

**Electronic Supporting Information**

**for mp-2019-00695n**

**BIOCONJUGATION OF GOLD(III) USING LIPOIC ACID TO LINEAR  
AND CYCLIC BREAST CANCER TARGETING PEPTIDES**

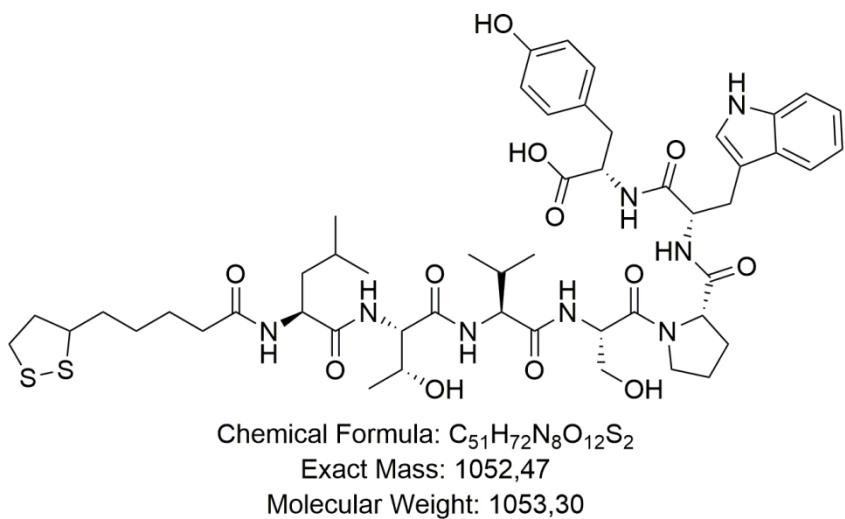
**by**

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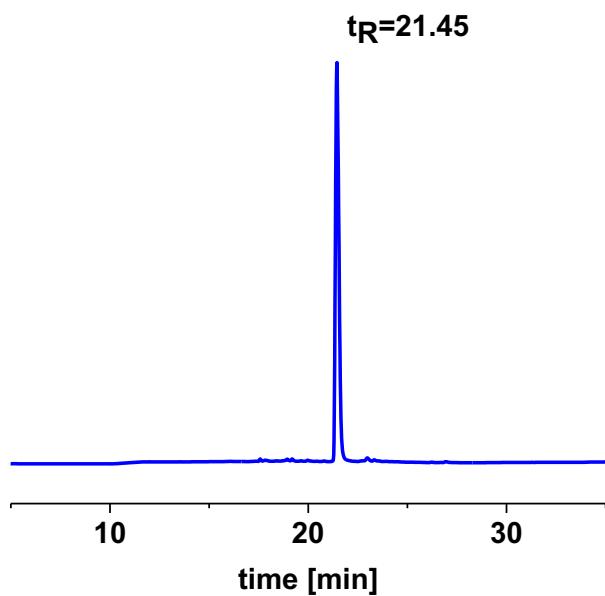
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**Figure S1.** Structure of linear LTVXPW<sub>X</sub> peptide (**2**).



**Figure S2.** HPLC chromatogram at 214 nm of linear LTVXPWX peptide (**2**).

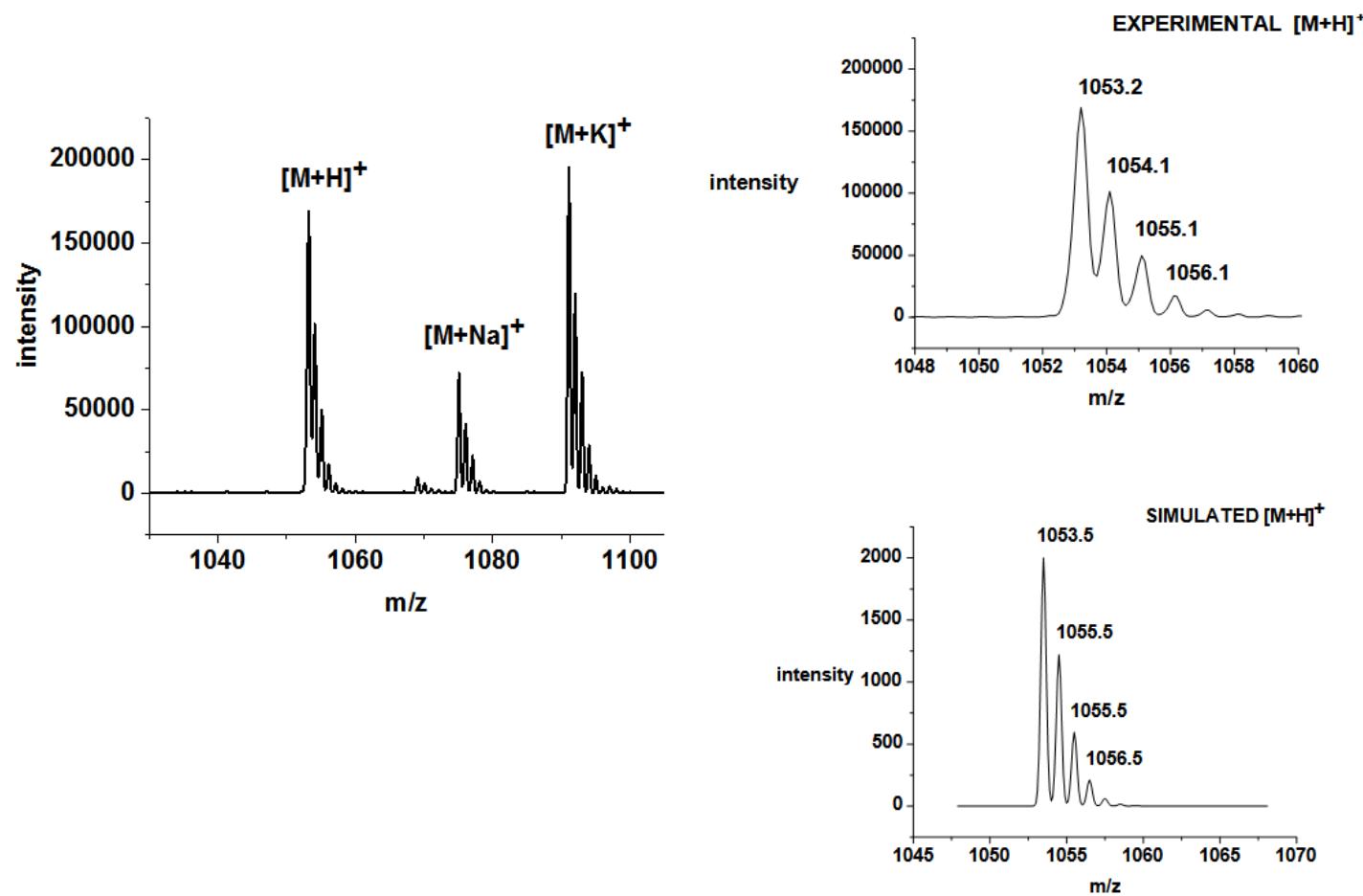
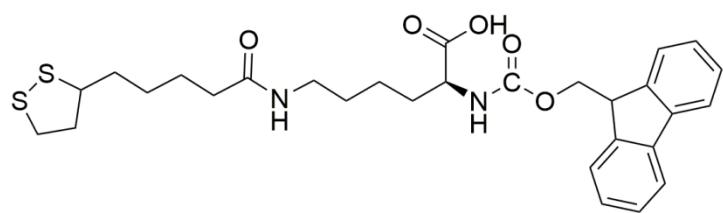


