Chemical modification improves stability and targeting function of DNA aptamer GBI-10 targeted Tenascin-C

Supporting Information

Kunfeng Li,[#] Jiali Deng,[#] Hongwei Jin, Xiantao Yang, Xinmeng Fan, Liyu Li, Yi Zhao, Zhu Guan,[*] Lihe Zhang, Zhenjun Yang[*]

State Key Laboratory of Natural and Biomimetic Drugs, School of Pharmaceutical Sciences, Peking University, Beijing 100191, PR China.

[*]To whom correspondence should be addressed. Tel & Fax: 86-10-82802503; Email: yangzj@bjmu.edu.cn (Prof. Z. J. Yang) and Tel & Fax: 86-10-82805023; guanzhu_gz@bjmu.edu.cn (Dr. Z. Guan)

[#]These authors contributed equally to this paper.

Table of Contents

The synthesize of the biotin labeled GBI-10 variants

Natural GBI-10 and D-/L-isoT modified GBI-10 were synthesized on ABI 394 automated DNA synthesizer (isoT phosphoramidite monomers and isoT-modified oligonucleotides were synthesized by our lab according to the literature1, 2 using standard phosphoramidite chemistry). All the GBI-10 variants were purified by C18 reverse high performance liquid chromatography (XBridgeTM OST C18, 2.5 μm, 10 mm × 50 mm) using a linear gradient of 15→35% eluent A in 35 min. Solutions of 0.1 M Et$_3$N-CH$_3$COOH in water, pH 7.7, were used as eluent B, and CH3CN was used as eluent A. Then the isolated DMT-on oligonucleotides were treated with 80% acetic acid for 10 min at room temperature. After neutralization with Et3N, the oligonucleotide solutions were desalted by Sephadex G25 column respectively. The oligonucleotide compositions were confirmed by MALDI-TOF-MS spectrometry.

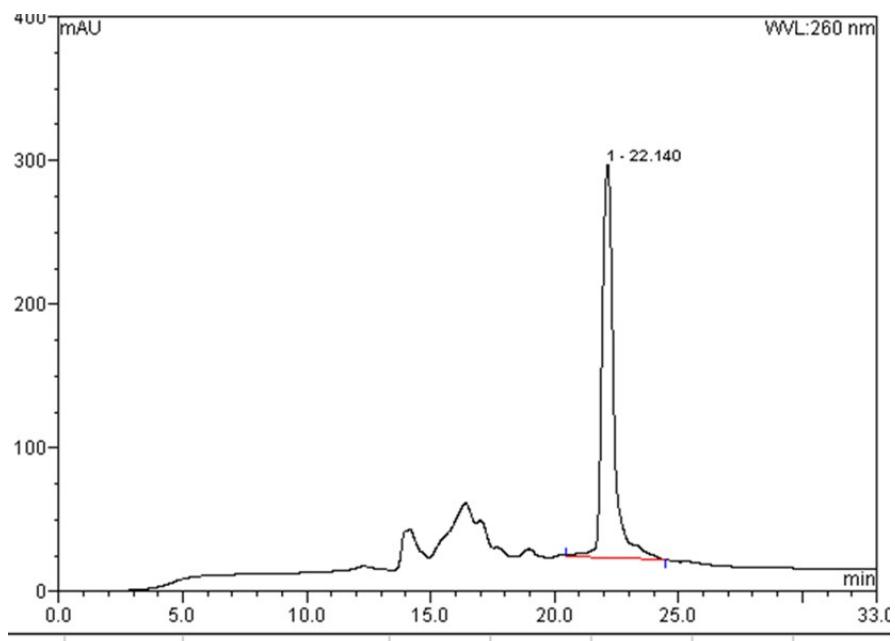**Figure S1.** The separation results of biotin labeled **GBI-10** with HPLC

Figure S2. MALDI-TOF-MS of biotin labeled GBI-10

Figure S3. MALDI-TOF-MS of biotin labeled GBI-10-15T$_D$
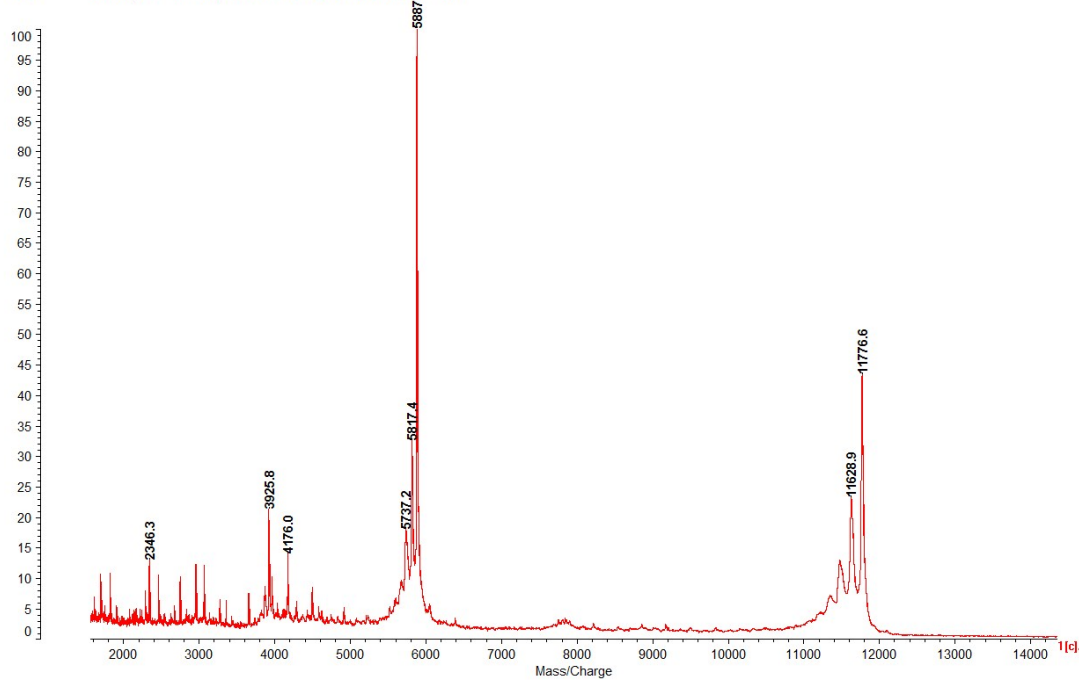
Figure S4. MALDI-TOF-MS of biotin labeled GBI-10-3C$_D$

