ELECTRONIC SUPPORTING INFORMATION

Toward predicting silver ion binding in proteins

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Table of contents

Experimental methods

Solid-Phase Peptide Synthesis

All tetrapeptide models were synthesized with a peptide synthesizer (Biotage Alstra + Initiator) by SPPS under stirring at room temperature.[1] The synthesis starts with the swelling of the dry Fmoc (9-fluoromethoxy-carbonyl) protected H-Rink-Amide resin (ChemMatrix, loading: 0.42-0.47 mmol/g) with DCM (dichloromethane, Fisher Chemical ≥99.8%) for 60 min. The Fmoc-deprotection step was then performed twice by using 20% piperidine (Thermo Scientific 99%) in DMF (N, N'-dimethylformamide, Fisher Chemical ≥99.5%) for 3- and 10-min. Free amines were coupled with Fmoc-protected amino acid (all from Iris Biotech GMBH ≥98%, except histidine and alanine from Fluorochem ≥98%, and methionine from Carl Roth ≥98%) in DMF by using HCTU (O-(1H-6-Chlorobenzotriazole-1-yl)-1,1,3,3-hexafluorophosphate, Acros Organics ≥98%) in DMF and HOBt (1H-1,2,3-Benzotriazol-1-ol hydrate, Sigma-Aldrich ≥97%) in DMF as coupling agents and DiEA (N-Ethyl-N-(propan-2-yl)propan-2-amine, Acros Organics ≥99%) in NMP (1-Methylpyrrolidin-2-one, Sigma-Aldrich ≥99.9%) as organic base for 60 min. To avoid side products with similar properties to the desired tetrapeptide, the capping of the unreacted amines was performed with a mixture of acetic anhydride (Acros Organics ≥99%) in DMF, and DiEA in NMP for 10 min. At the end of the synthesis, the N-terminus was acetylated by using a mixture of acetic anhydride in DMF, and DiEA in NMP for 10 min, followed by a pre-cleavage wash with DCM. Side chains deprotection and cleavage from the resin were carried out by adding 6.3 mL of a mixture of 95.5% TFA (Trifluoroacetic acid, Thermo Scientific ≥99%), 1.5% bidistillated H_2O, 1.5% TIPS (Tri(propan-2-yl)silane, Thermo Scientific ≥98%), and 1.5% EDT (ethane-1,2-dithiol, Sigma-Aldrich ≥98%) for 2 h. Then, a filtration was done with TFA followed by precipitation with cold diethylether (Fisher Chemical ≥99.5%). The product was centrifuged at 7500 g for 6 min. The precipitate was dried and purified by semi-preparative reverse-phase HPLC (Waters Delta 600) on a NucleoDurTM C18 HTec column (Macherynagel) with a linear gradient from 95% to 70% of A in B, at a flow rate of 5 mL/min for 25 min, where A is a solution of 0.1% TFA in H_2O, and B is a solution of 0.1% TFA in ACN (acetonitrile, Riedel-de-Haën ≥99.9%). Finally, the collected product was lyophilized (Christ Alpha 1-2 LDplus) for 2 days.[2,3]

Formation of Ag^+/tetrapeptide complexes

To obtain Ag^+/tetrapeptide complexes, around 5 mg of each lyophilized tetrapeptide was dissolved in 200-300 µL of bidistillated H_2O. Then, 20 µL of $AgNO_3$ solution 1M in bidistillated H_2O was added, and the solution was lyophilized for 1-2 days.

Electrospray ionization mass spectrometry

The ESI-MS (Brucker Esquire HCT) in positive ion mode was performed on all the tetrapeptides immediately after the purification by semi-preparative HPLC to verify that the correct tetrapeptide was obtained (Fig. S58-S112). This technique was also used to confirm the formation of Ag^+/tetrapeptide complexes.

Ultraviolet-visible spectroscopy

The concentrations of the tetrapeptide solutions were accurately determined by UV-Vis spectroscopy (Perkin Elmer Lambda 25) and the Beer-Lambert law: $A_\lambda = \varepsilon_\lambda cl$, where *A* is the absorbance, ε_λ is the molar extinction coefficient at wavelength λ, *c* is the concentration, and *l* is the length of the cuvette (1 cm in this research). The molar extinction coefficient at 205 nm (ε_{205}) of each peptide was determined by using the formula of Anthis *et al.*:[4]

$$\varepsilon_{205} = \sum(\varepsilon_i n_i) + \varepsilon_{bb}(r-1),$$

where for each amino acid *i*, ε_i is the molar extinction coefficient of the amino acid side chain (from Goldfarb *et al.*)[5], n_i is the number of occurrences of that amino acid in the peptide sequence, ε_{bb} is the molar extinction coefficient for a single backbone peptide bond, and *r* is the number of amino acid residues in the peptide sequence. In the case of the HEWM probe, the exact concentration was determined from the molar extinction coefficient at 280 nm (ε_{280} = 5540 $M^{-1}\cdot cm^{-1}$).[6] This was achieved by dissolving approximately 1 mg of each lyophilized tetrapeptide in 700 µL of bidistillated H_2O and measuring.

Determination of Ag^+/tetrapeptides secondary structure

The study of the secondary structure was performed by using a circular dichroism (CD) spectrometer (Applied Photophysics Chirascan V100). The CD spectra of the peptides (Fig. S113-S114) were measured by adding a solution of $AgNO_3$ (silver nitrate, Fisher Chemical ≥99.9%) in bidistillated H_2O (0 to 8 equivalents) at 25°C.

Determination of Ag^+/tetrapeptides binding constants

The silver binding constants ($\log(K_{ass})$) of each tetrapeptide were determined by using a fluorescence spectrometer (Perkin Elmer LS 50 B). Each tetrapeptide studied was titrated

three times at two different concentrations ($5.0 \cdot 10^{-6}$ M and $1.0 \cdot 10^{-5}$ M) using a competition titration strategy with HEWM probe (1 equivalent) in MOPS (3-(N-morpholino)propanesulfonic acid, Alfa Aesar ≥99%) buffer (20 equivalents, pH 7.4-7.5) by addition of $AgNO_3$ (silver nitrate, Fisher Chemical ≥99.9%) solution in bidistillated H_2O (0 to 3.0 equivalents) at 25°C.[3,7,8]

Dynafit coding

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  M + P     <==> MP       :   Kd2    dissoc
  MP + M    <==> MMP      :   Kd3    dissoc
[constants]
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  Kd2 = 1.2e-06 ??
  Kd3 = 1.2e-07 ??
[responses]
 P* = 133638.76 ?, MP* = 70201.37 ?
[data]
  variable M, P, P*
  plot titration ;