Figure S3. ESI-MS spectrum of linear LTVXPWX peptide (**2**).

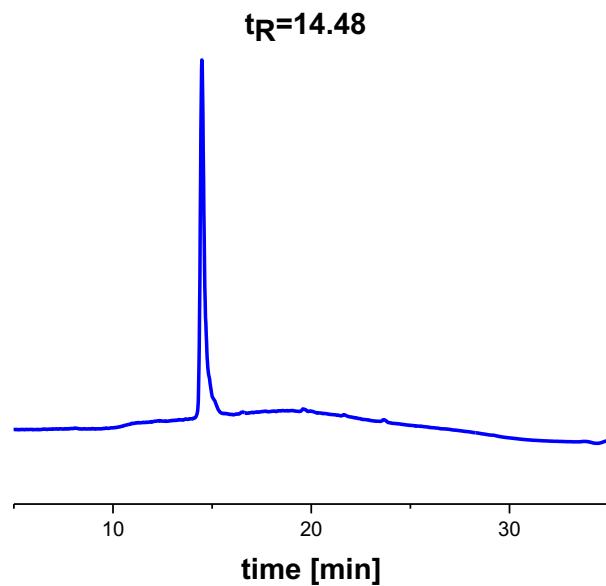


Chemical Formula: C<sub>29</sub>H<sub>36</sub>N<sub>2</sub>O<sub>5</sub>S<sub>2</sub>

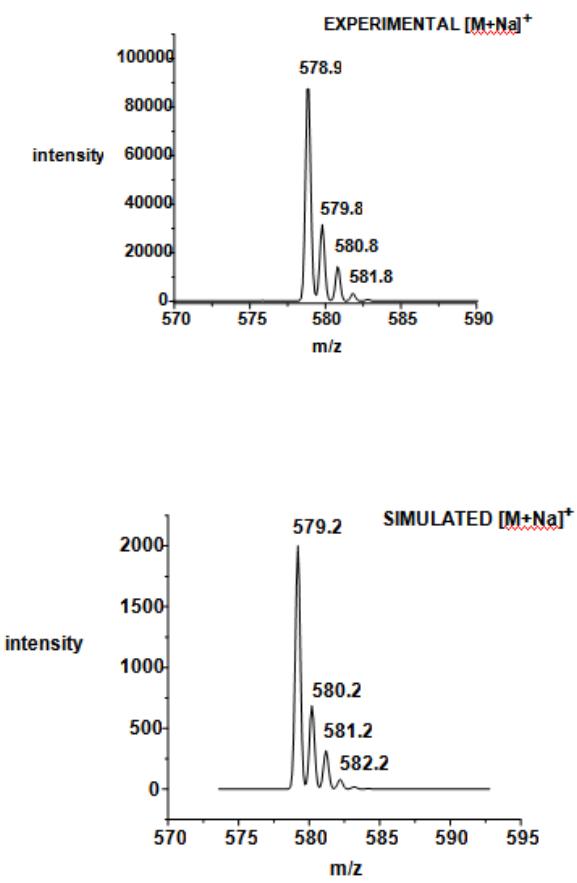
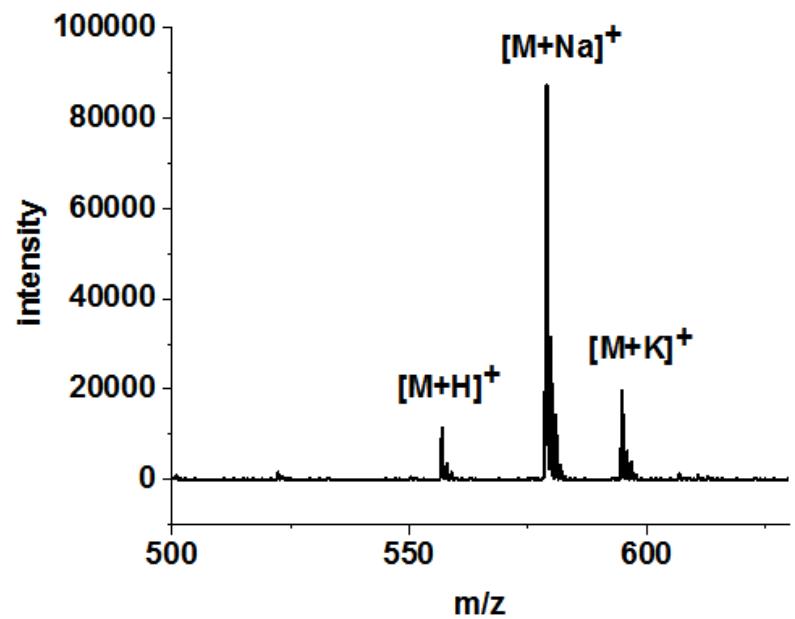
Exact Mass: 556,21