Figure S5. MALDI-TOF-MS of biotin labeled GBI-10-10A$_L$

Figure S6. MALDI-TOF-MS of biotin labeled GBI-10-18A$_L$

Data: G-19TD0001.J9 22 Nov 2013 17:25 Cal: tof 22 Nov 2013 17:22
Kratos PC Axima CFRplus V2.4.0: Mode Linear, Power: 95, Blanked, P.Ext. @ 11777 (bin 148)
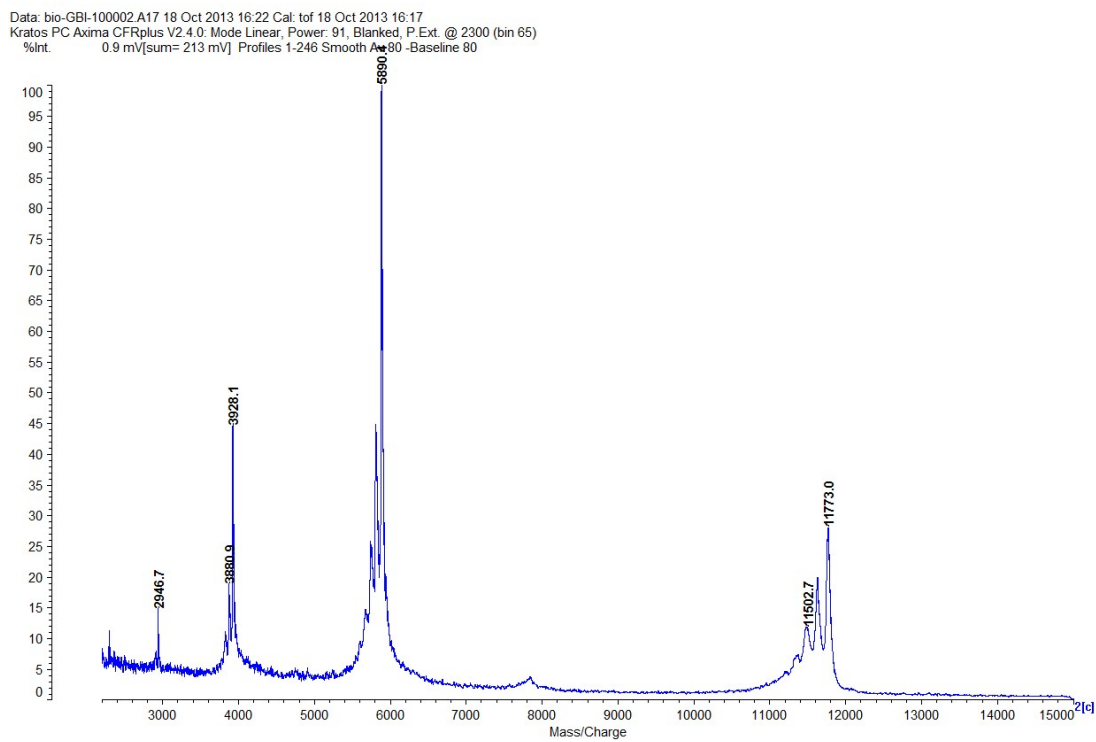%Int.   9.9 mV[sum= 1071 mV] Profiles 39-146 Smooth Av 50 -Baseline 80
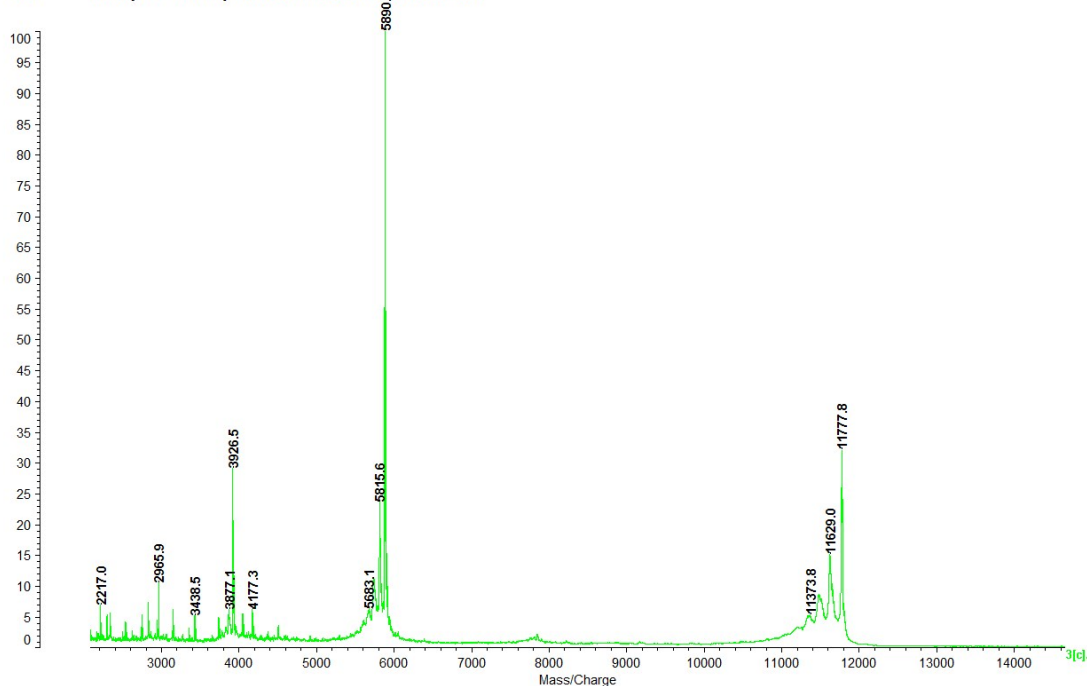
Figure S7. MALDI-TOF-MS of biotin labeled GBI-10-21T_D

