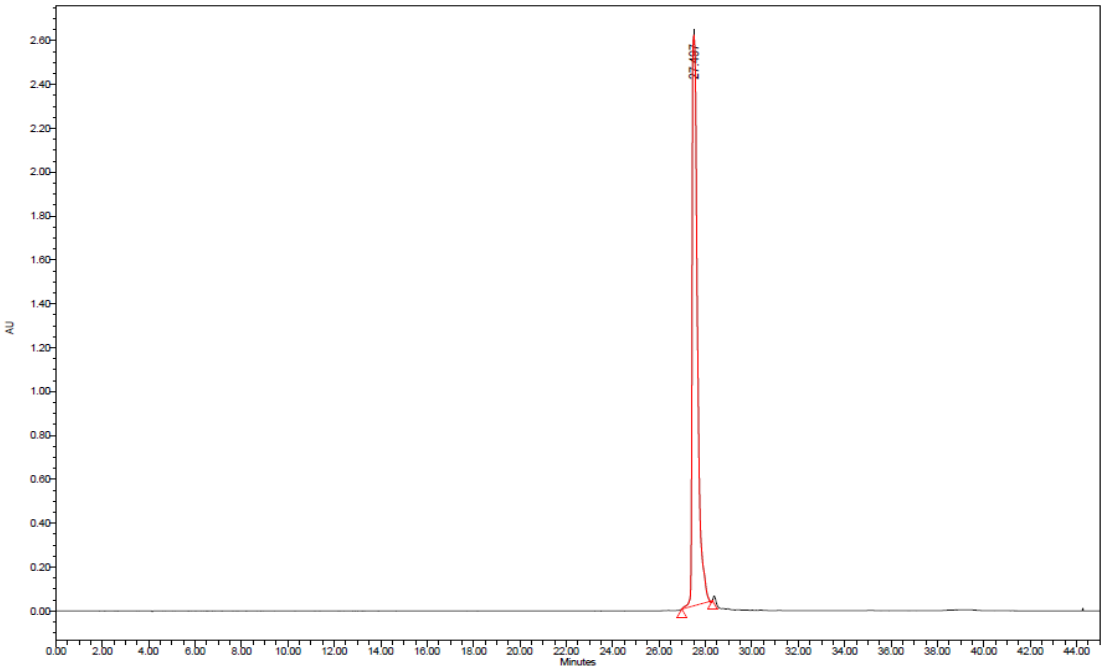


(b)

Fig. S17. Analytical HPLC chromatogram (a) and MALDI-TOF mass spectrum (b) of internally PyBtl-labeled **M11_TAAT** (calcd. for $[M+H]^+$: m/z = 4132.42).