Molecular Weight: 556,74

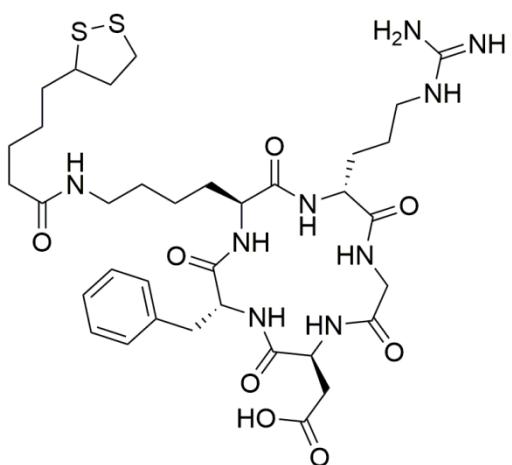
**Figure S4.** Structure of Fmoc-Lys(Lpa)-OH (**3**).



**Figure S5.** HPLC chromatogram at 214 nm of Fmoc-Lys(Lpa)-OH (**3**).



**Figure S6.** ESI-MS spectrum of Fmoc-Lys(Lpa)-OH (3).

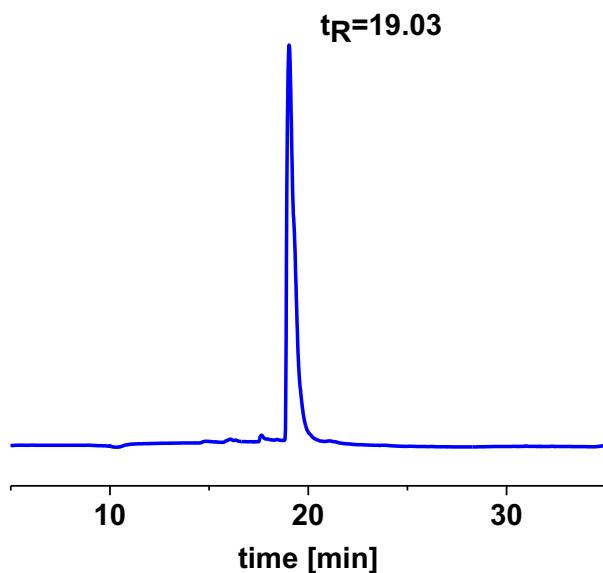


Chemical Formula:  $C_{35}H_{53}N_9O_8S_2$

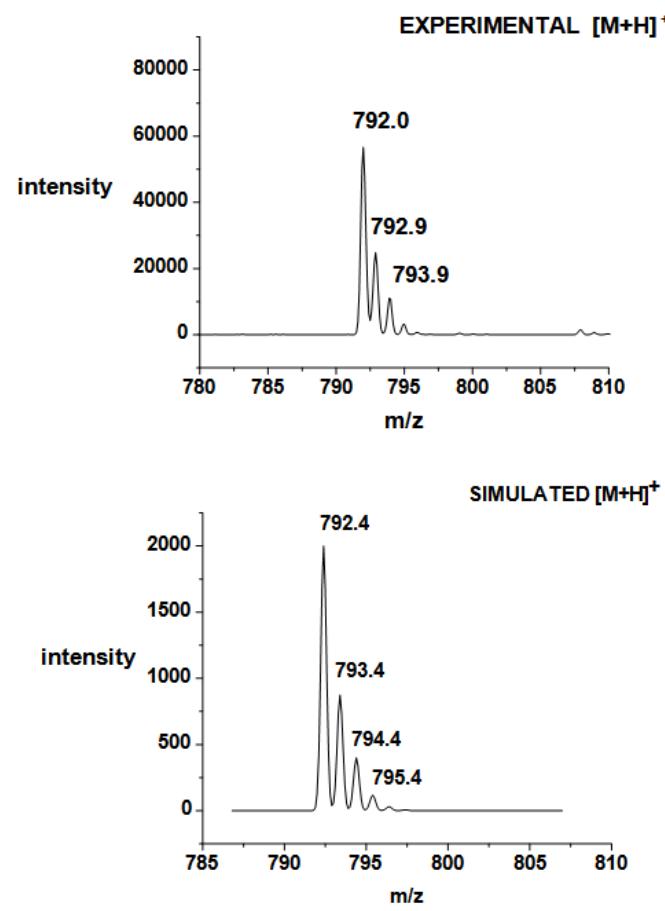
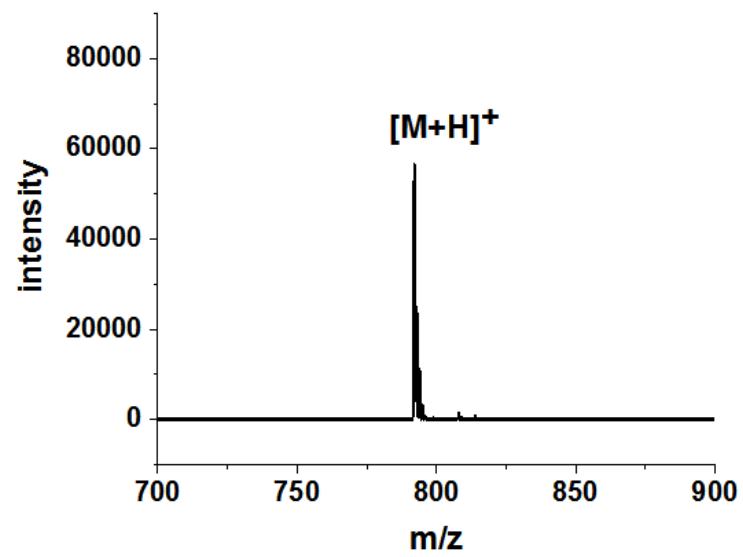
Exact Mass: 791,35