  set 1

[output]
  directory ./data/output/fit
[settings]
{Output}
  XAxisLabel = [Metal], M
  YAxisLabel = Fluorescence, A.U.
;_____________________________________________________________________
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0.000367853     0.005963388     0.005192444     682.17
0.000735412     0.005961005     0.005190368     662.1
0.001469649     0.005956244     0.005186223     632.93
0.002202713     0.00595149      0.005182084     611.14
0.00330012      0.005944374     0.005175887     569.03
0.004394904     0.005937275     0.005169706     526.97
0.005850556     0.005927836     0.005161487     484.02
0.007301587     0.005918426     0.005153294     427.12
0.010909091     0.005895033     0.005132925     383.63
0.014488189     0.005871825     0.005112717     370.39
0.018039216     0.005848798     0.005092667     362.07
0.025058366     0.005803282     0.005053036     354.73
[end]
;_____________________________________________________________________
;_____________________________________________________________________
```

Fig. S1 Example of *Dynafit* code used to determine the binding constant for the competition titrations between HAAH and HEWM, both at $5 \cdot 10^{-6}$ M. *M* represents the metal ion (Ag^+), *P* represents the peptide (HAAH), *P** represents the probe (HEWM). The K_{d1} of the probe was determined by Chabert *et al*.[3,9,10]

All-atom force field simulations

Constant-pH (cpH) computer simulations

GROMACS 2021-beta1-dev-UNCHECKED was used to perform *λ*-dynamics cpH-MD simulations of the apo forms of the five tetrapeptides.[11,12] An *ad-hoc* CHARMM36m modified force field is available for this purpose. The structure of each peptide was loaded on CHARMM-GUI webserver in order to obtain input files for GROMACS simulation package (with classical CHARMM36m forcefield).[13,14] After that, the atom classes of the titrable atoms in the forcefield .itp files were modified to be consistent with the constant-pH force field. The software Phbuilder.py was used to prepare input files for cpH simulations.[15] A minimization of 1000 steps with a force tolerance of 1000 kJ mol^{-1} nm^{-1} with steepest descent algorithm was used to relax the initial structure of the system. It was followed by 10 ps of NVT equilibration with a timestep of 2 fs and 10 ps of NPT equilibration with the same timestep. LINCS algorithm was used to constrain hydrogen bonds.[16] The equations of motion were integrated with the Leap-Frog algorithm.[17] Velocity rescale thermostat was used to keep the temperature at 300 K using the whole system as one coupling group.