

Supporting Information

Development of peptide based bifunctional chelator conjugated to a cytotoxic drug for the treatment of melanotic melanoma

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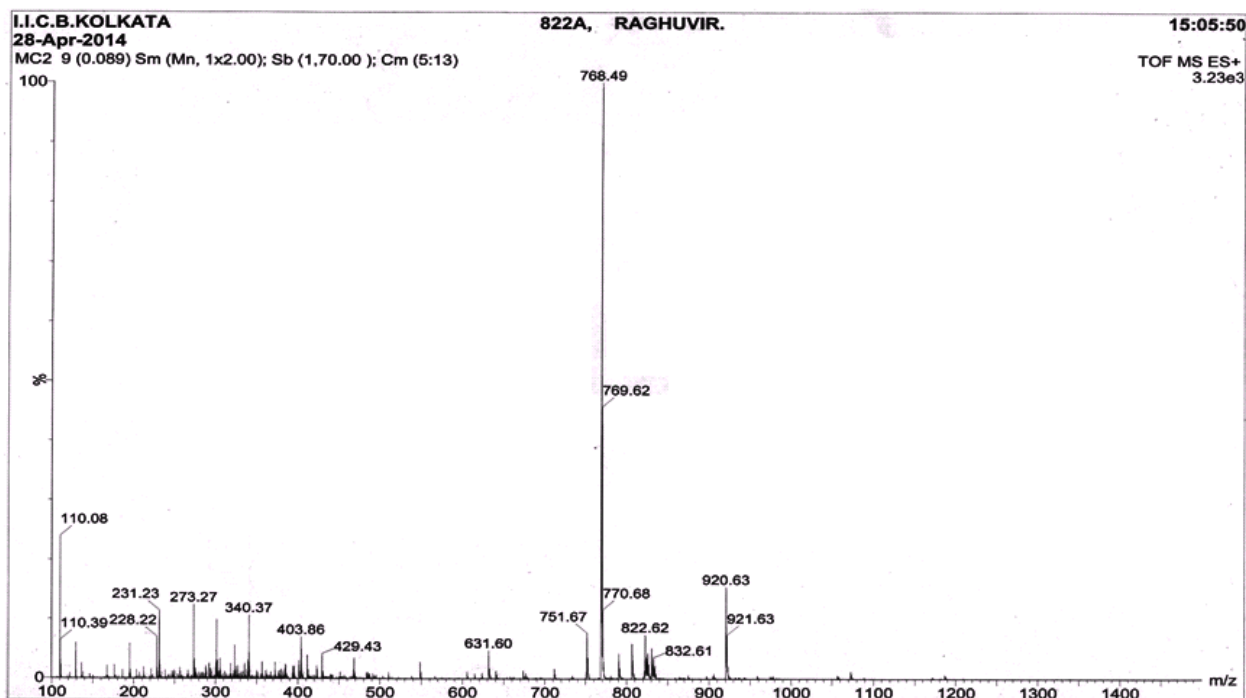


