Effective conjugation strategy for designing short peptide-based HIV-1 fusion inhibitors

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Supporting Information

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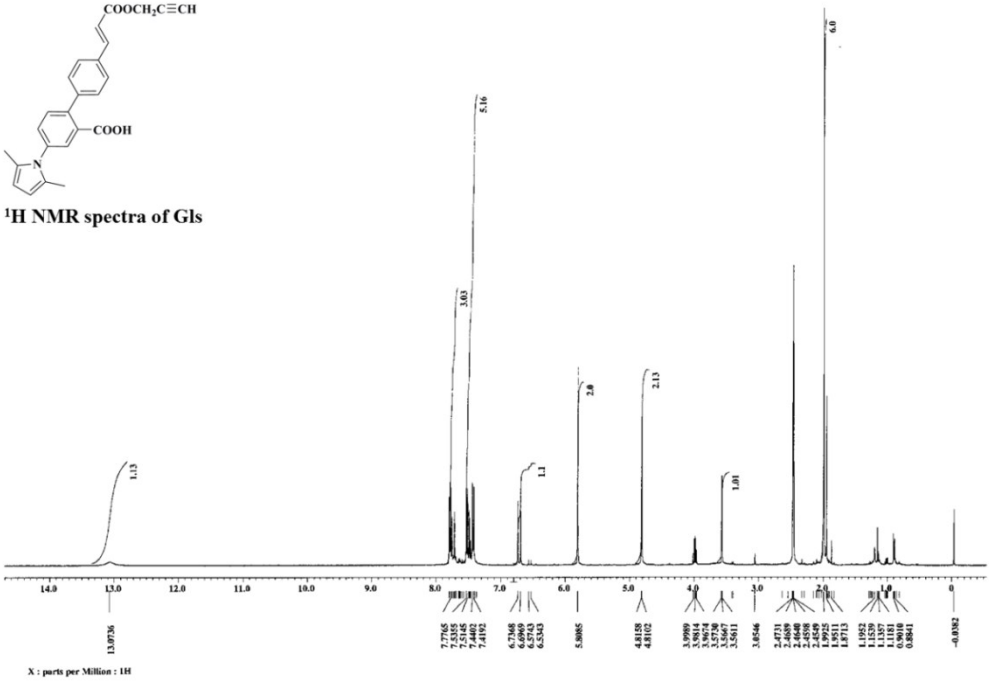
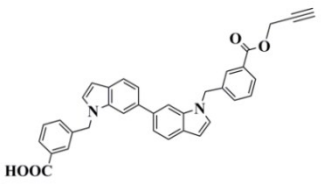
Table S1. The α-helicity of peptides and small molecule-peptide conjugates

Compound	θ (degree·cm^2·dmol^{-1})	Helicity %
T26	-16012	48.5%
T22	-8057	24.4%
T19	-8352	25.3%
Indole-T26	-9148	27.7%
Indole-T22	-7197	21.8%
Indole-T19	-9556	29.0%