Data: G-20TL0001.J10 22 Nov 2013 17:30 Cal: tof 22 Nov 2013 17:29
Kratos PC Axima CFRplus V2.4.0: Mode Linear, Power: 95, Blanked, P.Ext. @ 11777 (bin 148)
%Int.   7.8 mV[sum= 1132 mV] Profiles 1-145 Smooth Av 50 -Baseline 80
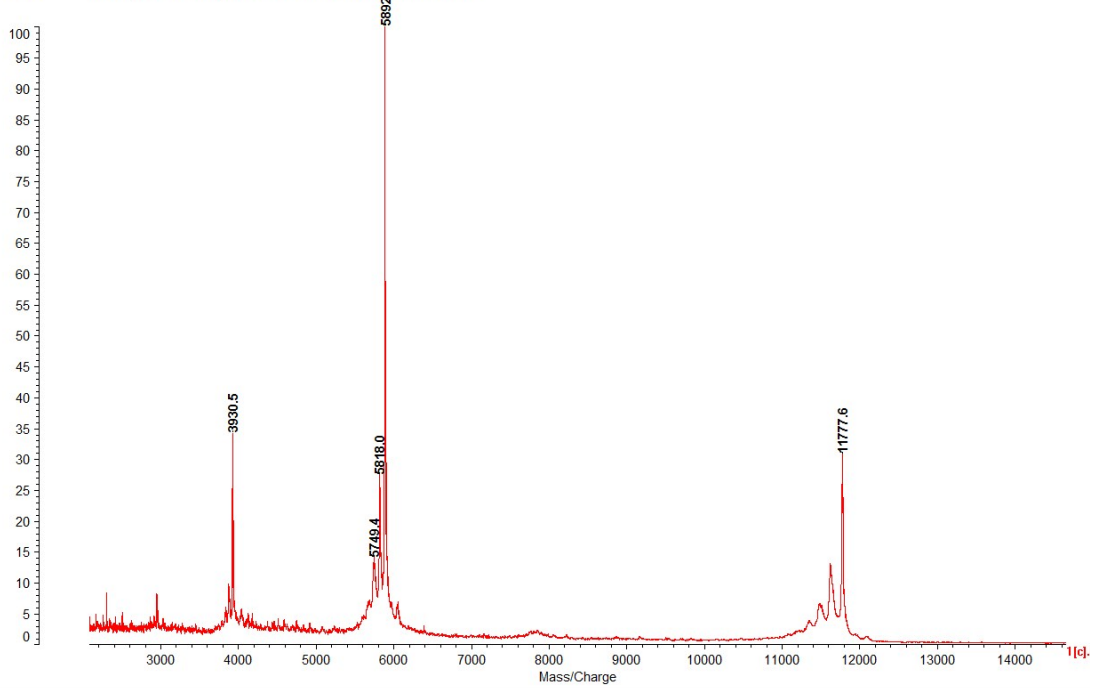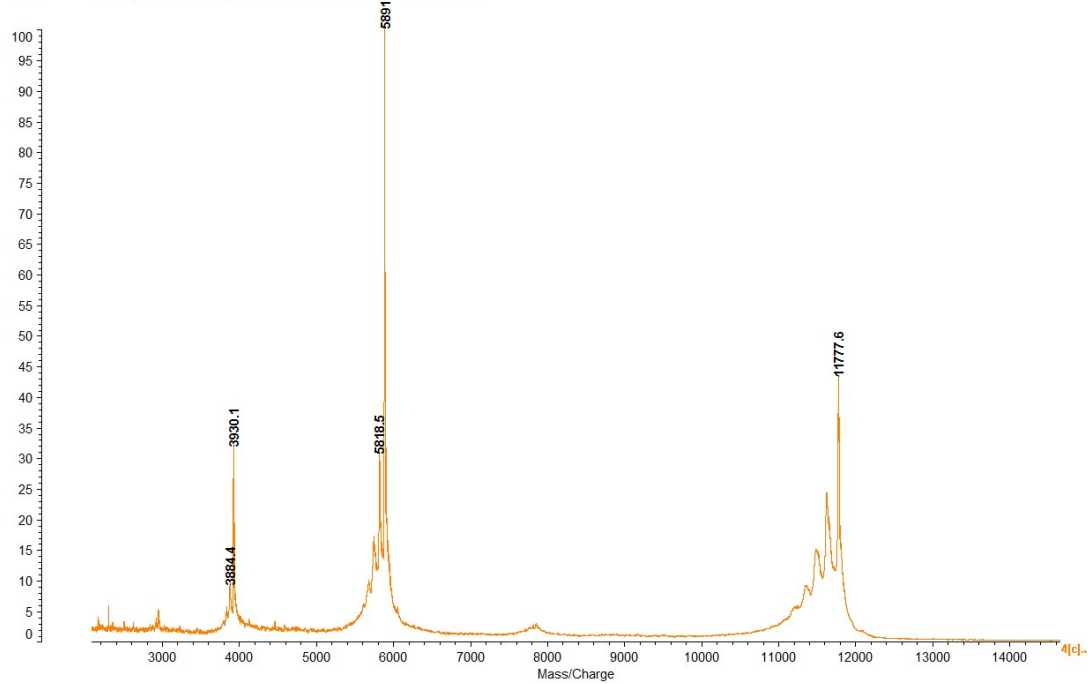
Figure S8. MALDI-TOF-MS of biotin labeled GBI-10-23C_L
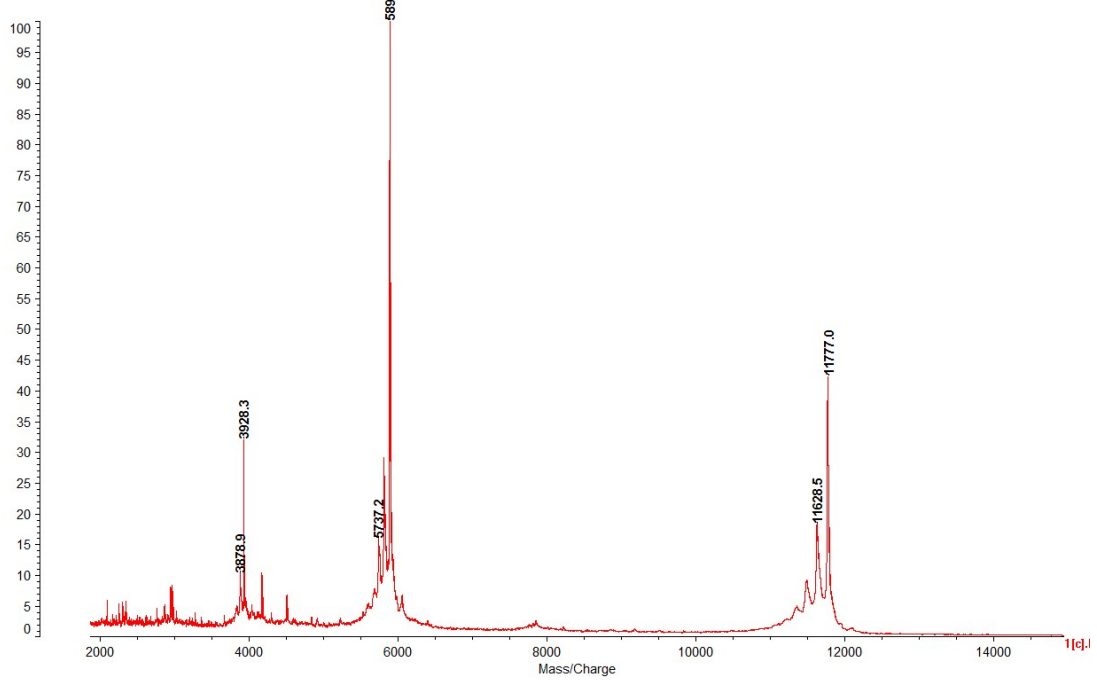
Figure S9. MALDI-TOF-MS of biotin labeled GBI-10-22T$_D$