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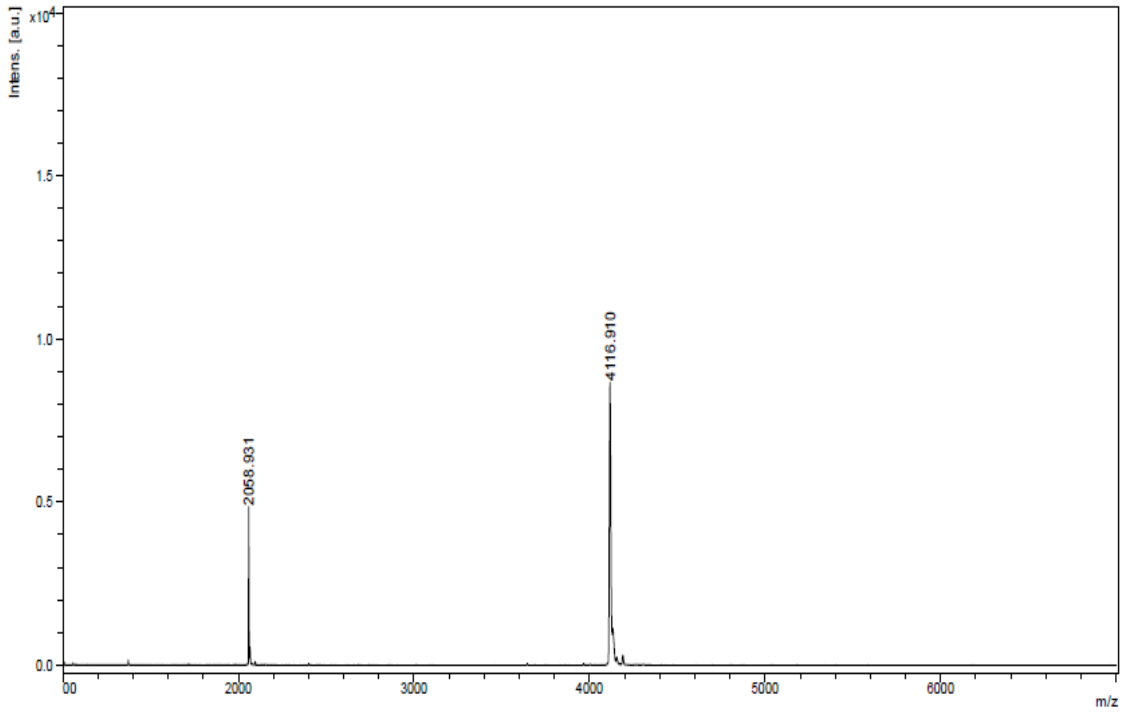
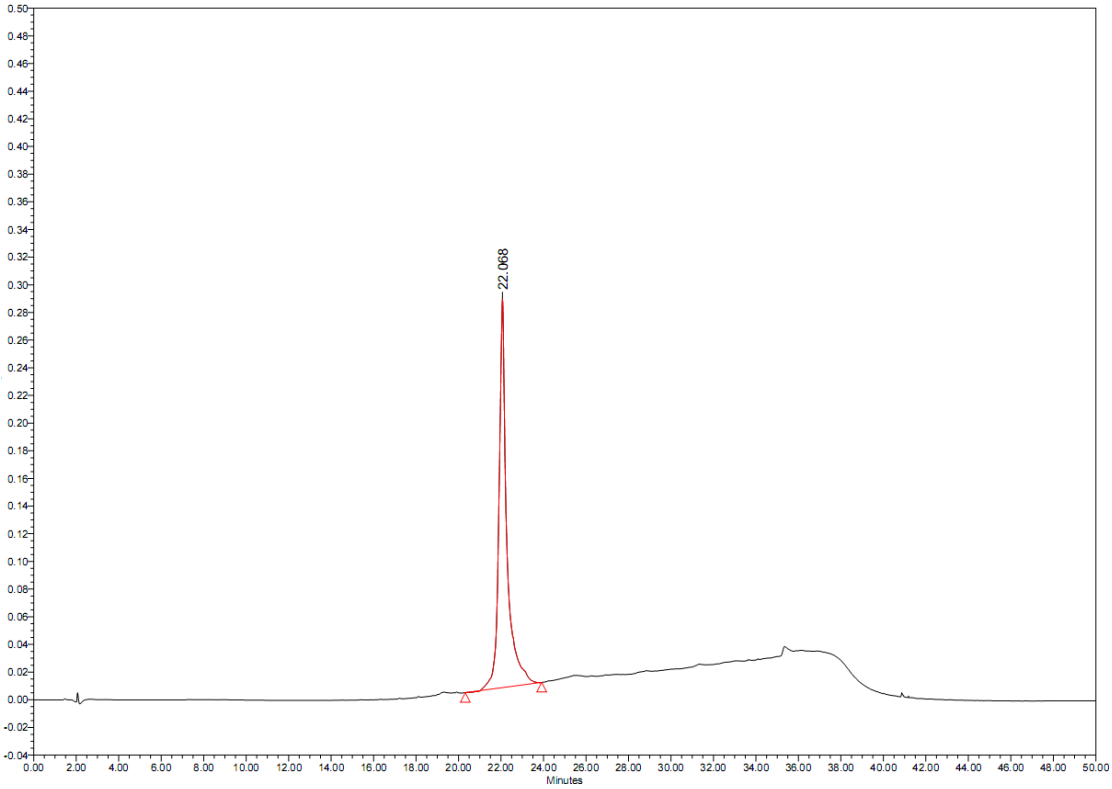


(b)

Fig. S18. Analytical HPLC chromatogram (a) and MALDI-TOF mass spectrum (b) of internally PyBtl-labeled **M11_TTTT** (calcd. for $[M+H]^+$: m/z = 4114.49).