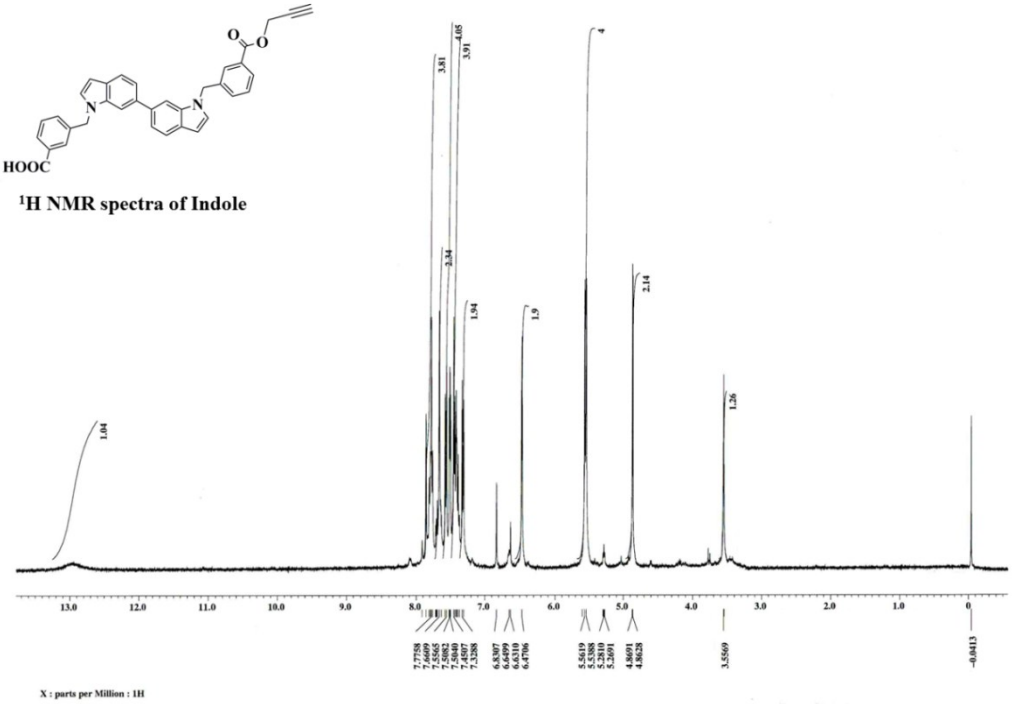
[1]H-NMR Spectra of Gls and Indole

[1]H NMR spectra of Gls



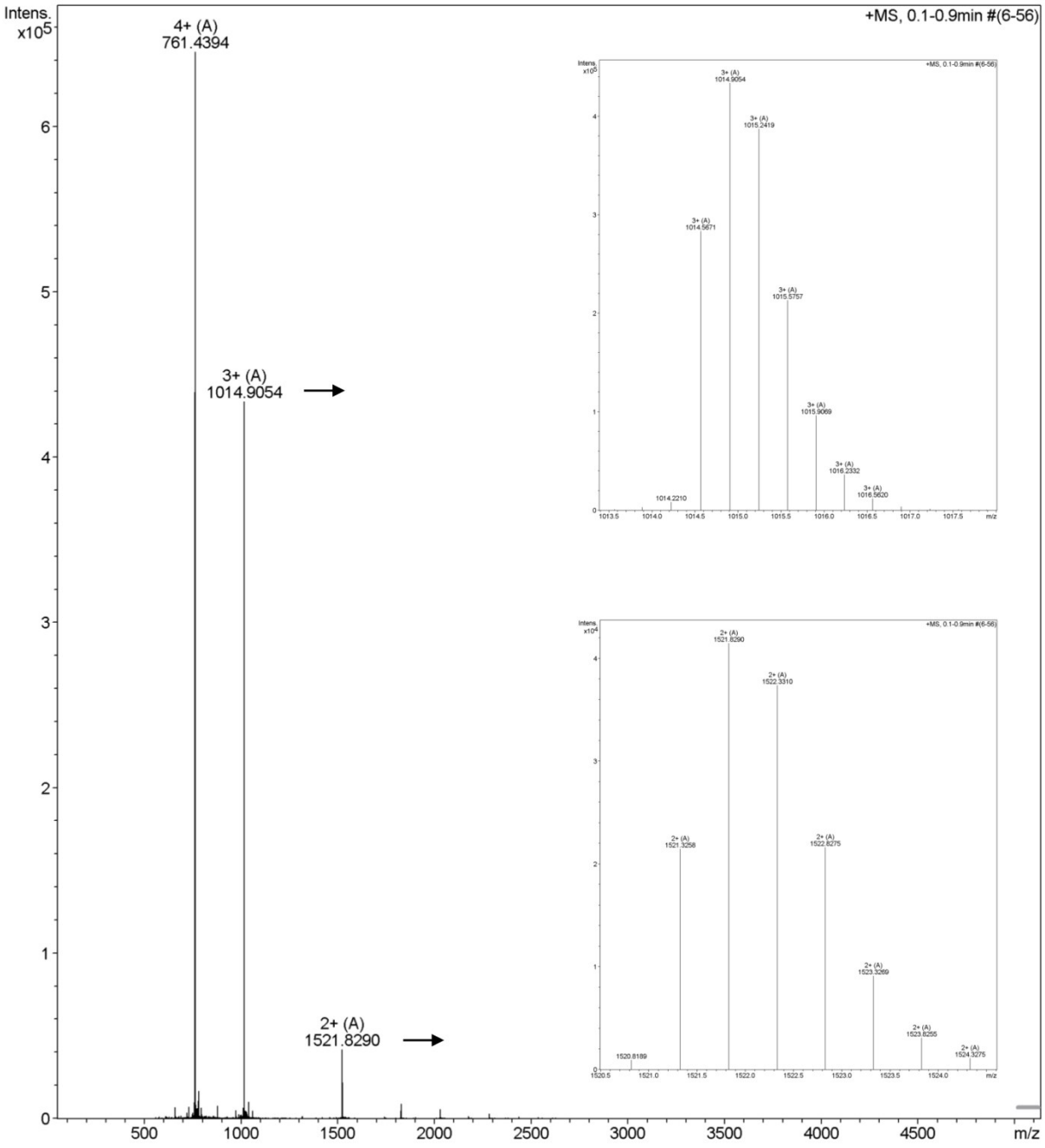


[1]H NMR spectra of Indole

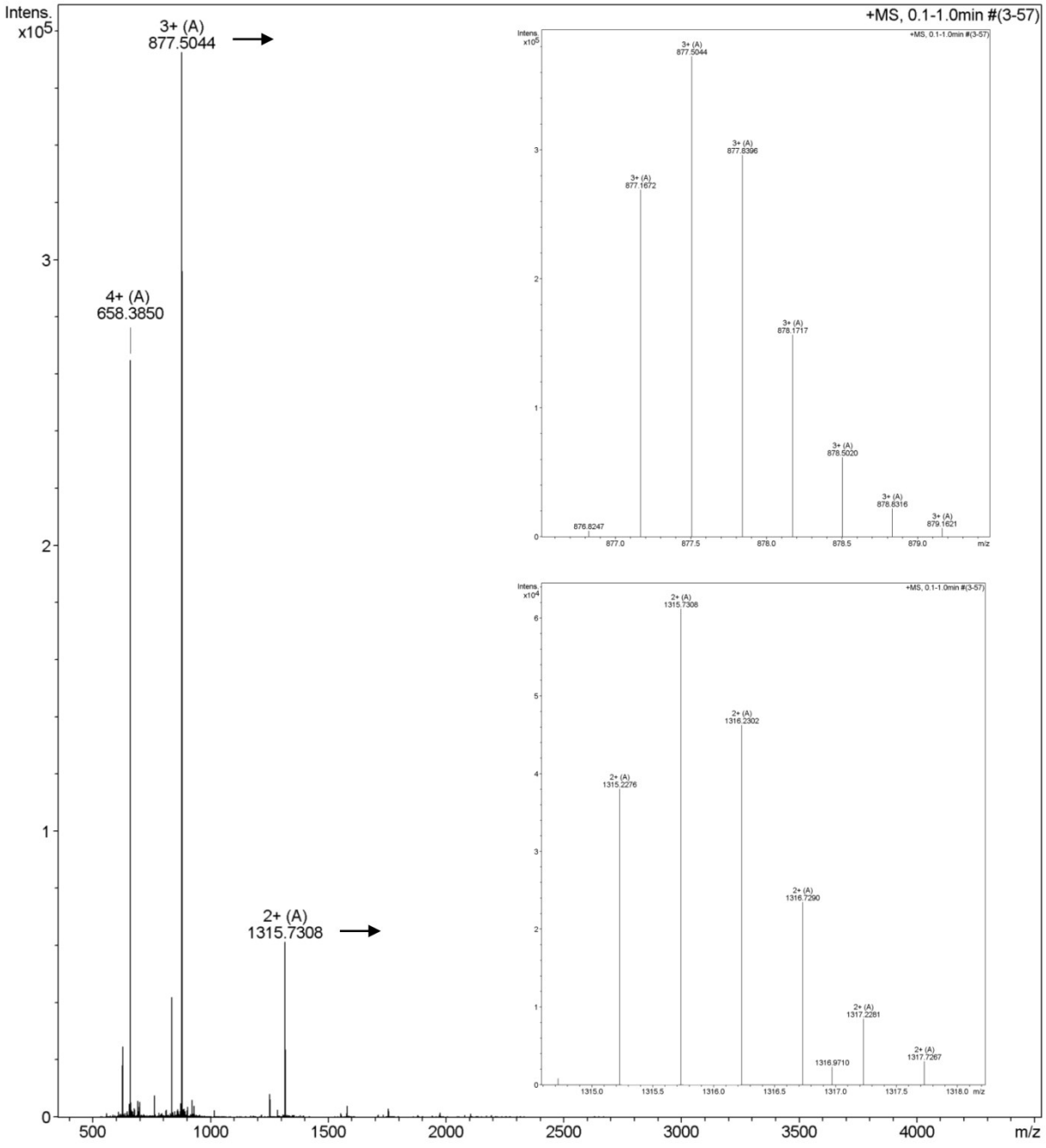