Molecular Weight: 791,98

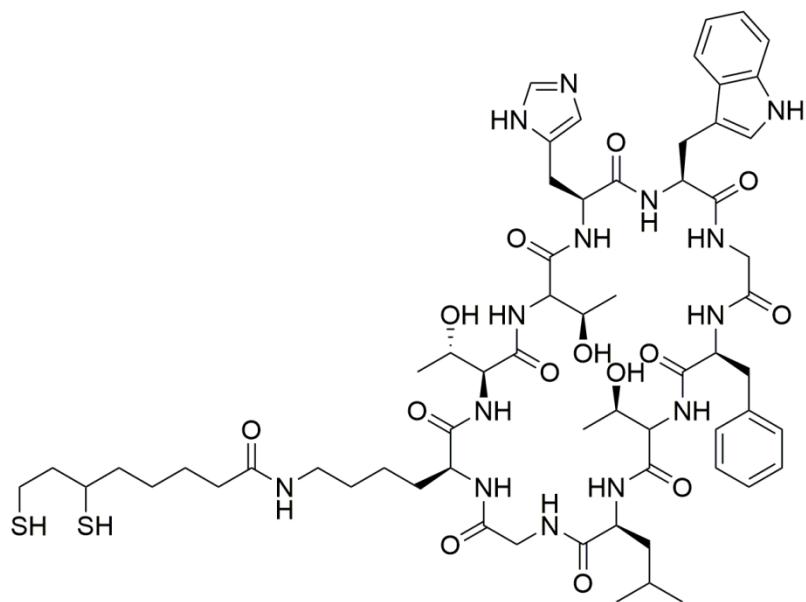
**Figure S7.** Structure of cyclic RGDFK peptide (4).



**Figure S8.** HPLC chromatogram at 214 nm of cyclic RGDFK peptide (4).

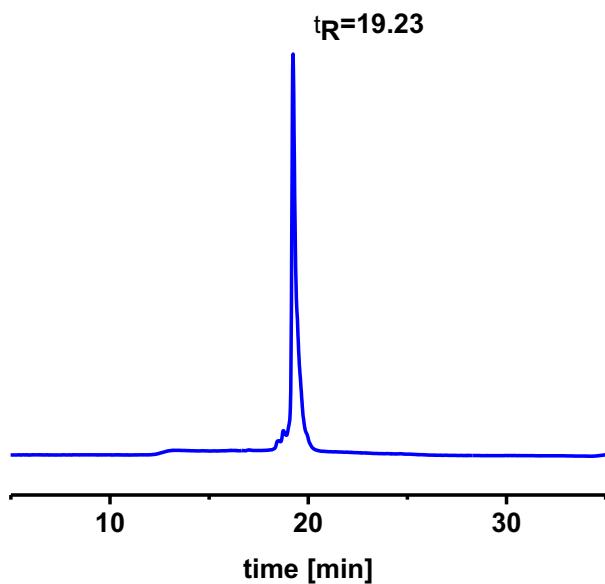


**Figure S9.** ESI-MS spectrum of cyclic RGDFK peptide (**4**).



Chemical Formula:  $C_{62}H_{90}N_{14}O_{14}S_2$   
Exact Mass: 1318,62  
Molecular Weight: 1319,61