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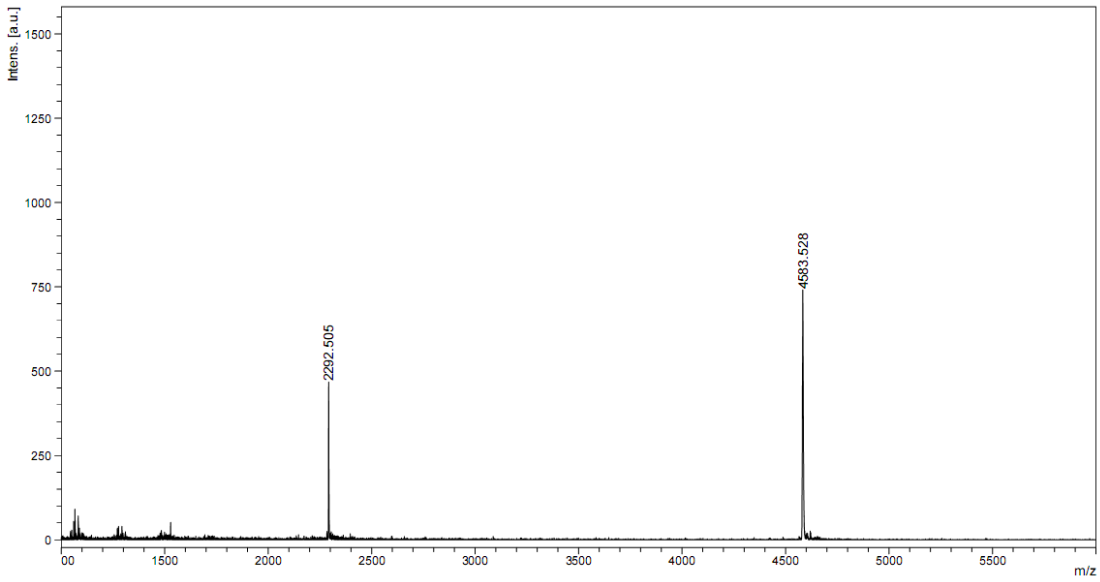
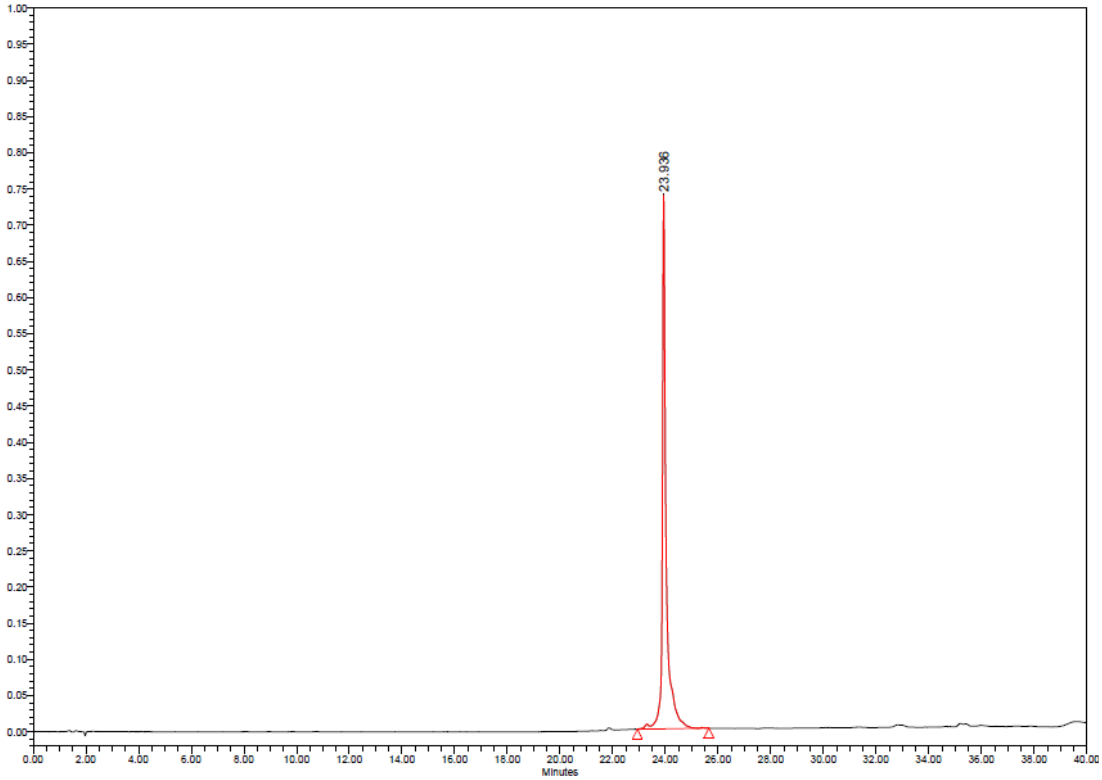