Figure S1-ESI MS spectra of pep-1

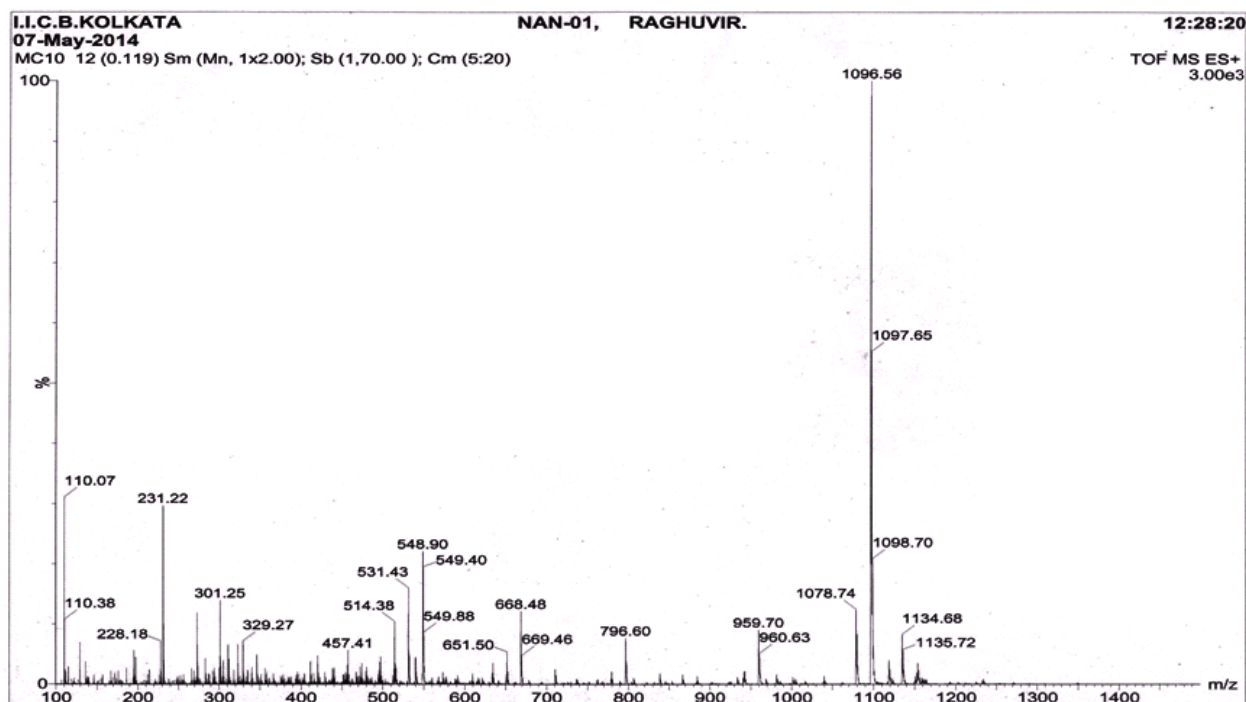


Figure S2-ESI MS spectra of pep-2

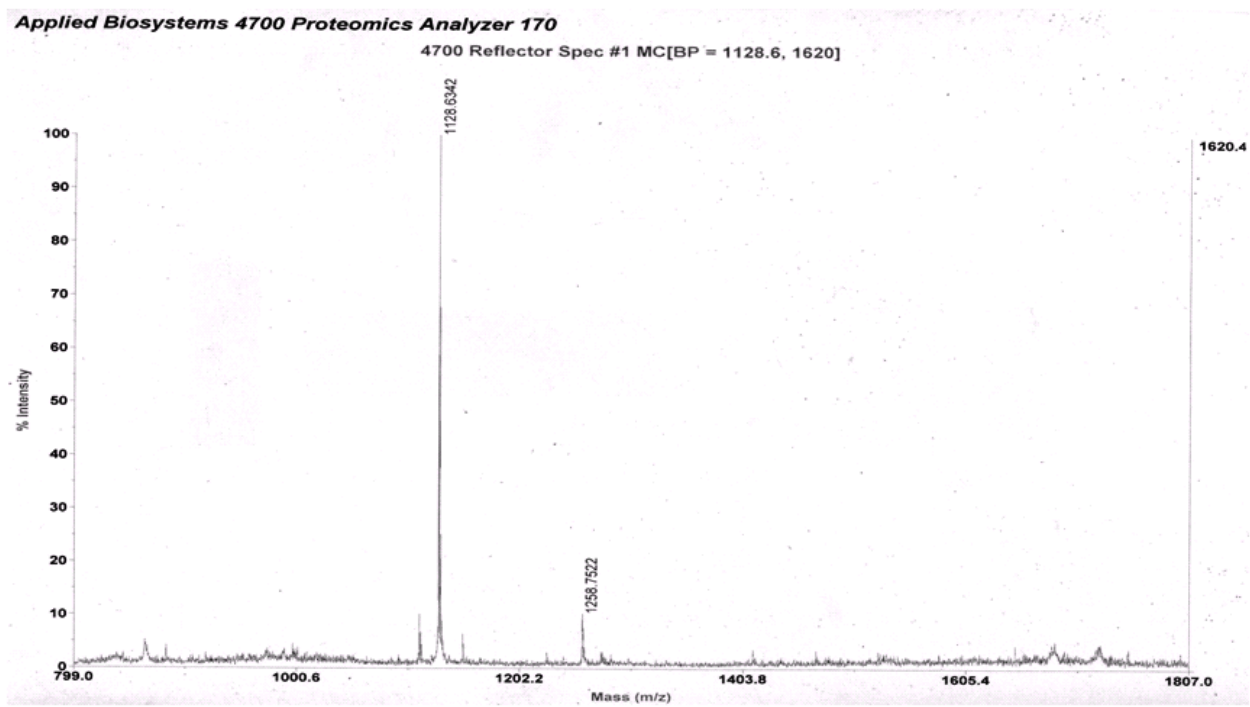