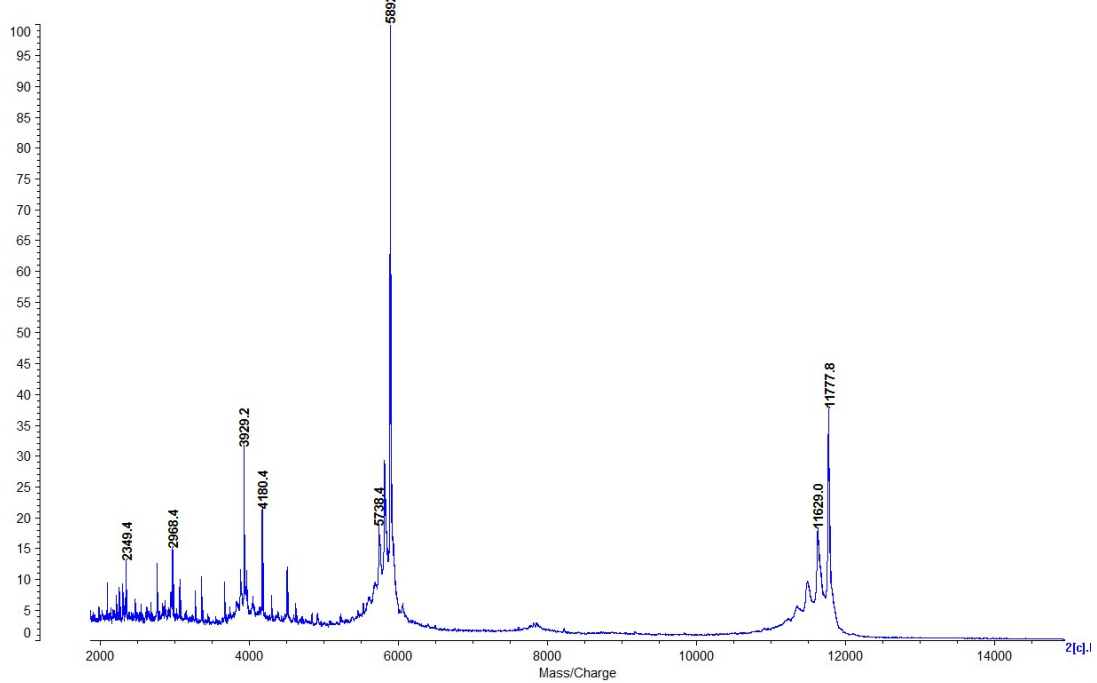
Figure S10. MALDI-TOF-MS of biotin labeled GBI-10-33C$_L$
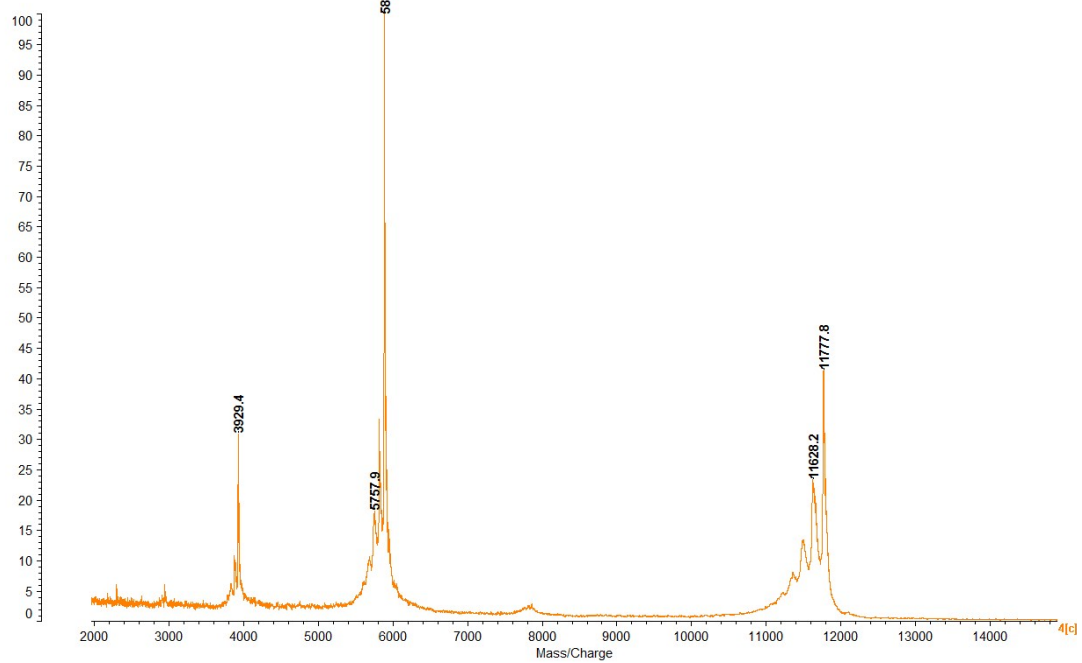
Figure S11. MALDI-TOF-MS of biotin labeled GBI-10-26T_L/32T_L