[18] C-rescale barostat was implemented to keep the pressure at 1 bar with a coupling constant of 5 ps to rescale the box size every 10 steps.[19] Coulomb interactions were managed with Particle Mesh Ewald (PME) scheme with a cutoff at 12 Å.[20] Lennard-Jones interactions were managed by means of a force-switch scheme to bring the interaction to zero between 10 and 12 Å. The box side was 30 Å filled with TIP3P water molecules. The simulations were performed at pH=7.4 to match experimental conditions. A mass of 5 a.m.u. was applied to the *λ*-particles. The thermostat coupling constant for the *λ*-particles tau was set to 2.0 ps. Three different replicas per peptide were simulated for 5 consecutive blocks of 100 ns each in NPT ensemble, for a total simulation time of 1.5 *μ*s for each system.

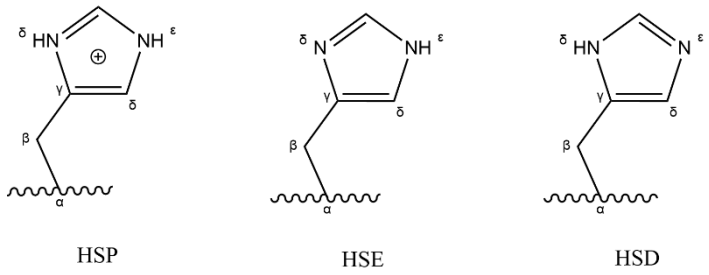

Fig. S2 Tautomers of the histidine side chains as defined in CHARMM force field family: HSP (left, positive), HSE (center, neutral), and HSD (right, neutral).

The fractions χ of the three tautomers HSP, HSE, and HSD (Fig. S2) calculated from cpH simulations of the apo-forms of the peptides are also reported. The fractions were calculated by counting the number of frames where the λ values corresponding to each tautomer were greater than a threshold value of 0.75, then dividing each count by the sum of counts of the tautomers in each trajectory. Averages were calculated over the three replicas (obtaining one value for each block) and then over the five blocks for each tetrapeptide. Standard errors of the mean were calculated over the averages of each block.

Association constants of tetrapeptides from MD-based enhanced sampling and cpH computer simulations

The association constants of holo-forms in Table S1 were calculated with the approach of Grubmüller using potential-scaled molecular dynamics and subsequent Hamiltonian reweighting; CHARMM36m force field was used with newly developed non-bonded parameters for Ag^+ ion based on the work of Merz and coworkers.[21-24] Details of the computational methods can be found in our companion article together with the methodology of the Ag^+ parametrization.[25]

First, the microscopic association constant $K_{ass,HSE}$ was determined for the HSE tautomer (Ag^+ can only bind on the N-δ atom, see Fig. S2). Then, the macroscopic association constant with tautomeric correction $K_{ass,corr}$ was calculated with:

$$\log_{10}(K_{ass,corr}) = \log_{10}(K_{ass,HSE}) + \log_{10}(\chi_{\mathrm{HSE}}),$$

where χ_{HSE} is the fraction of the HSE tautomer in the apo form (Table S1). This equation assumes that the HSE tautomer is the exclusive binder of Ag^+ as seen in experiments (see also main text).