ESI Q-TOF-MS of peptides and conjugates

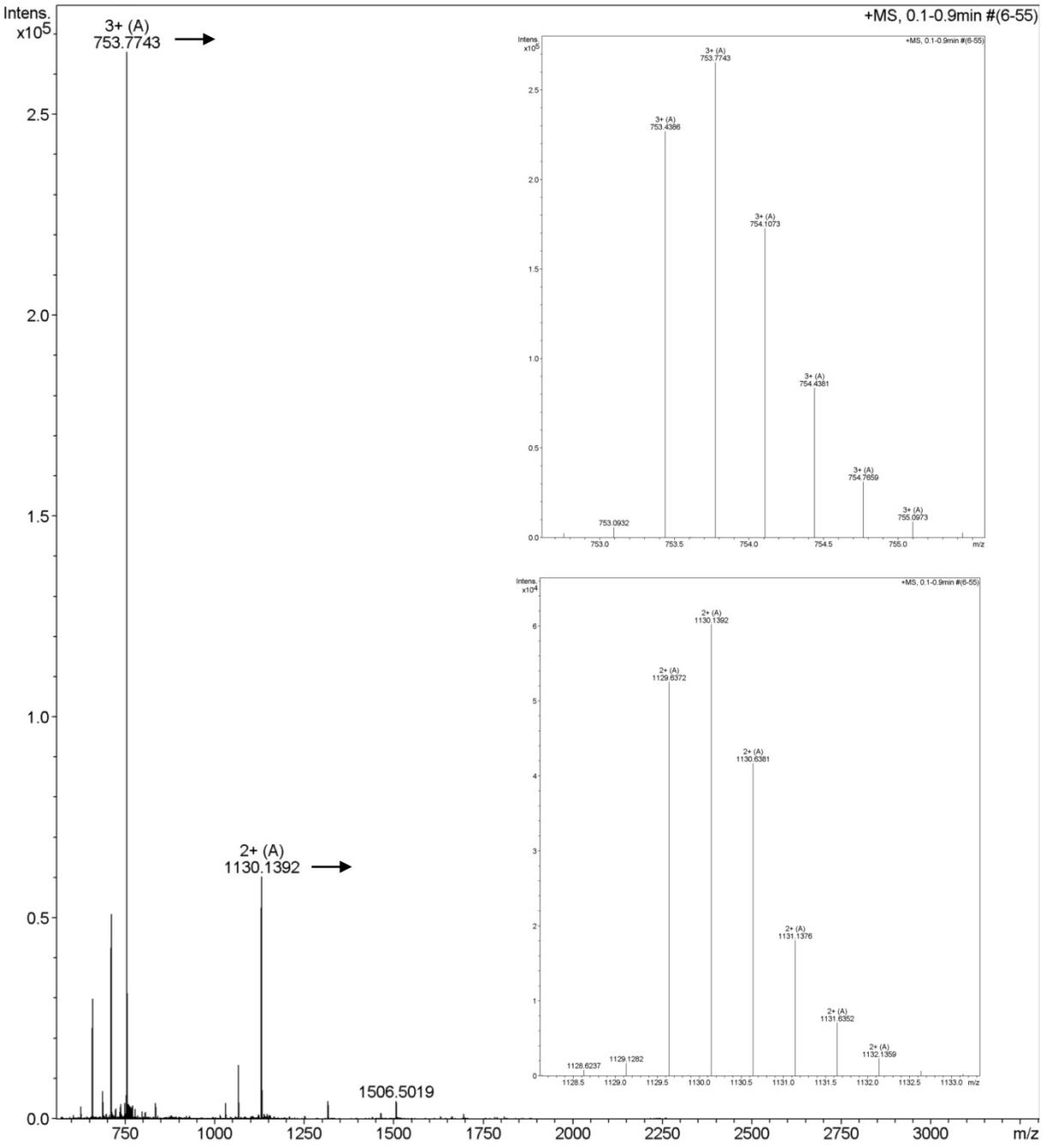
ESI Q-TOF-MS of T26



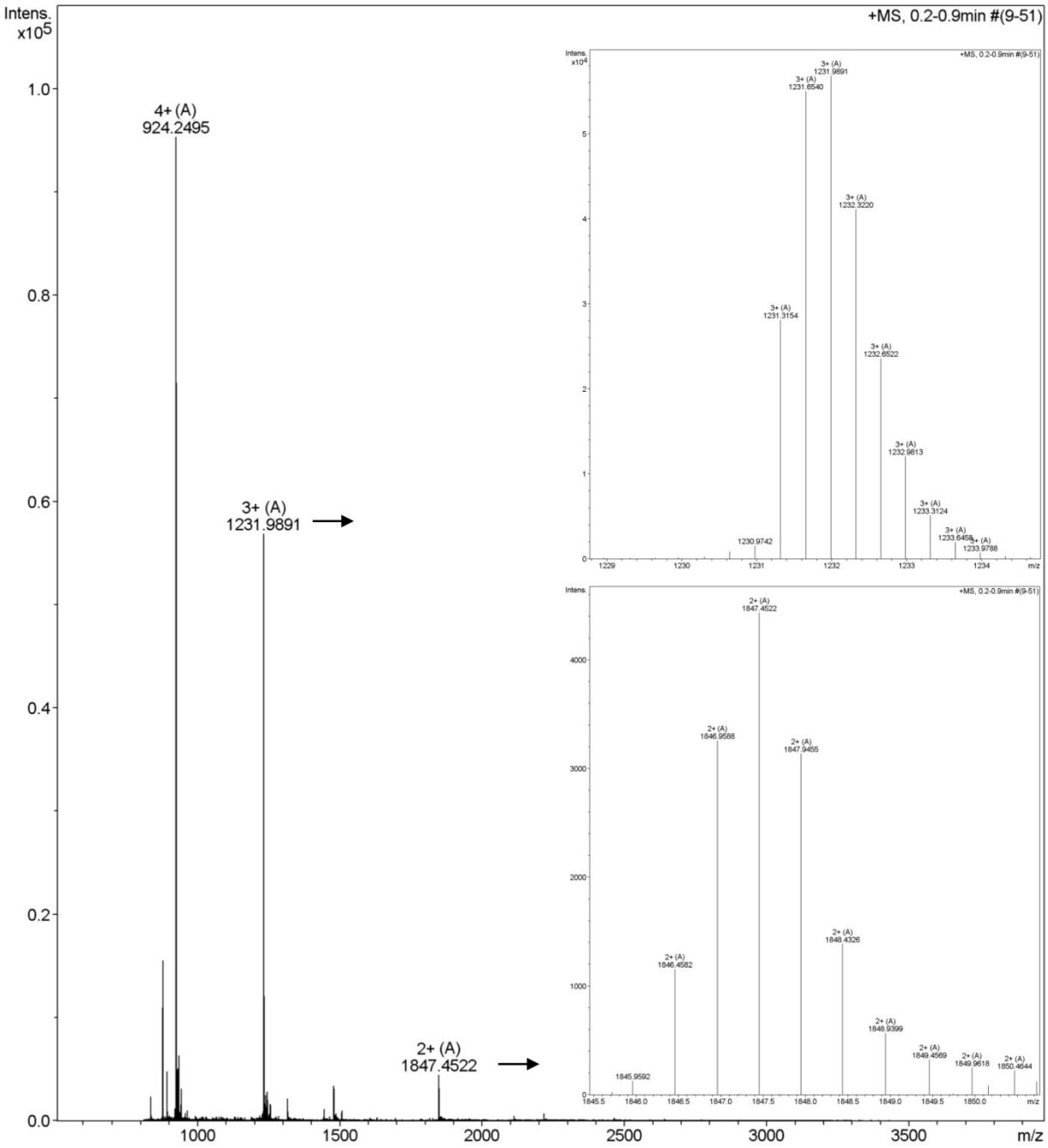
ESI Q-TOF–MS of T22



ESI Q-TOF-MS of T19