Figure S3-MALDI-TOF MS spectra of GEM-pep-3

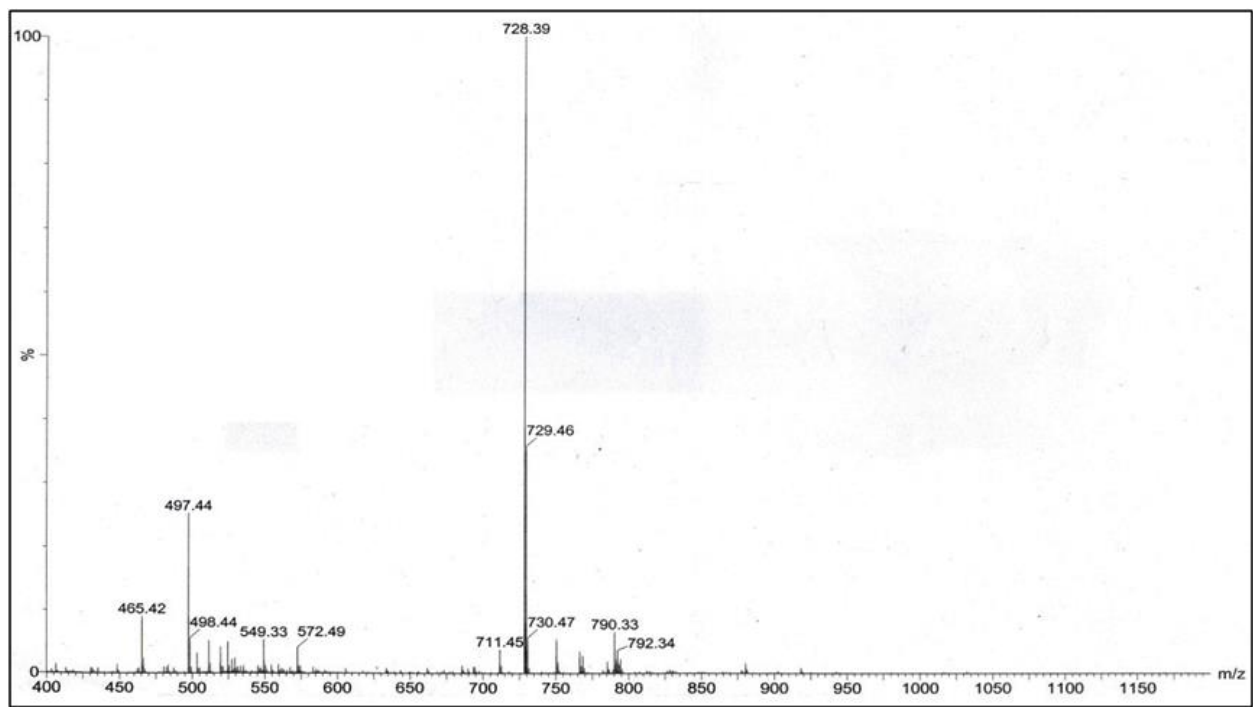


Figure S4-ESI MS spectra of GEM-pep-4

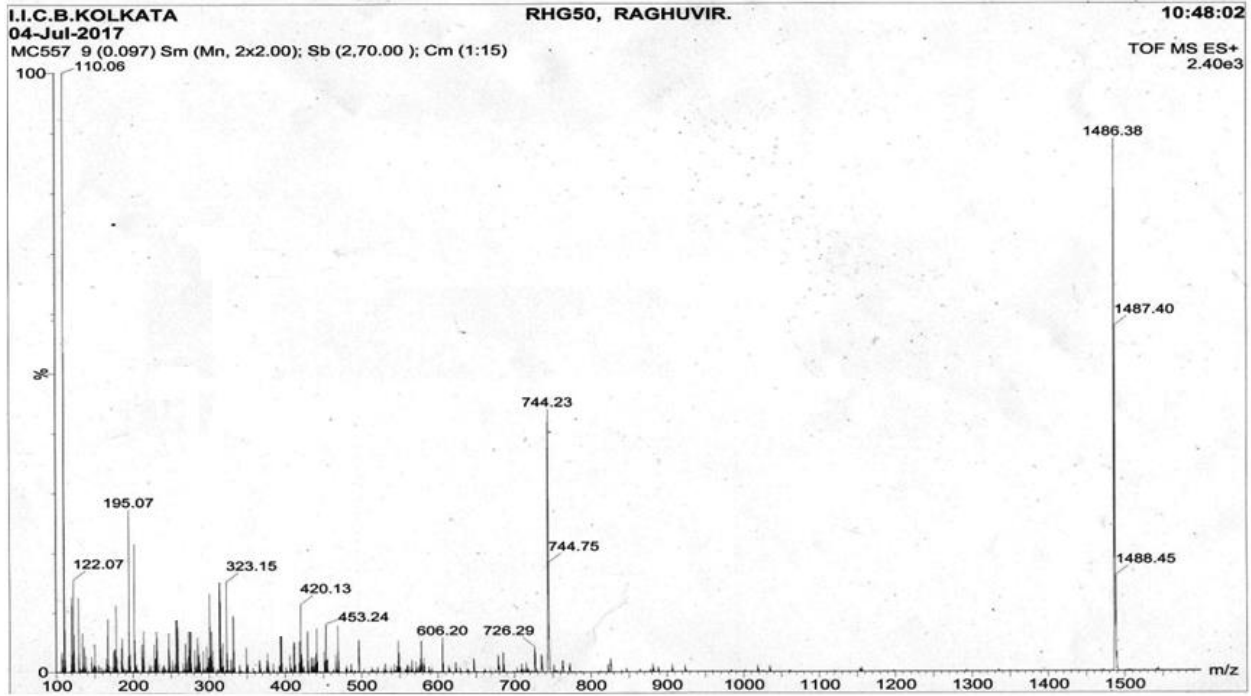


Figure S5- MALDI-TOF MS spectra of GEM-pep3-CF