Figure S12. MALDI-TOF-MS of biotin labeled GBI-10-4A_L/26T_L/32T_L

Table S1. Biotin labeled GBI-10 and 2′-dI, D-/L-isoNA modified variants

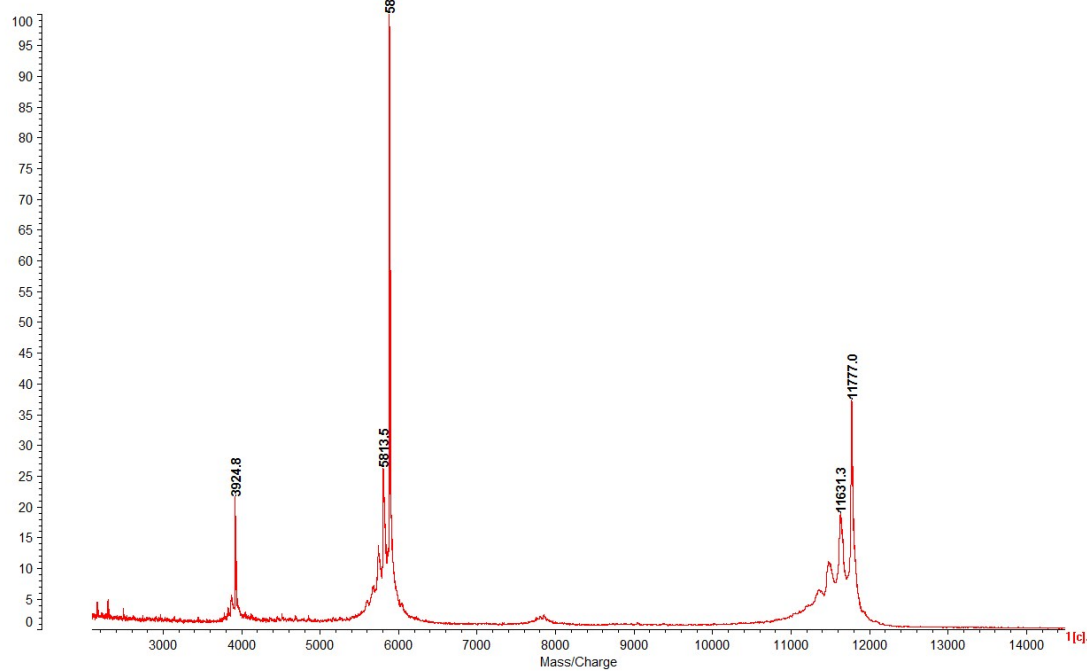| No.	Name	Sequence(5'-3')	MALDI-TOF-MS [M+H]$^+$ Calcd	Found
1	**GBI-10**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGGTTCACGTCC-3'	11777	11773
2	**GBI-10-1dI**	5'-biotin-TTT **dI**CCAGAGGGAAGACTTTAGGTTCGGTTCACGTCC-3'	11787	11787
3	**GBI-10-2dI**	5'-biotin-TTT C**dI**CAGAGGGAAGACTTTAGGTTCGGTTCACGTCC-3'	11787	11787
4	**GBI-10-3dI**	5'-biotin-TTT CC**dI**AGAGGGAAGACTTTAGGTTCGGTTCACGTCC-3'	11787	11787
5	**GBI-10-4dI**	5'-biotin-TTT CCC**dI**GAGGGAAGACTTTAGGTTCGGTTCACGTCC-3'	11787	11787
6	**GBI-10-6dI**	5'-biotin-TTT CCCAG**dI**GGGAAGACTTTAGGTTCGGTTCACGTCC-3'	11787	11787
7	**GBI-10-10dI**	5'-biotin-TTT CCCAGAGGG**dI**AGACTTTAGGTTCGGTTCACGTCC-3'	11787	11787
8	**GBI-10-11dI**	5'-biotin-TTT CCCAGAGGGA**dI**GACTTTAGGTTCGGTTCACGTCC-3'	11787	11787
9	**GBI-10-13dI**	5'-biotin-TTT CCCAGAGGGAAG**dI**CTTTAGGTTCGGTTCACGTCC-3'	11787	11787
10	**GBI-10-14dI**	5'-biotin-TTT CCCAGAGGGAAGA**dI**CTTTAGGTTCGGTTCACGTCC-3'	11787	11787
11	**GBI-10-15dI**	5'-biotin-TTT CCCAGAGGGAAGAC**dI**TTAGGTTCGGTTCACGTCC-3'	11787	11787
12	**GBI-10-16dI**	5'-biotin-TTT CCCAGAGGGAAGACT**dI**TAGGTTCGGTTCACGTCC-3'	11787	11787
13	**GBI-10-17dI**	5'-biotin-TTT CCCAGAGGGAAGACTT**dI**AGGTTCGGTTCACGTCC-3'	11787	11787
14	**GBI-10-18dI**	5'-biotin-TTT CCCAGAGGGAAGACTTT**dI**GGTTCGGTTCACGTCC-3'	11787	11787
15	**GBI-10-21dI**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGG**dI**TCGGTTCACGTCC-3'	11787	11787
16	**GBI-10-22dI**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGT**dI**CGGTTCACGTCC-3'	11787	11787
17	**GBI-10-23dI**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTT**dI**GGTTCACGTCC-3'	11787	11787
18	**GBI-10-26dI**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGG**dI**TCACGTCC-3'	11787	11787
19	**GBI-10-27dI**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGGT**dI**CACGTCC-3'	11787	11787
20	**GBI-10-28dI**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGGTT**dI**ACGTCC-3'	11787	11787
21	**GBI-10-29dI**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGGTTC**dI**CGTCC-3'	11787	11787
22	**GBI-10-30dI**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGGTTCA**dI**GTCC-3'	11787	11787
23	**GBI-10-32dI**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGGTTCACG**dI**CC-3'	11787	11787
24	**GBI-10-33dI**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGGTTCACGT**dI**C-3'	11787	11787
25	**GBI-10-34dI**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGGTTCACGTC**dI**-3'	11787	11787
26	**GBI-10-1C$_D$**	5'-biotin-TTT **C$_D$**CCAGAGGGAAGACTTTAGGTTCGGTTCACGTCC-3'	11777	11777
27	**GBI-10-2C$_D$**	5'-biotin-TTT CC$_D$CAGAGGGAAGACTTTAGGTTCGGTTCACGTCC-3'	11777	11777
28	**GBI-10-3C$_D$**	5'-biotin-TTT CCC$_D$AGAGGGAAGACTTTAGGTTCGGTTCACGTCC-3'	11777	11777
29	**GBI-10-14C$_D$**	5'-biotin-TTT CCCAGAGGGAAGAC$_D$TTTAGGTTCGGTTCACGTCC-3'	11777	11777
30	**GBI-10-23C$_D$**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTC$_D$GGTTCACGTCC-3'	11777	11777