ESI Q-TOF-MS of Indole-T26



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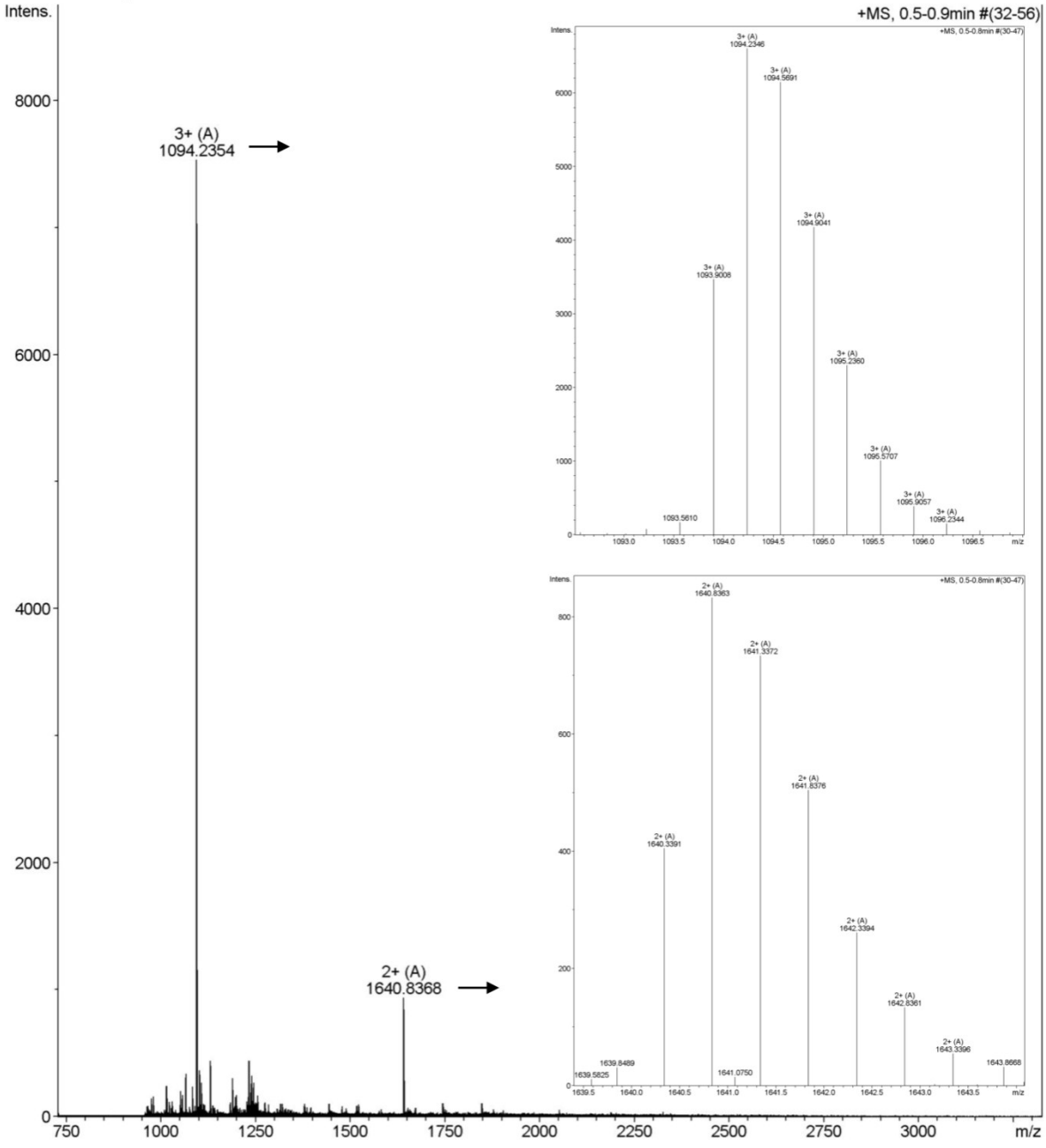

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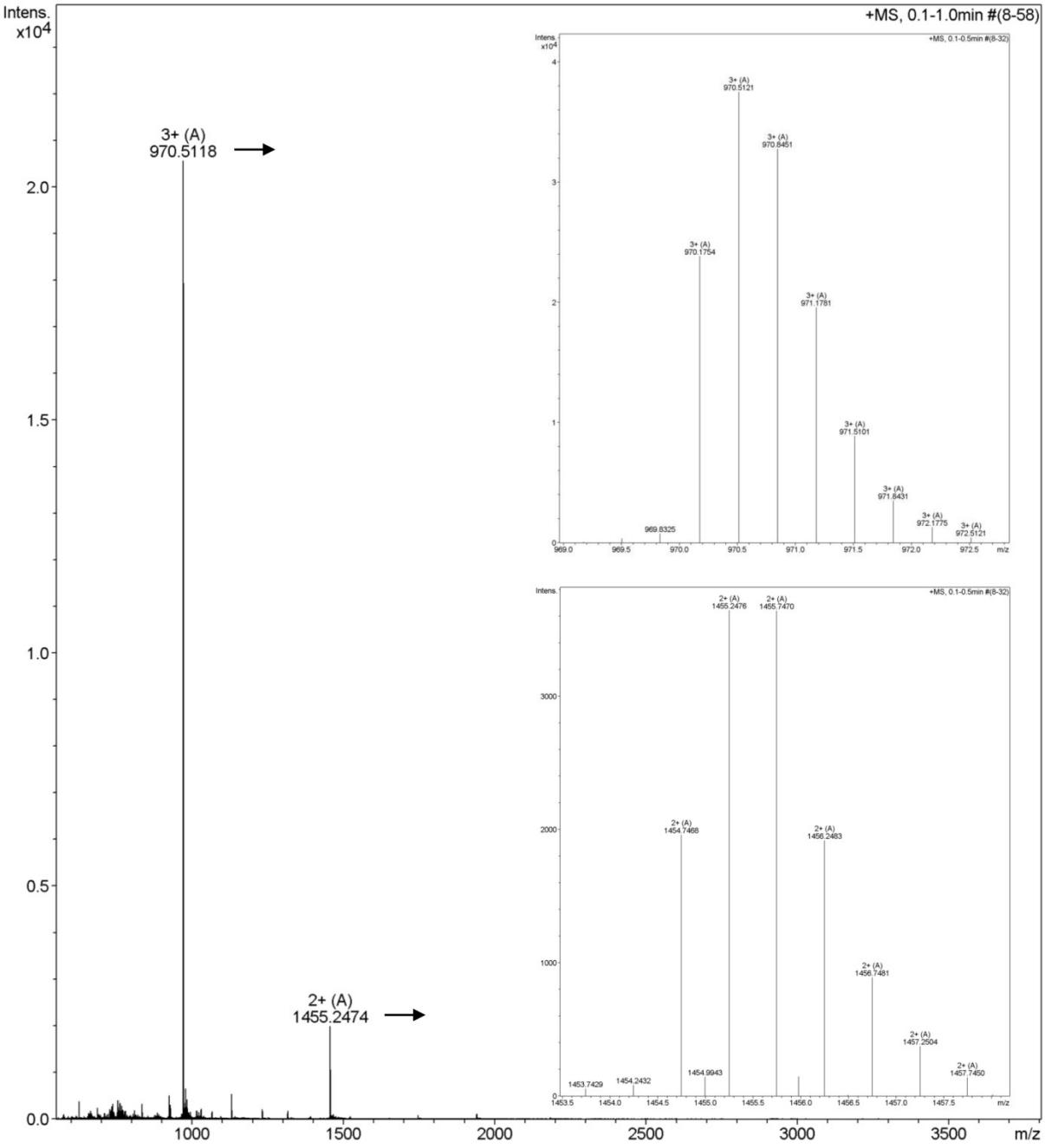