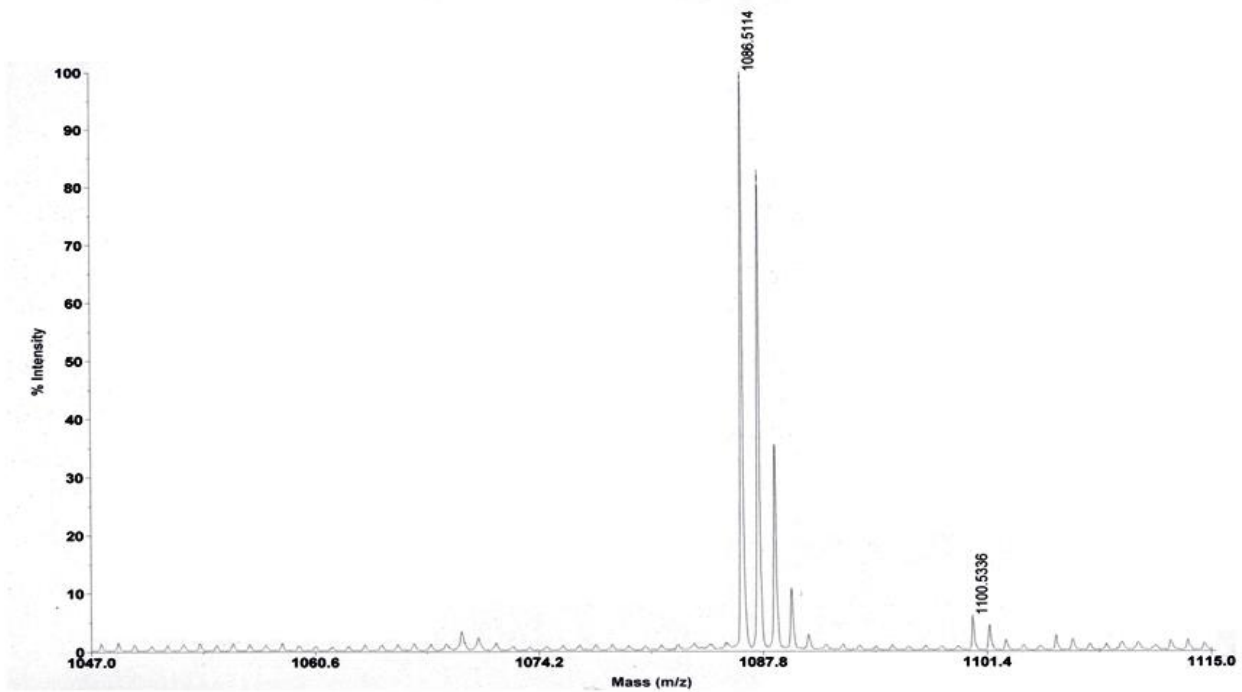


Figure S6- MALDI-TOF MS of GEM-pep4-CF

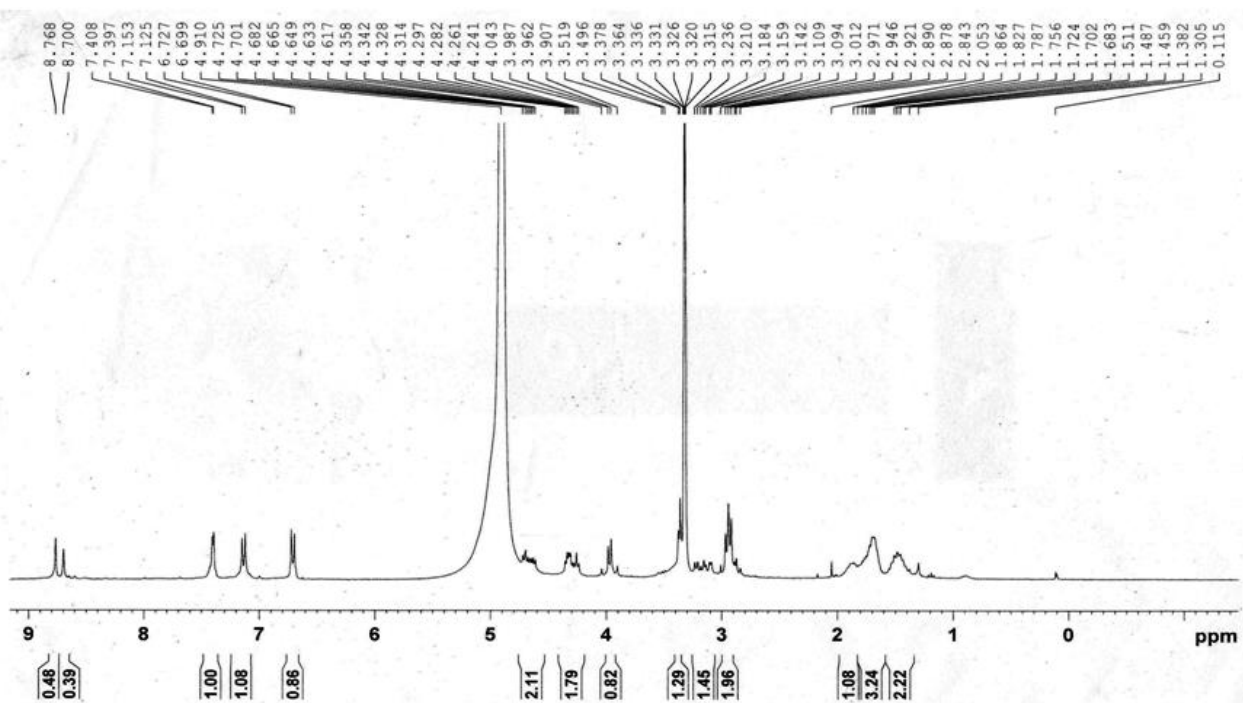


Figure S7- ^1H NMR spectra of pep-1