Table S1 Experimental and calculated association constants (in log scale) for the studied tetrapeptides (HEFM, MNEH, HAAM, MAAH, and HPPM) together with fractions of the three histidine tautomers and corrected association constants. The values are reported with the standard error of the mean.

Model	$\log_{10}(K_{ass,exp})$	$\log_{10}(K_{ass,HSE})$	$\log_{10}(\chi_{HSP})$	$\log_{10}(\chi_{HSE})$	$\log_{10}(\chi_{HSD})$	$\log_{10}(K_{ass,corr})$
HEFM	6.6 ± 0.1 [2]	6.0 ± 0.1	-0.72 ± 0.02	-0.28 ± 0.02	-0.56 ± 0.02	5.7 ± 0.1
MNEH	5.4 ± 0.1 [2]	5.75 ± 0.08	-0.253 ± 0.008	-0.651 ± 0.004	-0.66 ± 0.02	5.09 ± 0.08
HAAM	5.7 ± 0.1	5.91 ± 0.09	-1.046 ± 0.003	-0.231 ± 0.008	-0.49 ± 0.01	5.69 ± 0.09
MAAH	5.4 ± 0.1	5.91 ± 0.07	-0.466 ± 0.008	-0.451 ± 0.006	-0.518 ± 0.008	5.47 ± 0.07
HPPM	5.0 ± 0.1	6.2 ± 0.1	-0.91 ± 0.02	-0.50 ± 0.01	-0.251 ± 0.007	5.7 ± 0.1

Secondary structure determination of MPQH

The simulations were performed with two sets of eight replicas each, one set with Ag^+ and one set without Ag^+. For this analysis, we determined the RMSD of the backbone atoms with respect to a perfect α-helix for all sampled snapshots of each replica. A histogram was then generated for each of the eight replicas. The resulting eight histograms were used to calculate the average and standard error of the mean for the 25 bins (from 0.5 to 3.0 Ang). In the case of the holo-form, weighted histograms were generated based on the statistical weights.[25] The representative structures (Fig. 3e) correspond to the head of the most populated cluster as obtained by RMSD-based clustering (cutoff = 0.5 Å of the backbone atoms) using the leader algorithm of Wordom.[26]

Experimental data

HPLC: Retention times of tetrapeptides

Table S2 Retention times [min] of the peptides studied using semi-preparative reverse phase HPLC with a linear gradient from 95% to 70% of A in B, at a flow rate of 5 mL/min for 25 min, where A is a solution of 0.1% TFA in H_2O, and B is a solution of 0.1% TFA in ACN.

Model	Retention time [min]	Model	Retention time [min]	Model	Retention time [min]	Model	Retention time [min]
HQQM	4.80	MQQH	5.47	HQQH	2.57	MQQM	-
HRQM	4.53	MRQH	5.38	HRQH	2.47	MRQM	10.80
HQRM	4.52	MQRH	5.48	HQRH	2.60	MQRM	11.13
HPPM	11.60	MPPH	9.15	HPPH	3.62	MPPM	18.55
HQPM	6.70	MQPH	7.25	HQPH	2.57	MQPM	15.22
HPQM	7.17	MPQH	7.50	HPQH	2.60	MPQM	16.42
HKKM	4.00	MKKH	3.82	HKKH	2.62	MKKM	7.80
HRKM	4.45	MRKH	4.10	HRKH	2.55	MRKM	8.22
HKRM	4.17	MKRH	3.63	HKRH	2.53	MKRM	8.33
HAAM	6.18	MAAH	6.17	HAAH	2.58	MAAM	16.80
HRAM	5.10	MRAH	5.30	HRAH	2.60	MRAM	12.13