31	**GBI-10-28C$_D$**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGGTTC$_D$ACGTCC-3'	11777	11777
32	**GBI-10-30C$_D$**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGGTTCAC$_D$GTCC-3'	11777	11777
33	**GBI-10-33C$_D$**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGGTTCACGTC$_D$C-3'	11777	11777
34	**GBI-10-34C$_D$**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGGTTCACGTCC$_D$-3'	11777	11777
35	**GBI-10-1C$_L$**	5'-biotin-TTT **C$_L$**CCAGAGGGAAGACTTTAGGTTCGGTTCACGTCC-3'	11777	11777
36	**GBI-10-2C$_L$**	5'-biotin-TTT CC$_L$CAGAGGGAAGACTTTAGGTTCGGTTCACGTCC-3'	11777	11777
37	**GBI-10-3C$_L$**	5'-biotin-TTT CCC$_L$AGAGGGAAGACTTTAGGTTCGGTTCACGTCC-3'	11777	11777
38	**GBI-10-14C$_L$**	5'-biotin-TTT CCCAGAGGGAAGAC$_L$TTTAGGTTCGGTTCACGTCC-3'	11777	11777
39	**GBI-10-23C$_L$**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTC$_L$GGTTCACGTCC-3'	11777	11777
40	**GBI-10-28C$_L$**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGGTTC$_L$ACGTCC-3'	11777	11777
41	**GBI-10-30C$_L$**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGGTTCAC$_L$GTCC-3'	11777	11777
42	**GBI-10-33C$_L$**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGGTTCACGTC$_L$C-3'	11777	11777
43	**GBI-10-34C$_L$**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGGTTCACGTCC$_L$-3'	11777	11777
44	**GBI-10-4A$_D$**	5'-biotin-TTT CCCA$_D$GAGGGAAGACTTTAGGTTCGGTTCACGTCC-3'	11777	11777
45	**GBI-10-6A$_D$**	5'-biotin-TTT CCCAGA$_D$GGGAAGACTTTAGGTTCGGTTCACGTCC-3'	11777	11777
46	**GBI-10-10A$_D$**	5'-biotin-TTT CCCAGAGGGA$_D$AGACTTTAGGTTCGGTTCACGTCC-3'	11777	11777
47	**GBI-10-11A$_D$**	5'-biotin-TTT CCCAGAGGGAA$_D$GACTTTAGGTTCGGTTCACGTCC-3'	11777	11777
48	**GBI-10-13A$_D$**	5'-biotin-TTT CCCAGAGGGAAGA$_D$CTTTAGGTTCGGTTCACGTCC-3'	11777	11777
49	**GBI-10-18A$_D$**	5'-biotin-TTT CCCAGAGGGAAGACTTTA$_D$GGTTCGGTTCACGTCC-3'	11777	11777
50	**GBI-10-29A$_D$**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGGTTCA$_D$CGTCC-3'	11777	11777
51	**GBI-10-4A$_L$**	5'-biotin-TTT CCCA$_L$GAGGGAAGACTTTAGGTTCGGTTCACGTCC-3'	11777	11777
52	**GBI-10-6A$_L$**	5'-biotin-TTT CCCAGA$_L$GGGAAGACTTTAGGTTCGGTTCACGTCC-3'	11777	11777
53	**GBI-10-10A$_L$**	5'-biotin-TTT CCCAGAGGGA$_L$AGACTTTAGGTTCGGTTCACGTCC-3'	11777	11777
54	**GBI-10-11A$_L$**	5'-biotin-TTT CCCAGAGGGAA$_L$GACTTTAGGTTCGGTTCACGTCC-3'	11777	11777
55	**GBI-10-13A$_L$**	5'-biotin-TTT CCCAGAGGGAAGA$_L$CTTTAGGTTCGGTTCACGTCC-3'	11777	11777
56	**GBI-10-18A$_L$**	5'-biotin-TTT CCCAGAGGGAAGACTTTA$_L$GGTTCGGTTCACGTCC-3'	11777	11777
57	**GBI-10-29A$_L$**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGGTTCA$_L$CGTCC-3'	11777	11777
58	**GBI-10-15T$_D$**	5'-biotin-TTT CCCAGAGGGAAGACT$_D$TTAGGTTCGGTTCACGTCC-3'	11777	11777
59	**GBI-10-16T$_D$**	5'-biotin-TTT CCCAGAGGGAAGACTT$_D$TAGGTTCGGTTCACGTCC-3'	11777	11777
60	**GBI-10-17T$_D$**	5'-biotin-TTT CCCAGAGGGAAGACTTT$_D$AGGTTCGGTTCACGTCC-3'	11777	11777
61	**GBI-10-21T$_D$**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGT$_D$TCGGTTCACGTCC-3'	11777	11777