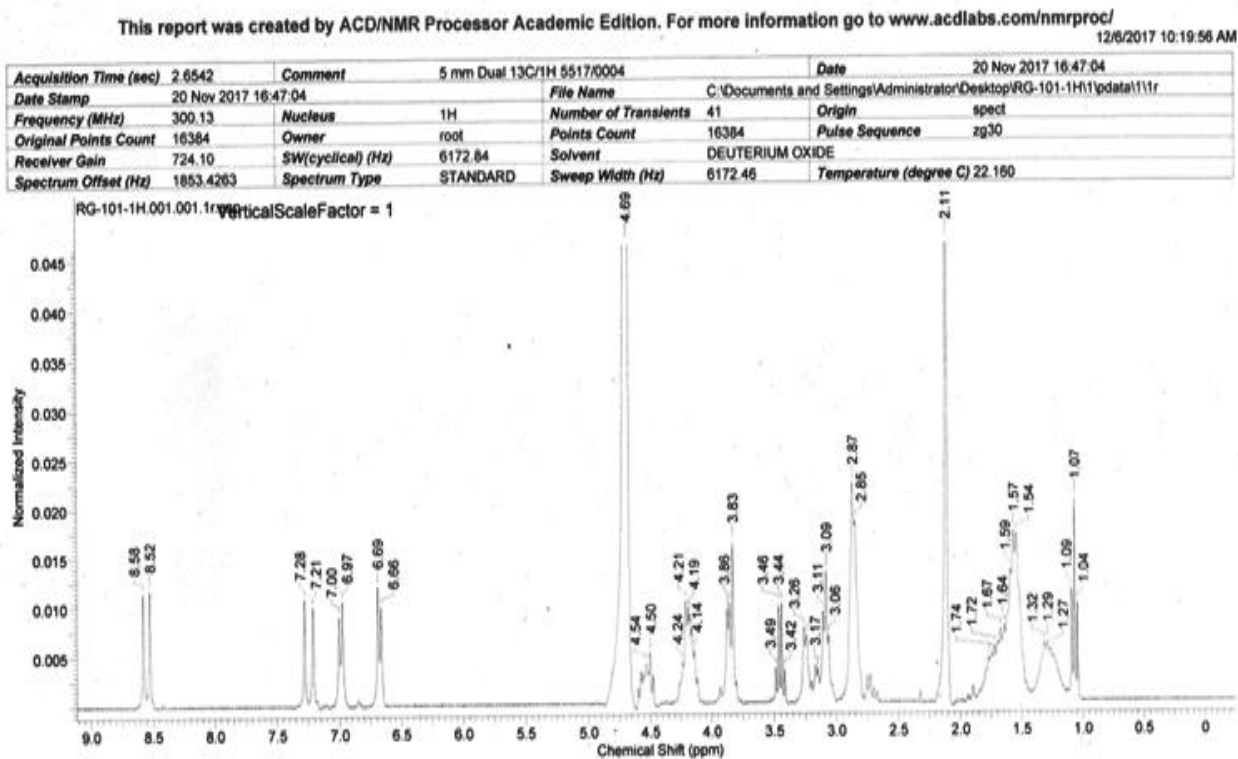


Figure S8- ^1H NMR spectra of pep-2

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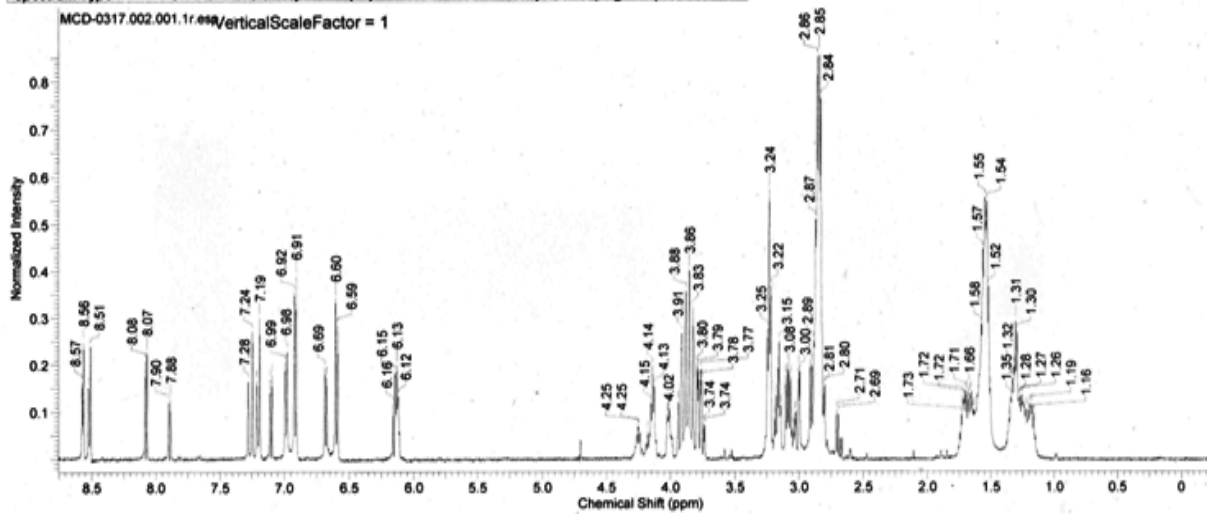