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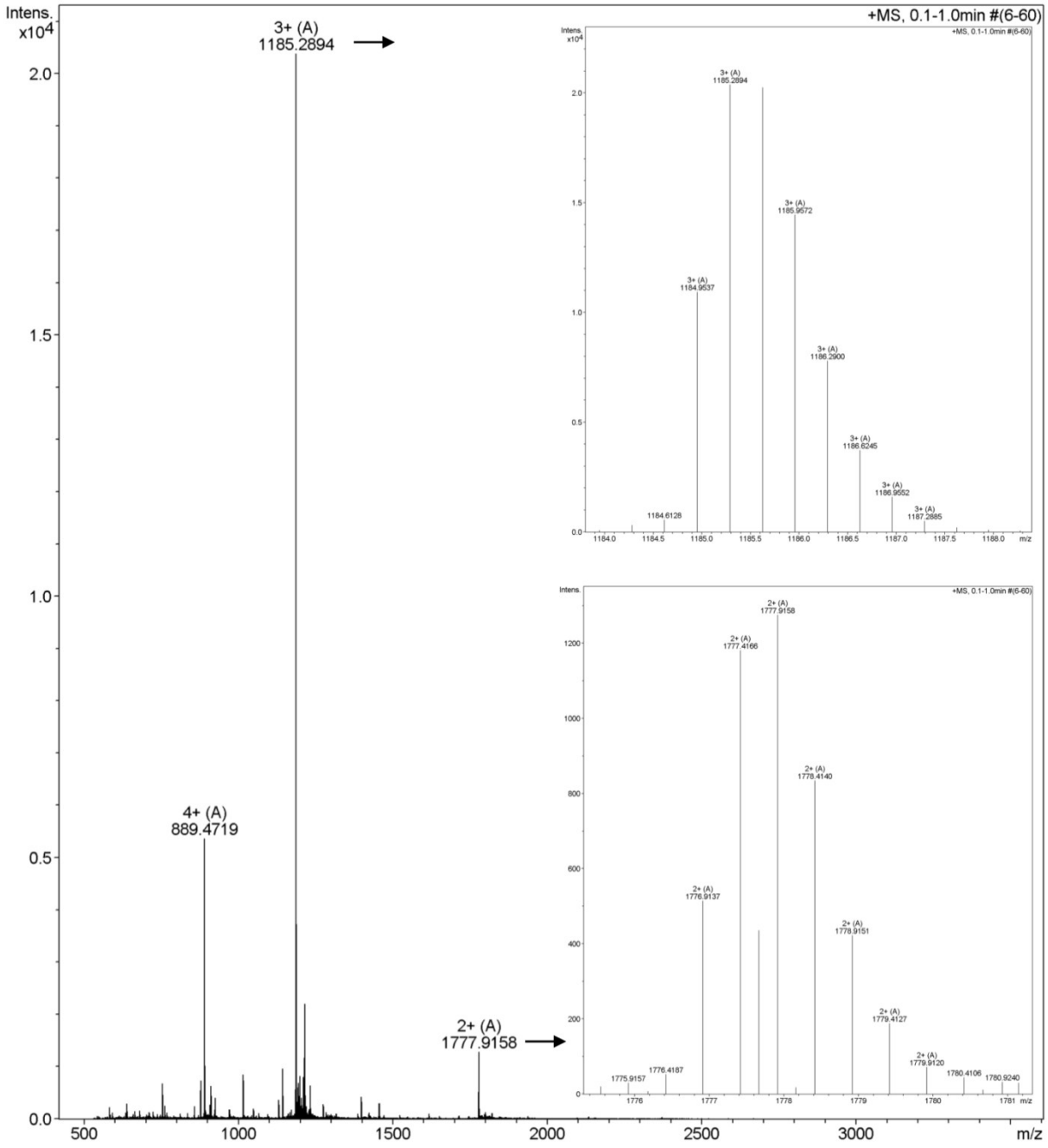