**Figure S10.** Structure of cyclic KTTHWGFTLG peptide (**5**).



**Figure S11.** HPLC chromatogram at 214 nm of cyclic KTTHWGFTLG peptide (**5**).

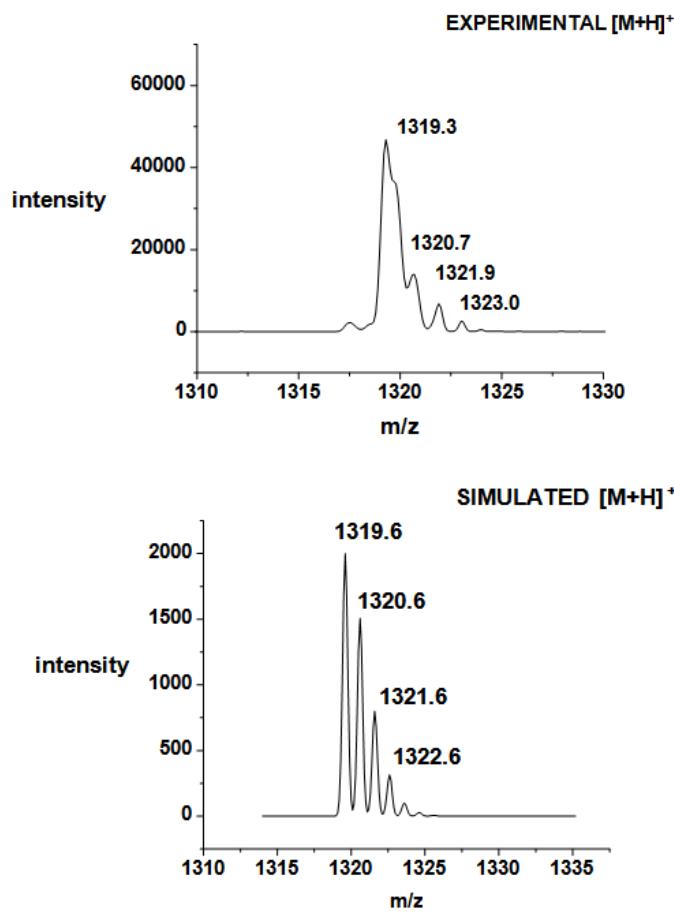
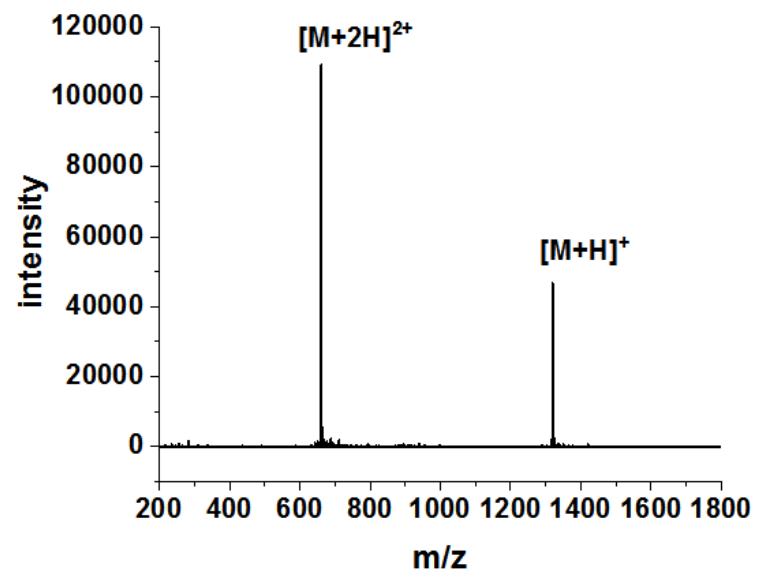
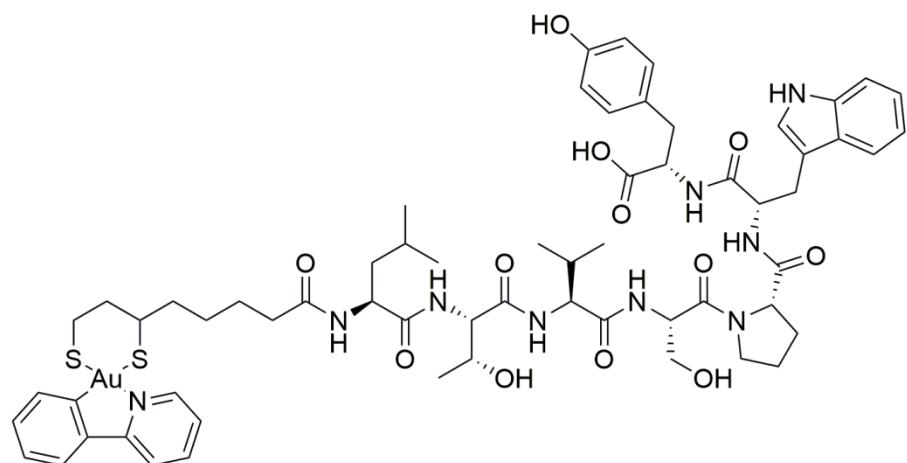
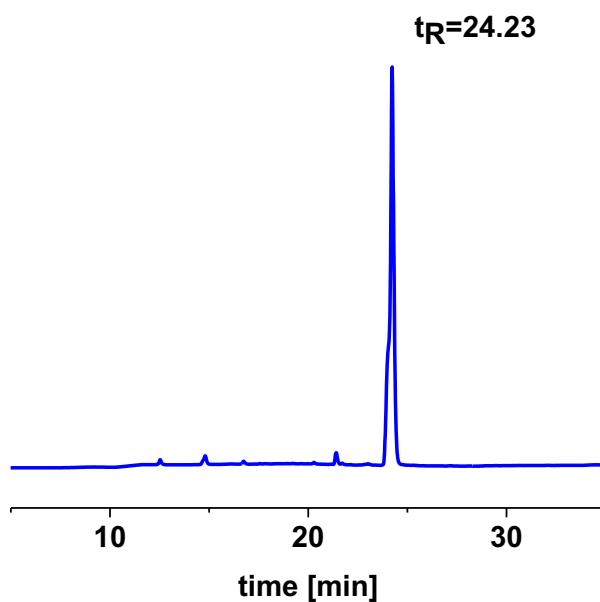


Figure S12. ESI-MS spectrum of cyclic KTTHWGFTLG peptide (**5**).