Figure S9-¹H NMR spectra of GEM-pep-3

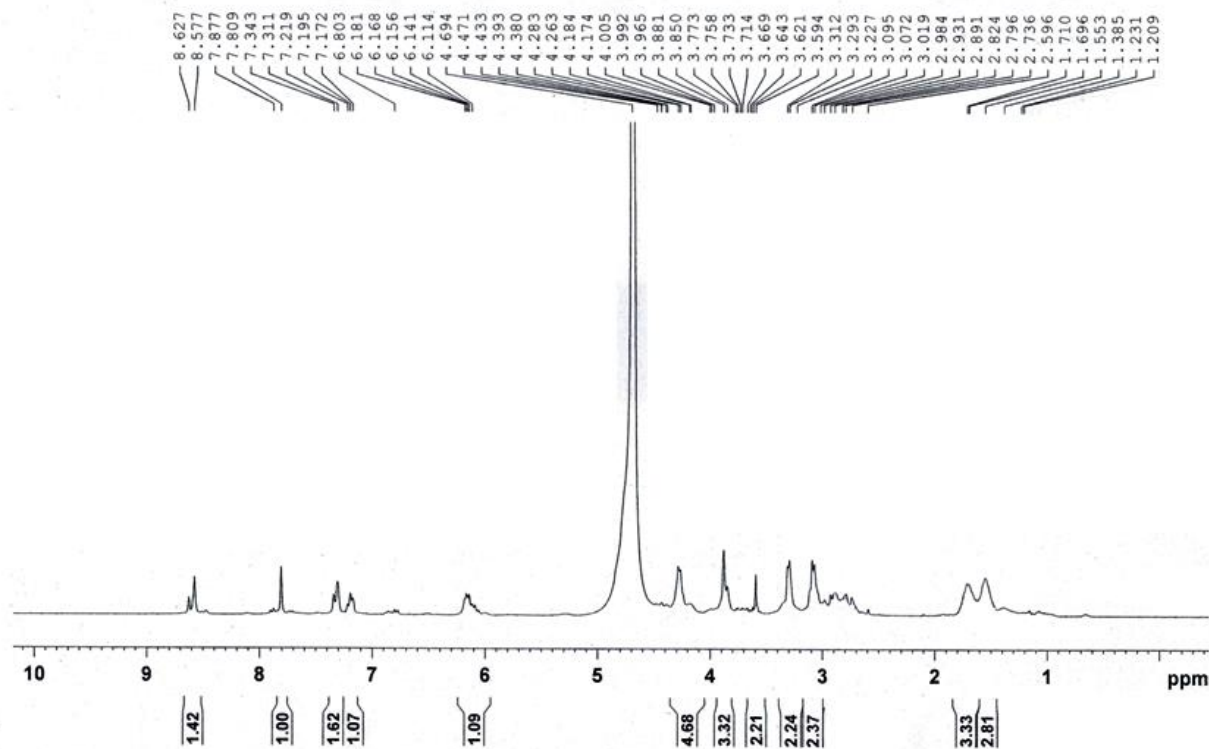


Figure S10-¹H NMR spectra of GEM-pep-4

Time	^{99m} Tc(CO) ₃ -pep-1		
	Saline	Serum	Histidine
0	98.23 ± 1.21	98.29 ± 1.18	97.43 ± 1.10
1	97.32 ± 1.11	96.52 ± 2.20	95.49 ± 1.19
2	96.39 ± 1.31	95.71 ± 2.13	94.81 ± 1.28
4	95.41 ± 1.10	94.17 ± 2.11	93.54 ± 1.91
24	92.13 ± 1.29	92.62 ± 1.71	92.52 ± 1.87
	^{99m} Tc(CO) ₃ -pep-2		
0	97.28 ± 1.31	97.61 ± 1.61	97.11 ± 1.31
1	96.54 ± 1.26	95.54 ± 1.59	95.25 ± 1.25
2	94.31 ± 1.61	93.72 ± 1.79	93.28 ± 1.37
4	92.15 ± 1.27	91.23 ± 1.37	92.15 ± 1.43
24	90.89 ± 1.23	90.25 ± 1.64	90.49 ± 1.39
	^{99m} Tc(CO) ₃ -GEM-pep-3		
0	98.26 ± 1.67	98.81 ± 1.39	98.34 ± 1.62
1	97.53 ± 1.58	96.28 ± 1.55	96.79 ± 1.38
2	96.67 ± 1.49	95.29 ± 1.36	94.86 ± 1.65
4	95.28 ± 1.63	93.37 ± 1.28	92.35 ± 1.75
24	92.49 ± 1.28	91.29 ± 1.37	91.34 ± 1.27
	^{99m} Tc(CO) ₃ -GEM-pep-4		
0	95.12 ± 3.213	94.21 ± 2.198	95.32 ± 1.290
1	95.12 ± 2.117	93.45 ± 2.109	94.23 ± 2.118
2	94.23 ± 1.110	93.76 ± 2.110	92.37 ± 1.198
4	93.21 ± 2.109	92.11 ± 2.117	90.34 ± 3.289
24	90.21 ± 1.920	90.67 ± 1.789	90.03 ± 2.276

Table S1-Stability study of ^{99m}Tc-labeled peptides

Compound	Retention time (min)	Yield (%)
Pep-1	5	80
Pep-2	5.8	76
Gem-pep-3	6.5	70
Gem-pep-4	12.5	73
^{99m} Tc(CO) ₃ -pep-1	12	>95
^{99m} Tc(CO) ₃ -pep-2	11	>95
^{99m} Tc(CO) ₃ -GEM-pep-3	14	>95
^{99m} Tc(CO) ₃ -GEM-pep-4	11.5	>95

Table S2- Analytical results with yield

Six-01_XT_00001_MHp_ #1 RT: 1.00 AV: 1 NL: 3.39E7
T: FTMS + p ESI Full ms [100.00-1400.00]

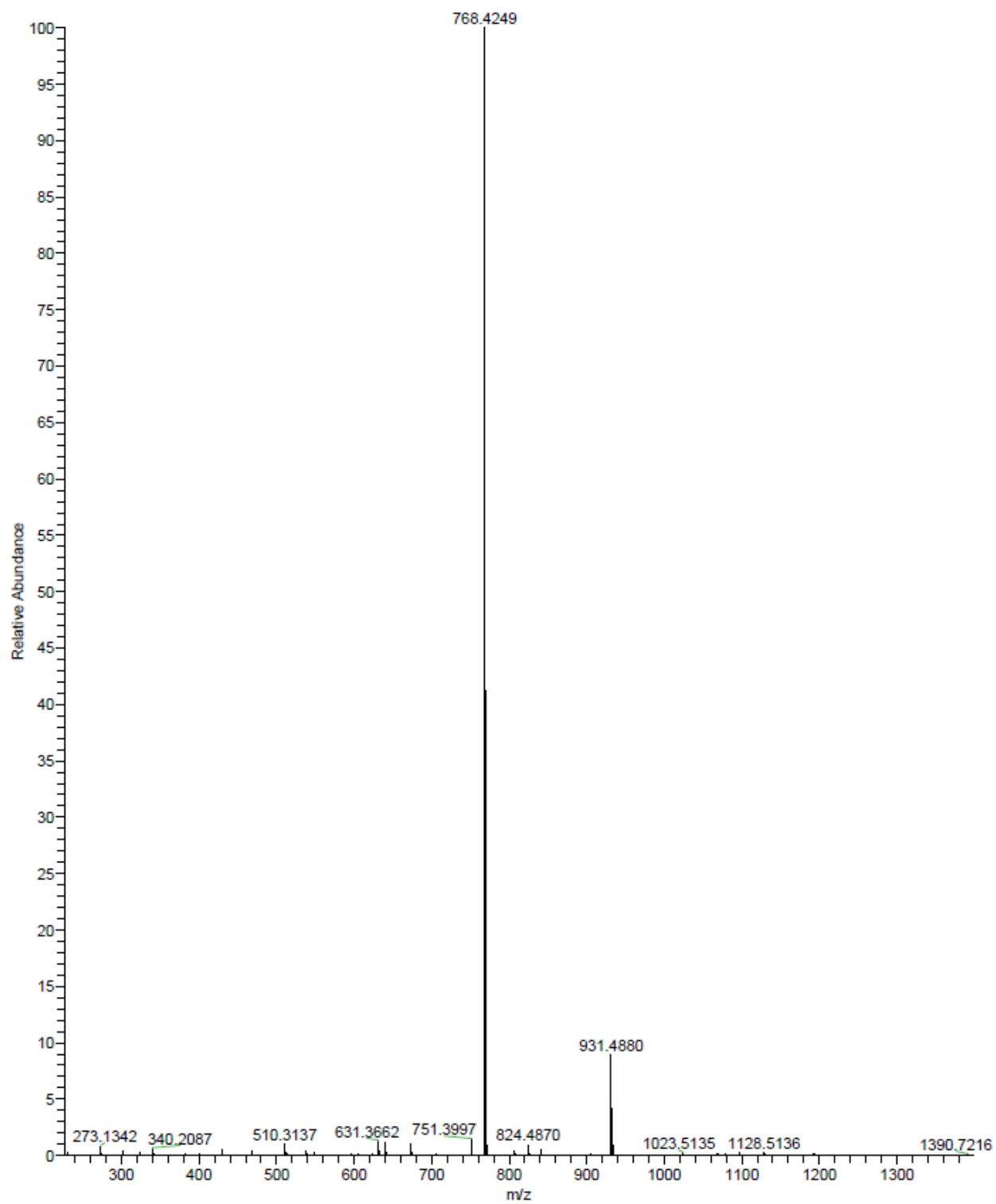


Figure S11-HRMS spectra of pep-1

Nine-01_XT_00001_MHp_ #1 RT: 1.00 AV: 1 NL: 1.75E7
T: FTMS + p ESI Full ms [100.00-1400.00]