(b)

Fig. S19. Analytical HPLC chromatogram (a) and MALDI-TOF mass spectrum (b) of internally PyBtr-labeled **M12_AT(Btr)** (calcd. for $[M+H]^+$: *m/z* = 4583.99).



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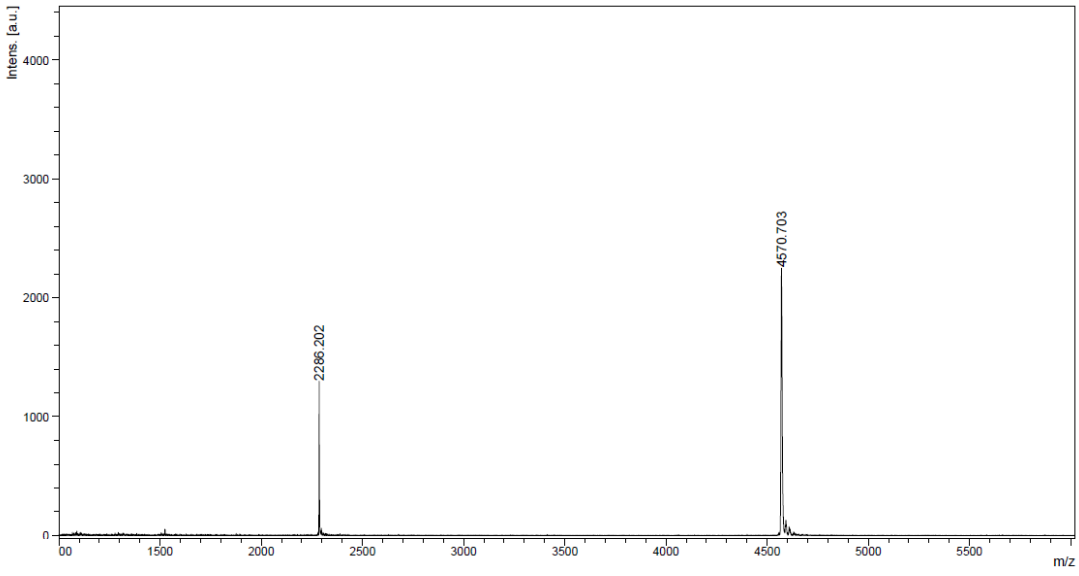

(b)

Fig. S20. Analytical HPLC chromatogram (a) and MALDI-TOF mass spectrum (b) of internally PyBtl-labeled **M12_AT(Btl)** (calcd. for $[M+H]^+$: m/z = 4569.03).