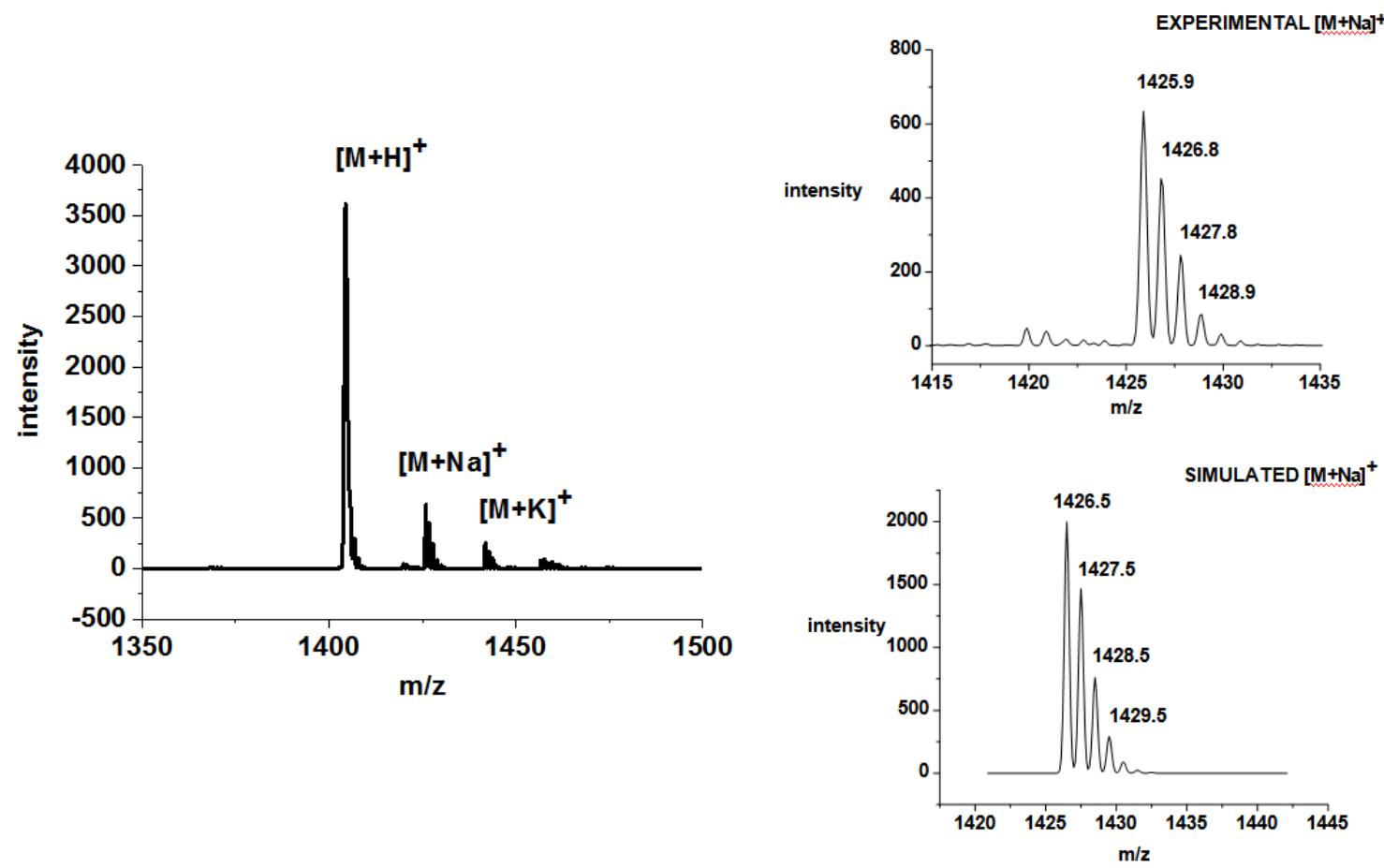


Chemical Formula:  $C_{62}H_{80}AuN_9O_{12}S_2$   
Exact Mass: 1403,50  
Molecular Weight: 1404,46

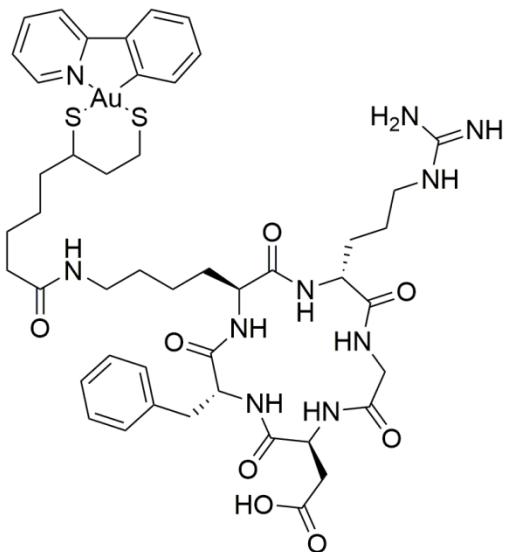
**Figure S13.** Structure of gold(III)- LTVXPWX bioconjugate (**6**).