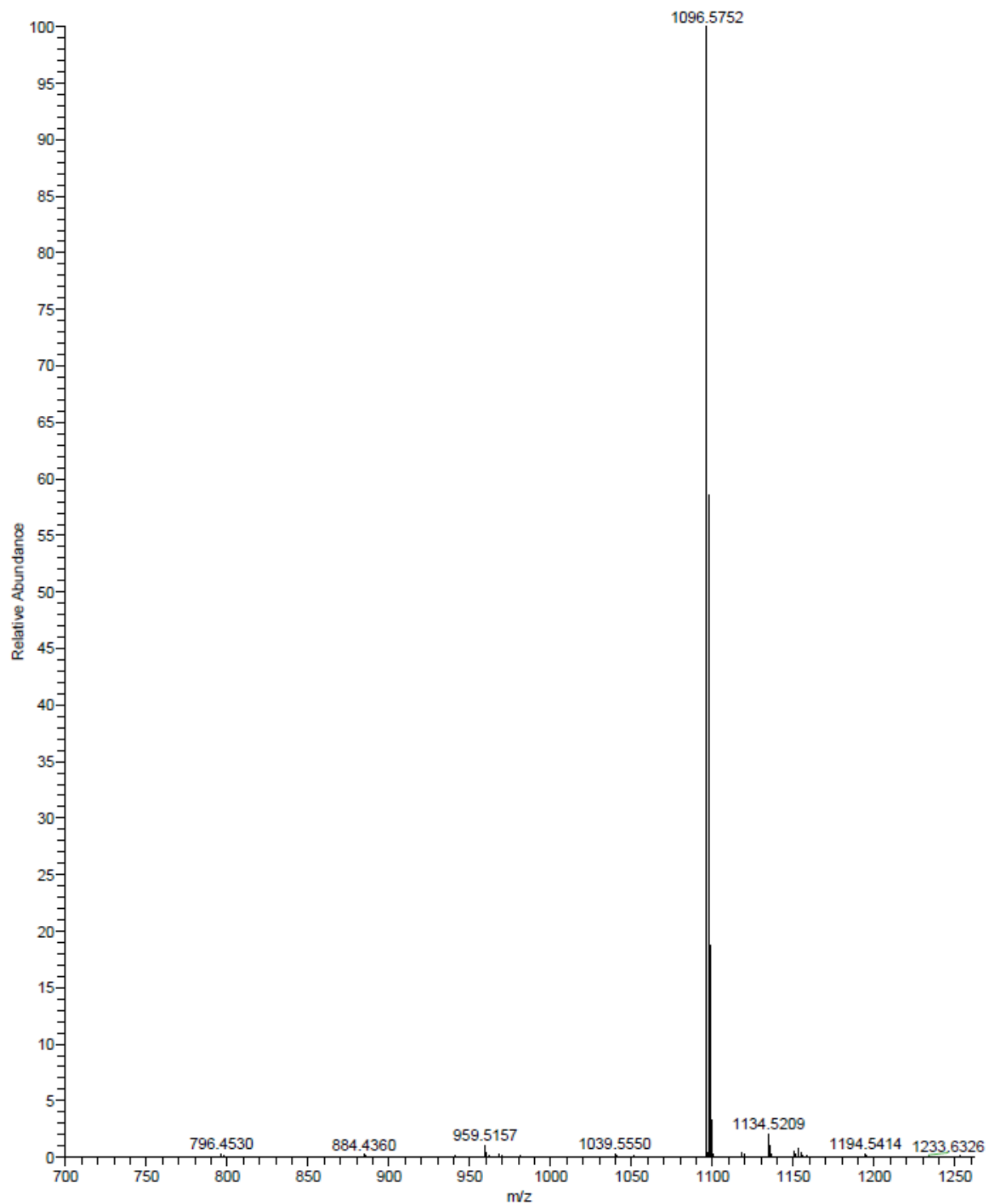


Figure S12-HRMS spectra of pep-1

Seven-01_XT_00001_MHp_ #1 RT: 1.00 AV: 1 NL: 2.67E6
T: FTMS + p ESI Full ms [100.00-1400.00]