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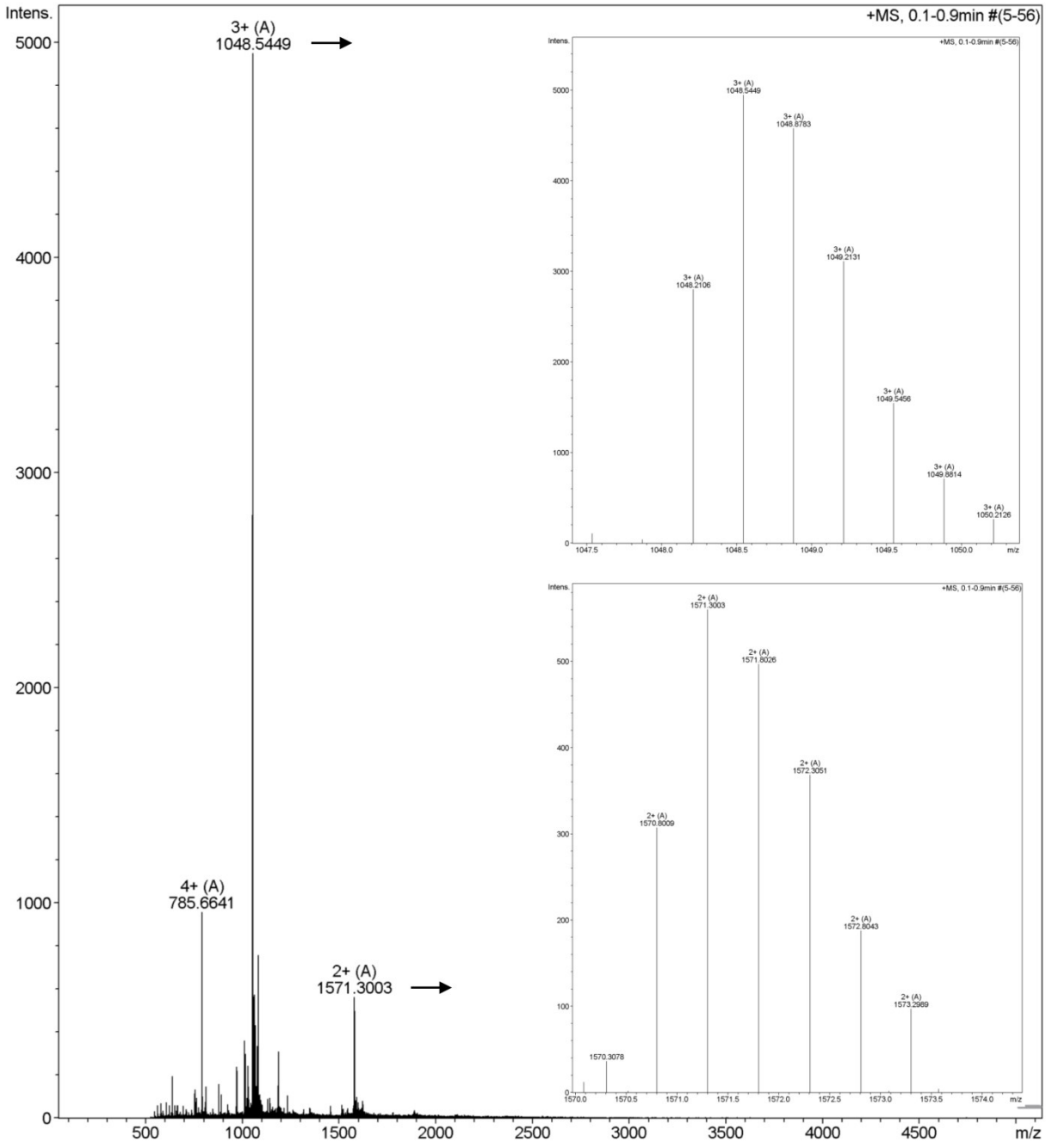

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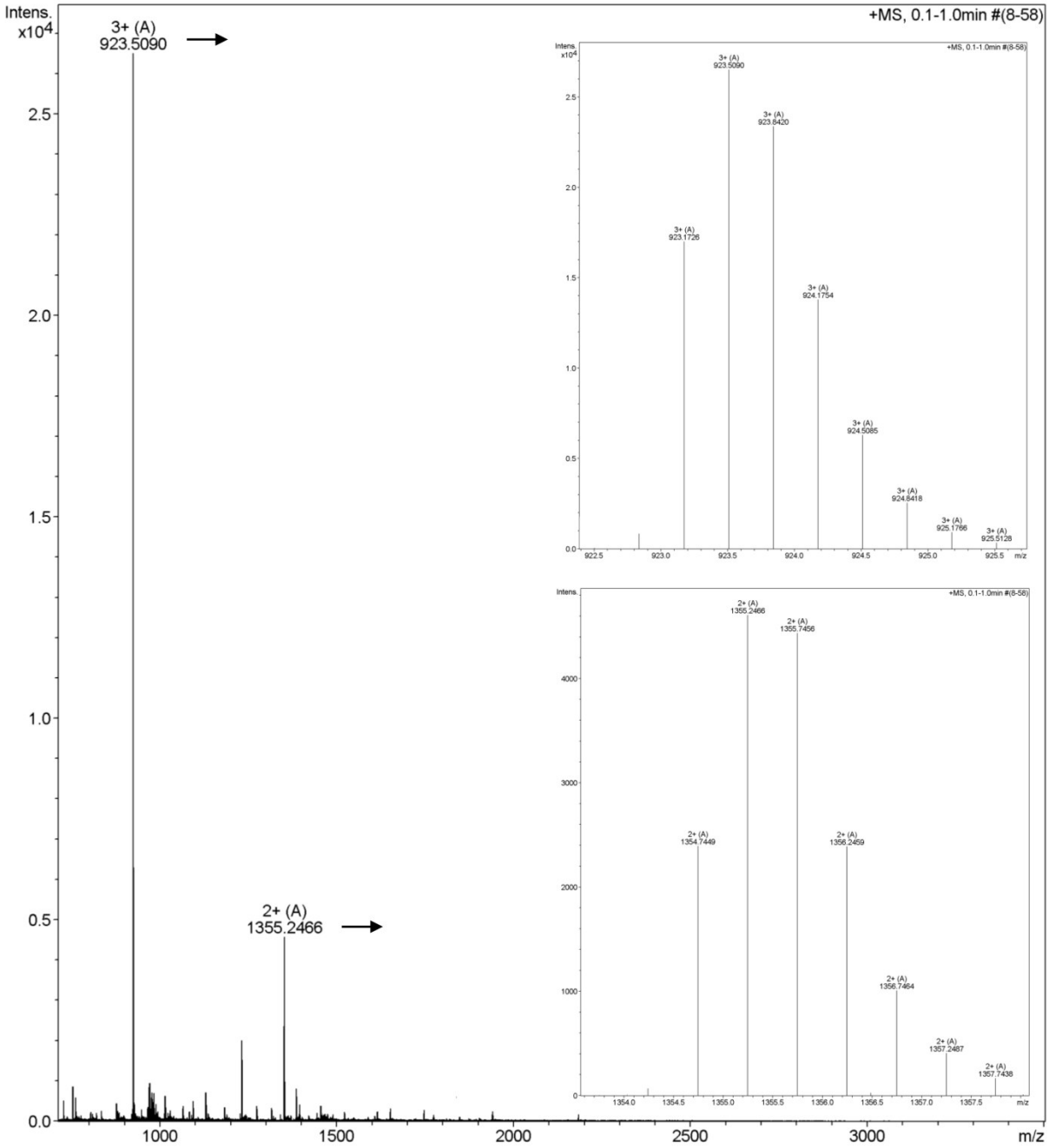
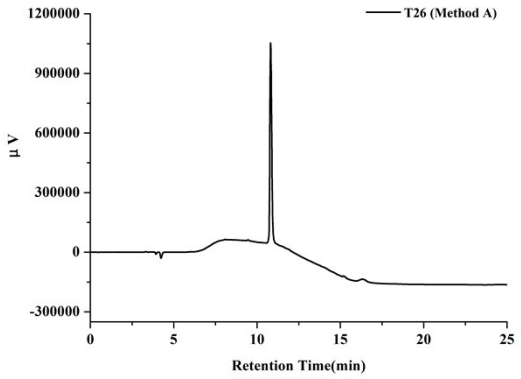