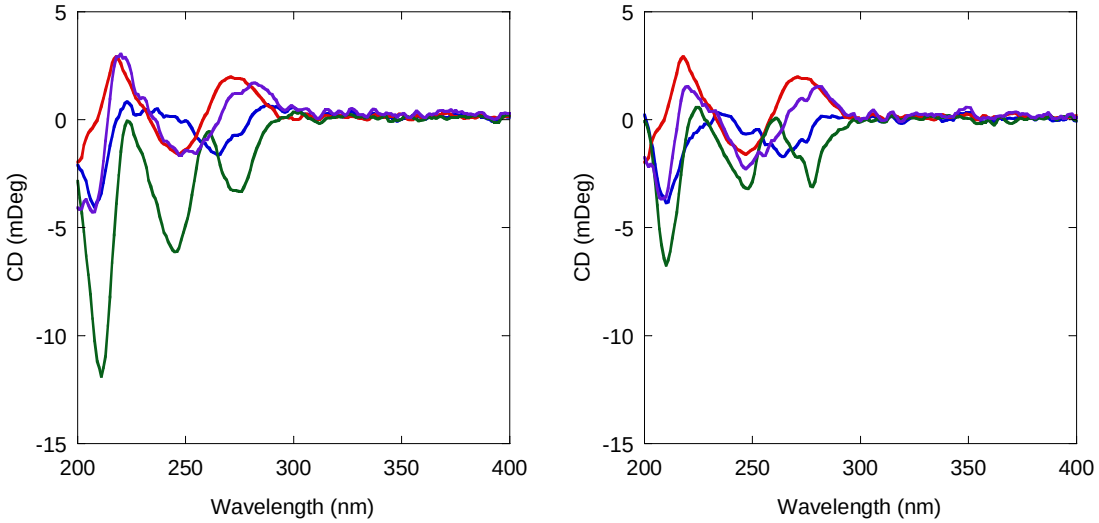

Fig. S21. CD spectra of unlabeled acpcPNA **M12** (a) and internally PyBtl-labeled acpcPNA **M12_AT(Btl)** (b) and their hybrids with complementary DNA (3′-TCAATAGGG ACG-5′): single stranded PNA (blue); single stranded DNA (red); mixture of acpcPNA:DNA (green); sum CD spectra of acpcPNA and DNA (purple). The CD spectra were measured in 10 mM sodium phosphate buffer, pH 7.0, [PNA] = 2.5 μM, [DNA] = 3.0 μM.

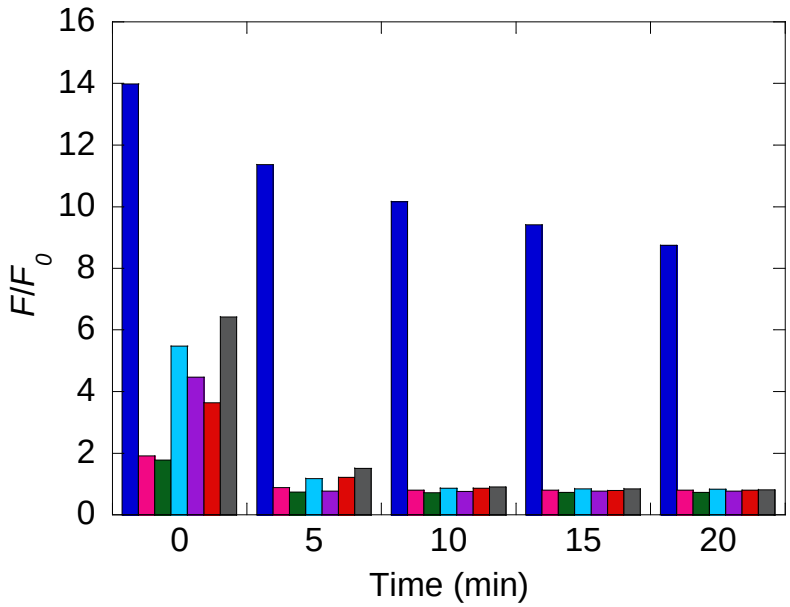

Fig. S22. Kinetics of nuclease S1 digestion of hybrids between internally PyBtr-labeled acpcPNA **M11_TT** with complementary and single base mismatched DNA; [PNA] = 1.0 μM, [DNA] = 1.0 μM in 30 mM sodium acetate buffer pH 4.6, 1 mM zinc acetate, 5% glycerol. Excitation wavelength was 345 nm. DNA sequence (3′→5′): GATTTAAGTCT ■; GATTTA*T*GTCT ■; GATTTAA*T*TCT ■; GATTT*T*AGTCT ■; GATTA*A*AGTCT ■; GATT*C*AAGTCT ■; GATT*G*AAGTCT ■.