HARM	6.53	MARH	4.15	HARH	2.00	MARM	13.62
HRRM	4.92	MRRH	5.05	HRRH	2.68	MRRM	10.30
HAQM	6.55	HKQM	3.75	H−Hex−QM	11.02	H−Dap−QM	3.58

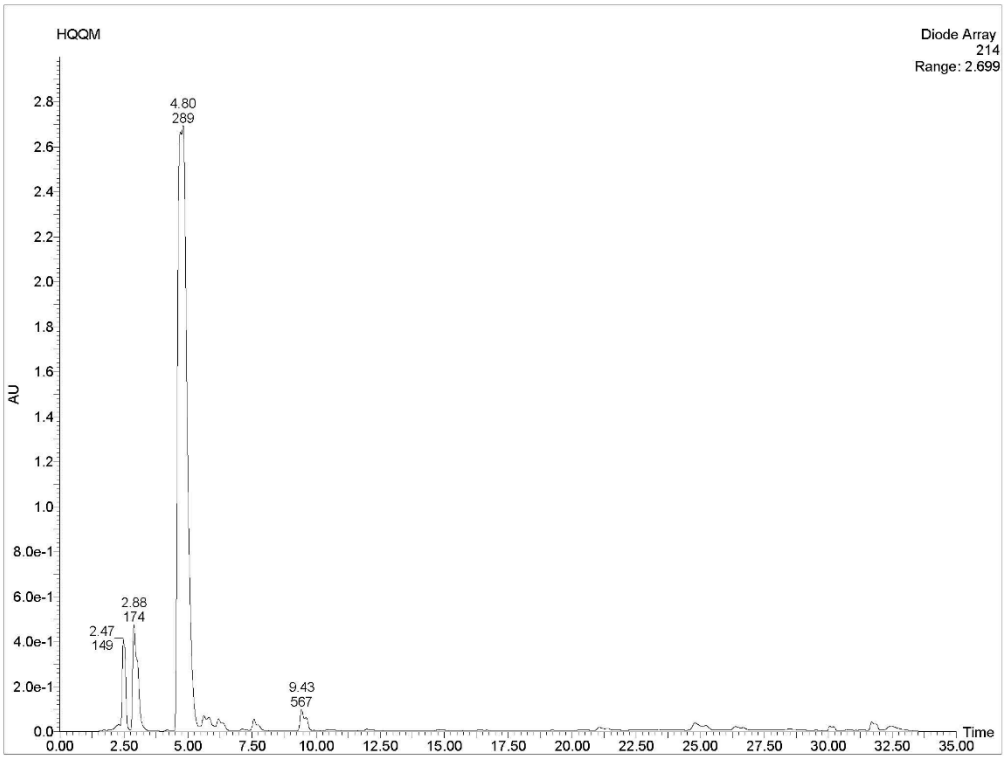

Fig. S3 HPLC chromatogram of HQQM

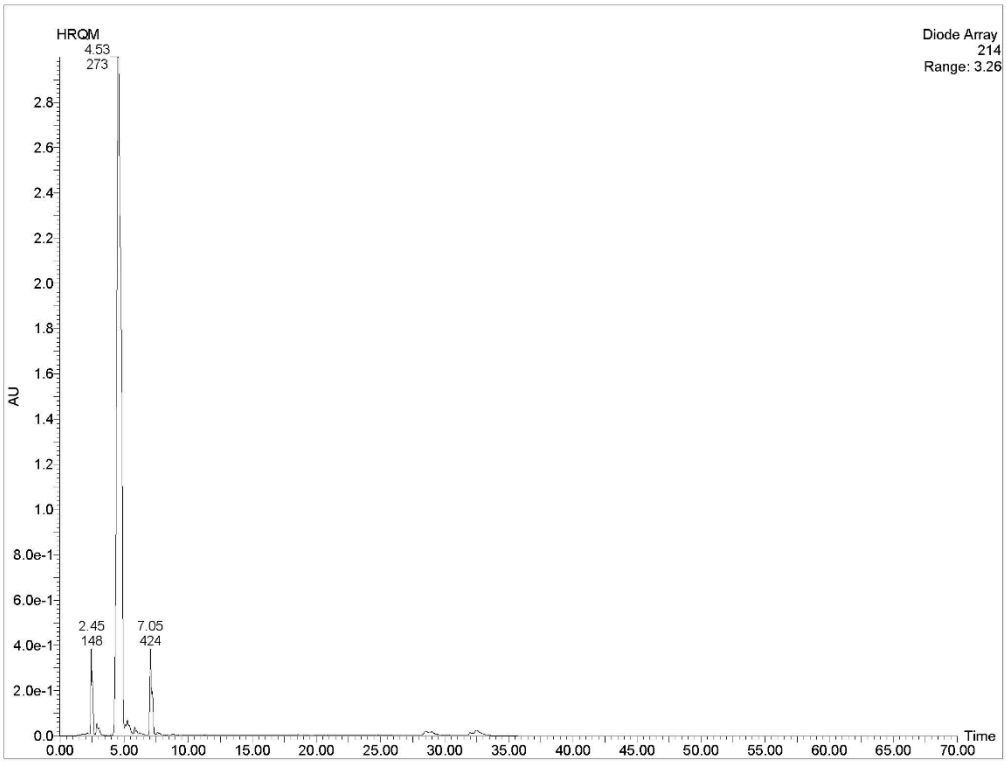

Fig. S4 HPLC chromatogram of HRQM

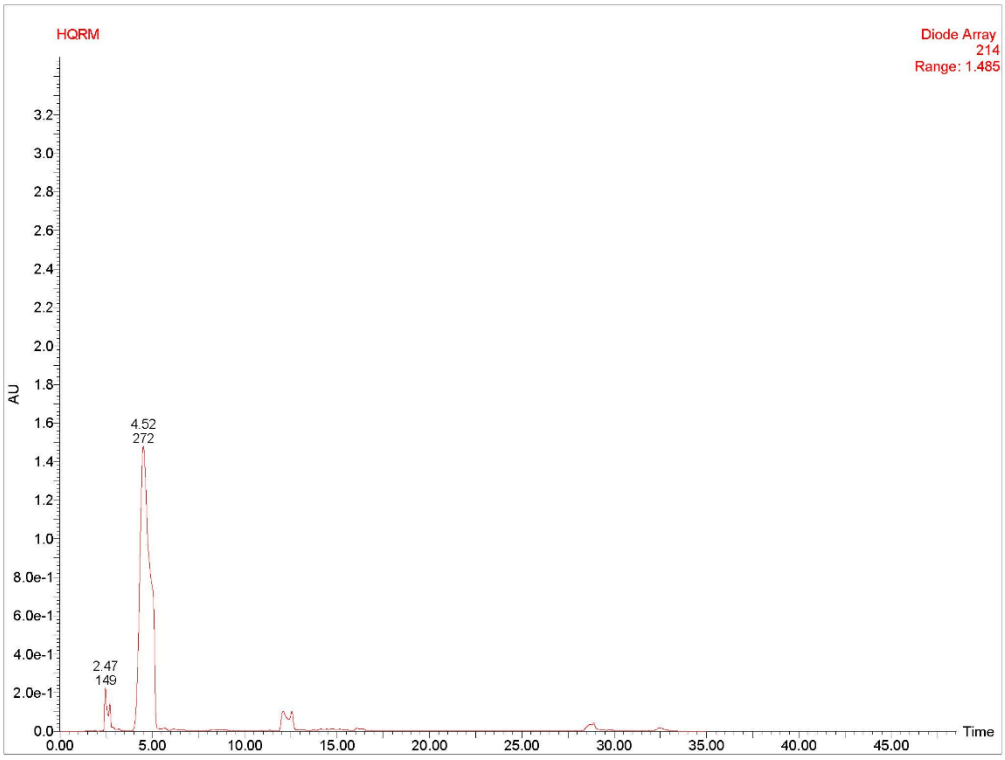

Fig. S5 HPLC chromatogram of HQRM

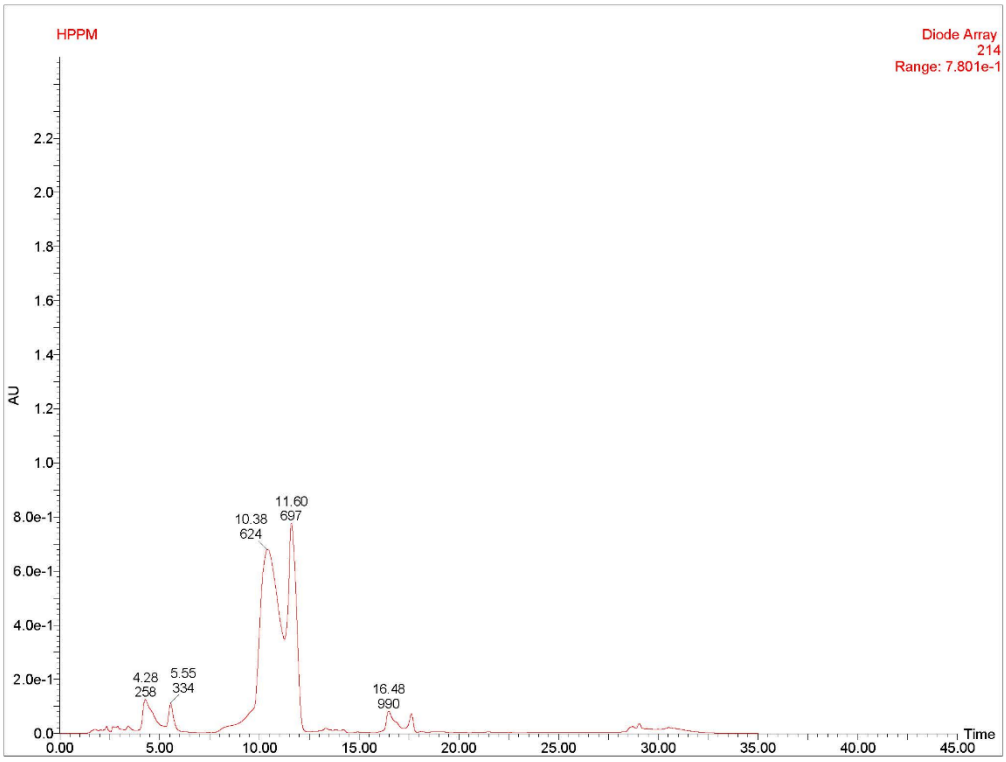

Fig. S6 HPLC chromatogram of HPPM

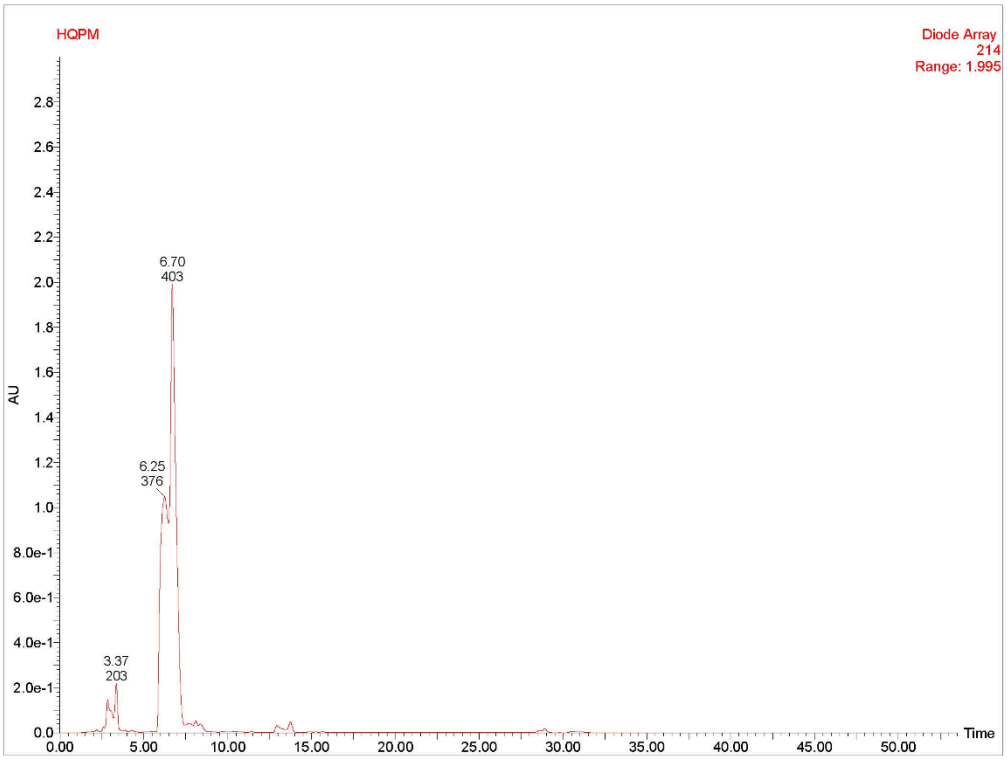

Fig. S7 HPLC chromatogram of HQPM

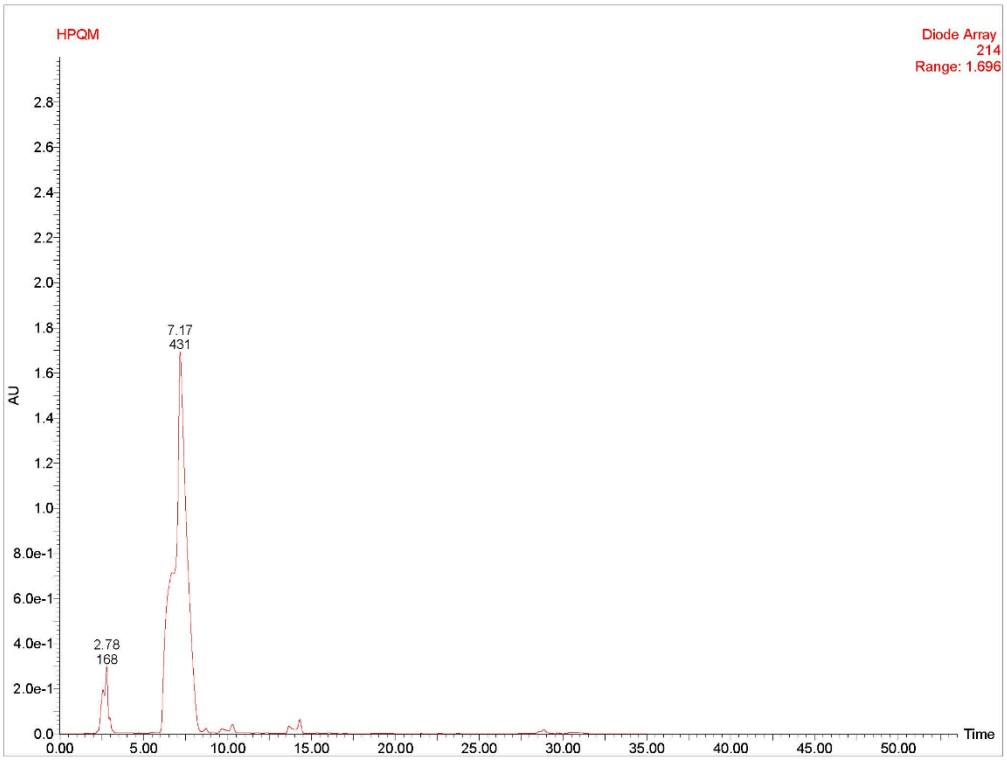

Fig. S8 HPLC chromatogram of HPQM

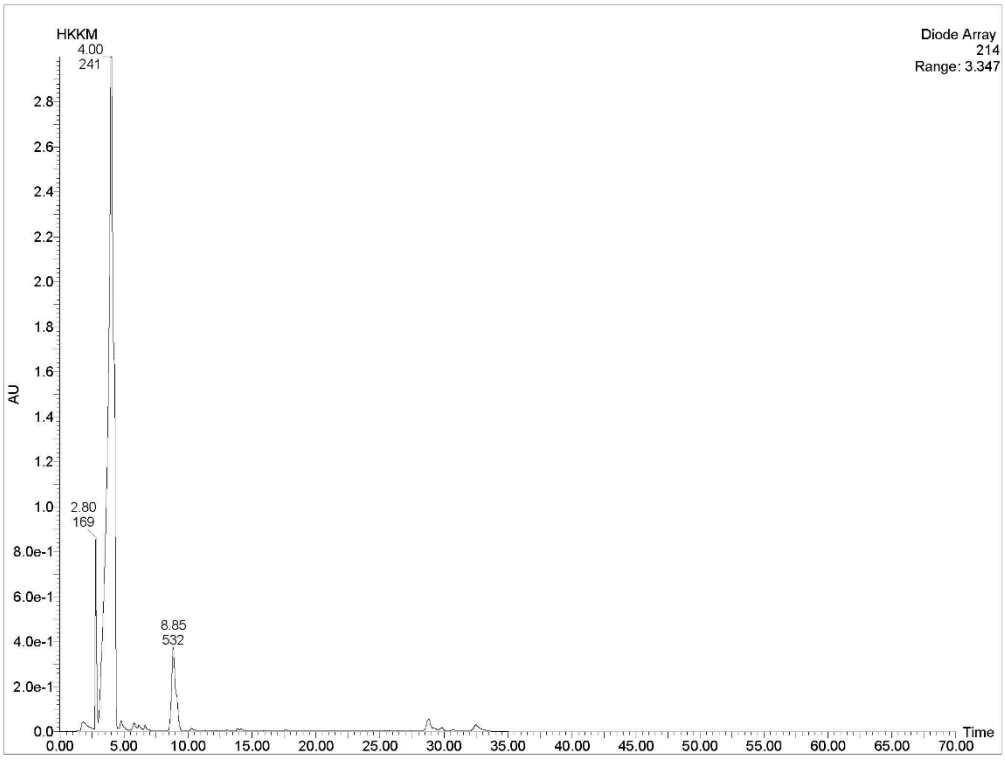

Fig. S9 HPLC chromatogram of HKKM

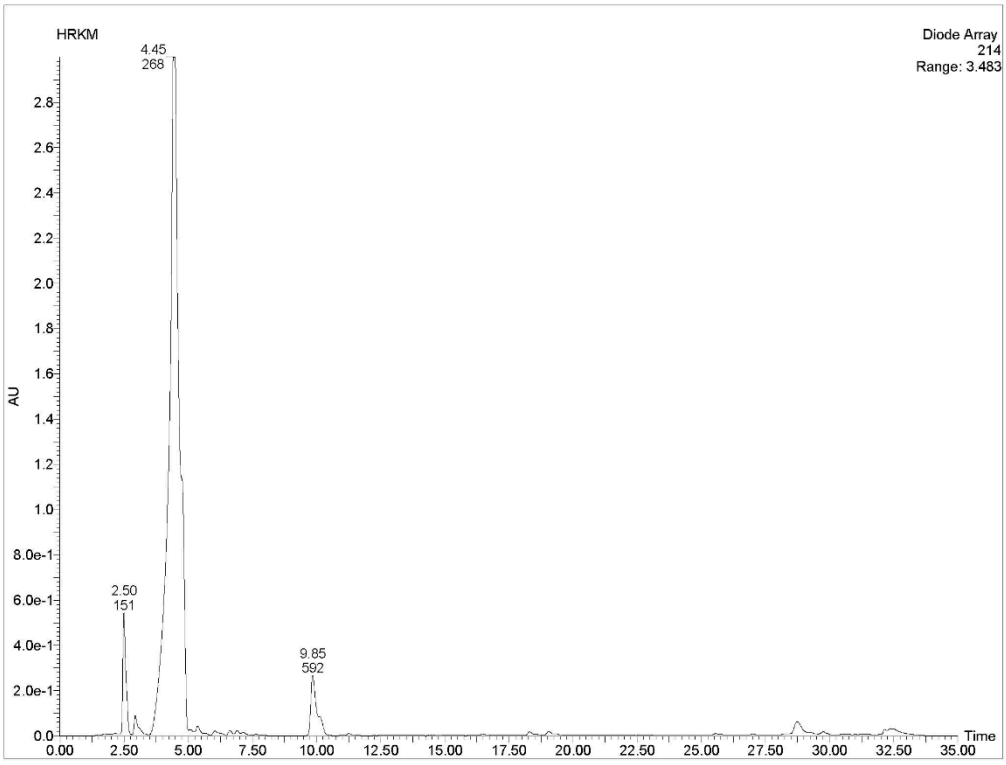

Fig. S10 HPLC chromatogram of HRKM

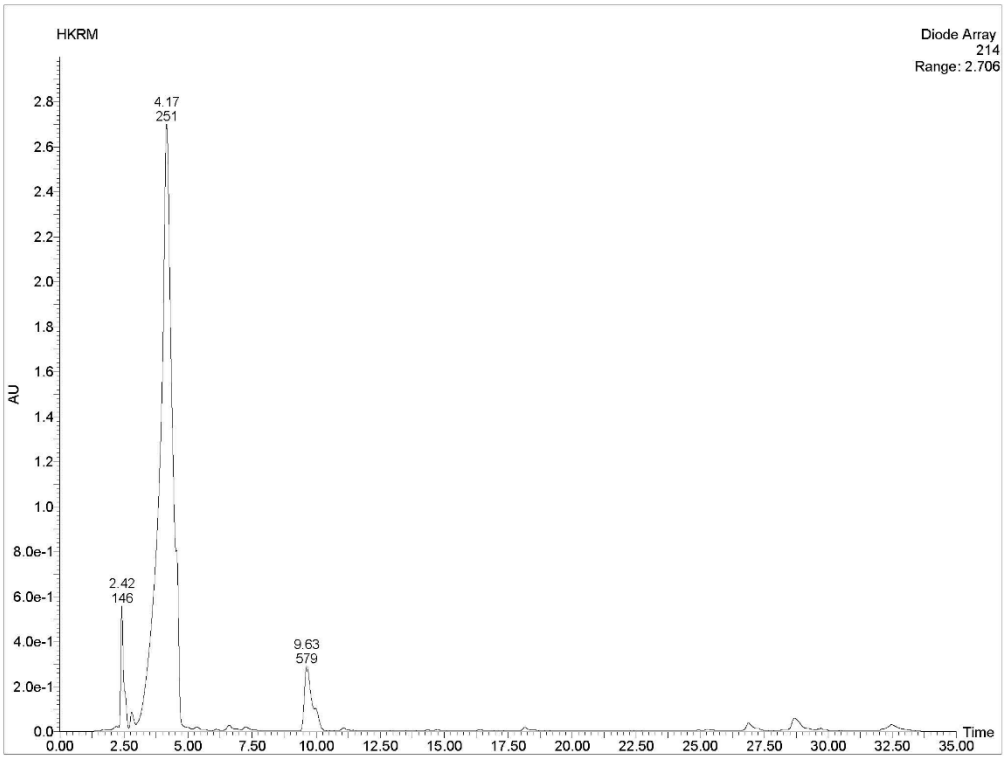

Fig. S11 HPLC chromatogram of HKRM

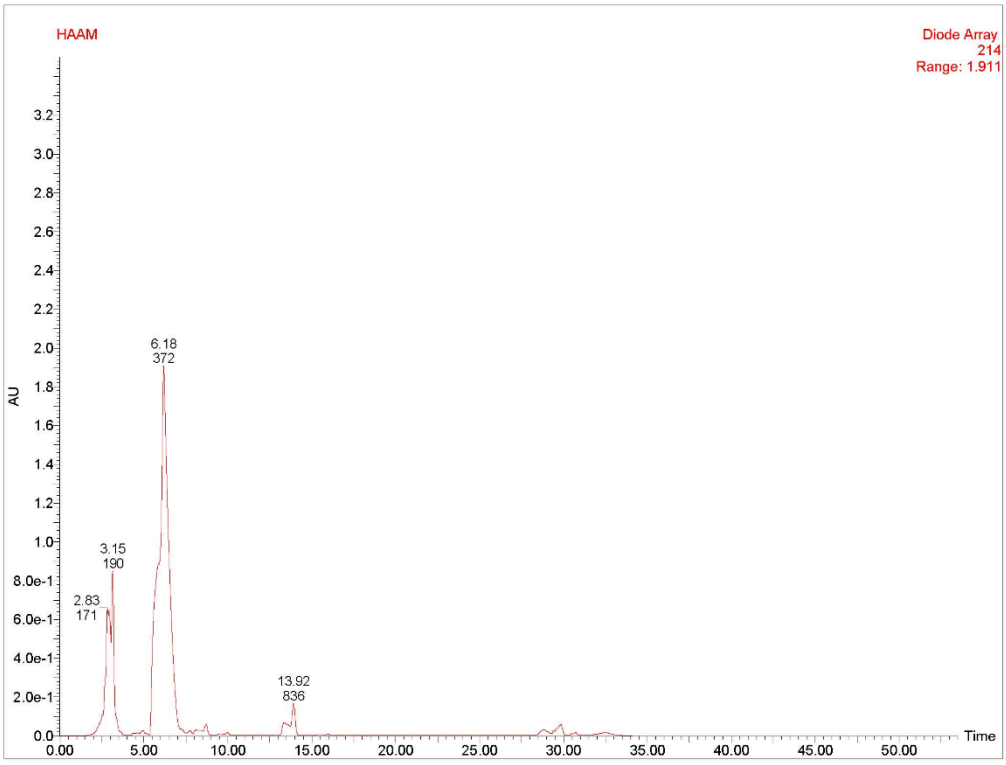

Fig. S12 HPLC chromatogram of HAAM

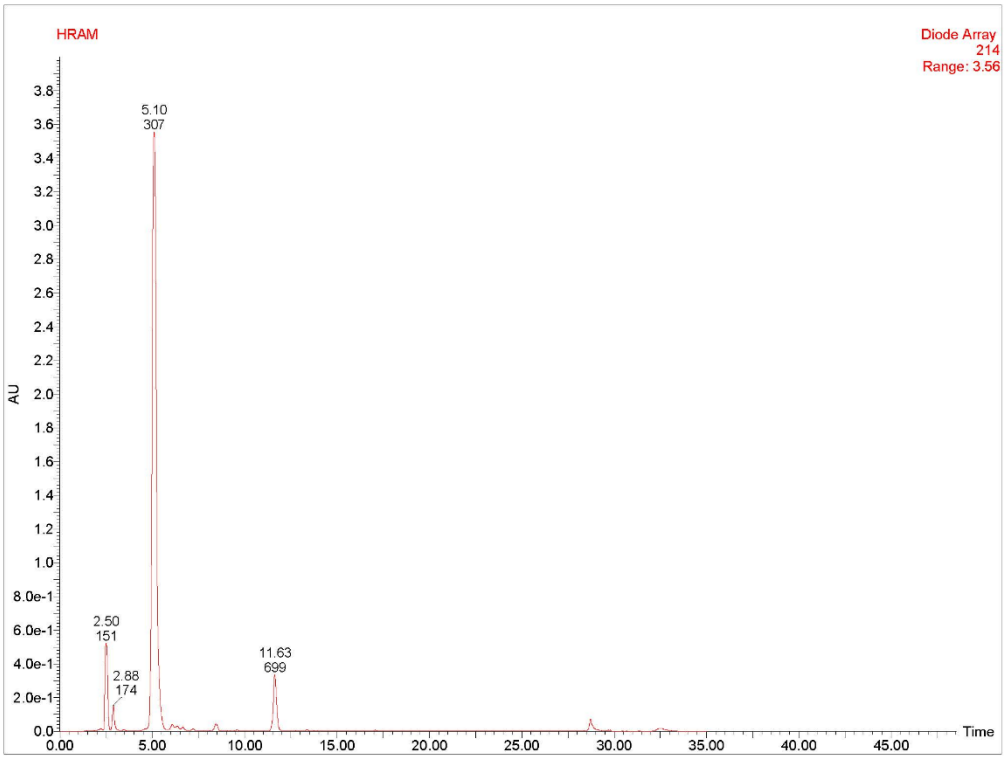

Fig. S13 HPLC chromatogram of HRAM

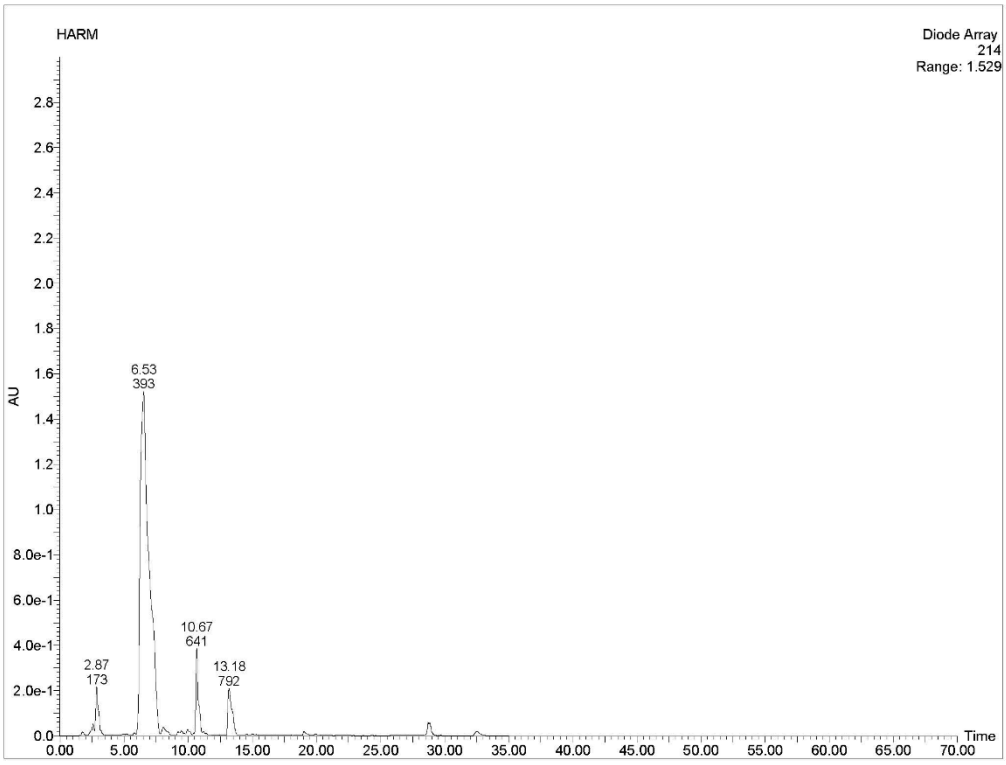

Fig. S14 HPLC chromatogram of HARM

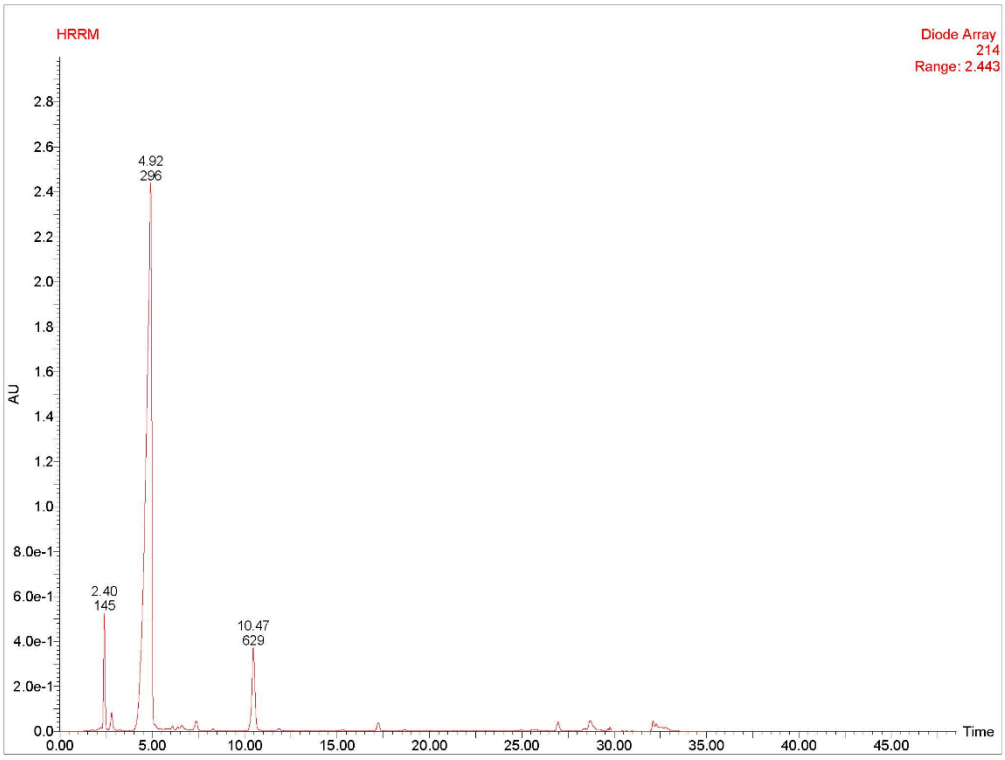

Fig. S15 HPLC chromatogram of HRRM

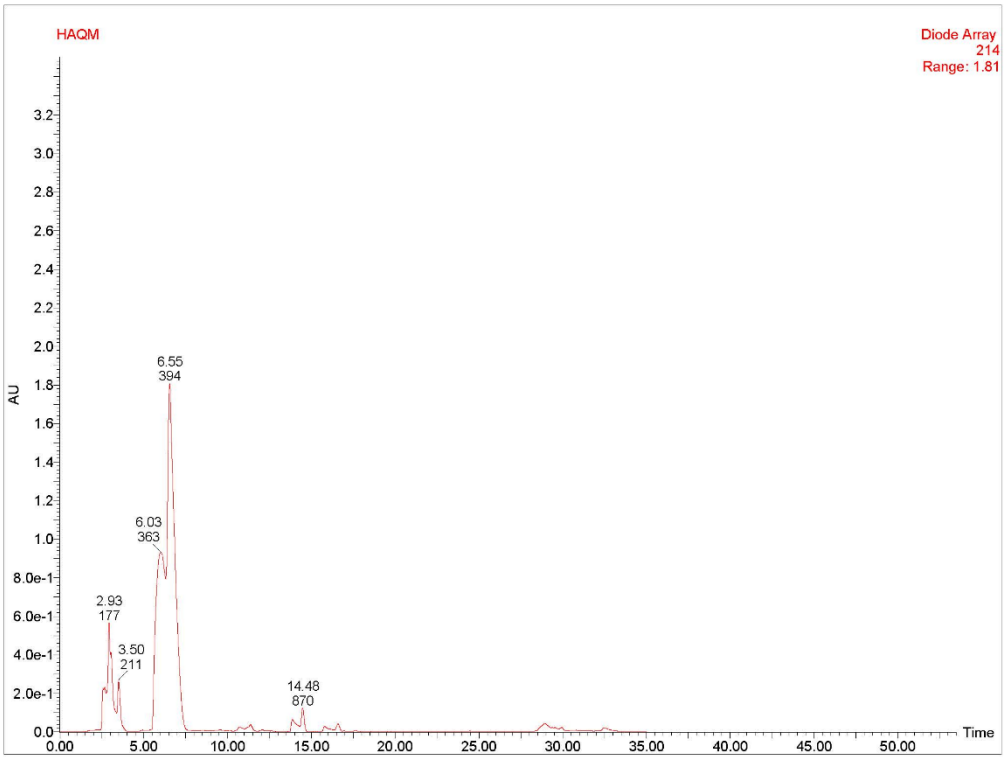

Fig. S16 HPLC chromatogram of HAQM

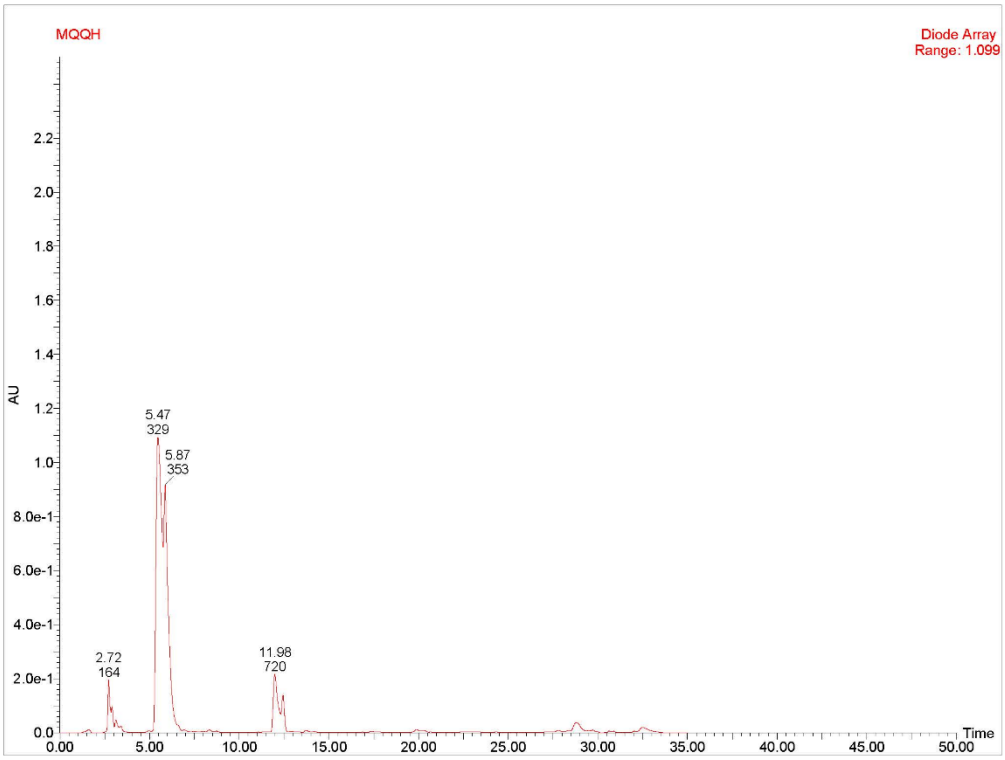

Fig. S17 HPLC chromatogram of MQQH

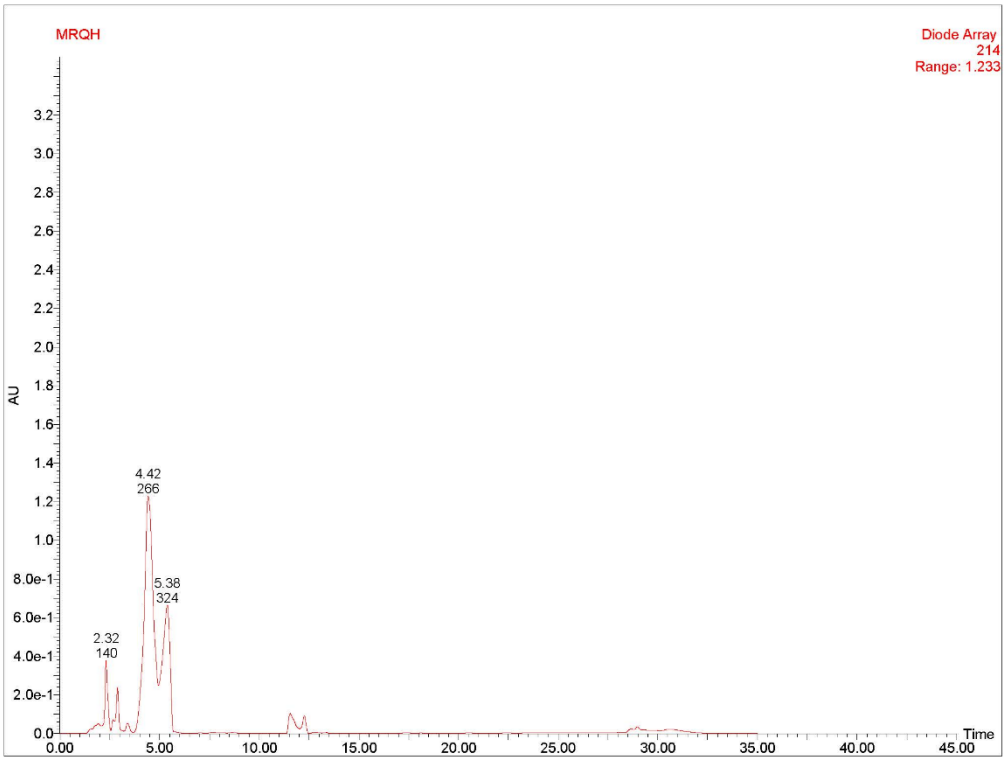

Fig. S18 HPLC chromatogram of MRQH

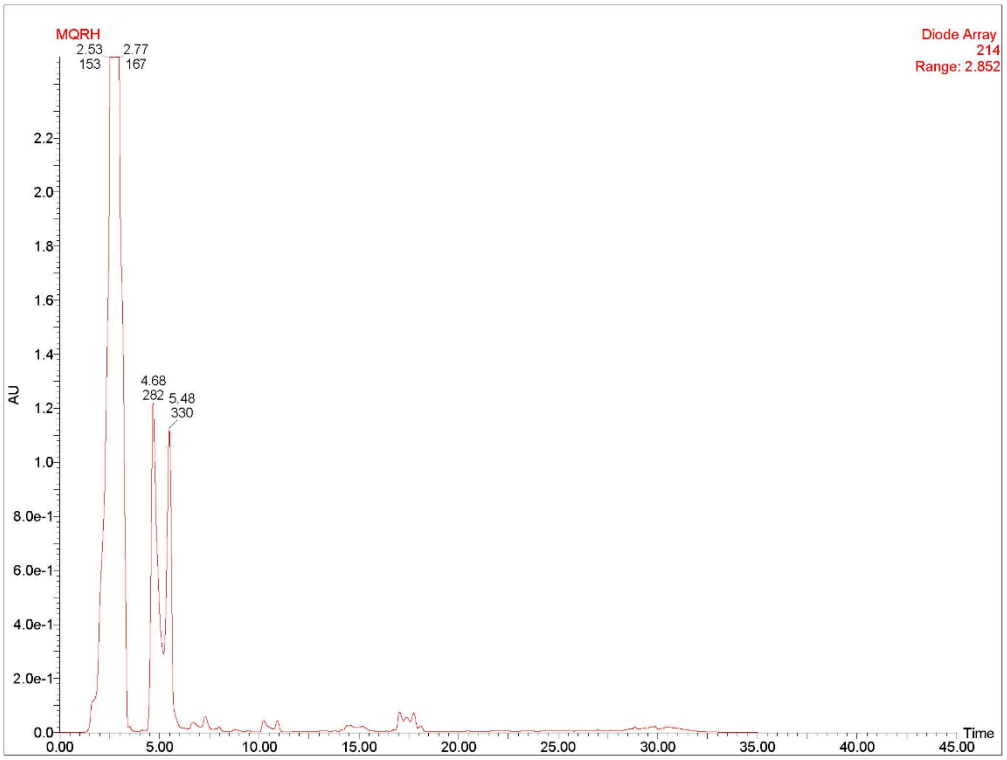

Fig. S19 HPLC chromatogram of MQRH

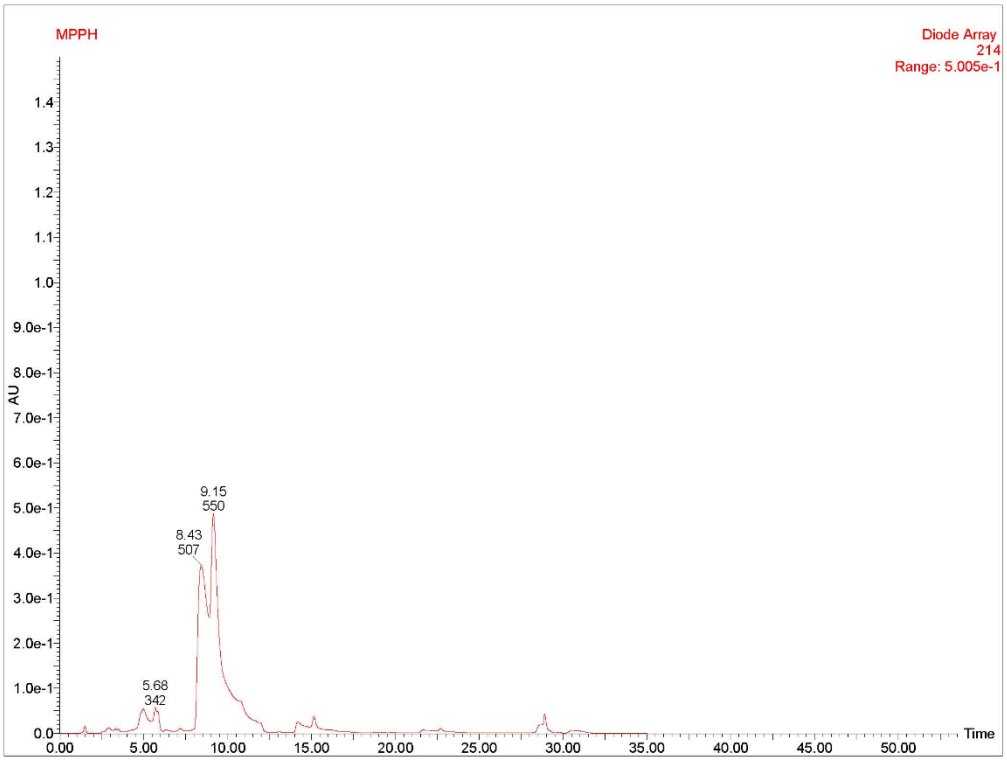

Fig. S20 HPLC chromatogram of MPPH

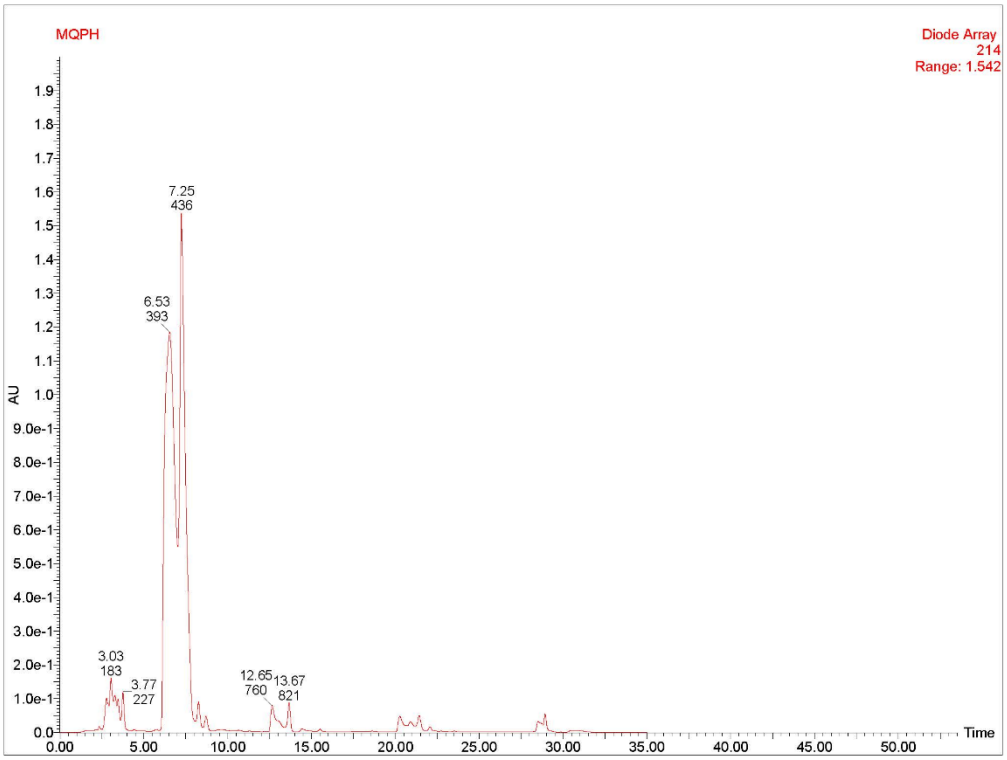

Fig. S21 HPLC chromatogram of MQPH

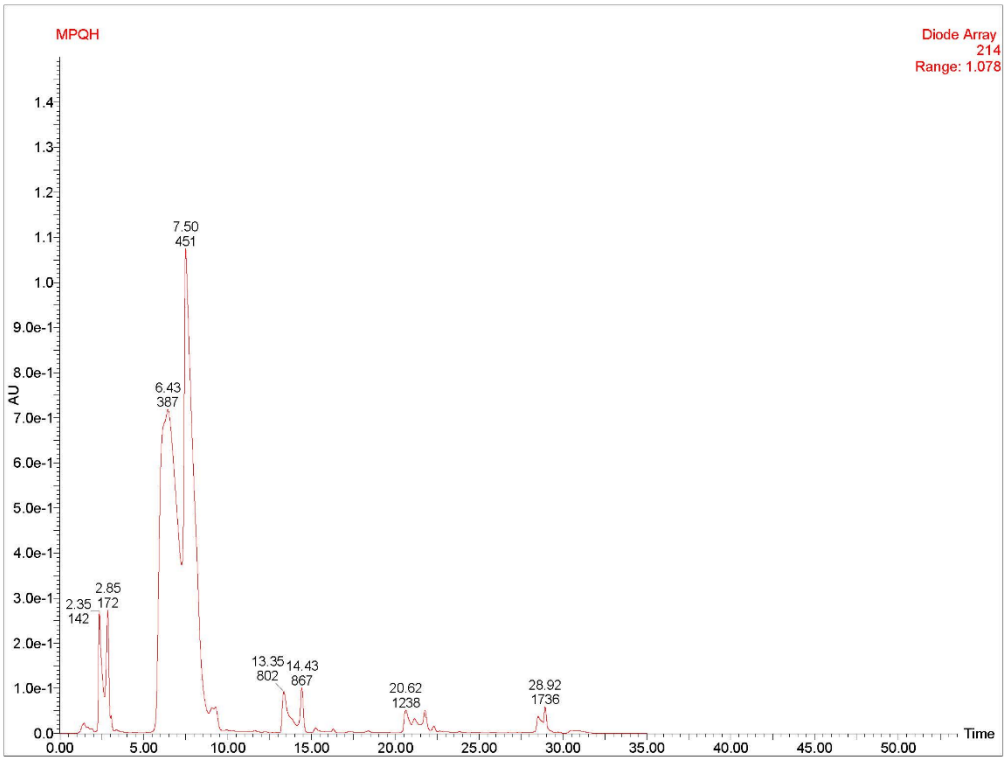

Fig. S22 HPLC chromatogram of MPQH

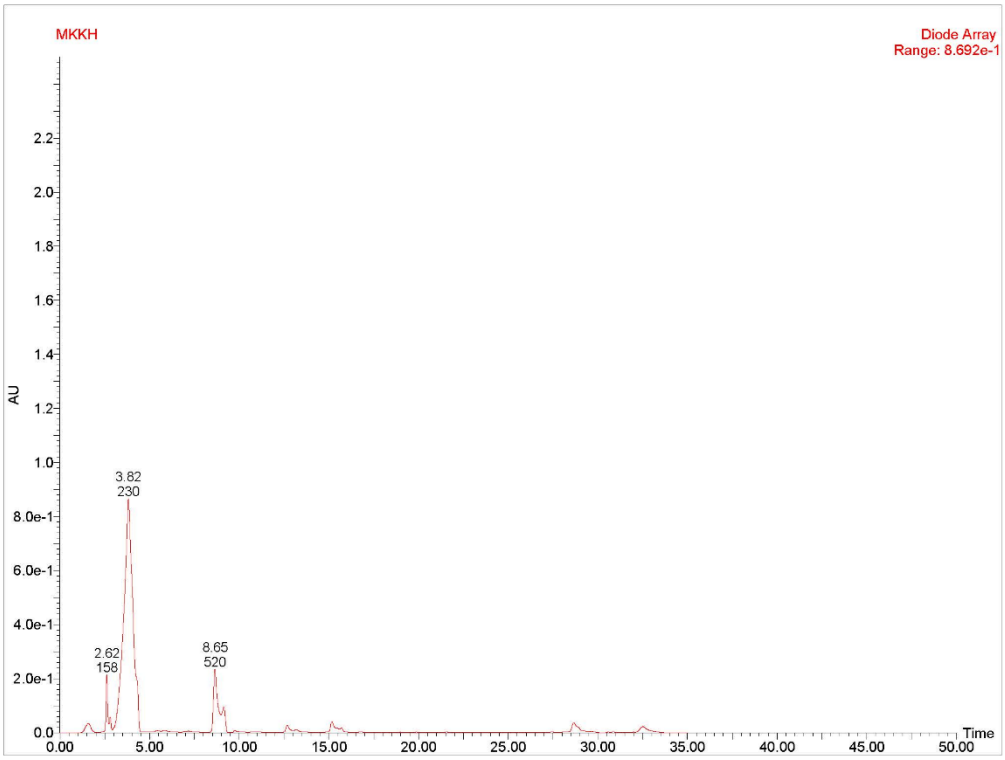

Fig. S23 HPLC chromatogram of MKKH

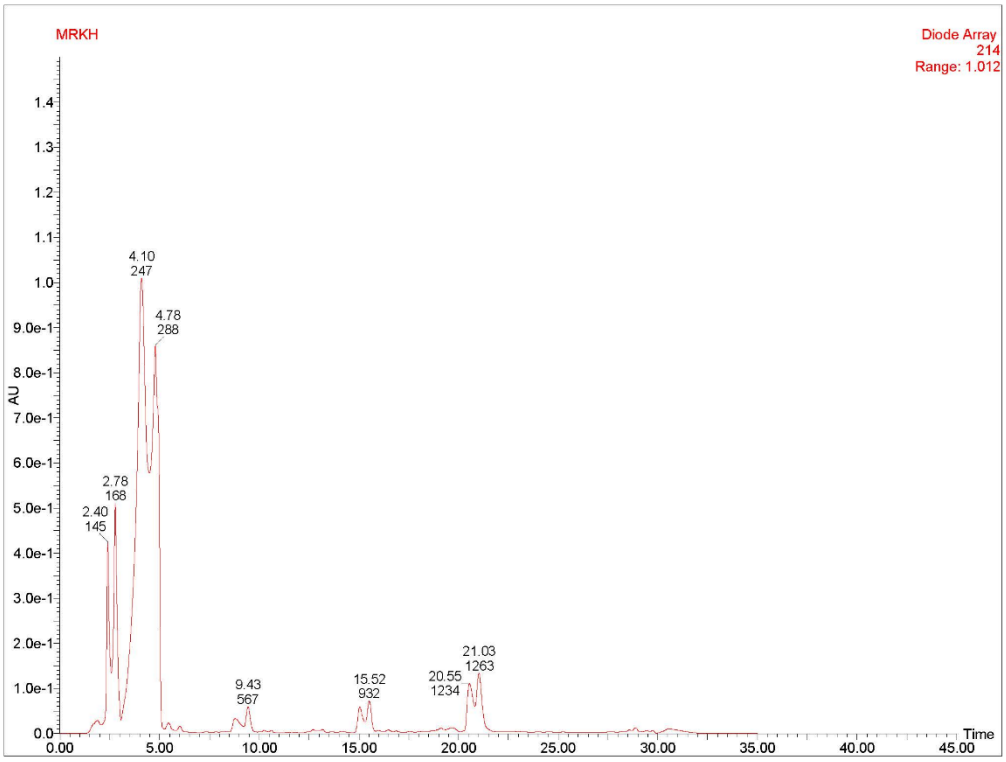

Fig. S24 HPLC chromatogram of MRKH

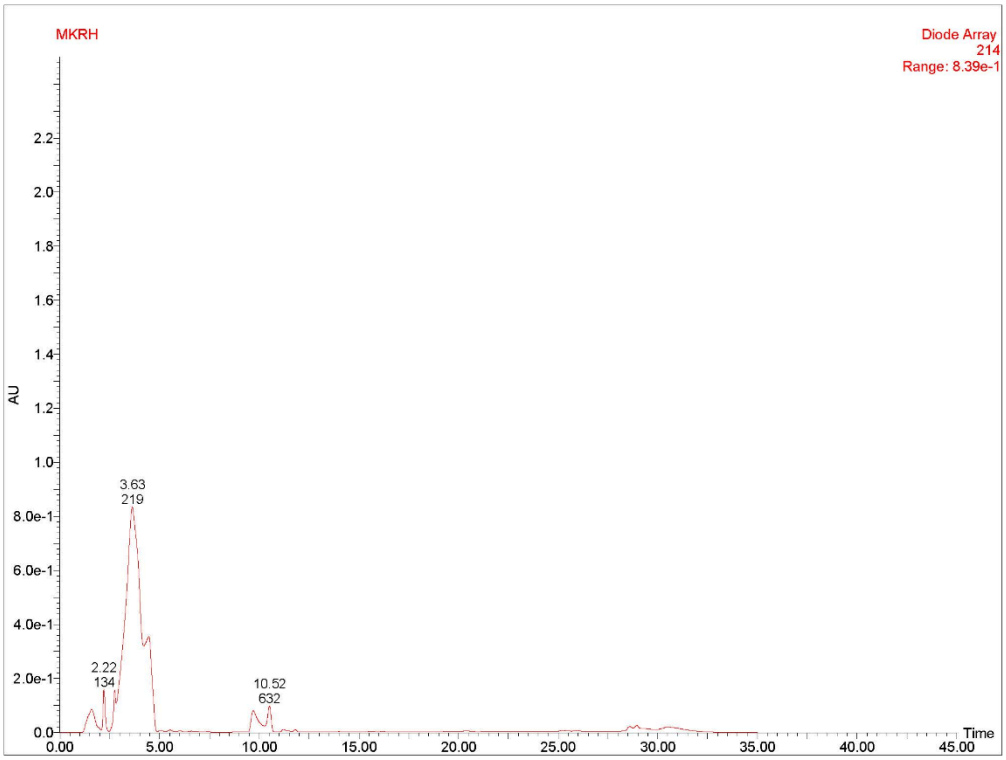

Fig. S25 HPLC chromatogram of MKRH

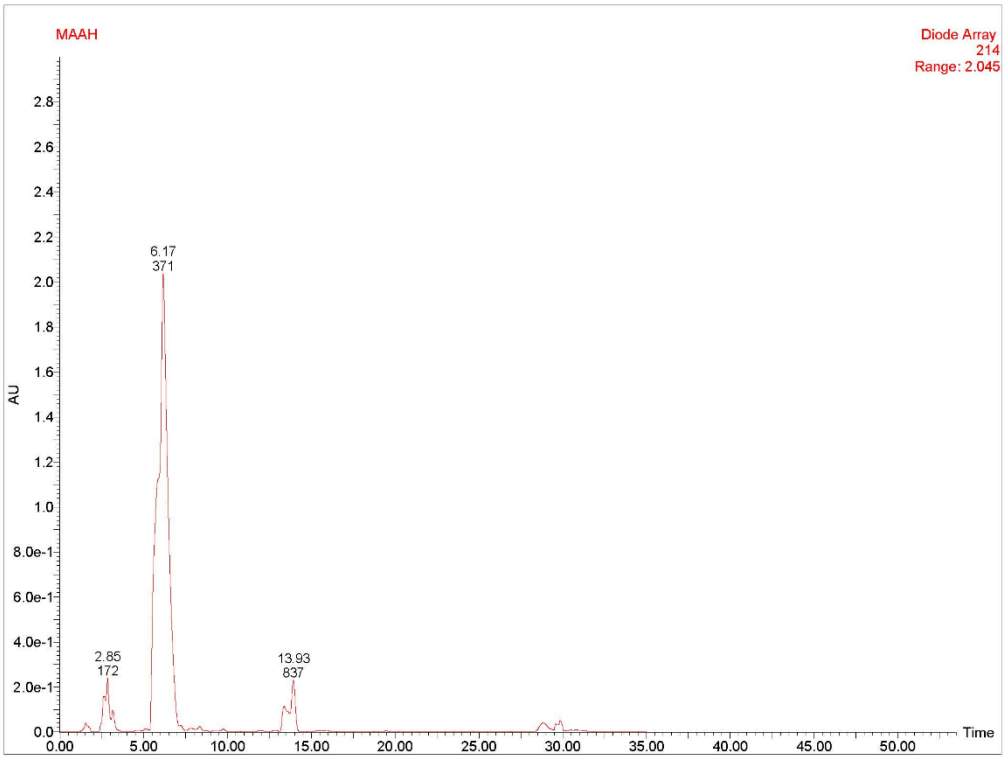

Fig. S26 HPLC chromatogram of MAAH

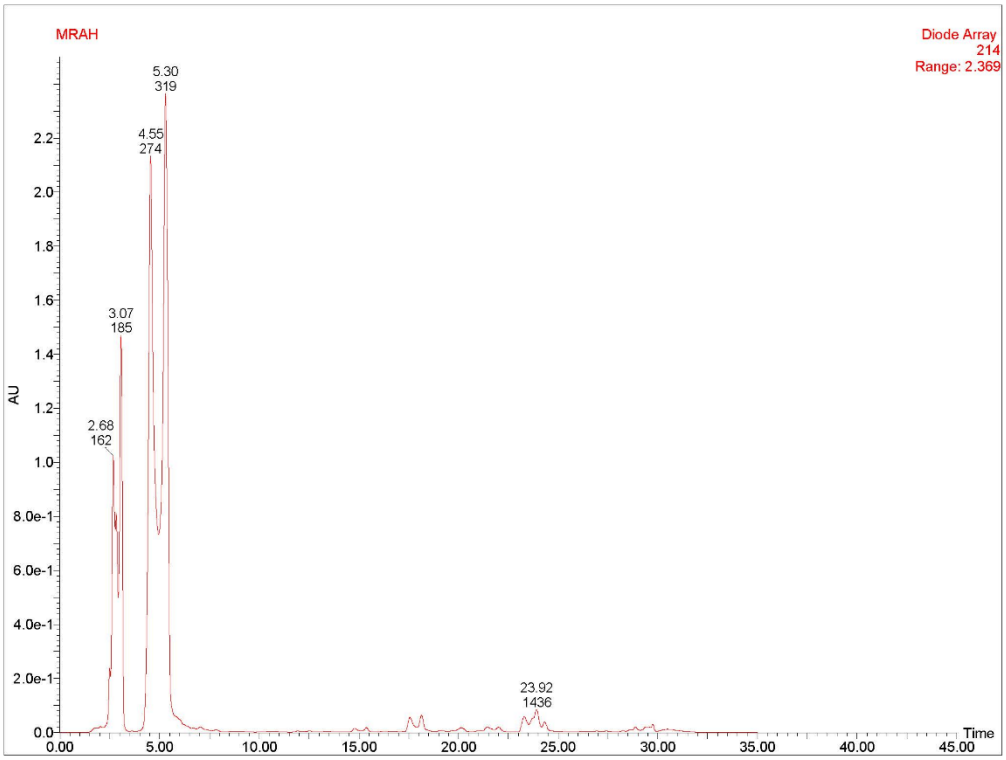

Fig. S27 HPLC chromatogram of MRAH

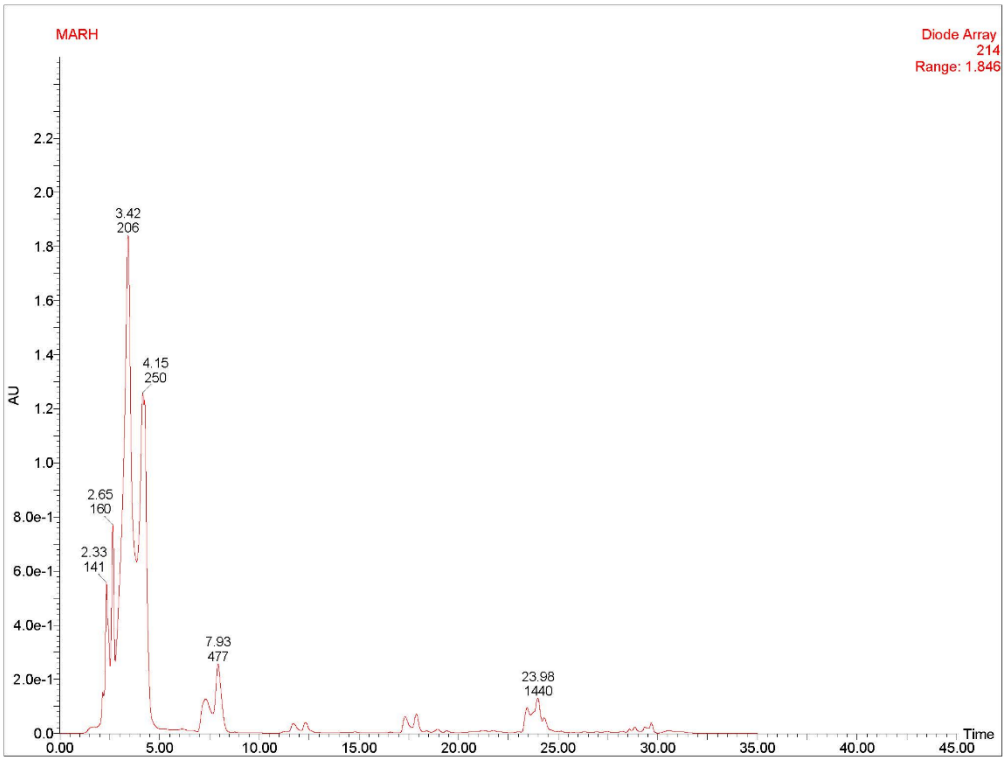

Fig. S28 HPLC chromatogram of MARH

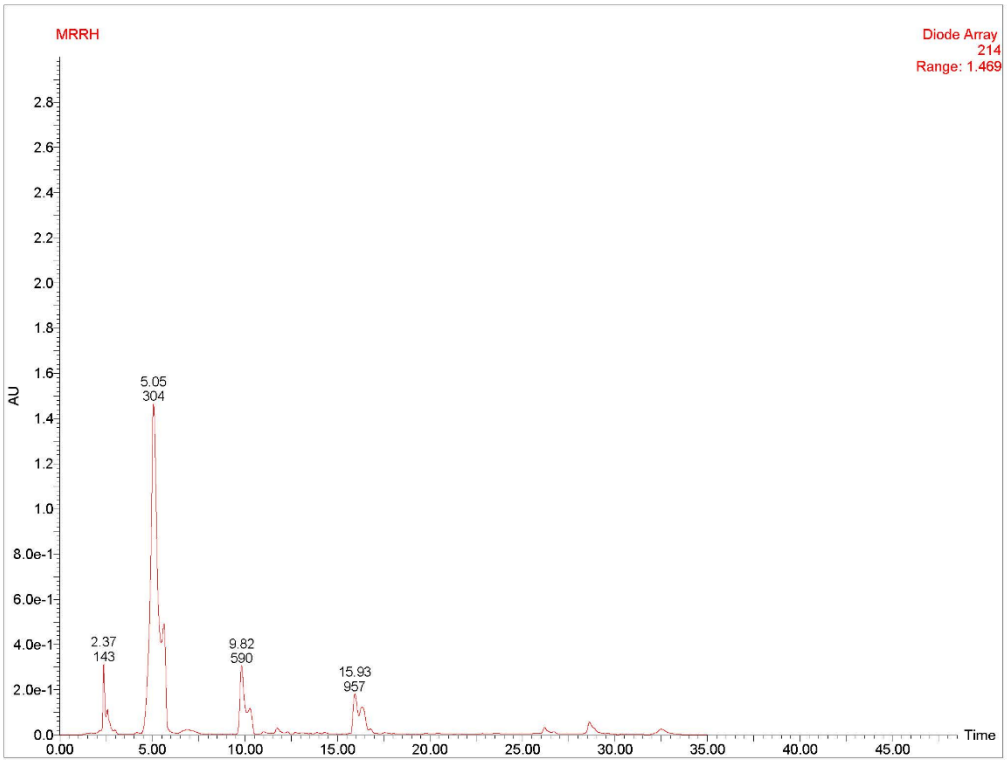

Fig. S29 HPLC chromatogram of MRRH

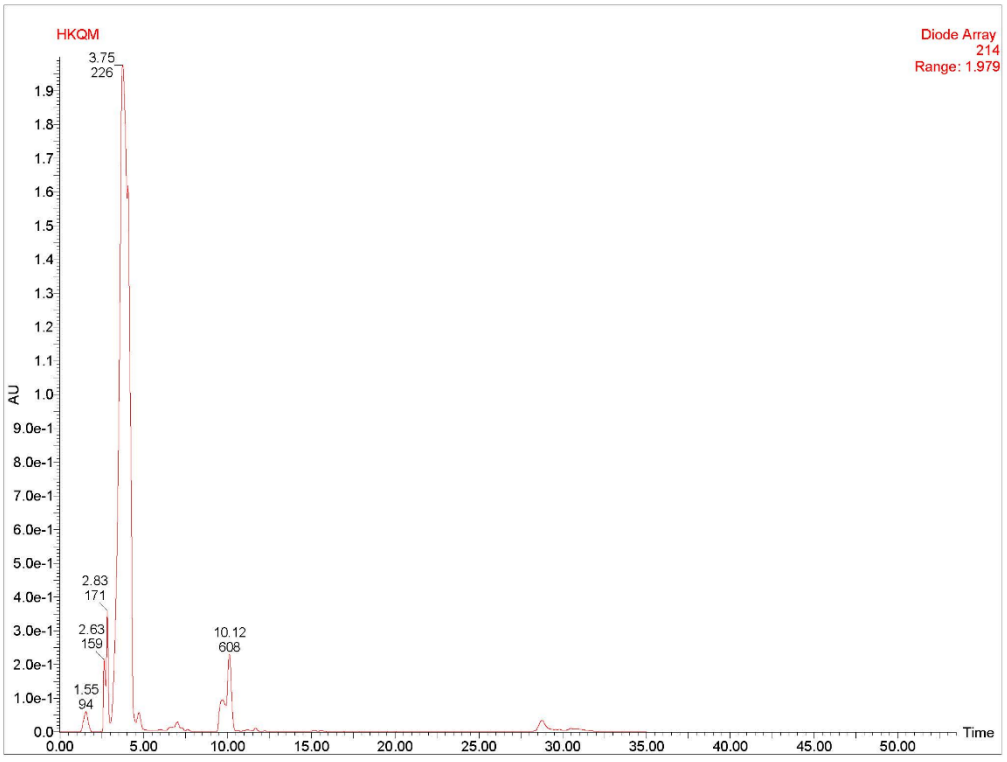

Fig. S30 HPLC chromatogram of HKQM

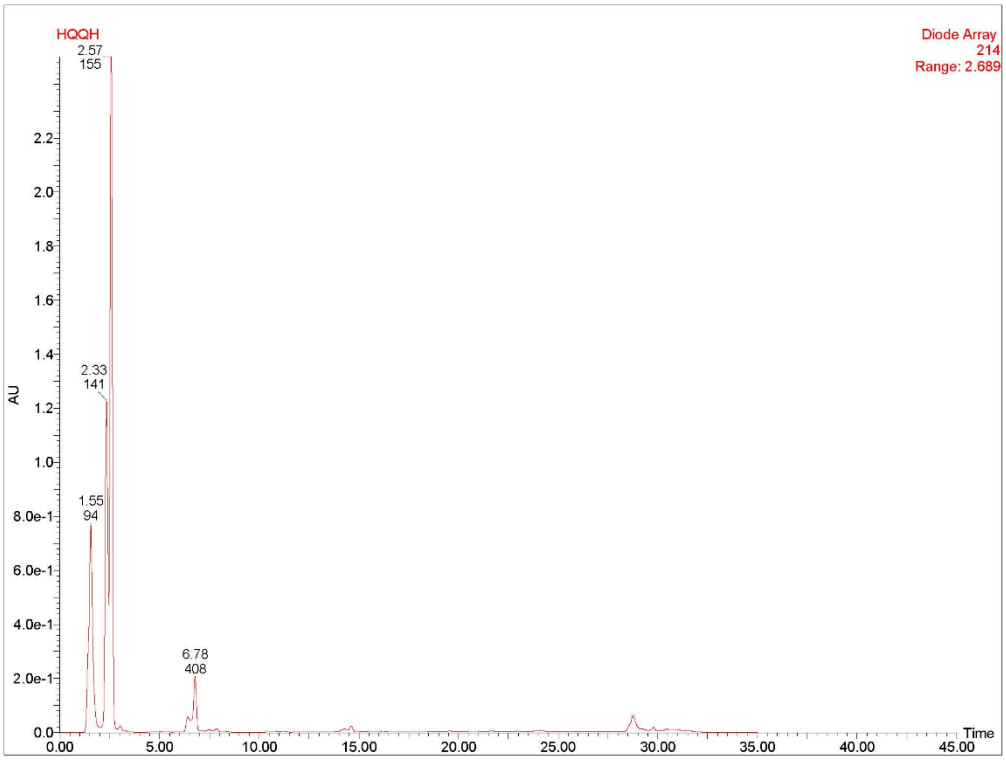

Fig. S31 HPLC chromatogram of HQQH

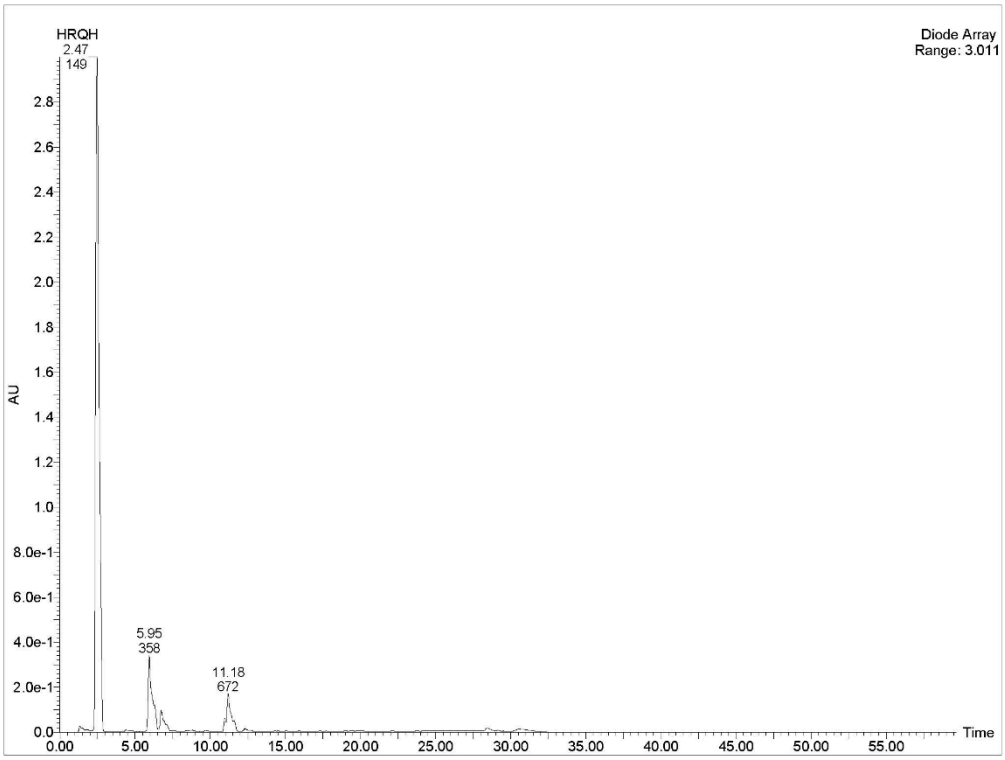

Fig. S32 HPLC chromatogram of HRQH

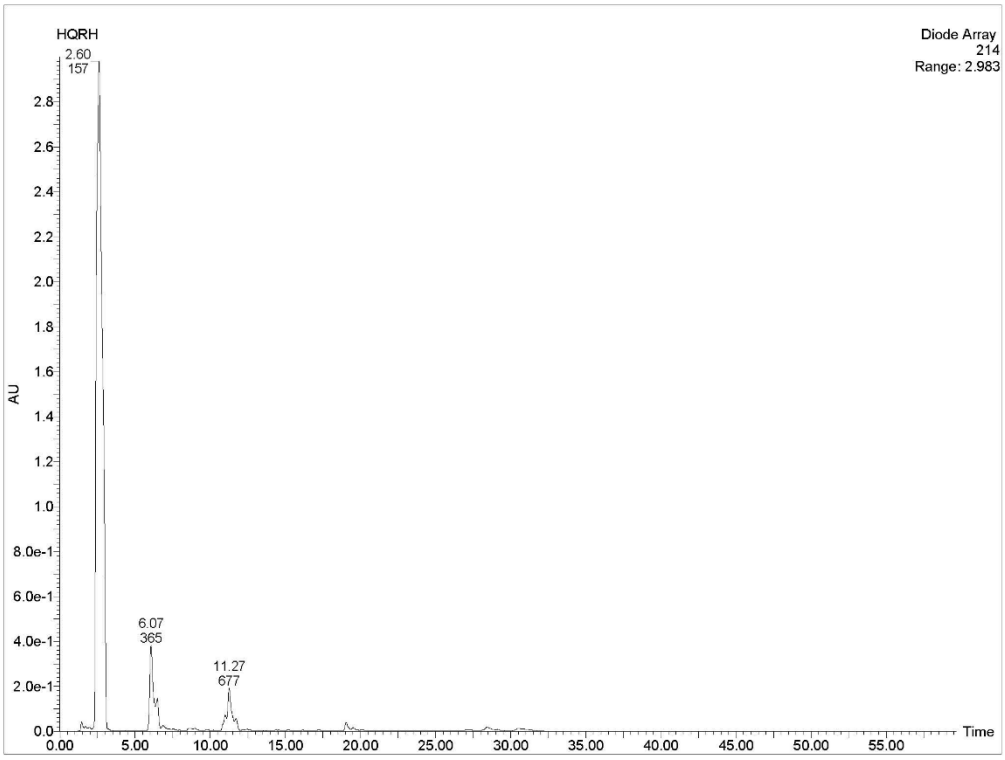

Fig. S33 HPLC chromatogram of HQRH

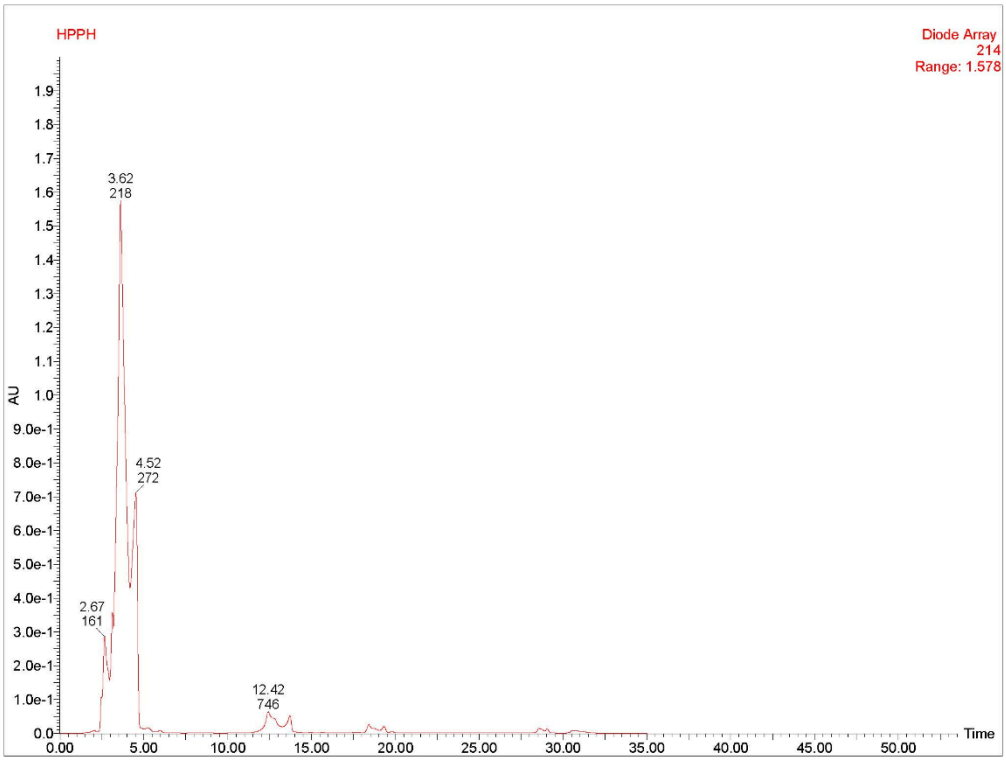

Fig. S34 HPLC chromatogram of HPPH