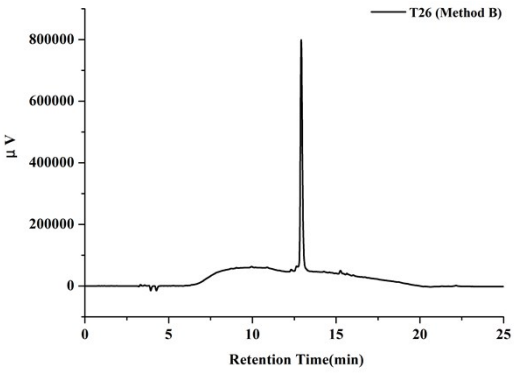
HPLC purity characterization of peptides and conjugates

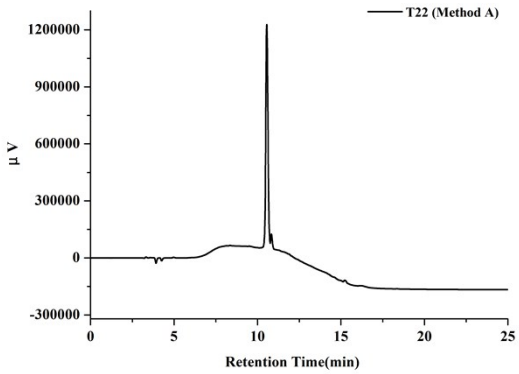
For conjugates, purity was determined by analytical RP-HPLC on a RP-C8 column (Zorbax Eclipse XDB-C8, 5 µm, 4.6 x 150 mm) using two different solvent systems (Method A and B, respectively), and a flow rate of 1 mL/min with detection wavelength at 210 nm. (Solvent A: 0.1% TFA in H_2O; Solvent B1: 0.1% TFA in 90% CH_3CN/H_2O; Solvent B2:0.1% TFA in 70% CH_3CN/H_2O).

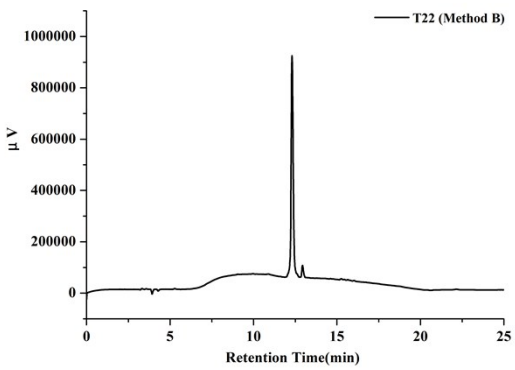
Table 1.HPLC methods used for the analysis of peptides and conjugates

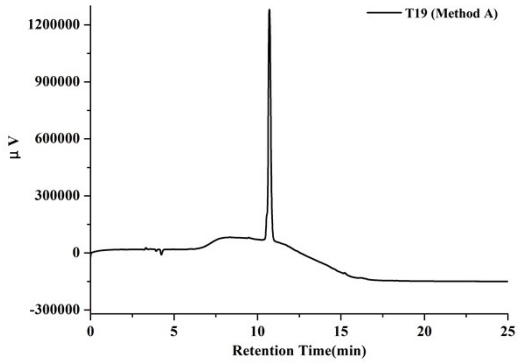
	Time (min)	Solvent A (%)	Solvent B1(%)
Method A	5	50	50
	10	0	100
	20	0	100
	23	90	10
	Time (min)	**Solvent A (%)**	**Solvent B2(%)**
Method B	5	50	50
	15	0	100
	20	0	100
	23	90	10

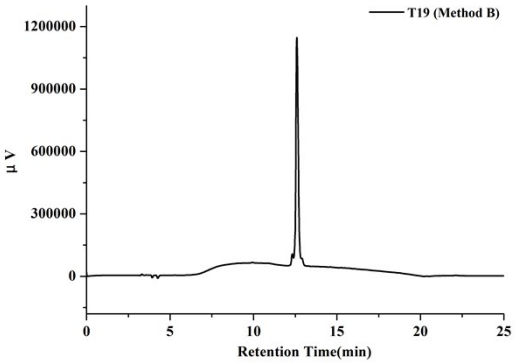


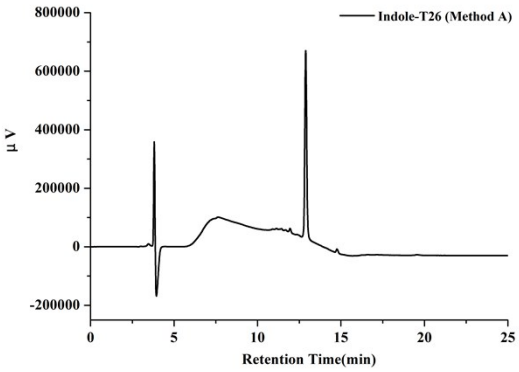


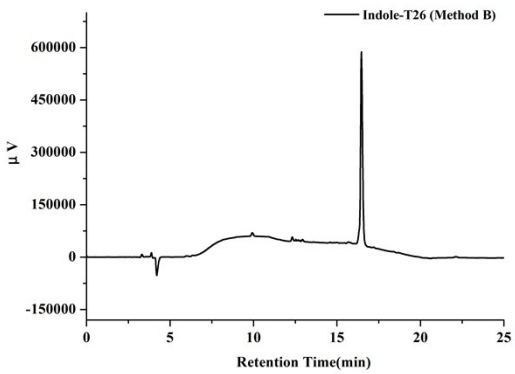

T22 (Method A)
μ V
Retention Time(min)

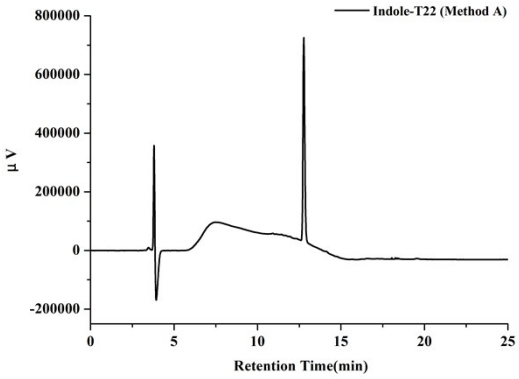

T22 (Method B)
μ V
Retention Time(min)