**Figure S14.** HPLC chromatogram at 214 nm of gold(III)- LTVXPWX bioconjugate (**6**).



**Figure S15.** ESI-MS spectrum of gold(III)- LTVXPWX bioconjugate (**6**).

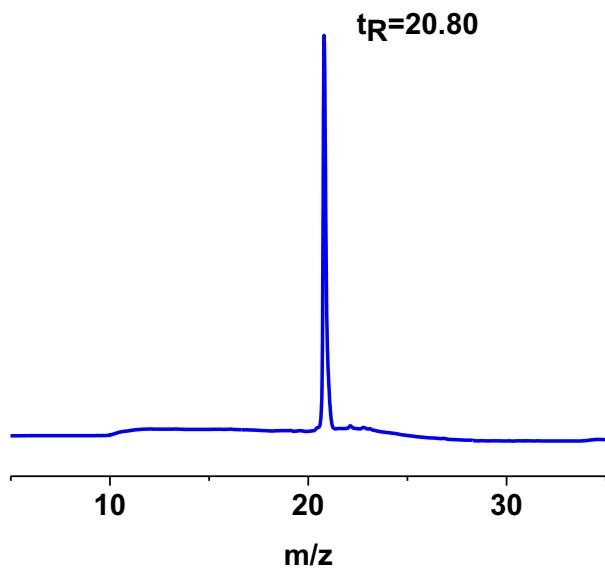


Chemical Formula:  $C_{46}H_{61}AuN_{10}O_8S_2$

Exact Mass: 1142,38

Molecular Weight: 1143,14

**Figure S16.** Structure of gold(III)- RGDFK bioconjugate (7).



**Figure S17.** HPLC chromatogram at 214 nm of gold(III)- RGDFK bioconjugate (7).

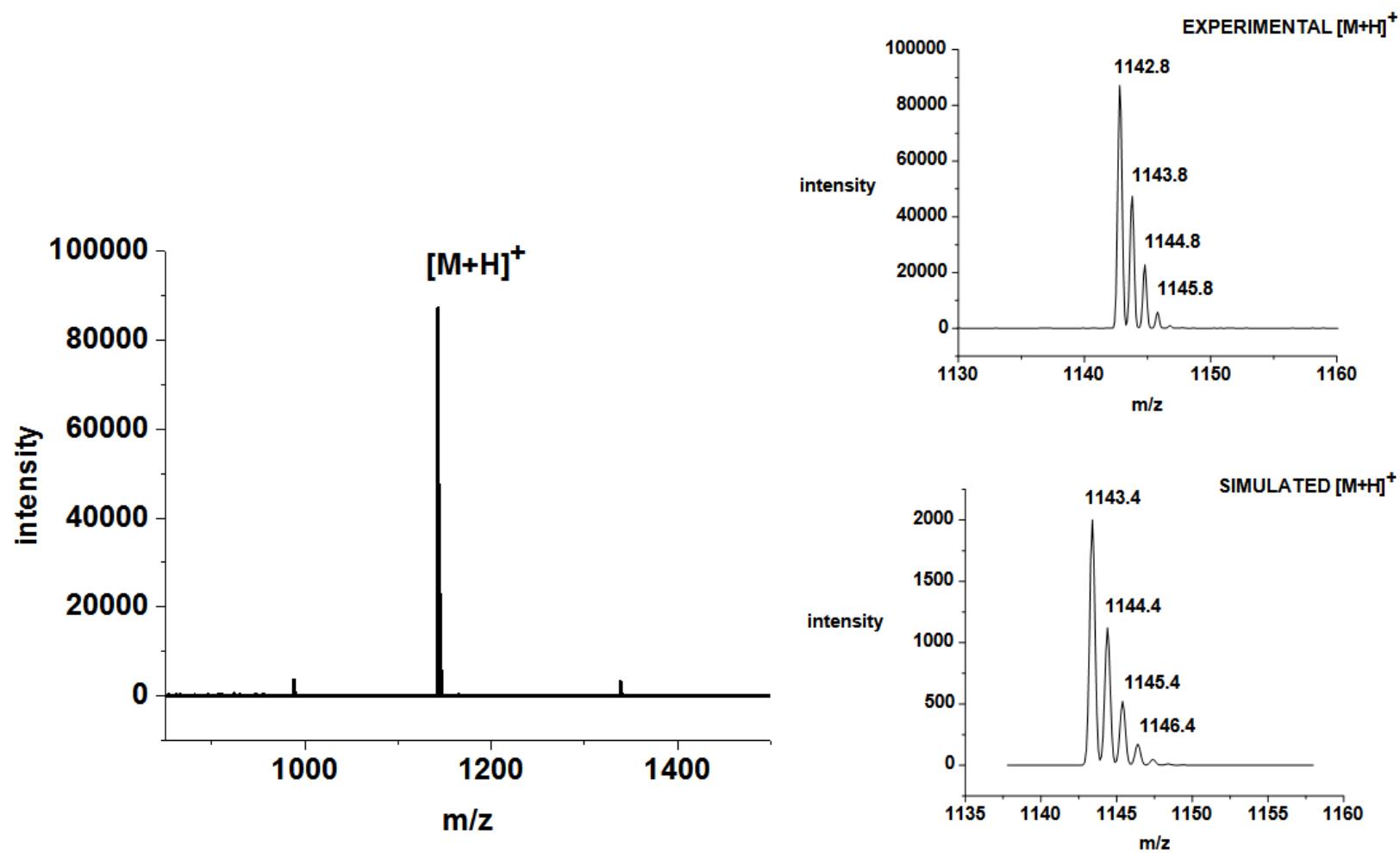
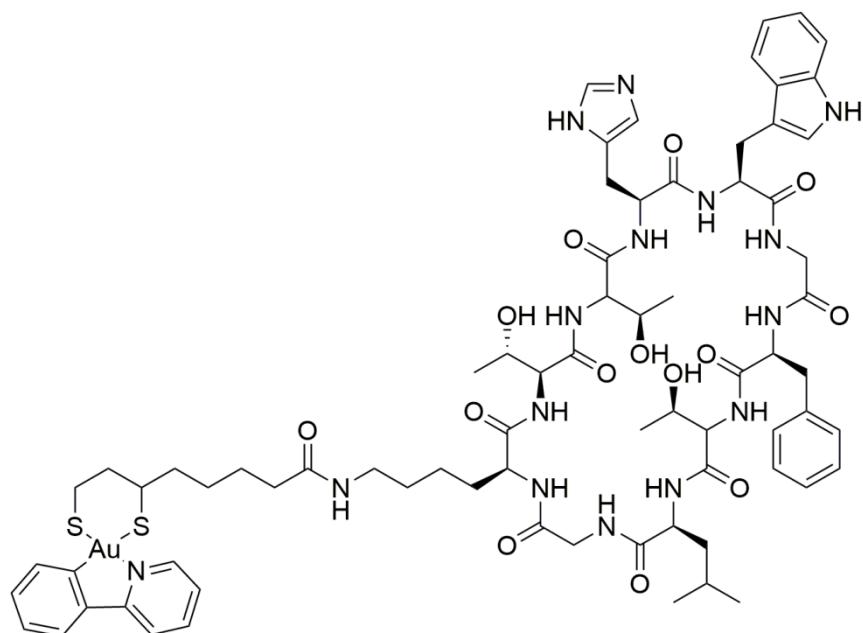
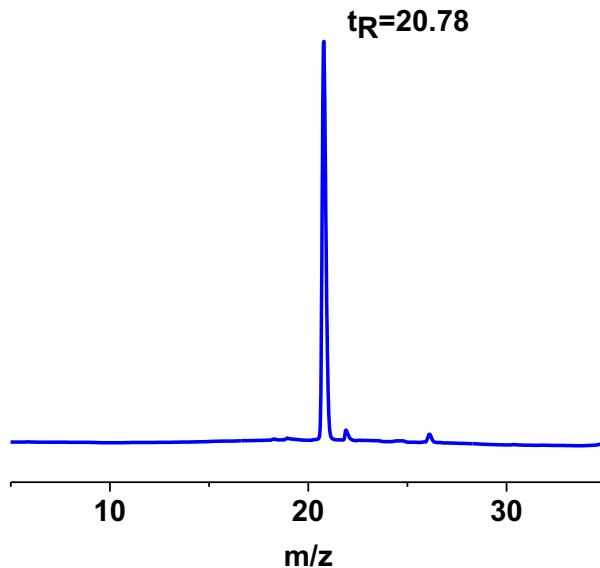


Figure S18. ESI-MS spectrum of gold(III)- RGDFK bioconjugate (7).