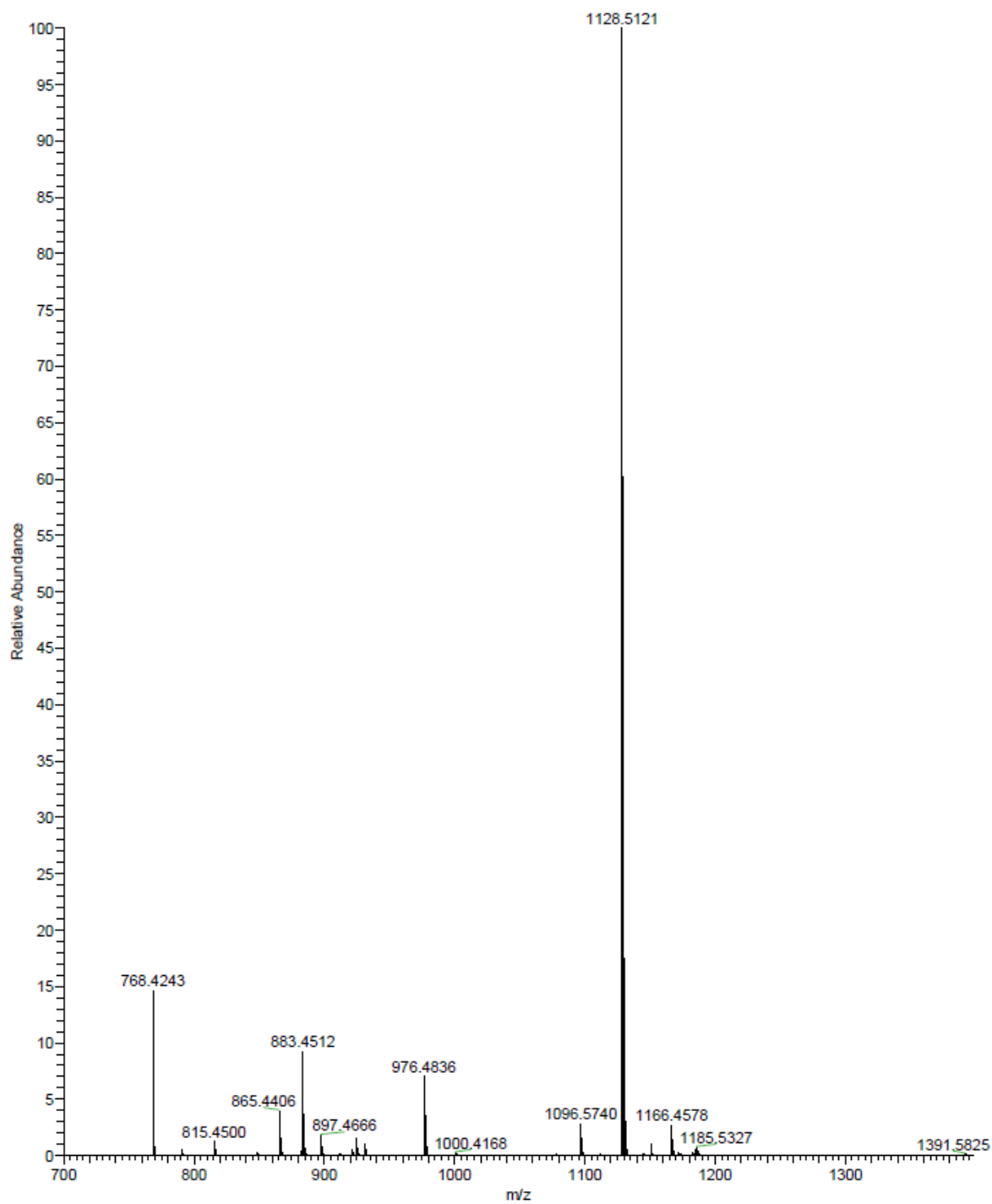


Figure S13-HRMS spectra of pep-1

Four-01 XT 00001 MHp #1 RT: 1.00 AV: 1 NL: 6.08E6
T: FTMS + p ESI Full ms [100.00-1400.00]

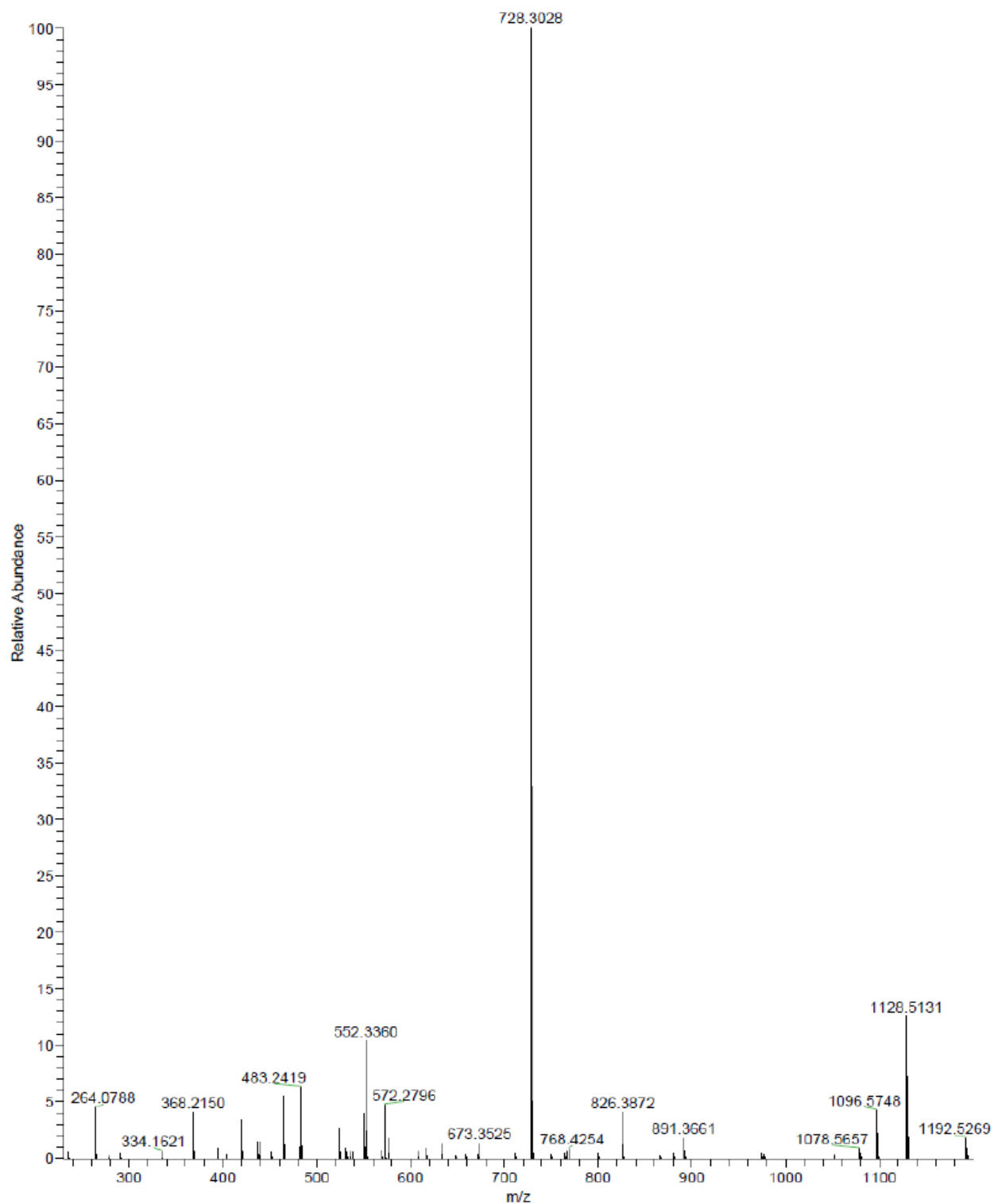


Figure S14-HRMS spectra of pep-1