Fig. S35 HPLC chromatogram of HQPH

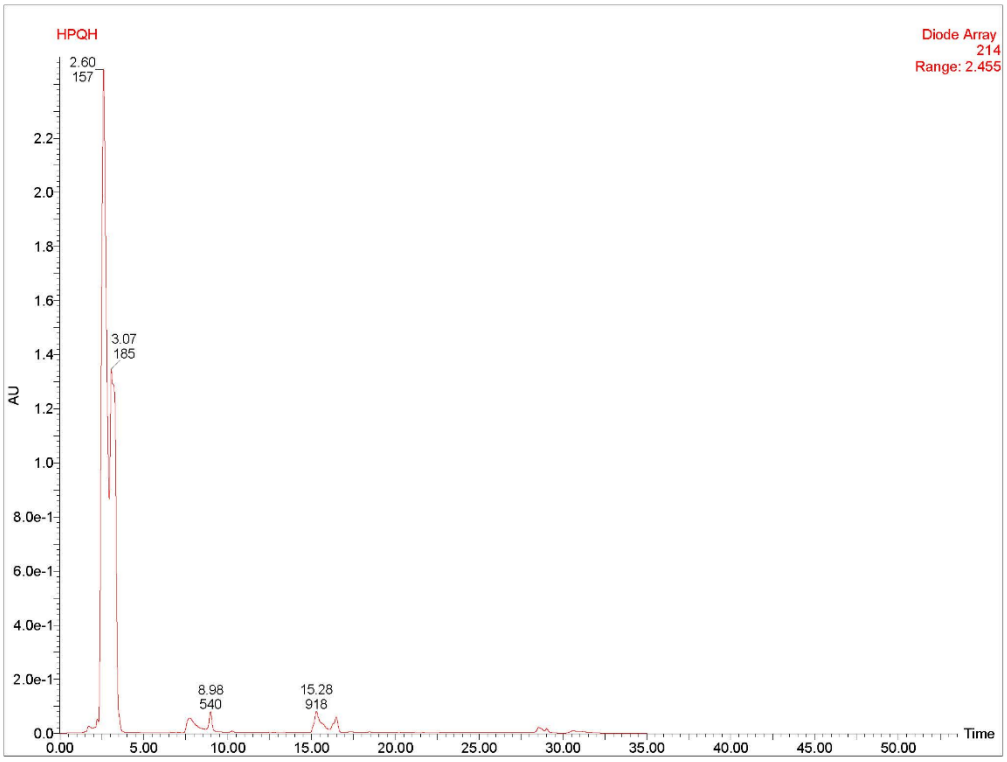

Fig. S36 HPLC chromatogram of HPQH

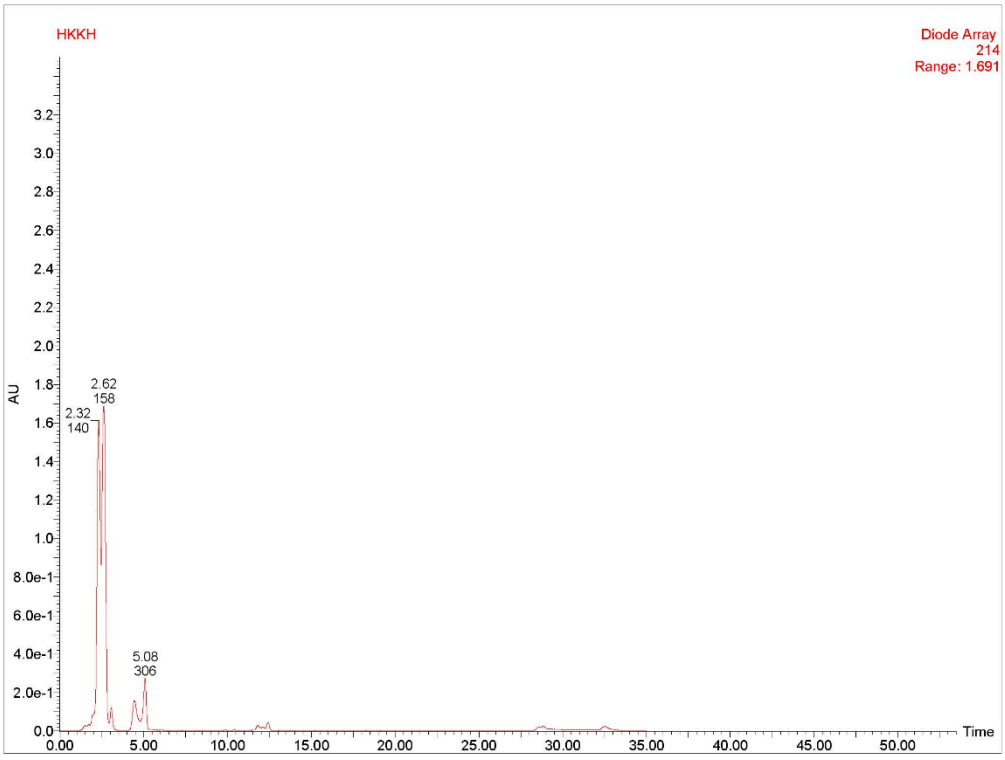

Fig. S37 HPLC chromatogram of HKKH

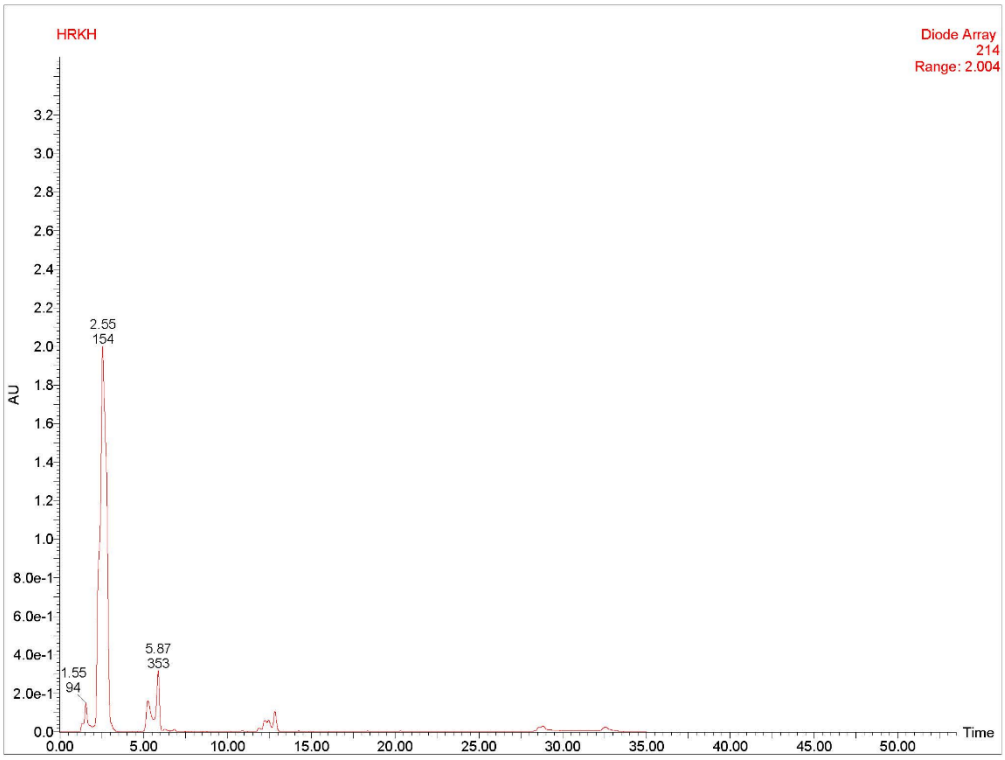

Fig. S38 HPLC chromatogram of HRKH

Fig. S39 HPLC chromatogram of HKRH

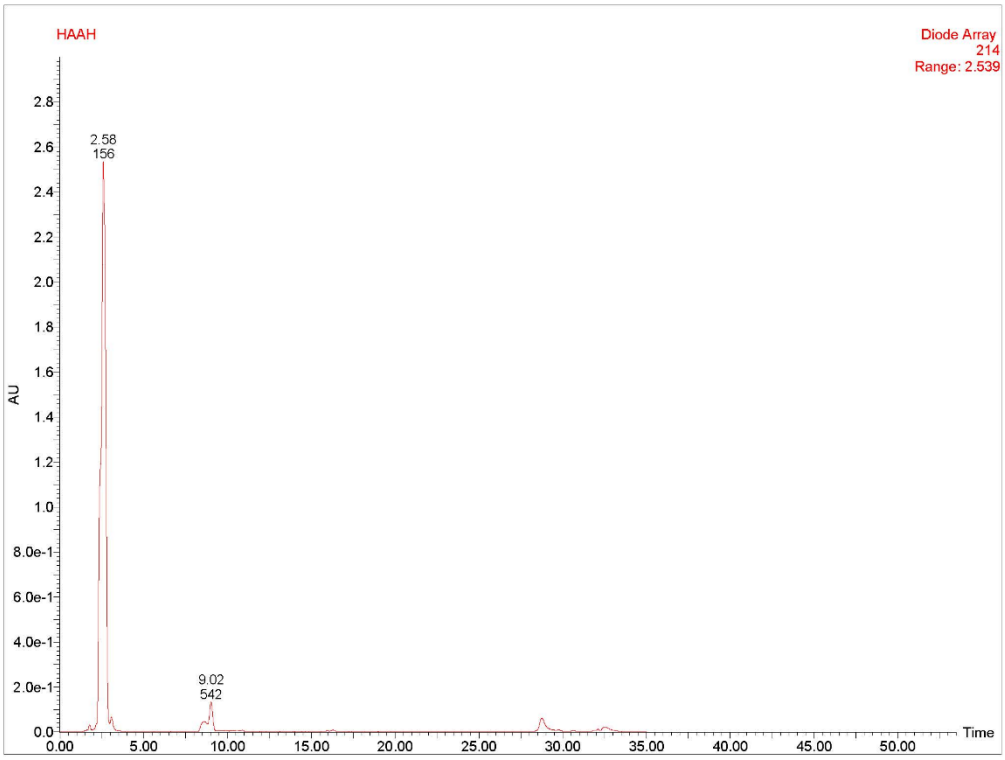

Fig. S40 HPLC chromatogram of HAAH

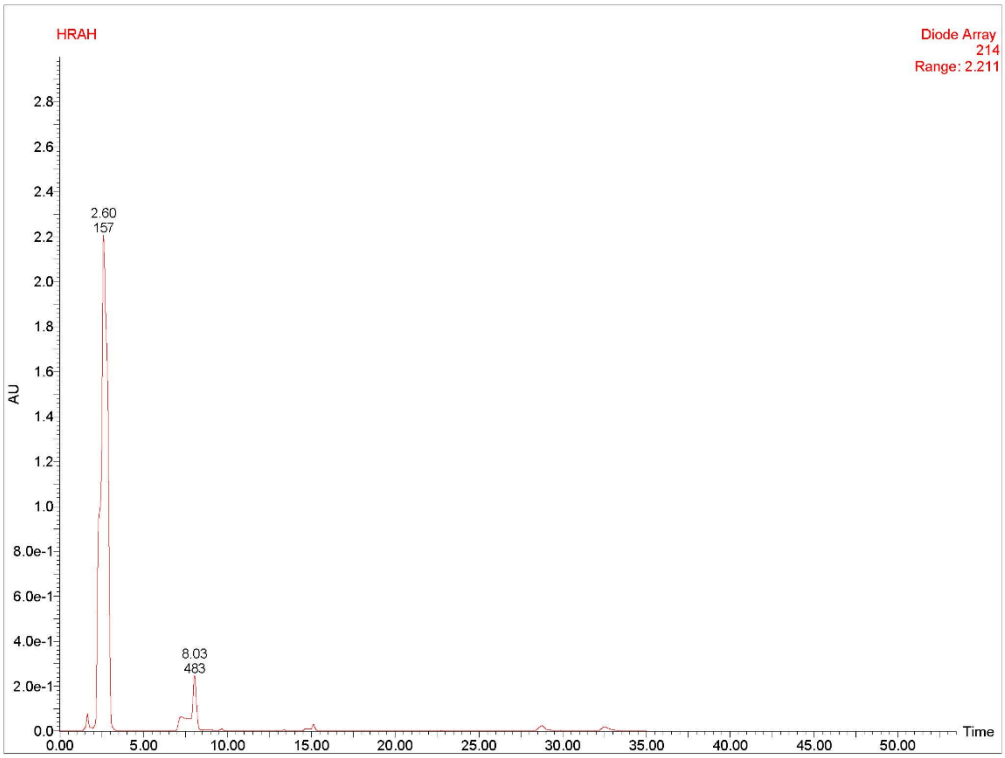

Fig. S41 HPLC chromatogram of HRAH

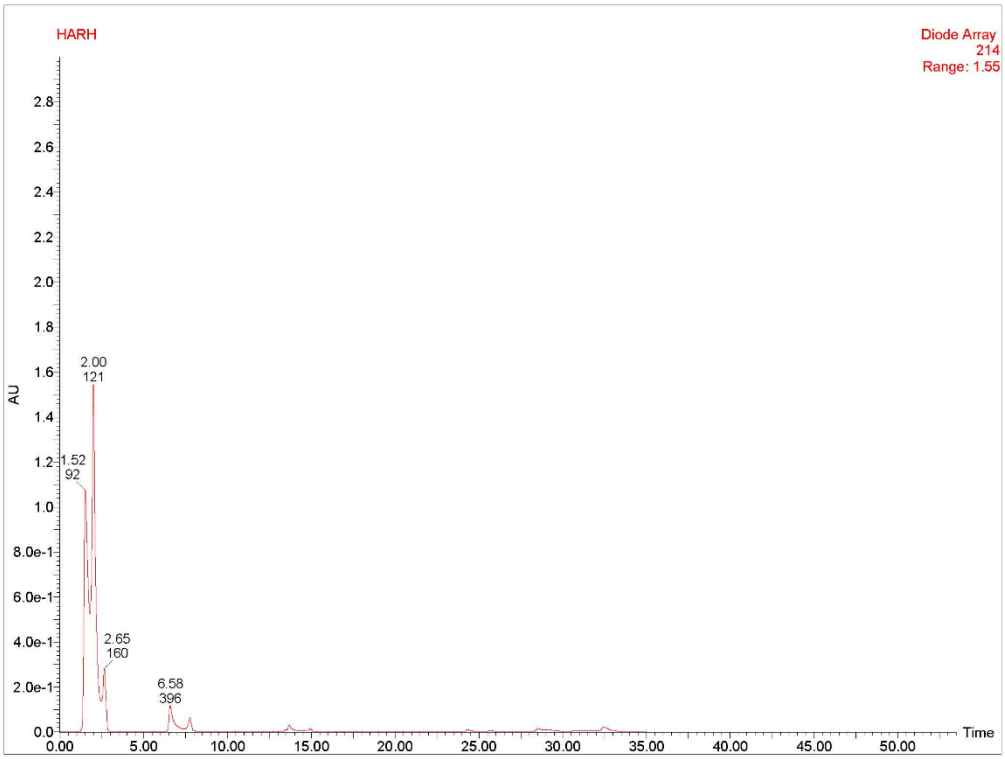

Fig. S42 HPLC chromatogram of HARH

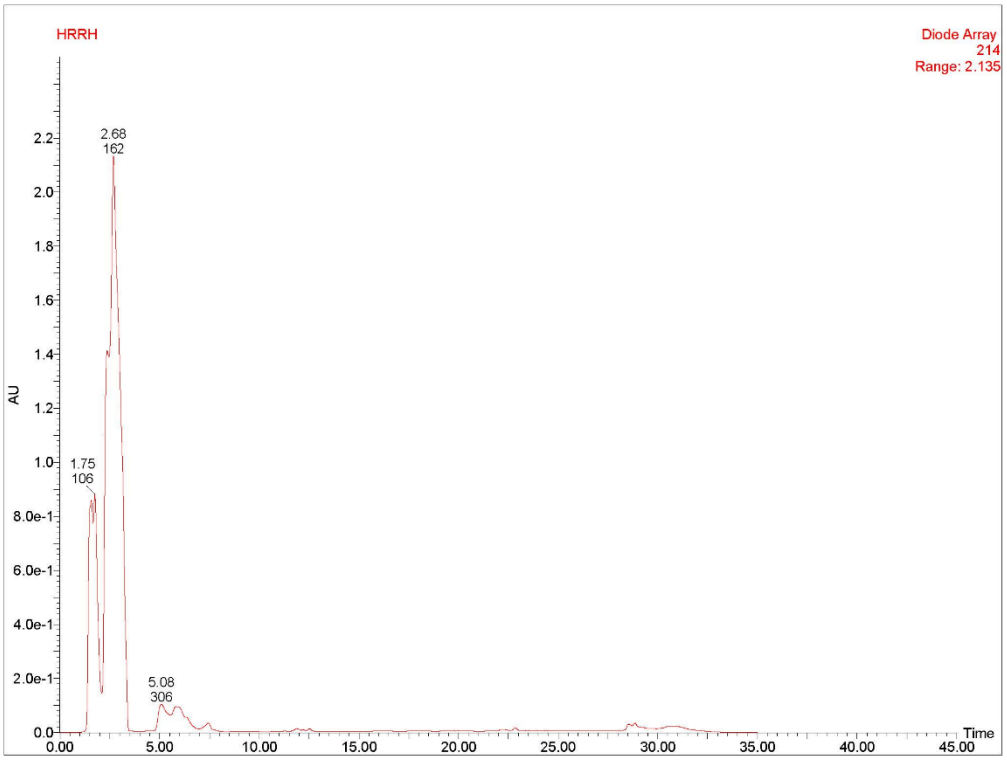

Fig. S43 HPLC chromatogram of HRRH

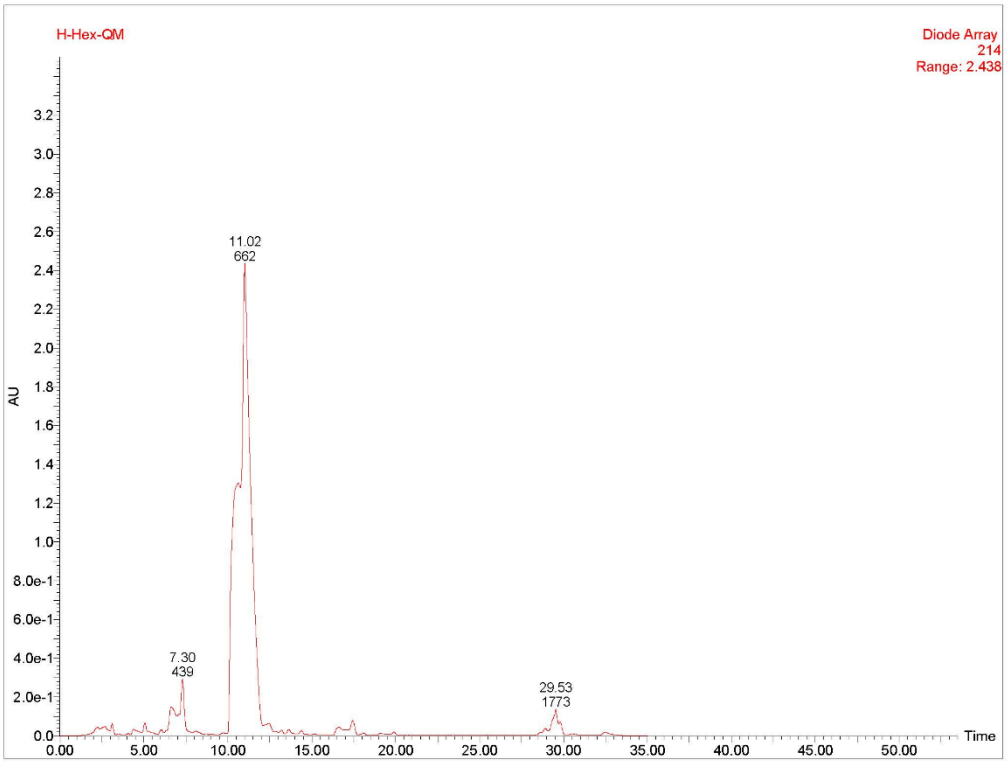

Fig. S44 HPLC chromatogram of H−Hex−QM

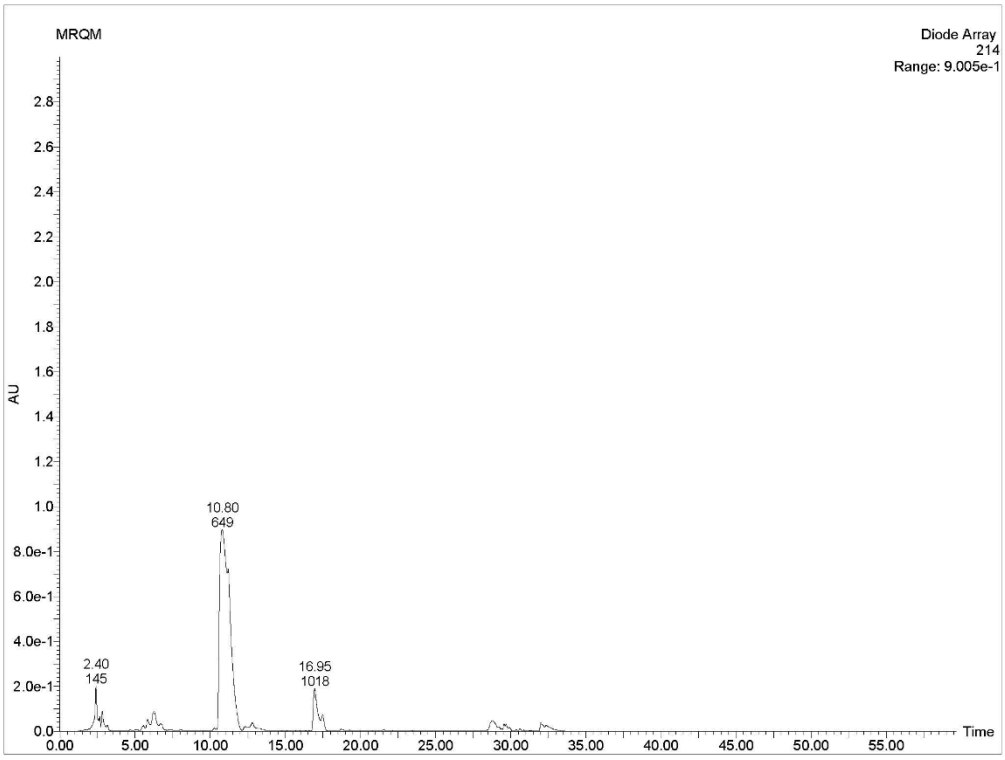

Fig. S45 HPLC chromatogram of MRQM

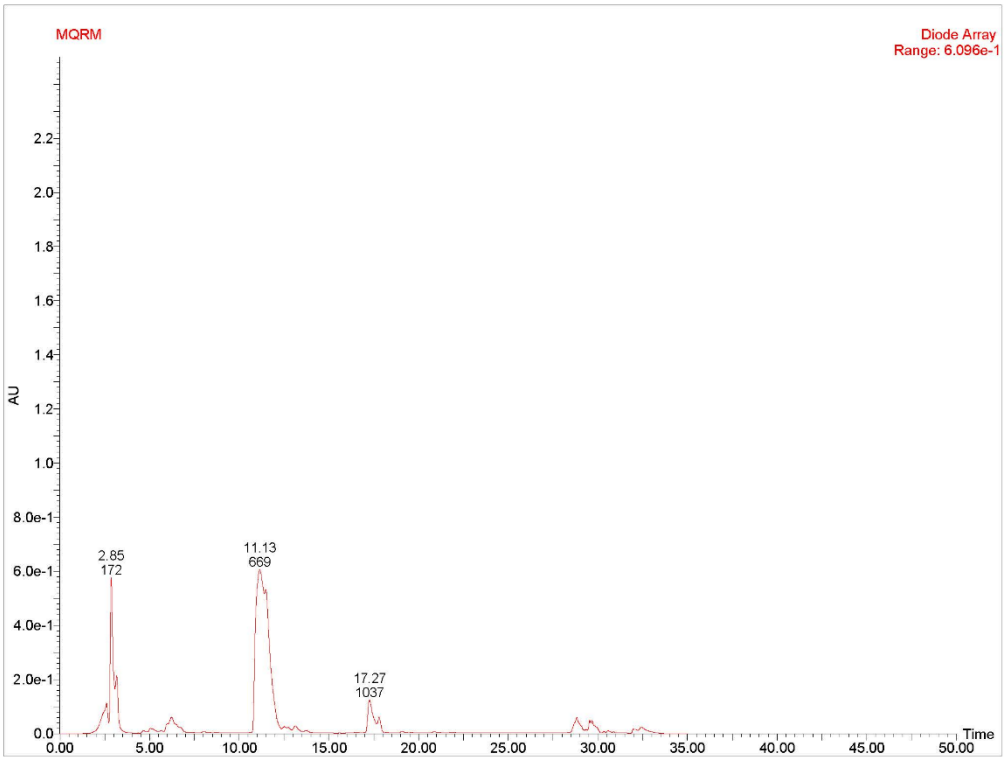

Fig. S46 HPLC chromatogram of MQRM

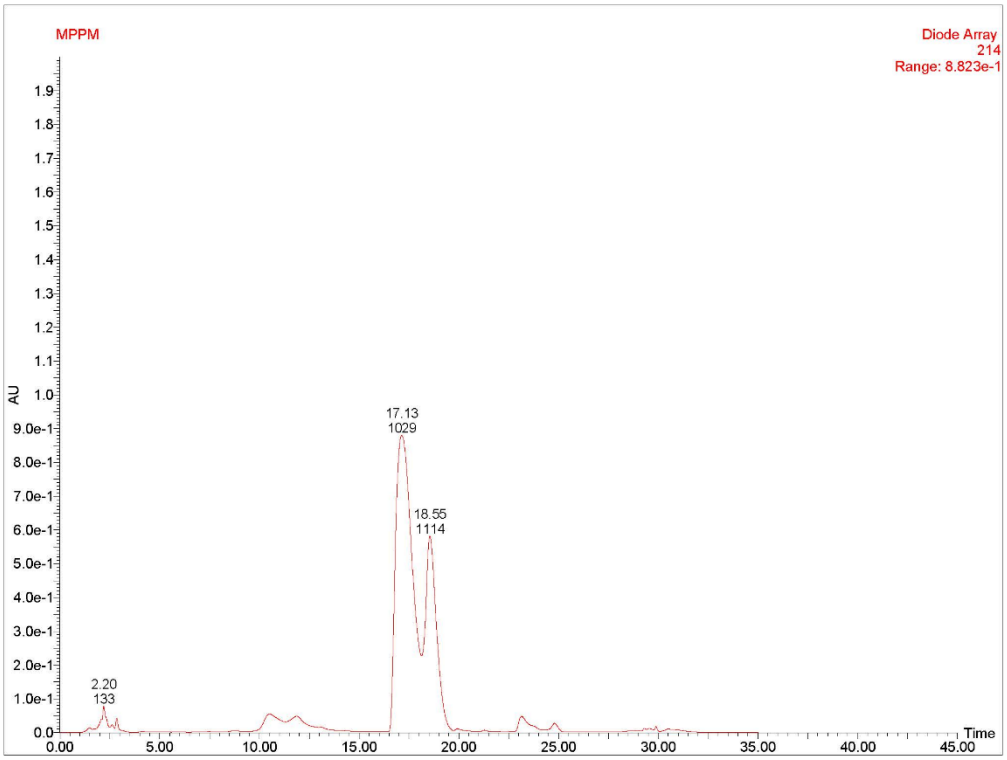

Fig. S47 HPLC chromatogram of MPPM

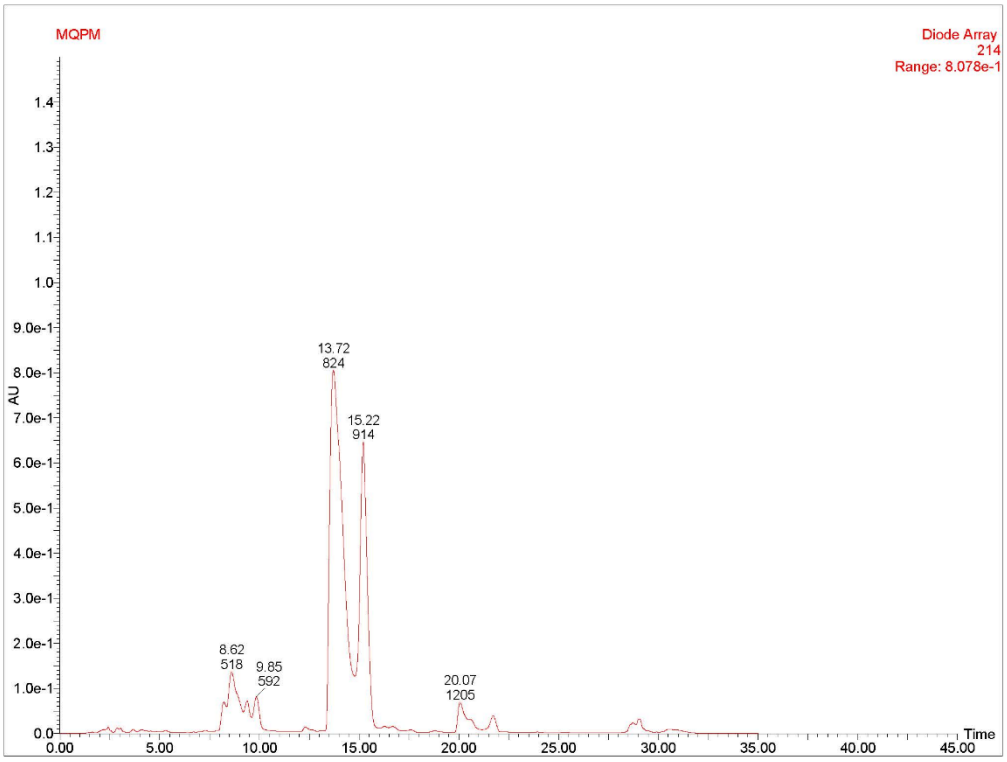

Fig. S48 HPLC chromatogram of MQPM

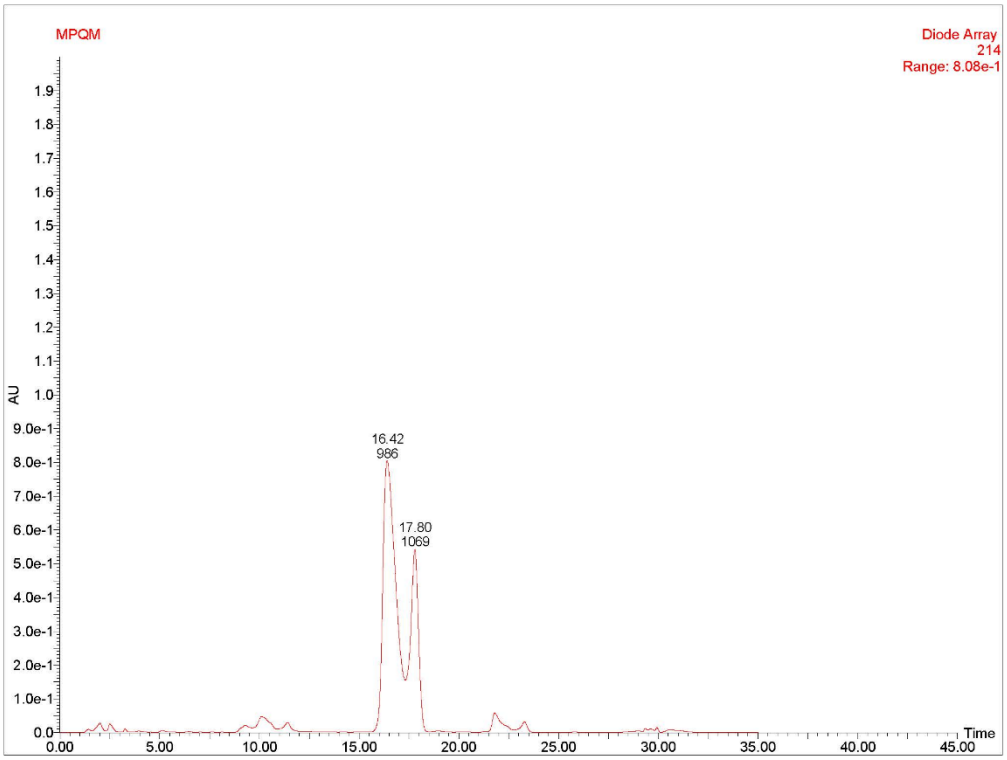

Fig. S49 HPLC chromatogram of MPQM

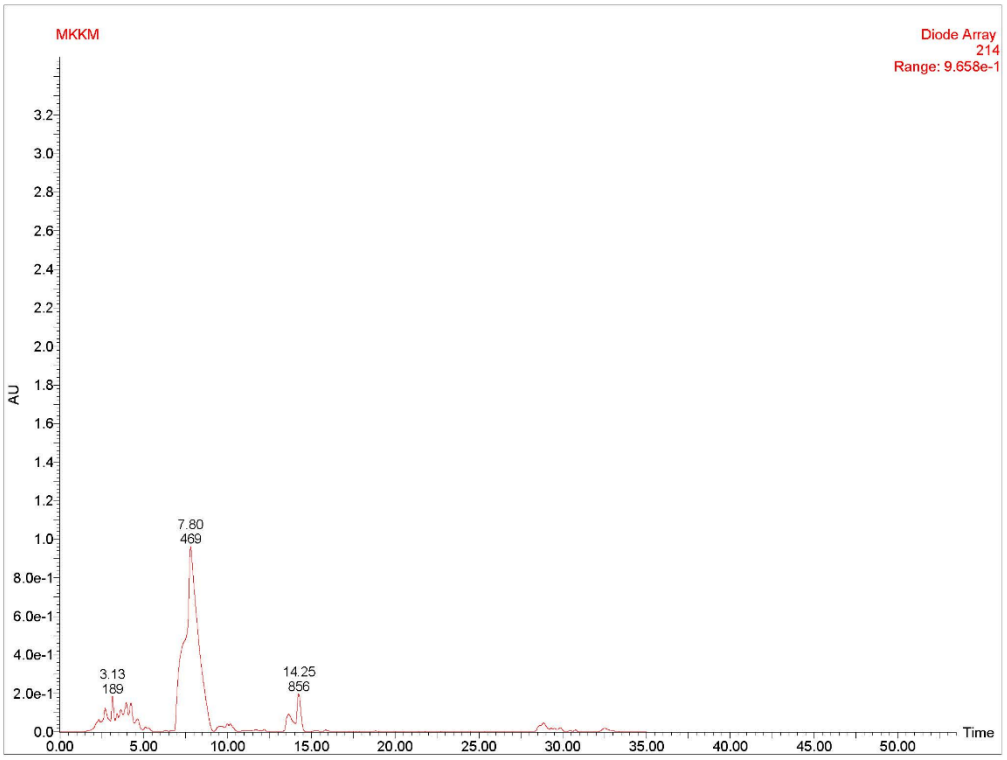

Fig. S50 HPLC chromatogram of MKKM

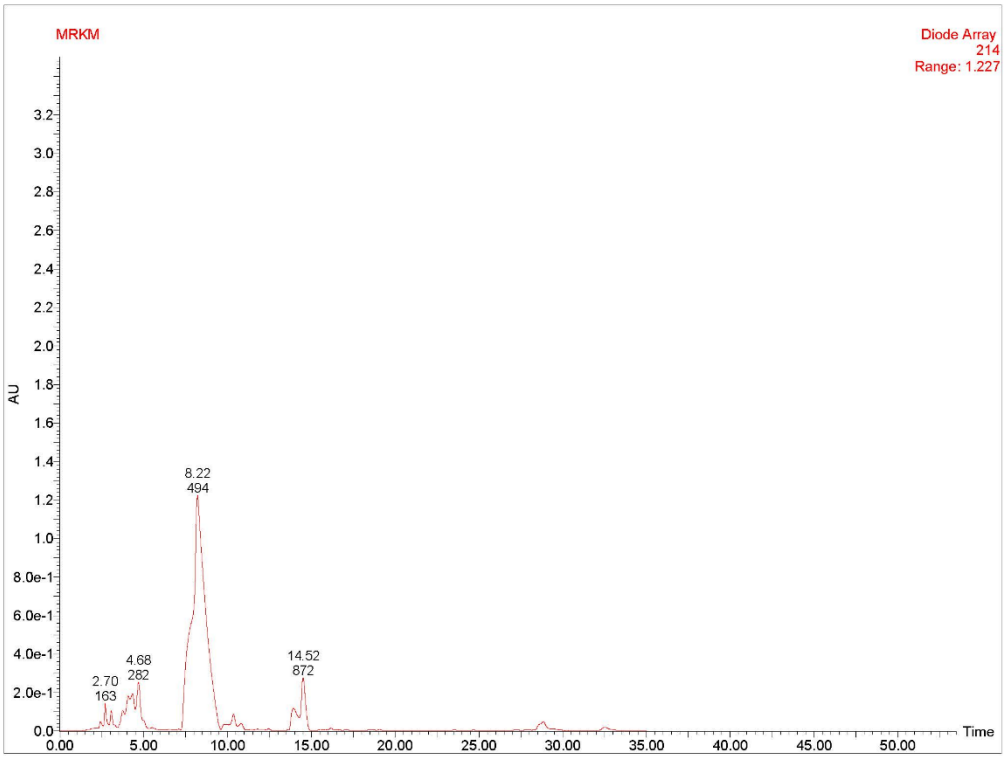

Fig. S51 HPLC chromatogram of MRKM

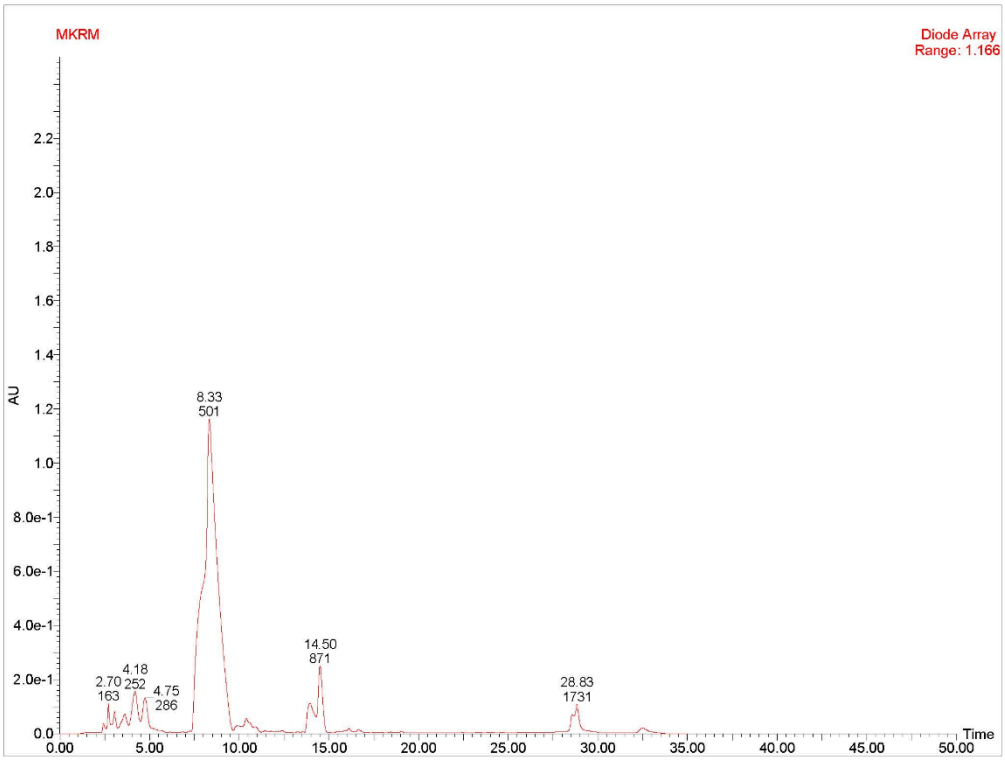

Fig. S52 HPLC chromatogram of MKRM

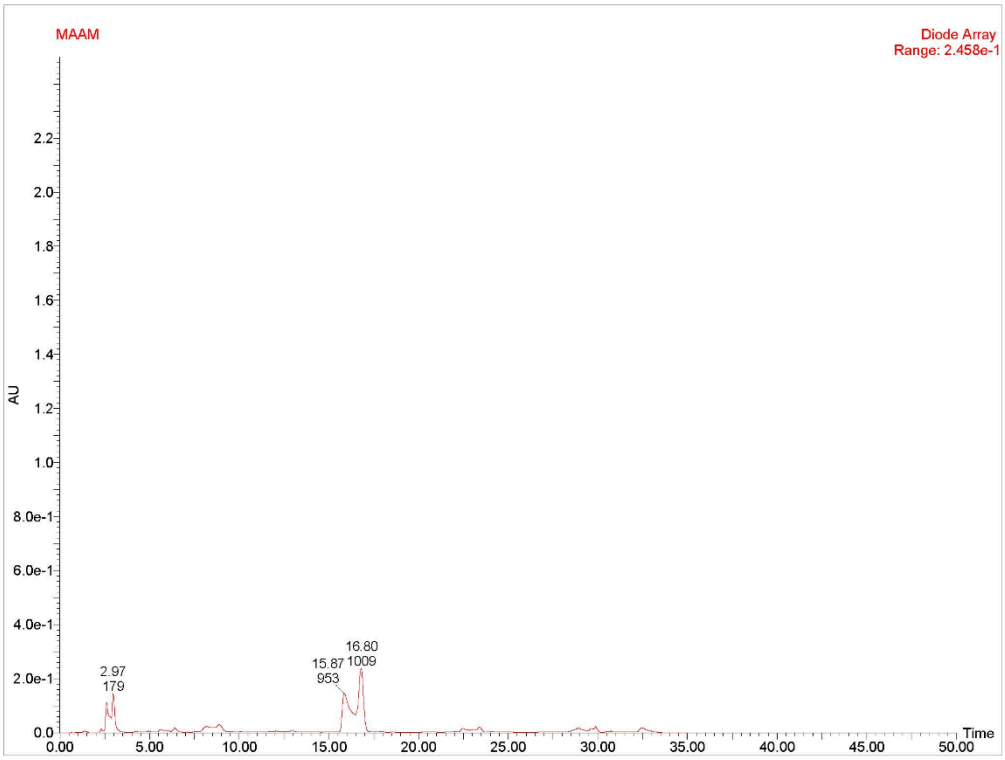

Fig. S53 HPLC chromatogram of MAAM

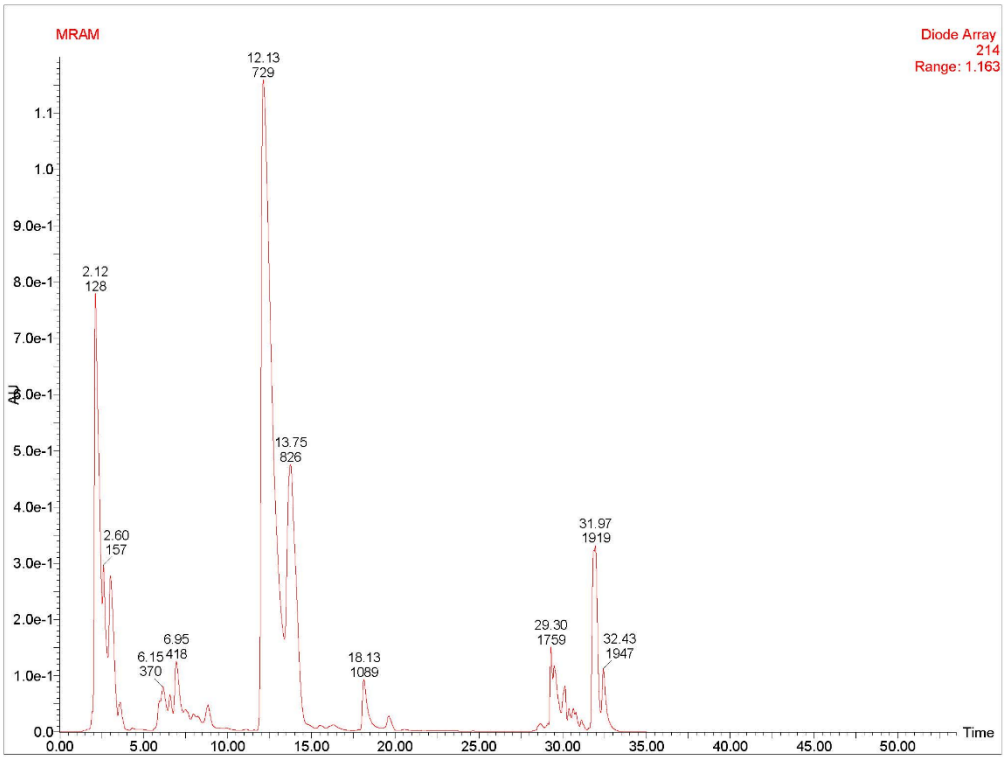

Fig. S54 HPLC chromatogram of MRAM

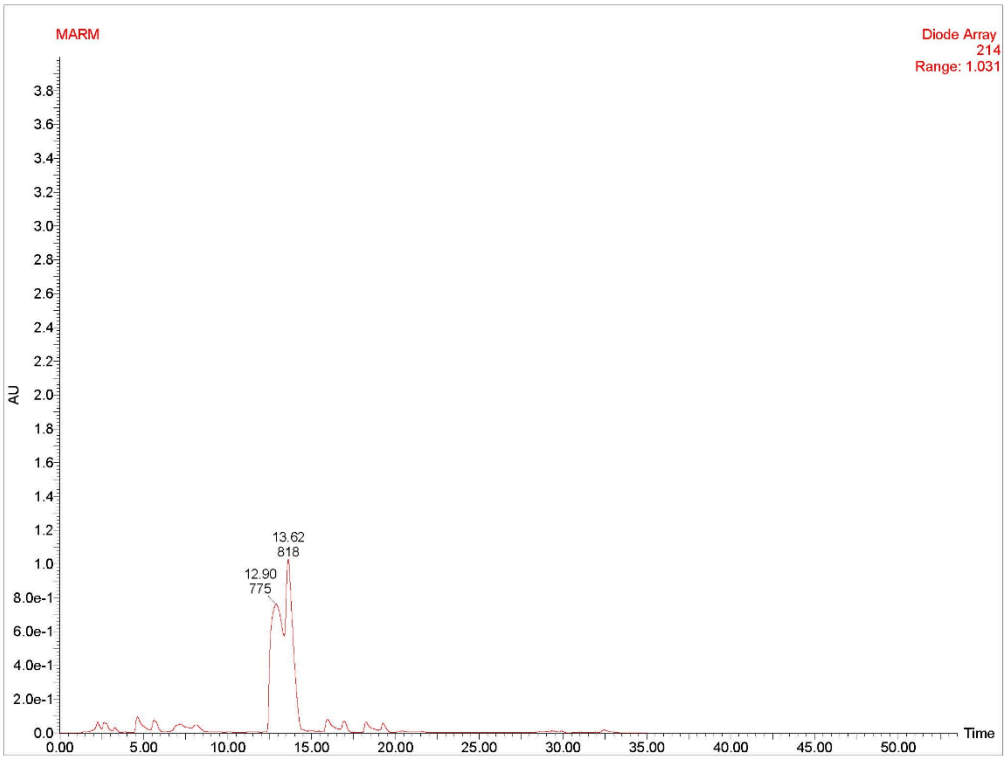

Fig. S55 HPLC chromatogram of MARM

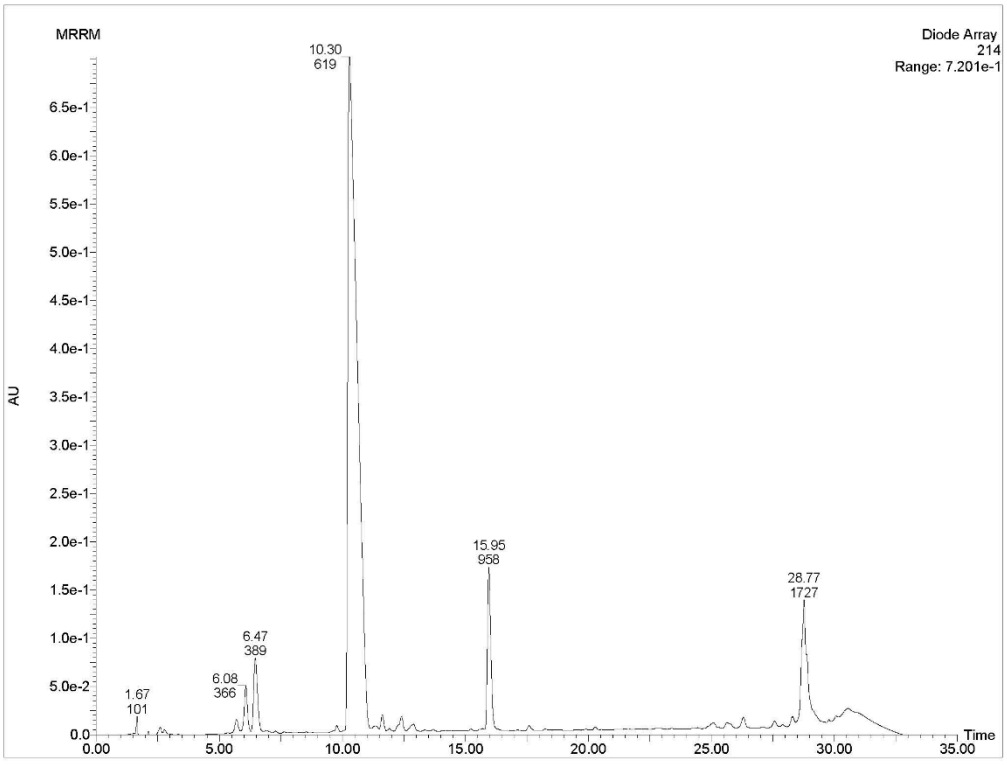

Fig. S56 HPLC chromatogram of MRRM

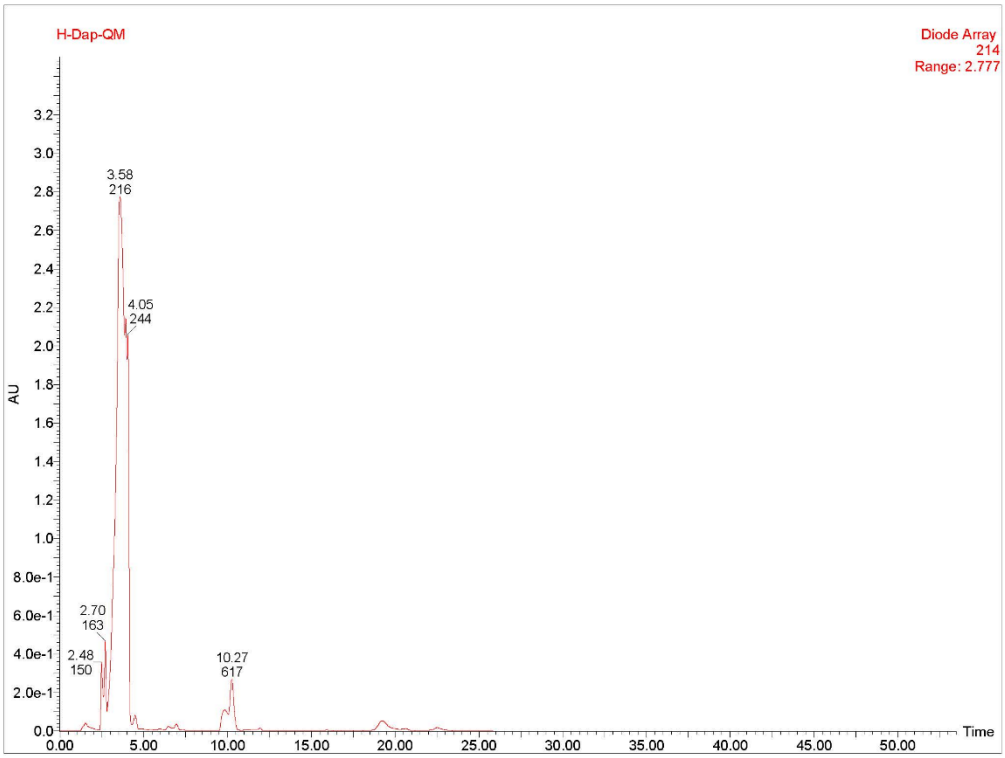

Fig. S57 HPLC chromatogram of H−Dap−QM

Electrospray ionization mass spectrometry

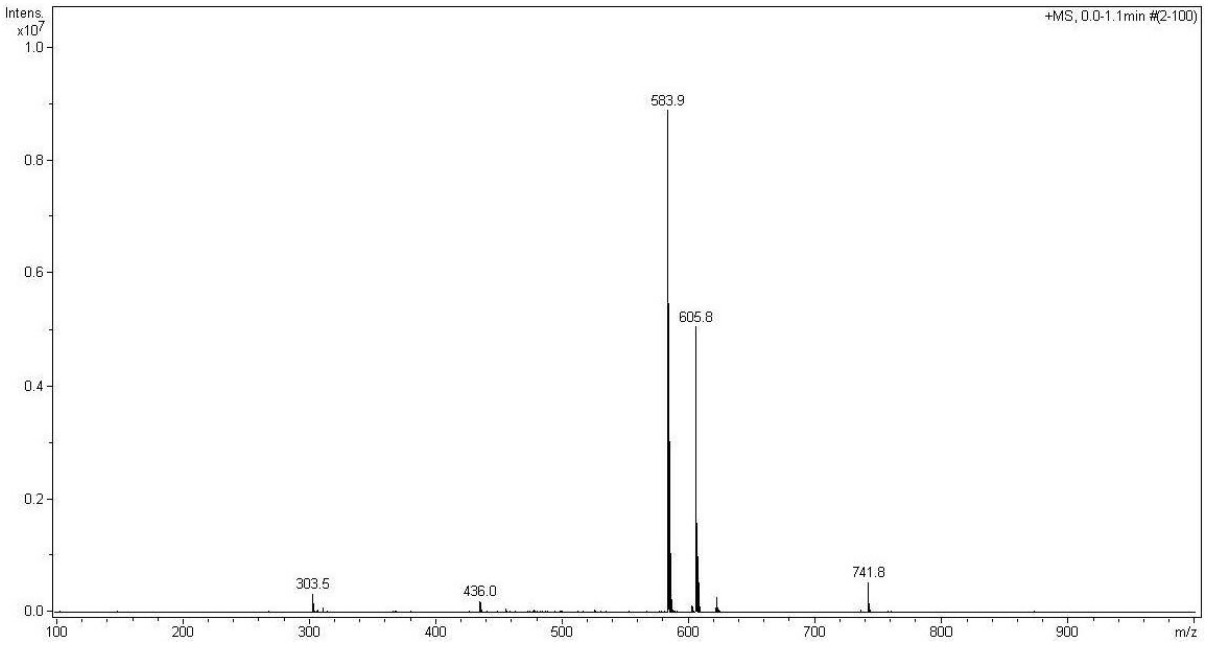

Fig. S58 ESI-MS spectrum of HQQM. $[M+H]^{+}_{calc}$ (m/z) : 584.3 ; $[M+H]^{+}_{exp}$ (m/z) : 583.9 ; $[M+Na]^{+}_{exp}$ (m/z) : 605.8 ; $[M+H+Na]^{2+}_{exp}$ (m/z) : 303.5

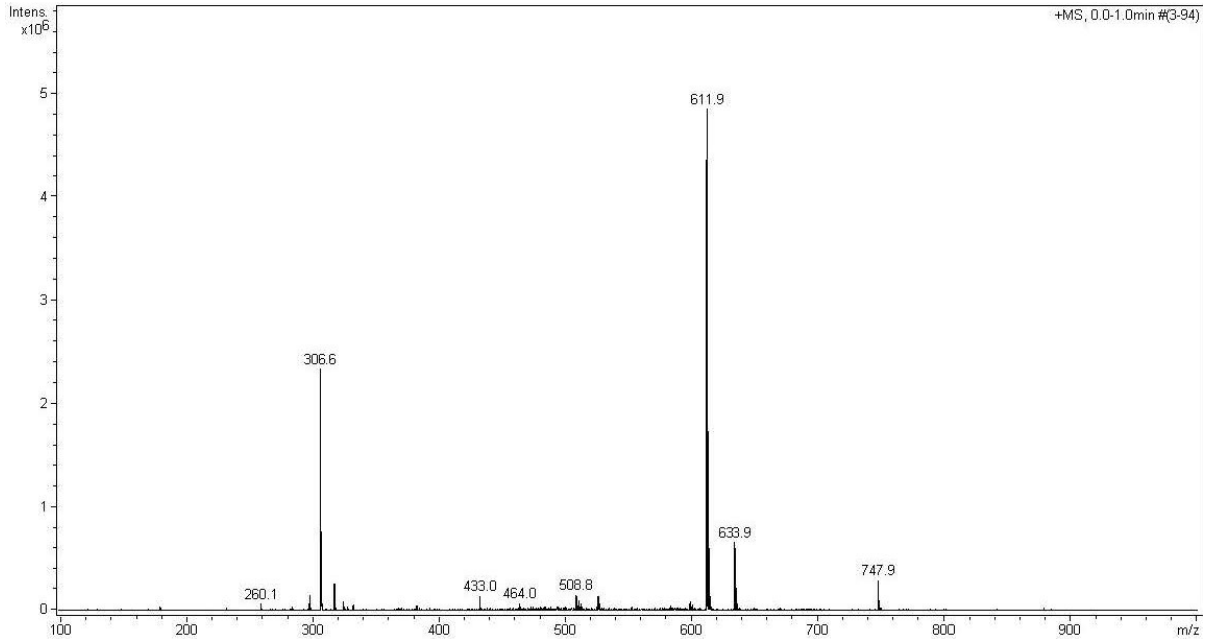

Fig. S59 ESI-MS spectrum of HRQM. $[M+H]^{+}_{calc}$ (m/z) : 612.3 ; $[M+H]^{+}_{exp}$ (m/z) : 611.9 ; $[M+Na]^{+}_{exp}$ (m/z) : 633.9 ; $[M+2H]^{2+}_{exp}$ (m/z) : 306.6

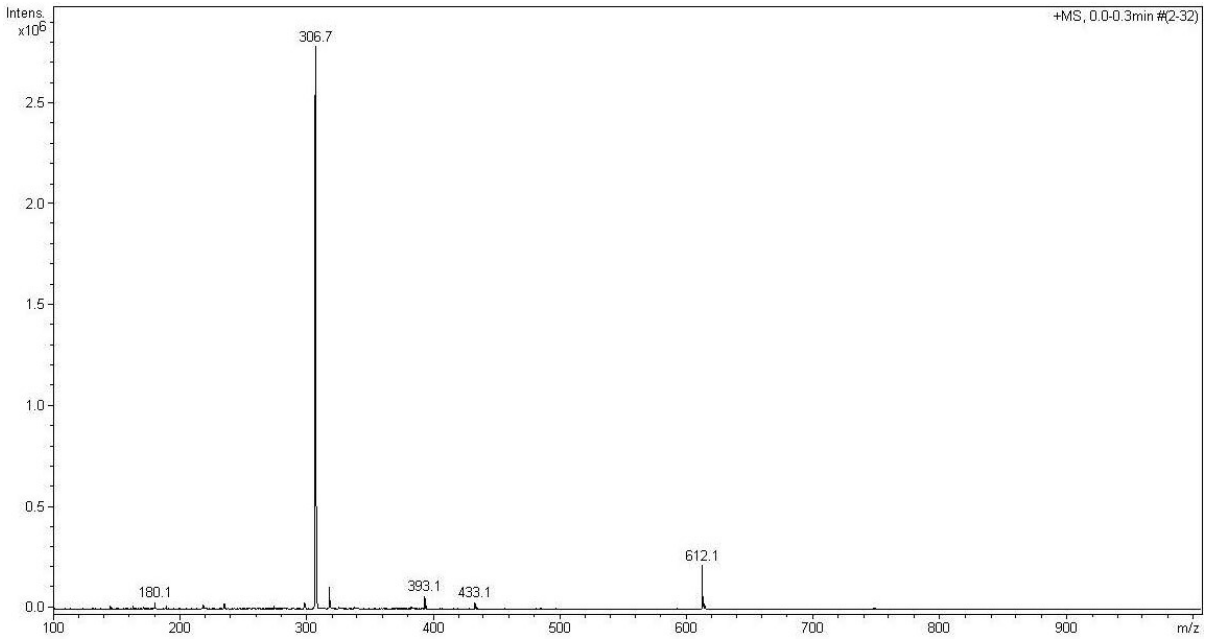

Fig. S60 ESI-MS spectrum of HQRM. $[M+H]^{+}_{calc}$ (m/z) : 612.3 ; $[M+H]^{+}_{exp}$ (m/z) : 612.1 ; $[M+2H]^{2+}_{exp}$ (m/z) : 306.7

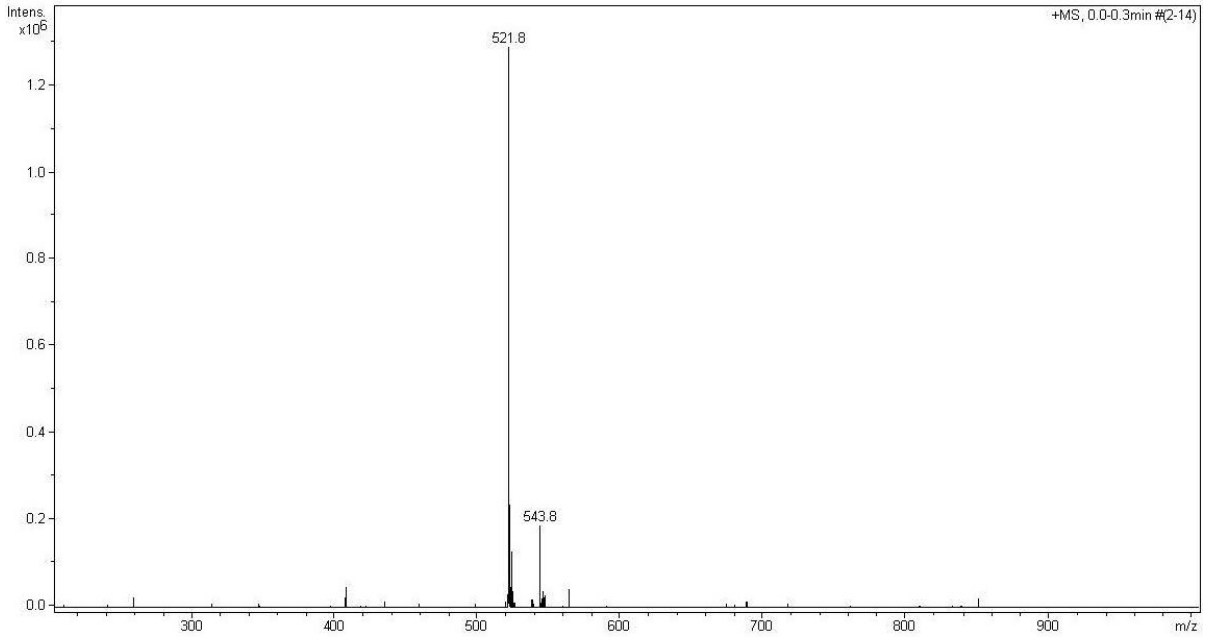

Fig. S61 ESI-MS spectrum of HPPM. $[M+H]^{+}_{calc}$ (m/z) : 522.2 ; $[M+H]^{+}_{exp}$ (m/z) : 521.8 ; $[M+Na]^{+}_{exp}$ (m/z) : 543.8

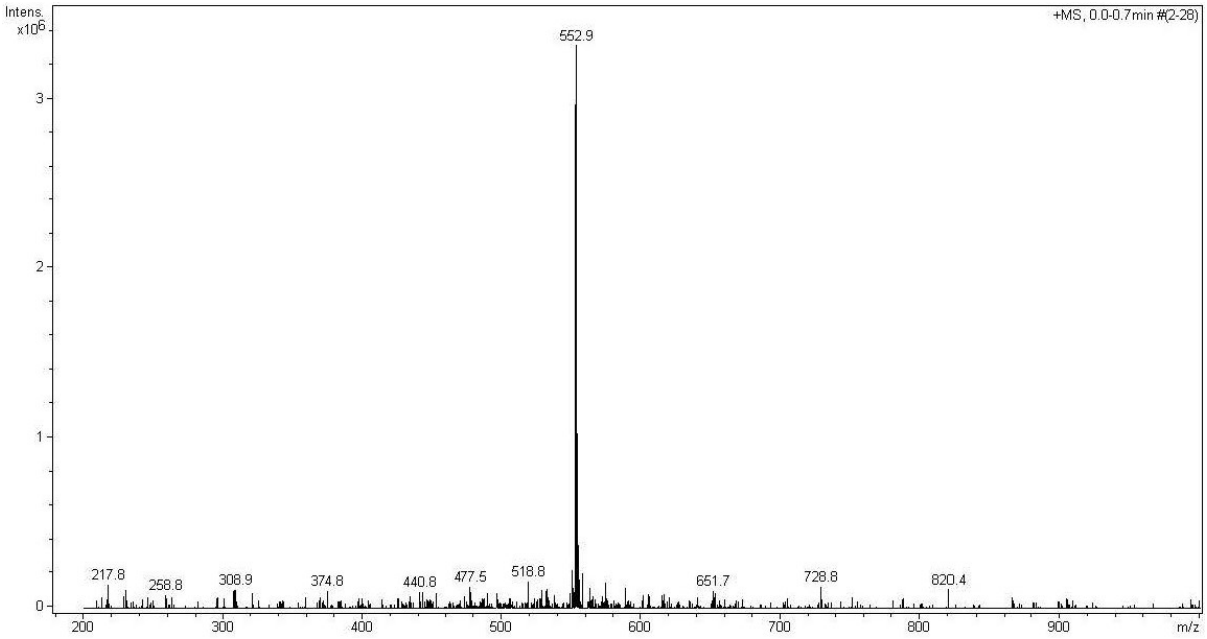