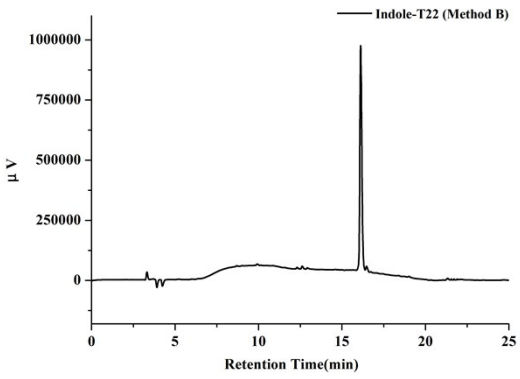

T19 (Method A)
μ V
Retention Time(min)

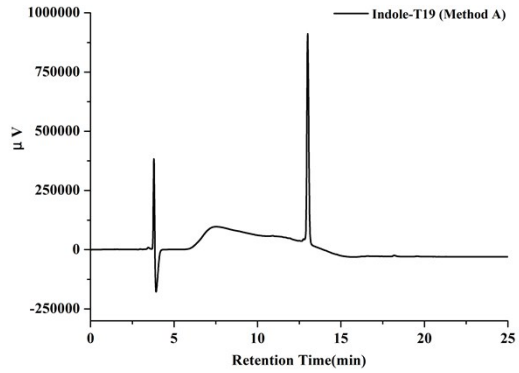

T19 (Method B)
μ V
Retention Time(min)

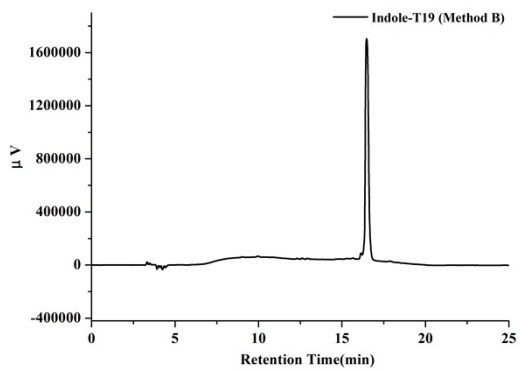

Indole-T26 (Method A)
μ V
Retention Time(min)

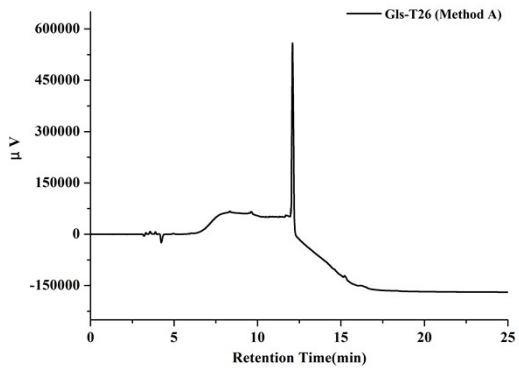

Indole-T26 (Method B)
μ V
Retention Time(min)

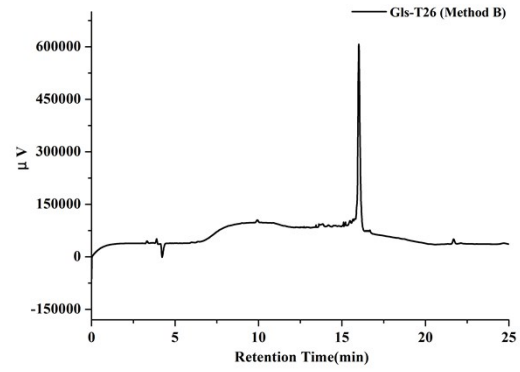

Indole-T22 (Method A)
μ V
Retention Time(min)


Indole-T22 (Method B)
μ V
Retention Time(min)


Indole-T19 (Method A)
μ V
Retention Time(min)


Indole-T19 (Method B)
μ V
Retention Time(min)


Gls-T26 (Method A)
μ V
Retention Time(min)


Gls-T26 (Method B)
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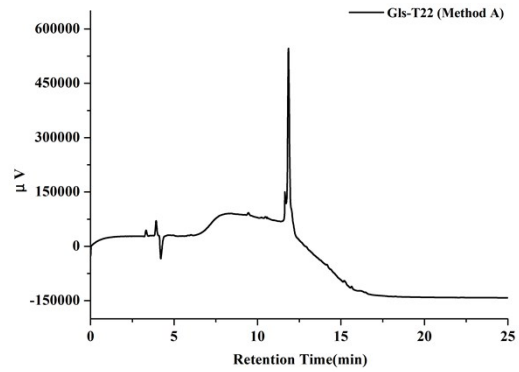
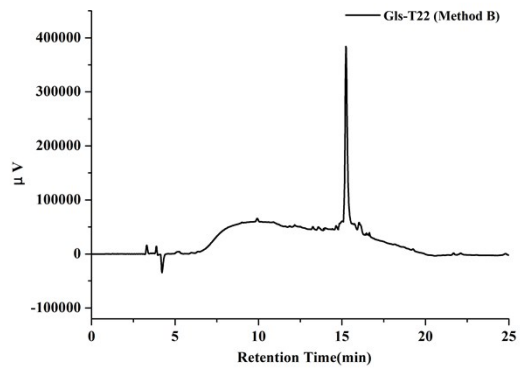
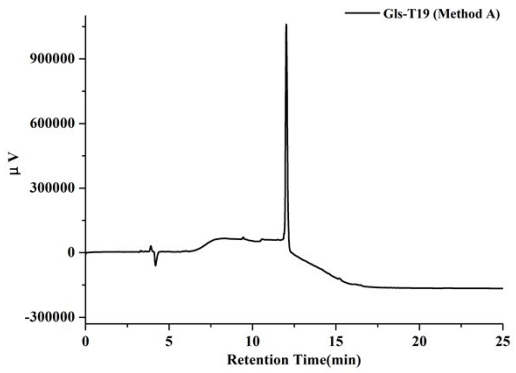
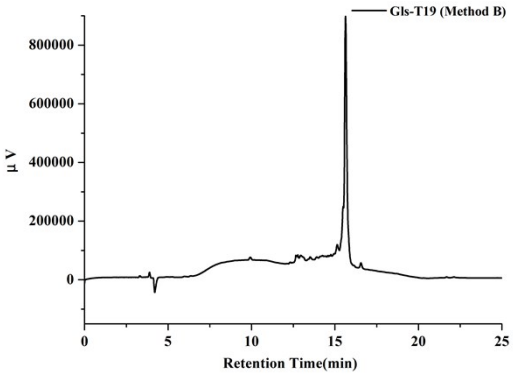
Retention Time(min)


Gls-T22 (Method A)
μ V
Retention Time(min)


Gls-T22 (Method B)
μ V
Retention Time(min)


Gls-T19 (Method A)
900000
600000
300000
0
-300000
μ V
0
5
10
15
20
25
Retention Time(min)


Gls-T19 (Method B)
800000
600000
400000
200000
0
μ V
0
5
10
15
20
25
Retention Time(min)