62	**GBI-10-22T$_D$**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTT**T$_D$**CGGTTCACGTCC-3'	11777	11777
63	**GBI-10-26T$_D$**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGG**T$_D$**TCACGTCC-3'	11777	11777
64	**GBI-10-27T$_D$**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGGT**T$_D$**CACGTCC-3'	11777	11777
65	**GBI-10-32T$_D$**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGGTTCACGT**T$_D$**CC-3'	11777	11777
66	**GBI-10-15T$_L$**	5'-biotin-TTT CCCAGAGGGAAGACT**T$_L$**TTAGGTTCGGTTCACGTCC-3'	11777	11777
67	**GBI-10-16T$_L$**	5'-biotin-TTT CCCAGAGGGAAGACTT**T$_L$**TAGGTTCGGTTCACGTCC-3'	11777	11777
68	**GBI-10-17T$_L$**	5'-biotin-TTT CCCAGAGGGAAGACTTT**T$_L$**AGGTTCGGTTCACGTCC-3'	11777	11777
69	**GBI-10-21T$_L$**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGG**T$_L$**TCGGTTCACGTCC-3'	11777	11777
70	**GBI-10-22T$_L$**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTT**T$_L$**CGGTTCACGTCC-3'	11777	11777
71	**GBI-10-26T$_L$**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGG**T$_L$**TCACGTCC-3'	11777	11777
72	**GBI-10-27T$_L$**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGGT**T$_L$**CACGTCC-3'	11777	11777
73	**GBI-10-32T$_L$**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGGTTCACG**T$_L$**CC-3'	11777	11777
74	**18A$_L$/26T$_L$**	5'-biotin-TTT CCCAGAGGGAAGACTTT**A$_L$**GGTTCGG**T$_L$**TCACGTCC-3'	11777	11777
75	**18A$_L$/32T$_L$**	5'-biotin-TTT CCCAGAGGGAAGACTTT**A$_L$**GGTTCGGTTCACGT**T$_L$**CC-3'	11777	11777
76	**26T$_L$/32T$_L$**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGGTTCGG**T$_L$**TCACGT**T$_L$**CC-3'	11777	11777
77	**21T$_D$/26T$_L$/32T$_L$**	5'-biotin-TTT CCCAGAGGGAAGACTTTAGG**T$_D$**TCGG**T$_L$**TCACGT**T$_L$**CC-3'	11777	11777
78	**4A$_L$/26T$_L$/32T$_L$**	5'-biotin-TTT CCC**A$_L$**GAGGGAAGACTTTAGGTTCGG**T$_L$**TCACGT**T$_L$**CC-3'	11777	11777
79	**4A$_L$/18A$_L$/26T$_L$**	5'-biotin-TTT CCC**A$_L$**GAGGGAAGACTTT**A$_L$**GGTTCGG**T$_L$**TCACGTCC-3'	11777	11777
80	**4A$_L$/18A$_L$/26T$_L$/32T$_L$**	5'-biotin-TTT CCC**A$_L$**GAGGGAAGACTTT**A$_L$**GGTTCGG**T$_L$**TCACGT**T$_L$**CC-3'	11777	11777
81	**18A$_L$/26T$_L$/32T$_L$**	5'-biotin-TTT CCCAGAGGGAAGACTTT**A$_L$**GGTTCGG**T$_L$**TCACGT**T$_L$**CC-3'	11777	11777
82	**18A$_L$/26T$_L$/32T$_D$**	5'-biotin-TTT CCCAGAGGGAAGACTTT**A$_L$**GGTTCGG**T$_L$**TCACGT**T$_D$**CC-3'	11777	11777
83	**18A$_L$/26T$_L$/32dI**	5'-biotin-TTT CCCAGAGGGAAGACTTT**A$_L$**GGTTCGG**T$_L$**TCACG**dI**CC-3'	11787	11787
84	**11A$_L$/26T$_L$/32T$_L$**	5'-biotin-TTT CCCAGAGGGAA**A$_L$**GACTTTAGGTTCGG**T$_L$**TCACGT**T$_L$**CC-3'	11777	11777
85	**15T$_L$/26T$_L$/32T$_L$**	5'-biotin-TTT CCCAGAGGGAAGACT**T$_L$**TTAGGTTCGG**T$_L$**TCACGT**T$_L$**CC-3'	11777	11777