Fig. S62 ESI-MS spectrum of HQPM. $[M+H]^+_{calc}$ (m/z) : 553.2 ; $[M+H]^+_{exp}$ (m/z) : 552.9

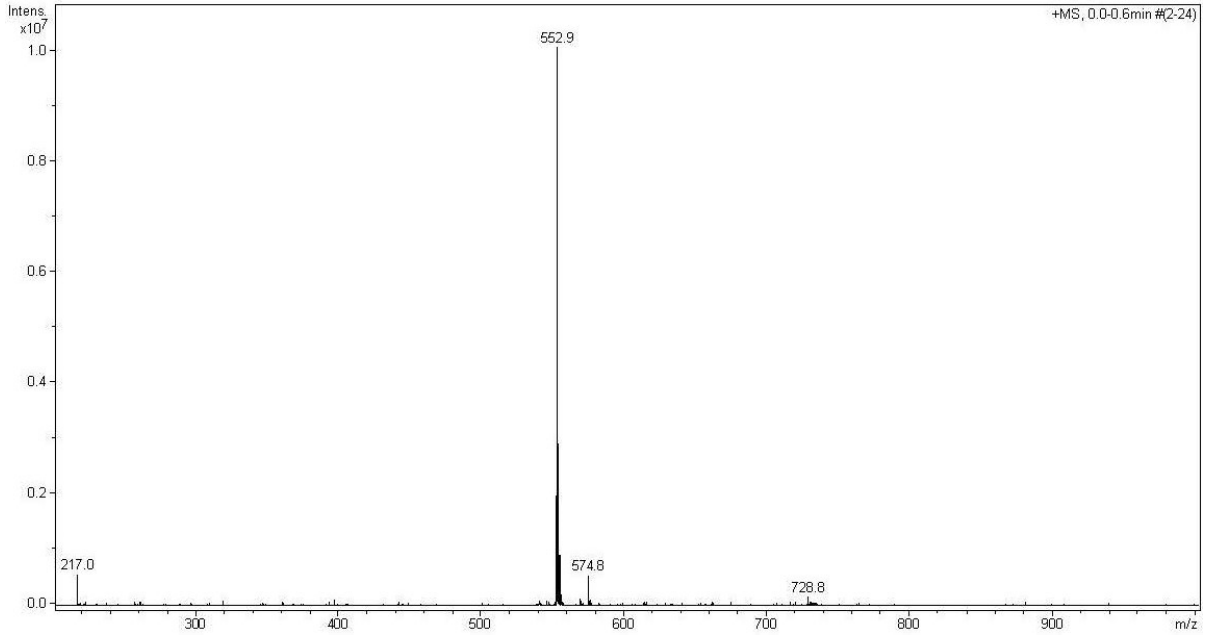

Fig. S63 ESI-MS spectrum of HPQM. $[M+H]^+_{calc}$ (m/z) : 553.2 ; $[M+H]^+_{exp}$ (m/z) : 552.9 ; $[M+Na]^+_{exp}$ (m/z) : 574.8

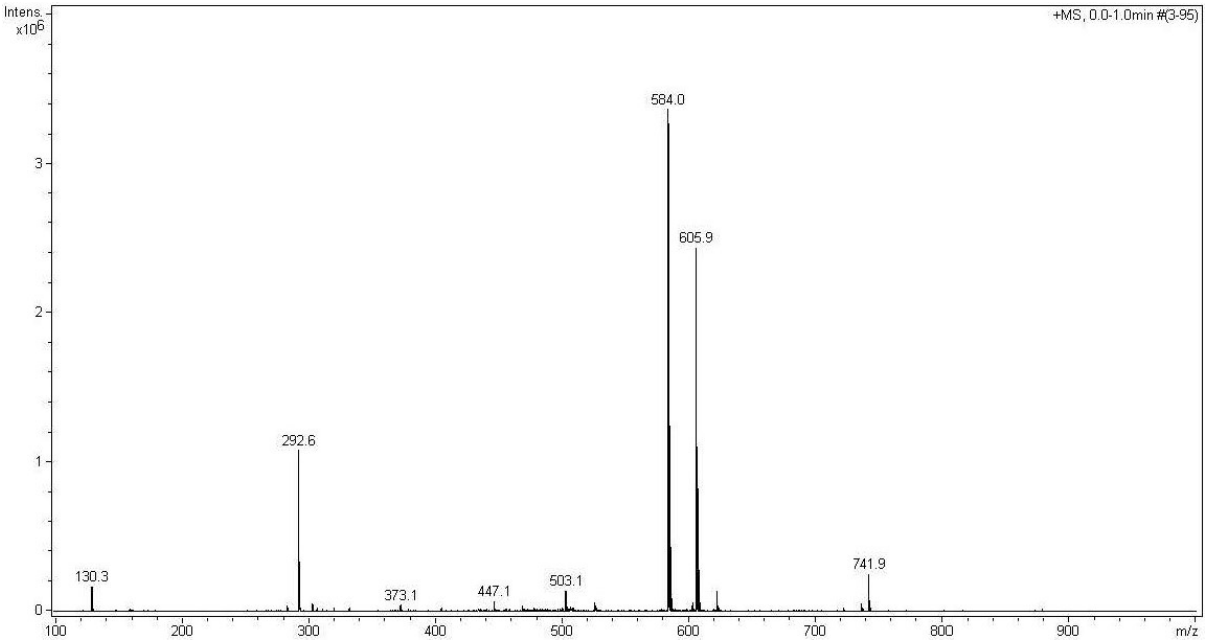

Fig. S64 ESI-MS spectrum of HKKM. $[M+H]^{+}_{calc}$ (m/z) : 583.3 ; $[M+H]^{+}_{exp}$ (m/z) : 584.0 ; $[M+Na]^{+}_{exp}$ (m/z) : 605.9 ; $[M+2H]^{2+}_{exp}$ (m/z) : 292.6

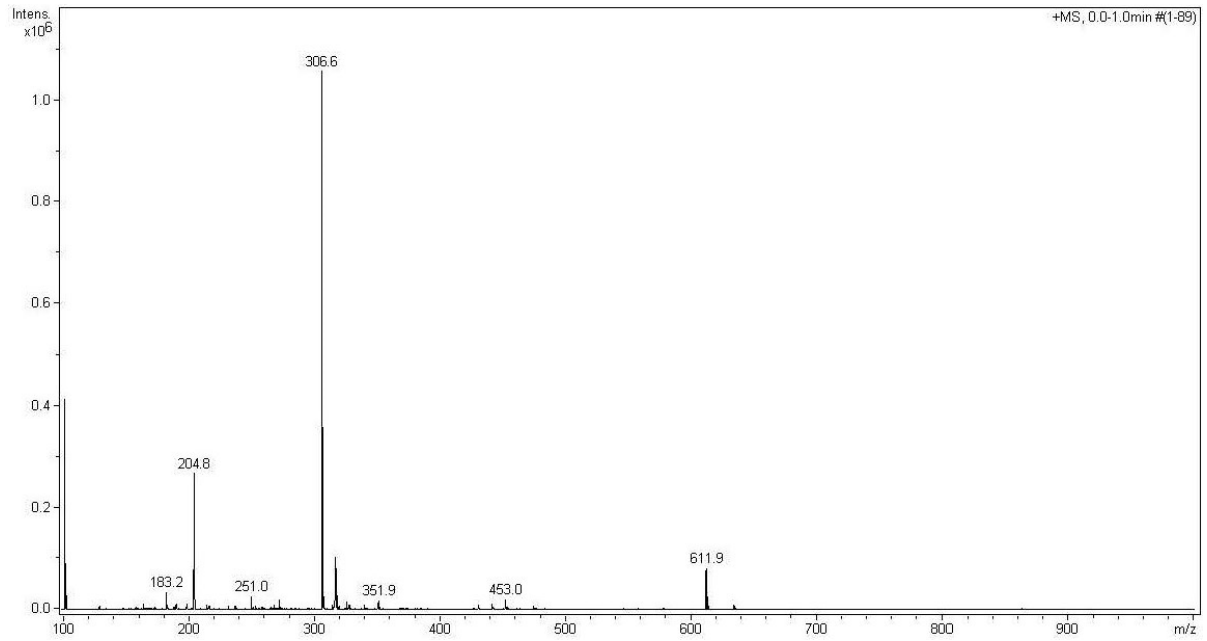

Fig. S65 ESI-MS spectrum of HRKM. $[M+H]^{+}_{calc}$ (m/z) : 612.3 ; $[M+H]^{+}_{exp}$ (m/z) : 611.9 ; $[M+2H]^{2+}_{exp}$ (m/z) : 306.6 ; $[M+3H]^{3+}_{exp}$ (m/z) : 204.8

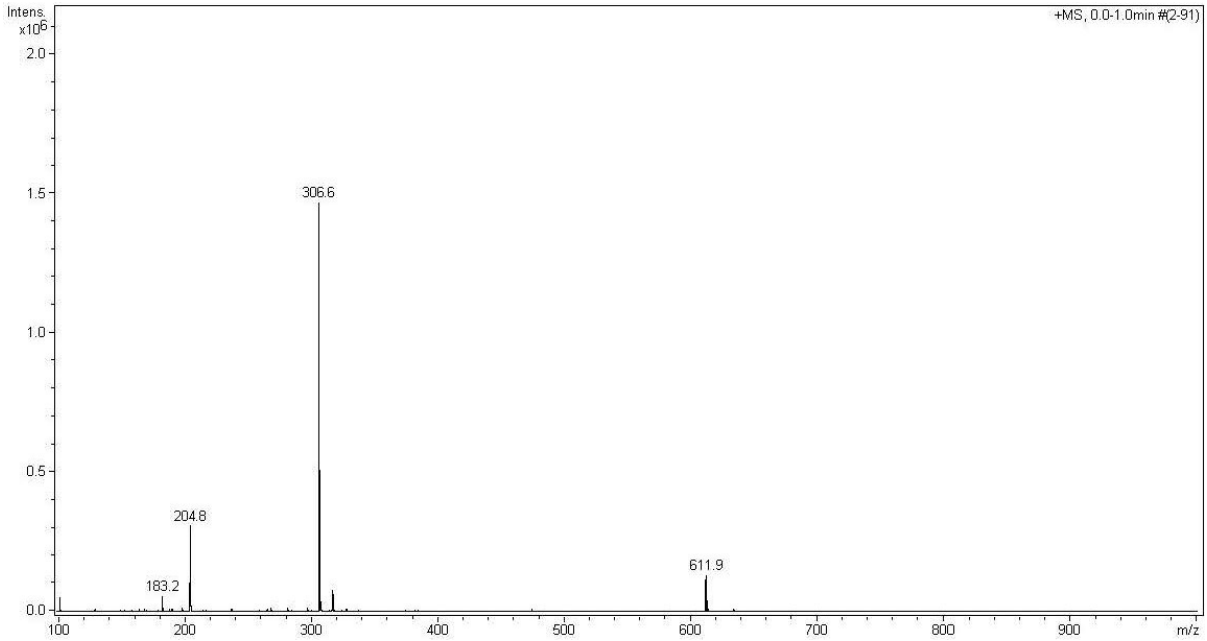

Fig. S66 ESI-MS spectrum of HKRM. $[M+H]^{+}_{calc}$ (m/z) : 612.3 ; $[M+H]^{+}_{exp}$ (m/z) : 611.9 ; $[M+2H]^{2+}_{exp}$ (m/z) : 306.6; $[M+3H]^{3+}_{exp}$ (m/z) : 204.8

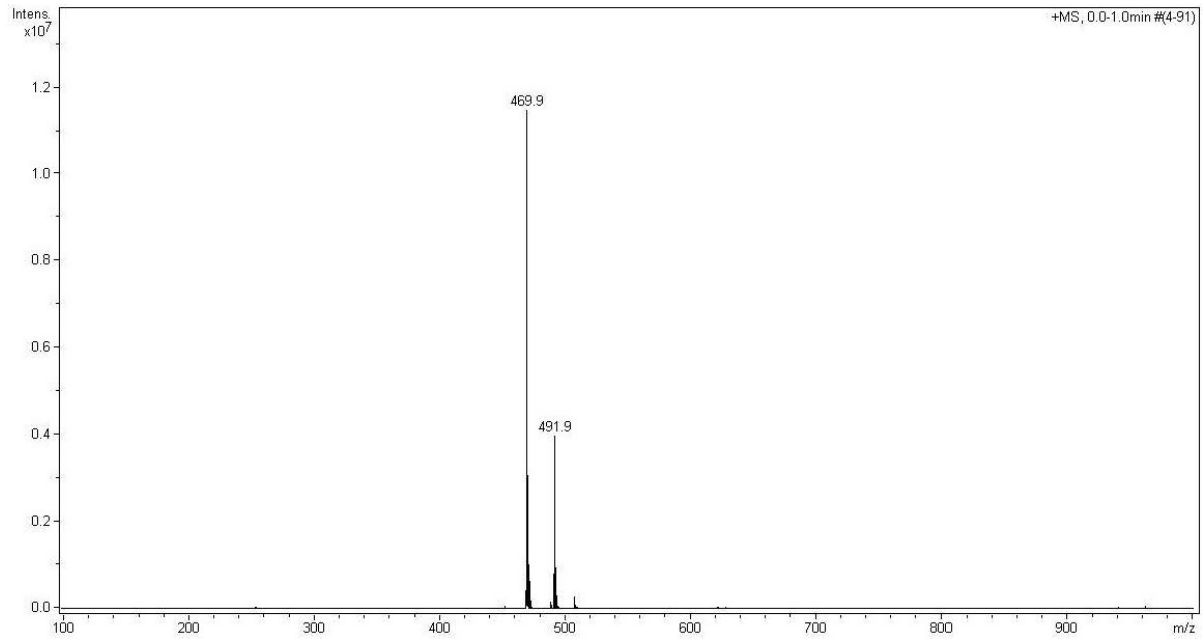

Fig. S67 ESI-MS spectrum of HAAM. $[M+H]^{+}_{calc}$ (m/z) : 470.2 ; $[M+H]^{+}_{exp}$ (m/z) : 469.9 ; $[M+Na]^{+}_{exp}$ (m/z) : 491.9

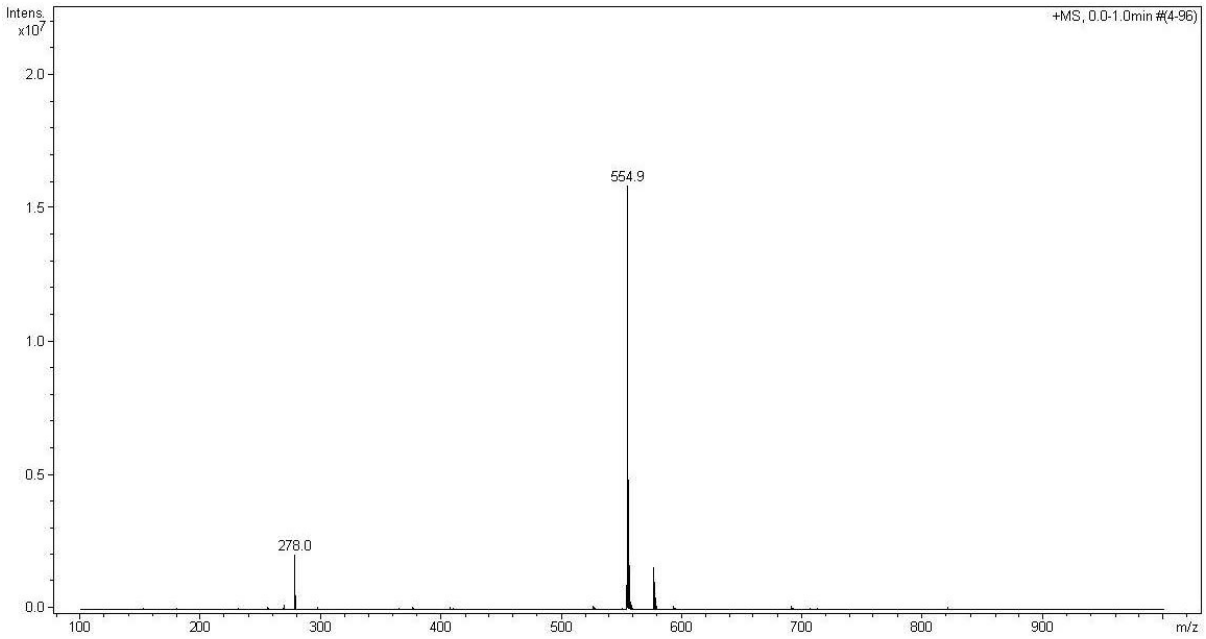

Fig. S68 ESI-MS spectrum of HRAM. $[M+H]^{+}_{calc}$ (m/z) : 555.3 ; $[M+H]^{+}_{exp}$ (m/z) : 554.9 ; $[M+2H]^{2+}_{exp}$ (m/z) : 278.0

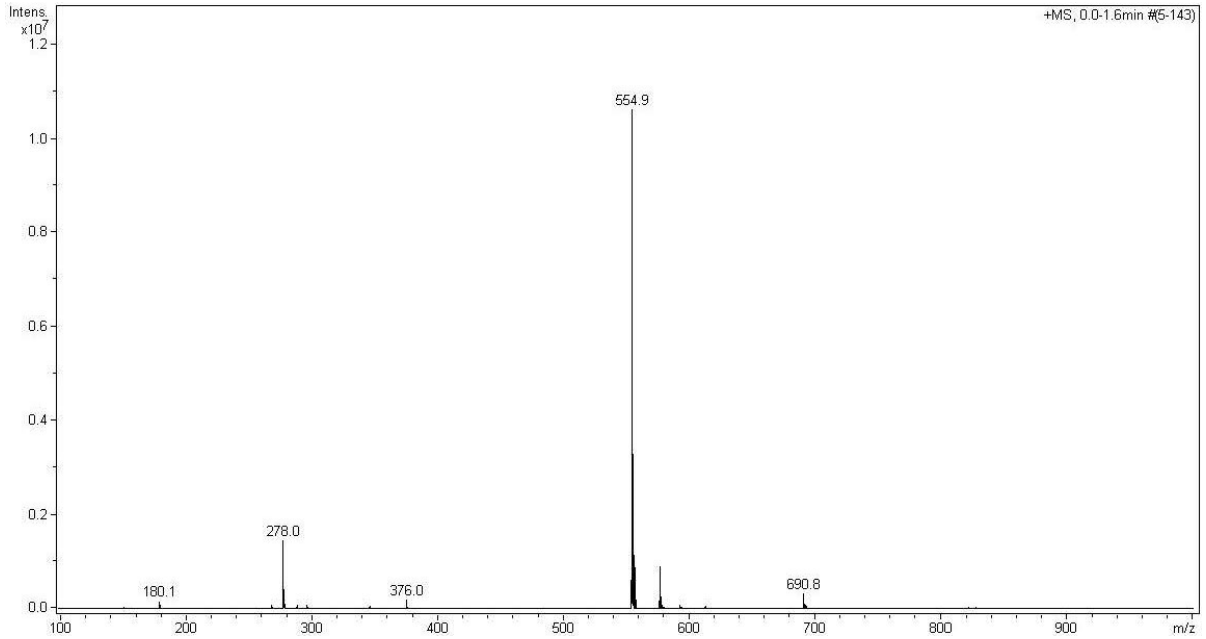

Fig. S69 ESI-MS spectrum of HARM. $[M+H]^{+}_{calc}$ (m/z) : 555.3 ; $[M+H]^{+}_{exp}$ (m/z) : 554.9 ; $[M+2H]^{2+}_{exp}$ (m/z) : 278.0

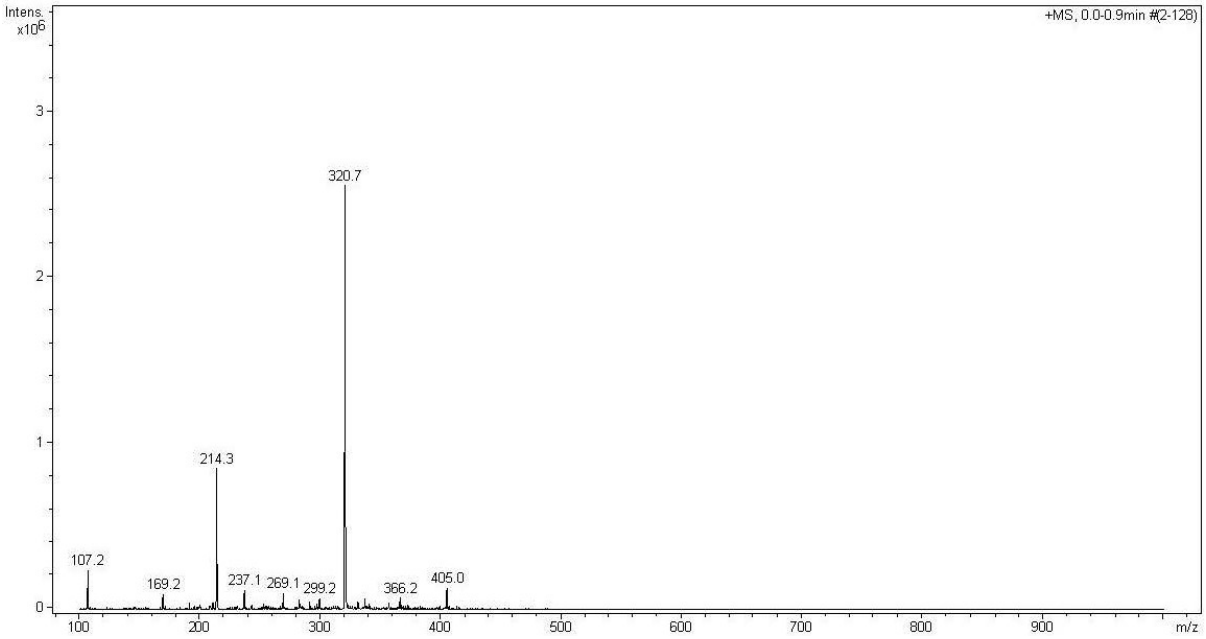

Fig. S70 ESI-MS spectrum of HRRM. $[M+H]^{+}_{calc}$ (m/z) : 640.3 ; $[M+2H]^{2+}_{exp}$ (m/z) : 320.7 ; $[M+3H]^{3+}_{exp}$ (m/z) : 214.3

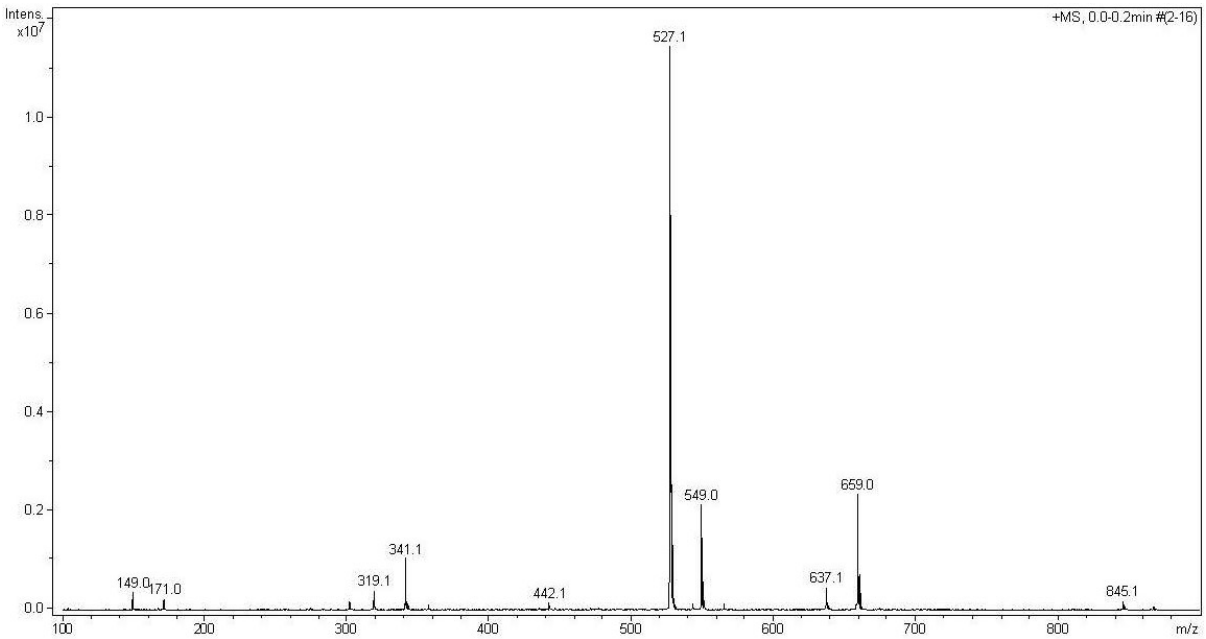

Fig. S71 ESI-MS spectrum of HAQM. $[M+H]^{+}_{calc}$ (m/z) : 527.2 ; $[M+H]^{+}_{exp}$ (m/z) : 527.1 ; $[M+Na]^{+}_{exp}$ (m/z) : 549.0

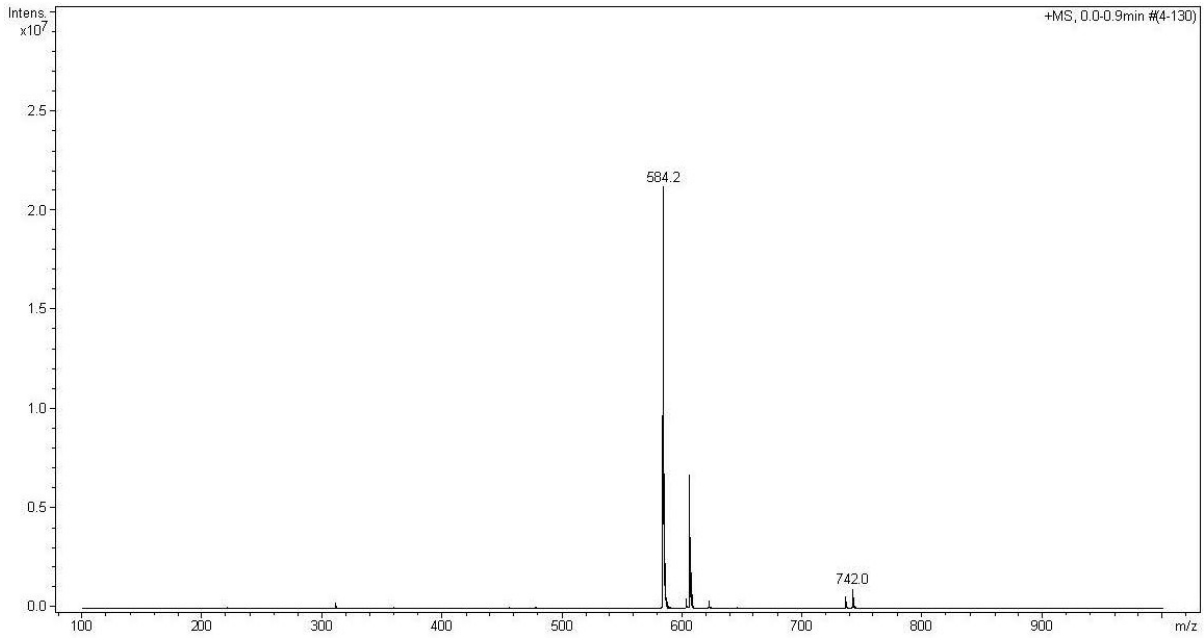

Fig. S72 ESI-MS spectrum of MQQH. $[M+H]^{+}_{calc}$ (m/z) : 584.3 ; $[M+H]^{+}_{exp}$ (m/z) : 584.2

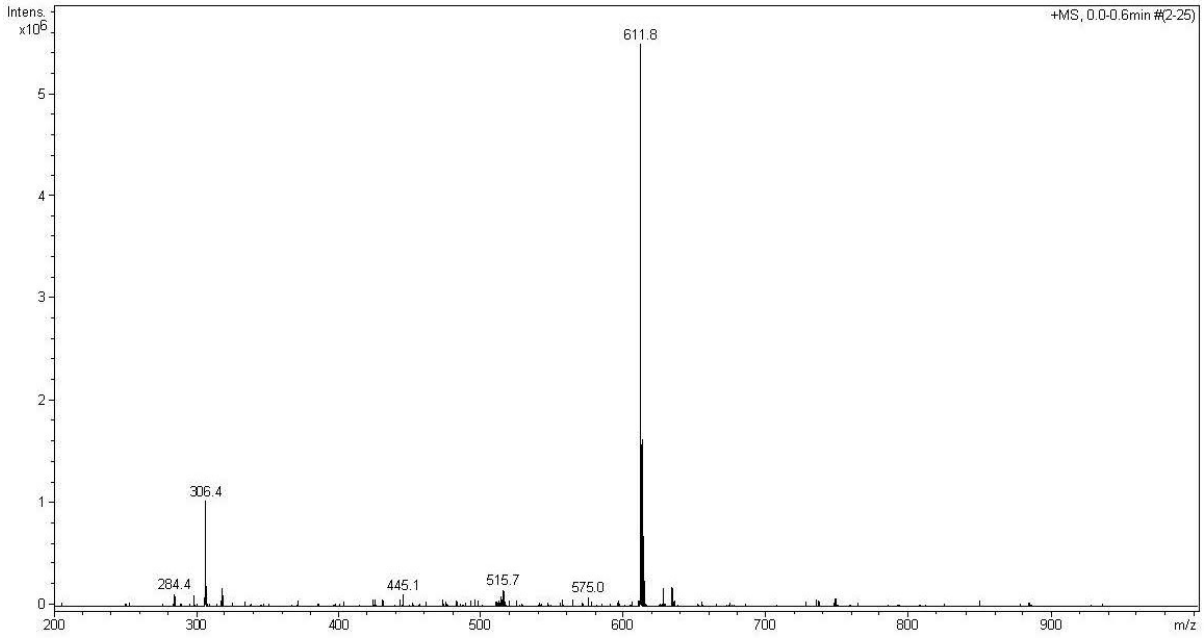

Fig. S73 ESI-MS spectrum of MRQH. $[M+H]^{+}_{calc}$ (m/z) : 612.3 ; $[M+H]^{+}_{exp}$ (m/z) : 611.8 ; $[M+2H]^{2+}_{exp}$ (m/z) : 306.4

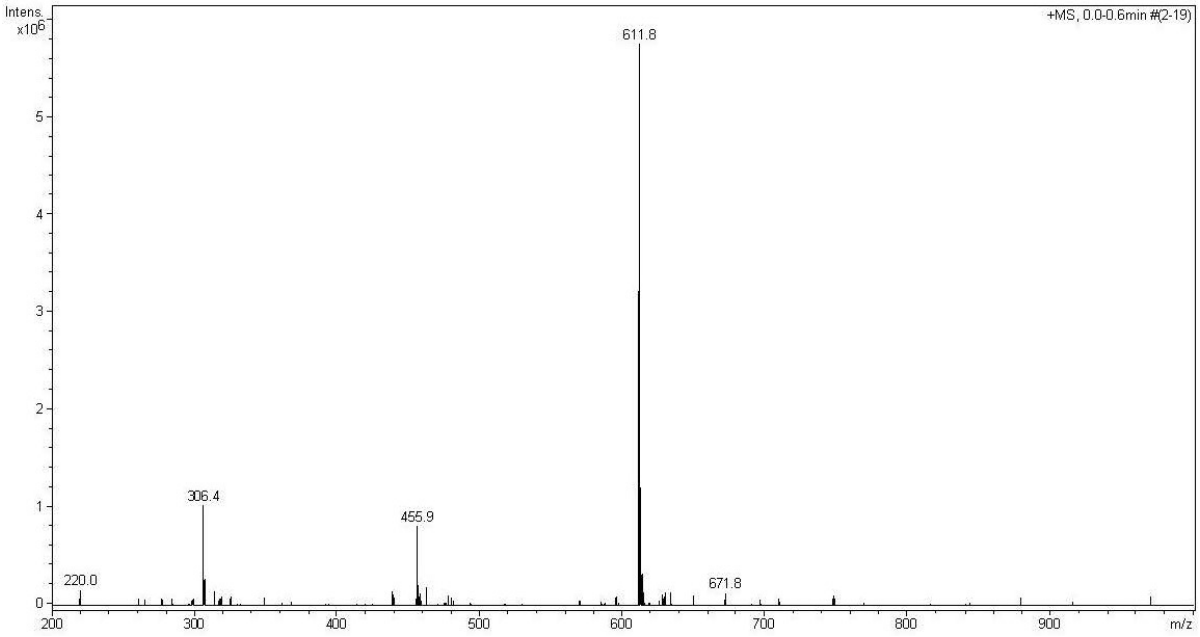

Fig. S74 ESI-MS spectrum of MQRH. $[M+H]^{+}_{calc}$ (m/z) : 612.3 ; $[M+H]^{+}_{exp}$ (m/z) : 611.8 ; $[M+2H]^{2+}_{exp}$ (m/z) : 306.4

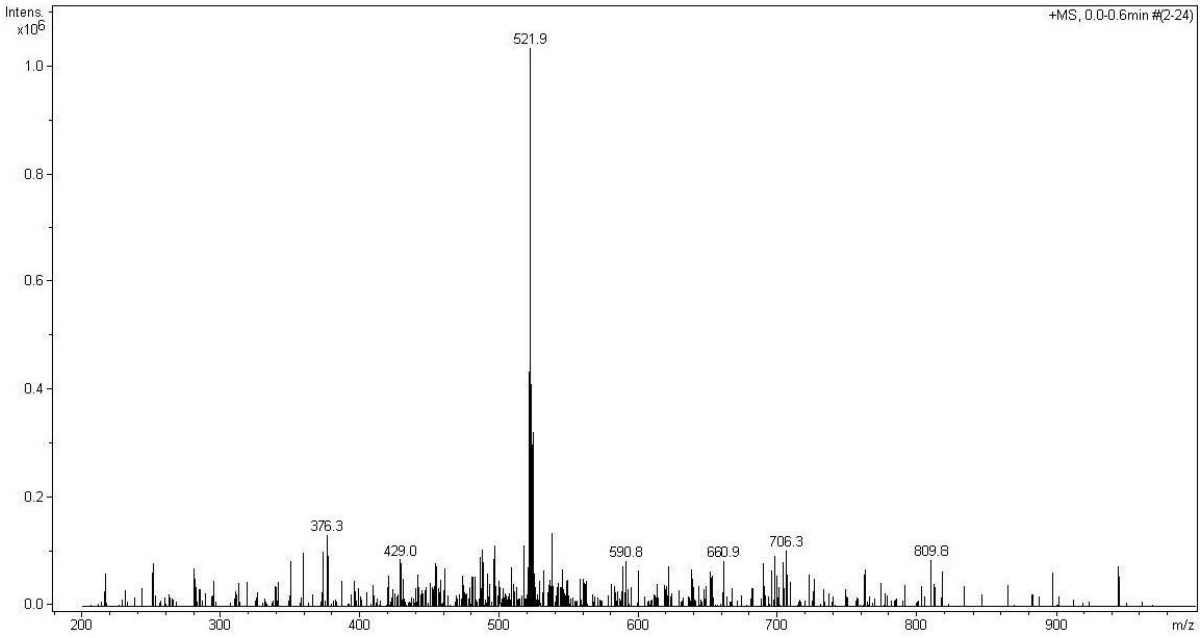

Fig. S75 ESI-MS spectrum of MPPH. $[M+H]^{+}_{calc}$ (m/z) : 522.2 ; $[M+H]^{+}_{exp}$ (m/z) : 521.9

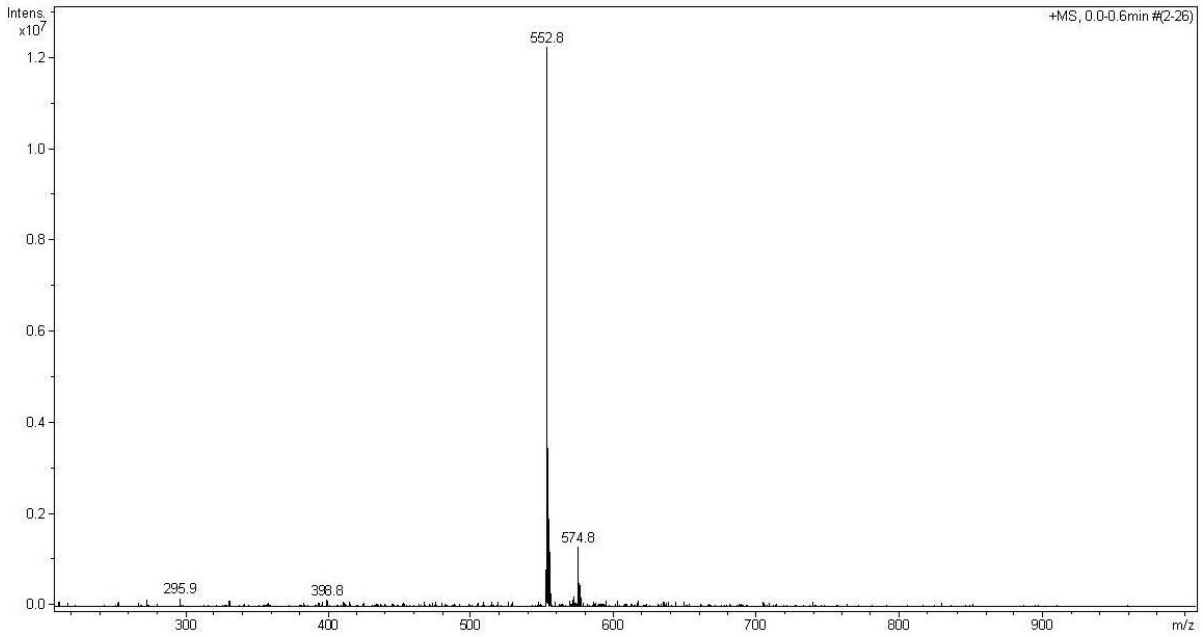

Fig. S76 ESI-MS spectrum of MQPH. $[M+H]^+_{calc}$ (m/z) : 553.2 ; $[M+H]^+_{exp}$ (m/z) : 552.8 ; $[M+Na]^+_{exp}$ (m/z) : 574.8