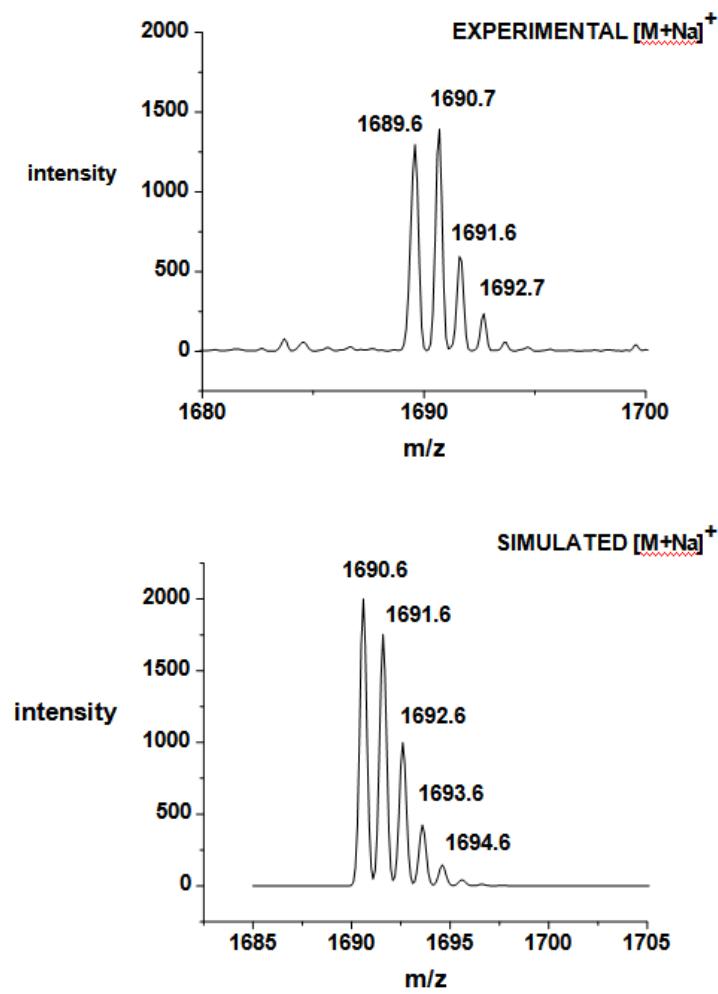
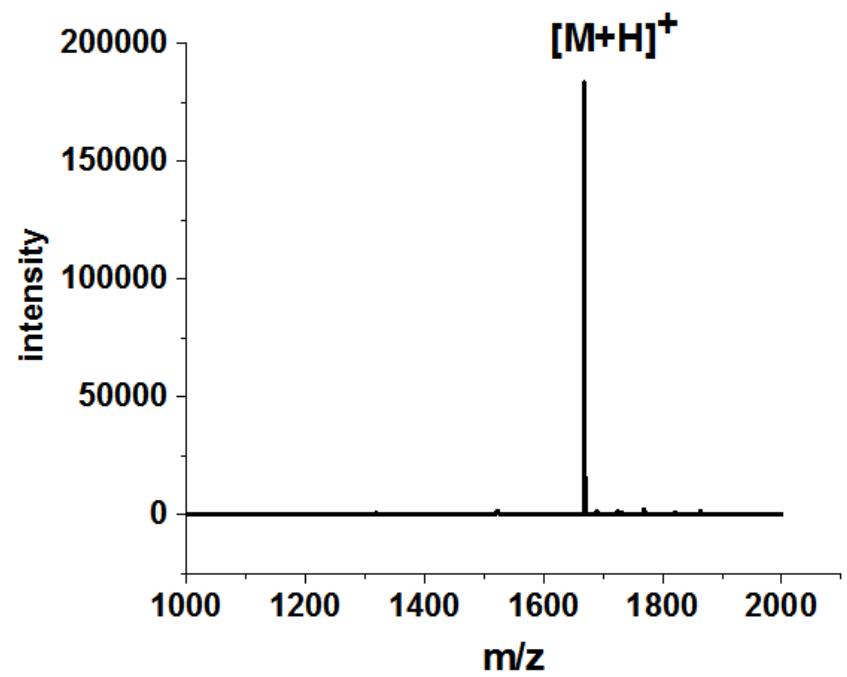


Chemical Formula:  $C_{73}H_{96}AuN_{15}O_{14}S_2$   
 Exact Mass: 1667,64  
 Molecular Weight: 1668,75

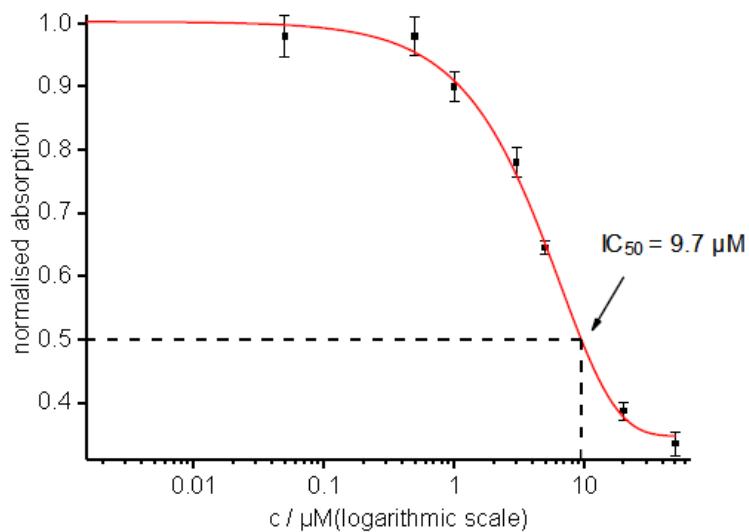
**Figure S19.** Structure of gold(III)- KTTHWGFTLG bioconjugate (8).



**Figure S20.** HPLC chromatogram at 214 nm of gold(III)- KTTHWGFTLG bioconjugate (8).



**Figure S21.** ESI-MS spectrum of gold(III)- KTTHWGFTLG bioconjugate (**8**).



**Figure S22.** The dose-response curve for the determination of the IC<sub>50</sub> value of bioconjugate **7** on MDA-MB-231 cells.

**Table S1.** Cytotoxicity data determined by MTT after 48 h of incubation.

IC <sub>50</sub> [ $\mu$ M] <sup>a</sup>	Cell lines		
	MCF7	MDA-MB-231	GM5657T
<b>CDDP</b>	8.9±2.3	22.4±2.5	10.2±2.1
<b>1</b>	44.3±3.6	77.9±5.1	50.8±4.1
<b>6</b>	24.8±2.9	12.5±0.5	11.5±0.8
<b>7</b>	6.3±1.3	9.7±1.6	7.2±1.3
<b>8</b>	36.3±4.3	50.1±4.6	40.2±3.2
<b>4</b>	80.6±12.6	106.7±15.1	110.5±6.1
<b>9</b>	>250	>250	>250
<b>10</b>	129±5.3	174.2±6.5	151.3±4.1

<sup>a</sup> The IC<sub>50</sub> values are averages of three independent determinations. All compounds were dissolved in DMSO (final concentration 0.5 %).