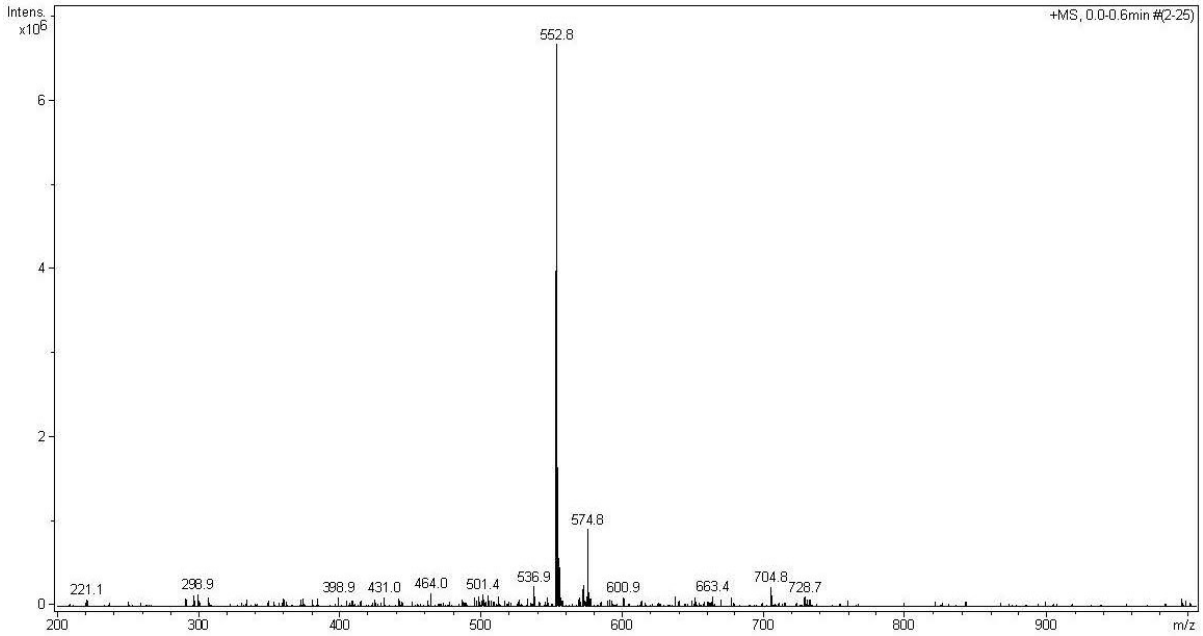

Fig. S77 ESI-MS spectrum of MPQH. $[M+H]^+_{calc}$ (m/z) : 553.2 ; $[M+H]^+_{exp}$ (m/z) : 552.8 ; $[M+Na]^+_{exp}$ (m/z) : 574.8

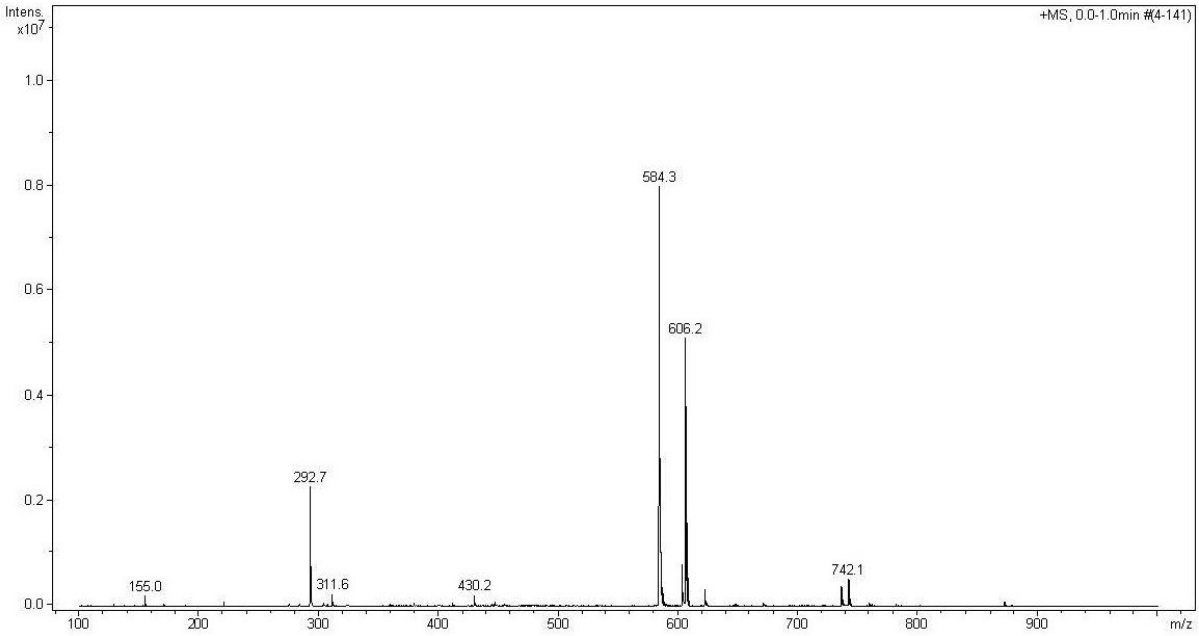

Fig. S78 ESI-MS spectrum of MKKH. $[M+H]^{+}_{calc}$ (m/z) : 584.3 ; $[M+H]^{+}_{exp}$ (m/z) : 584.3 ; $[M+Na]^{+}_{exp}$ (m/z) : 606.2 ; $[M+2H]^{2+}_{exp}$ (m/z) : 292.7

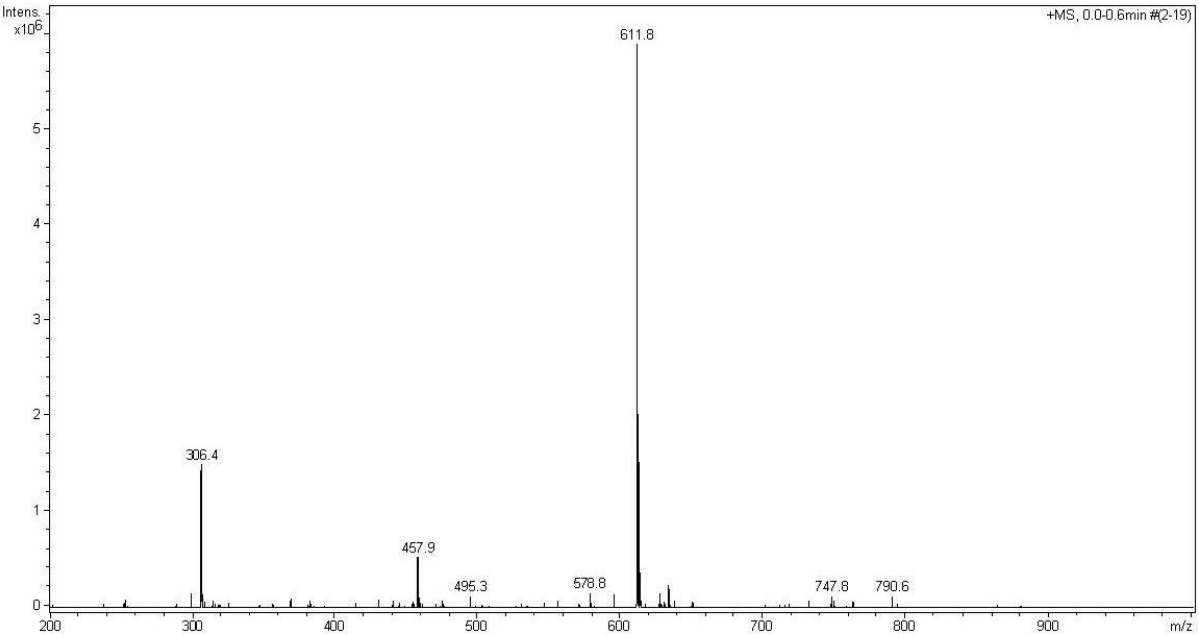

Fig. S79 ESI-MS spectrum of MRKH. $[M+H]^{+}_{calc}$ (m/z) : 612.3 ; $[M+H]^{+}_{exp}$ (m/z) : 611.8 ; $[M+2H]^{2+}_{exp}$ (m/z) : 306.4

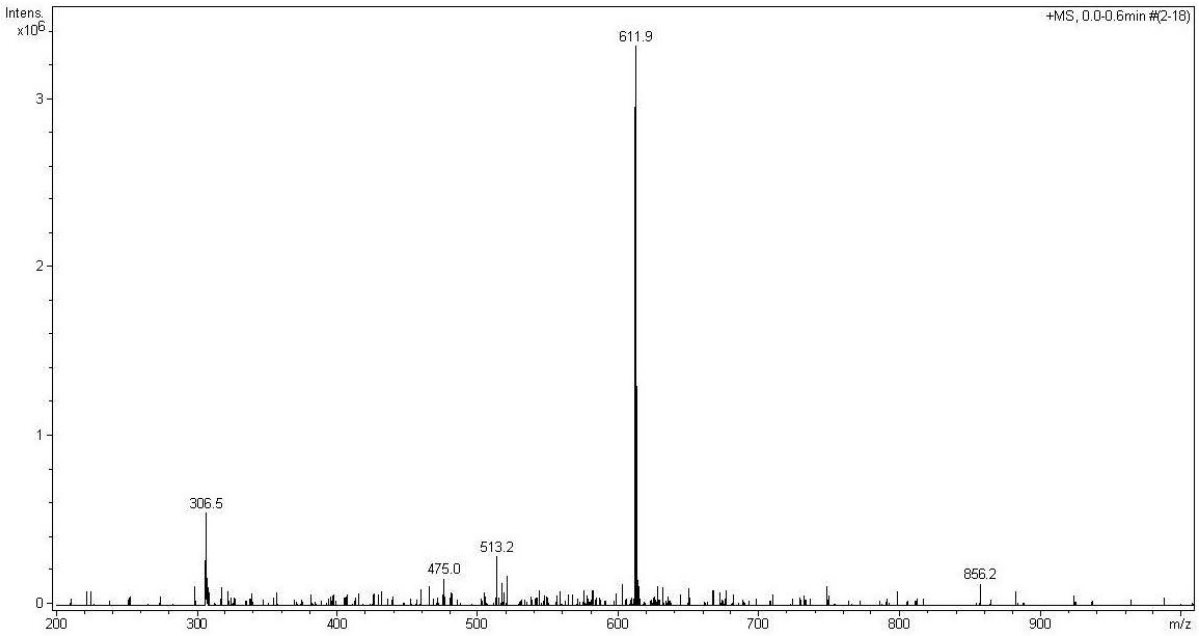

Fig. S80 ESI-MS spectrum of MKRH. $[M+H]^{+}_{calc}$ (m/z) : 612.3 ; $[M+H]^{+}_{exp}$ (m/z) : 611.9 ; $[M+2H]^{2+}_{exp}$ (m/z) : 306.5

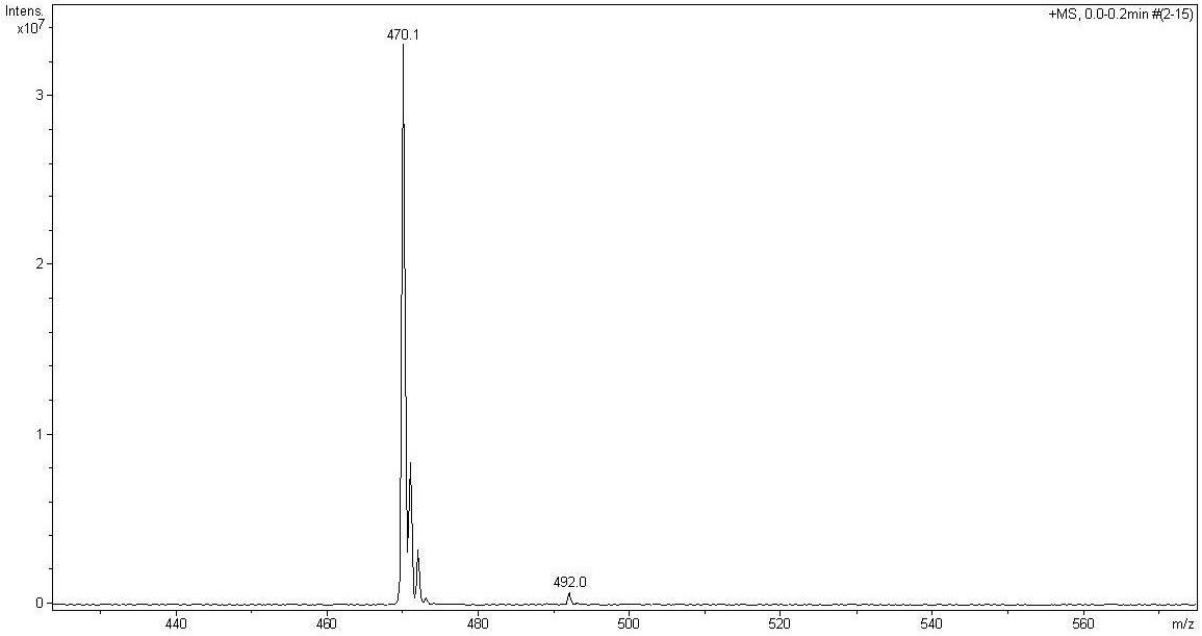

Fig. S81 ESI-MS spectrum of MAAH. $[M+H]^{+}_{calc}$ (m/z) : 470.2 ; $[M+H]^{+}_{exp}$ (m/z) : 470.1

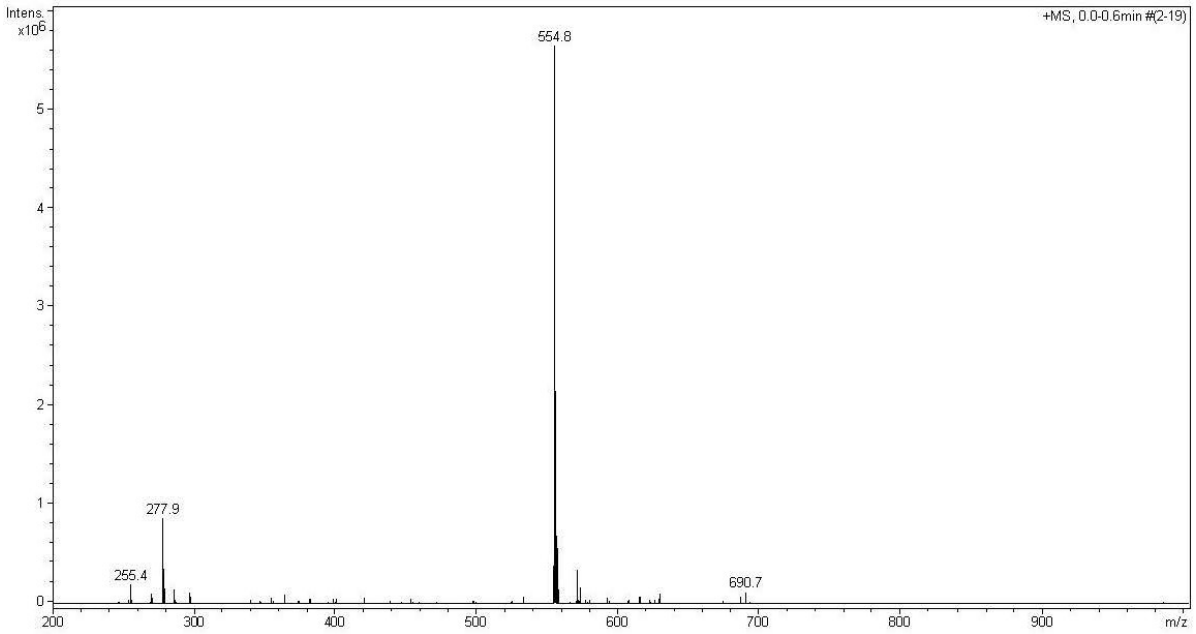

Fig. S82 ESI-MS spectrum of MRAH. $[M+H]^{+}_{calc}$ (m/z) : 555.3 ; $[M+H]^{+}_{exp}$ (m/z) : 554.8 ; $[M+2H]^{2+}_{exp}$ (m/z) : 277.9

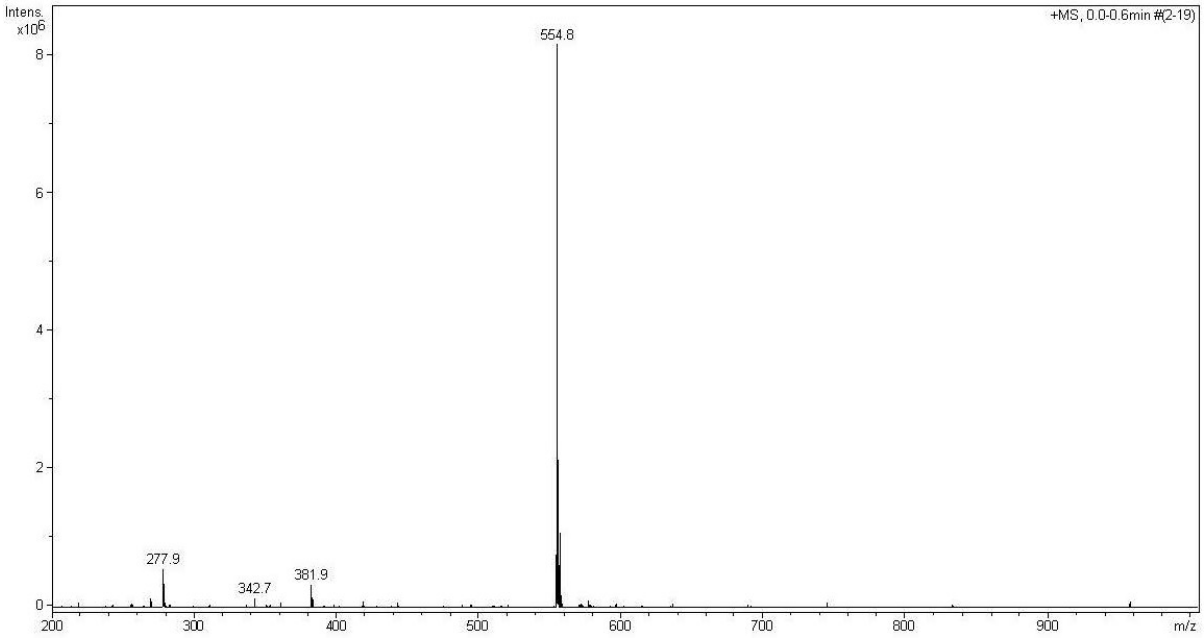

Fig. S83 ESI-MS spectrum of MARH. $[M+H]^{+}_{calc}$ (m/z) : 555.3 ; $[M+H]^{+}_{exp}$ (m/z) : 554.8 ; $[M+2H]^{2+}_{exp}$ (m/z) : 277.9

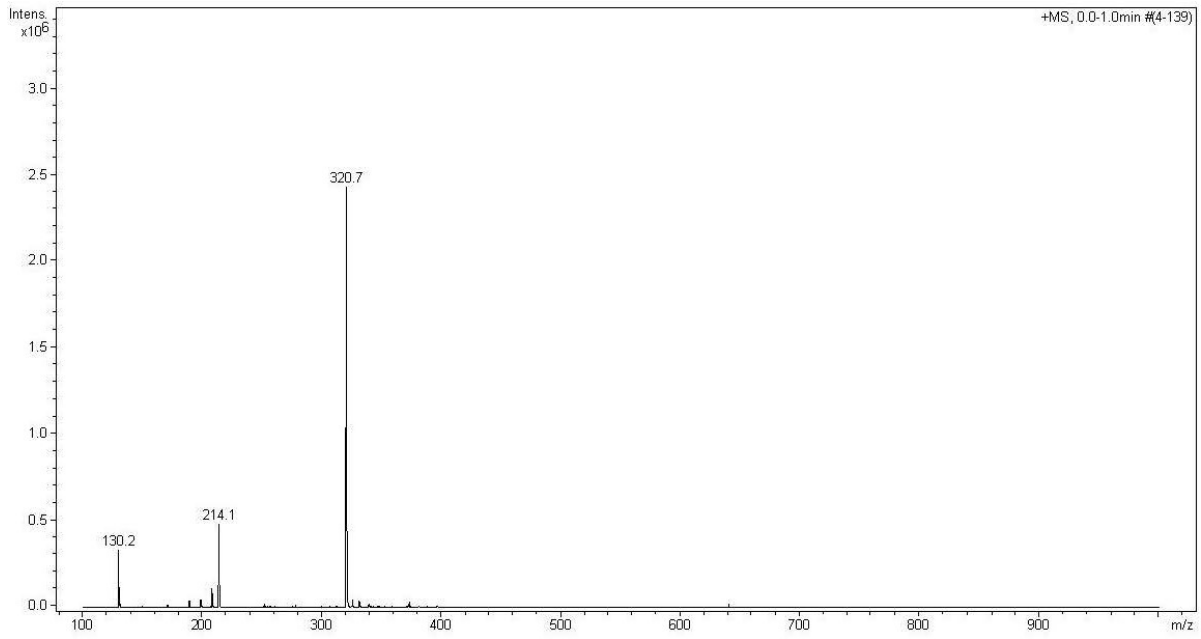

Fig. S84 ESI-MS spectrum of MRRH. $[M+H]^{+}_{calc}$ (m/z) : 640.3 ; $[M+2H]^{2+}_{exp}$ (m/z) : 320.7 ; $[M+3H]^{3+}_{exp}$ (m/z) : 214.1

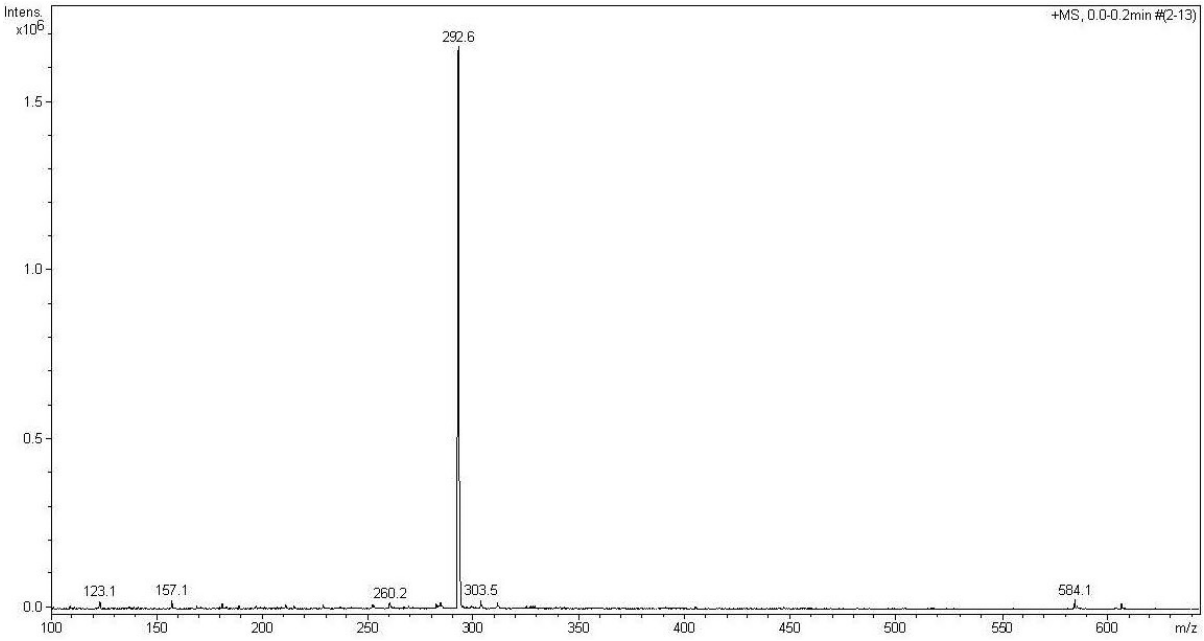

Fig. S85 ESI-MS spectrum of HKQM. $[M+H]^{+}_{calc}$ (m/z) : 584.3 ; $[M+H]^{+}_{exp}$ (m/z) : 584.1 ; $[M+2H]^{2+}_{exp}$ (m/z) : 292.6

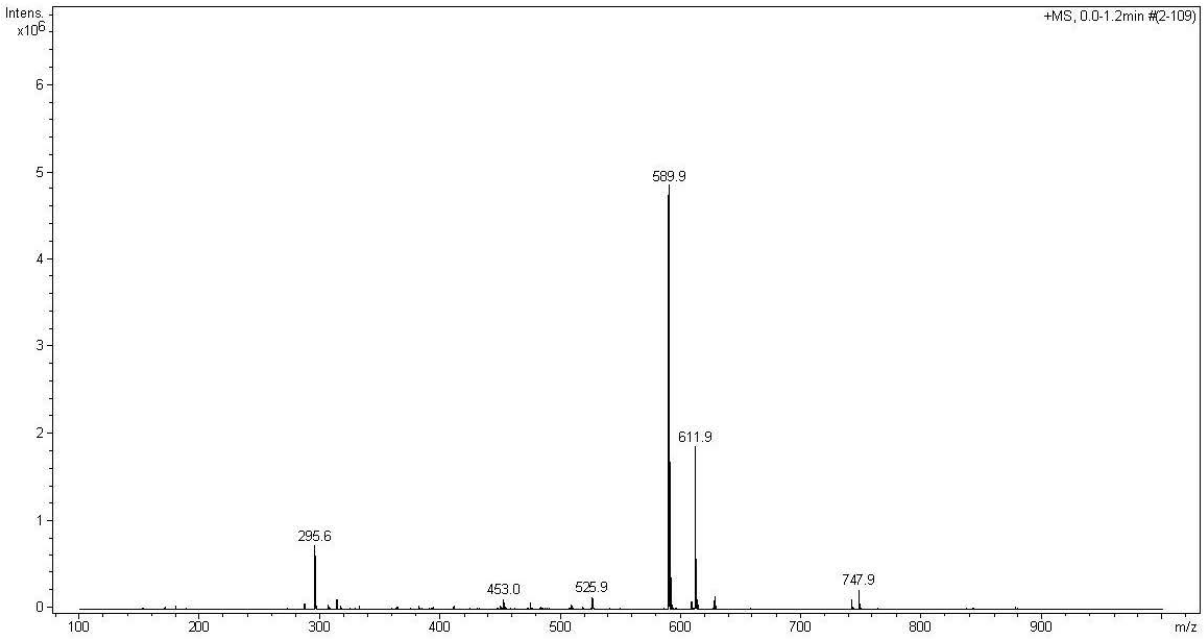

Fig. S86 ESI-MS spectrum of HQQH. $[M+H]^{+}_{calc}$ (m/z) : 590.3 ; $[M+H]^{+}_{exp}$ (m/z) : 589.9 ; $[M+Na]^{+}_{exp}$ (m/z) : 611.9 ; $[M+2H]^{2+}_{exp}$ (m/z) : 295.6

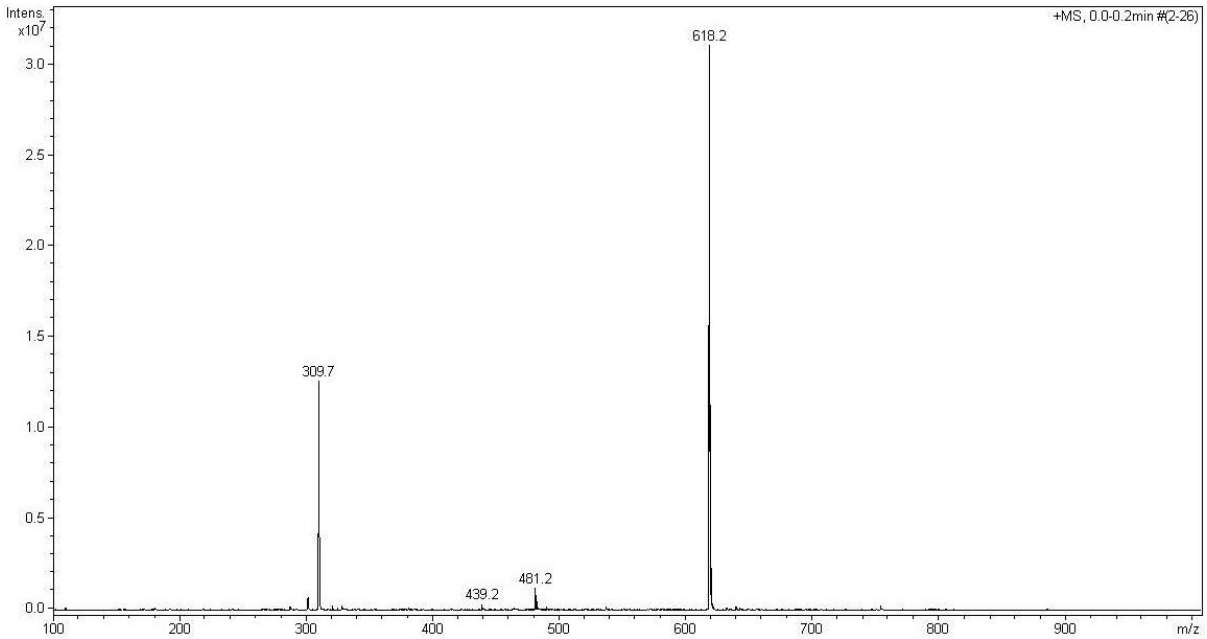

Fig. S87 ESI-MS spectrum of HRQH. $[M+H]^{+}_{calc}$ (m/z) : 618.3 ; $[M+H]^{+}_{exp}$ (m/z) : 618.2 ; $[M+2H]^{2+}_{exp}$ (m/z) : 309.7

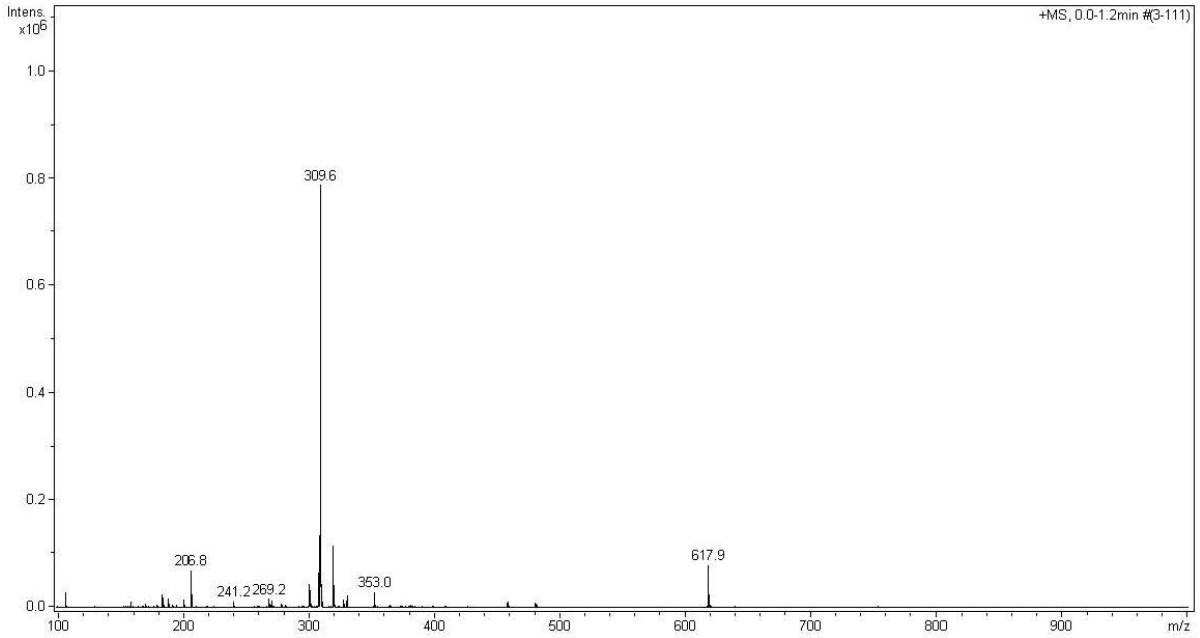

Fig. S88 ESI-MS spectrum of HQRH. $[M+H]^{+}_{calc}$ (m/z) : 618.3 ; $[M+H]^{+}_{exp}$ (m/z) : 617.9 ; $[M+2H]^{2+}_{exp}$ (m/z) : 309.6

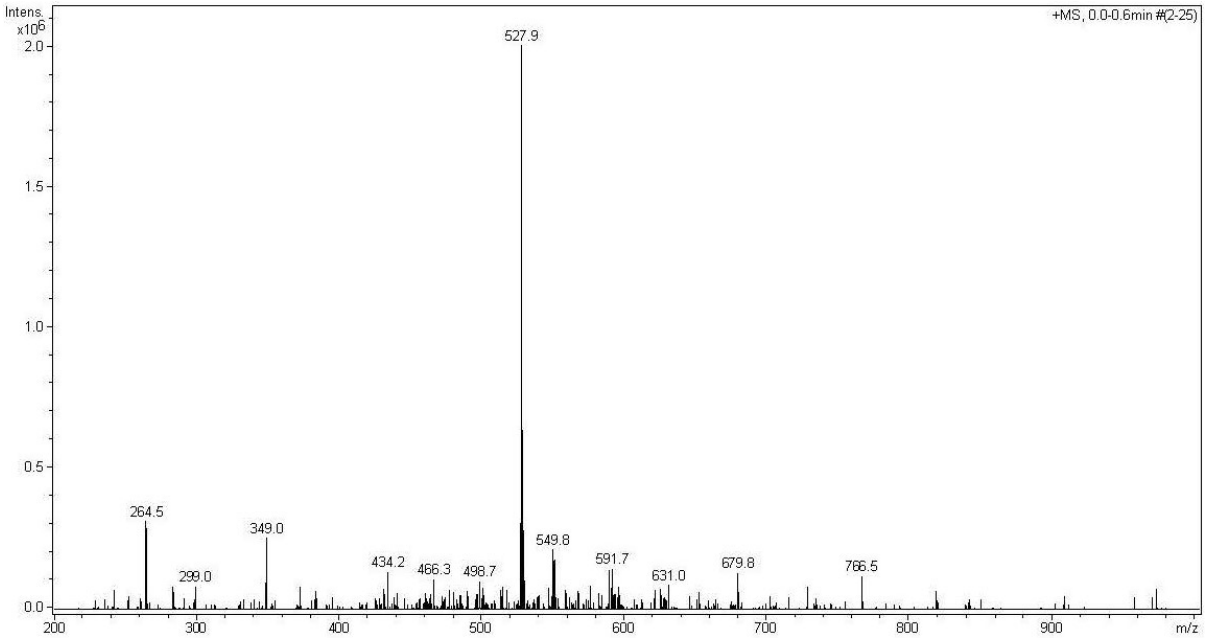

Fig. S89 ESI-MS spectrum of HPPH. $[M+H]^{+}_{calc}$ (m/z) : 528.3 ; $[M+H]^{+}_{exp}$ (m/z) : 527.9 ; $[M+Na]^{+}_{exp}$ (m/z) : 549.8 ; $[M+2H]^{2+}_{exp}$ (m/z) : 264.5

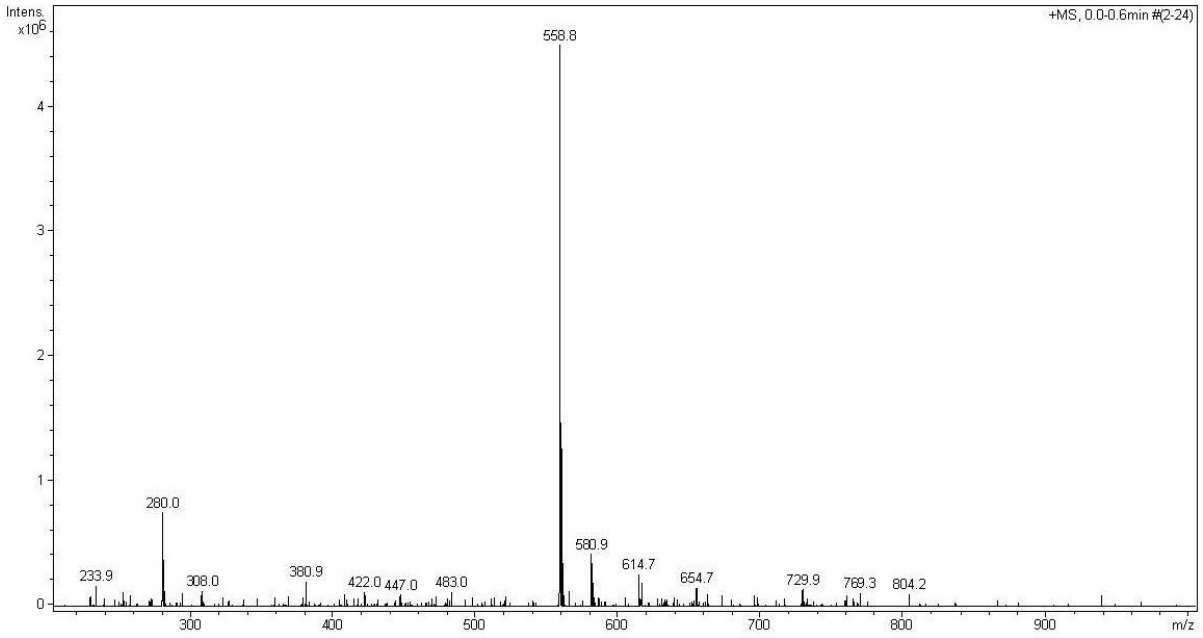

Fig. S90 ESI-MS spectrum of HQPH. $[M+H]^{+}_{calc}$ (m/z) : 559.3 ; $[M+H]^{+}_{exp}$ (m/z) : 558.8 ; $[M+Na]^{+}_{exp}$ (m/z) : 580.9 ; $[M+2H]^{2+}_{exp}$ (m/z) : 280.0

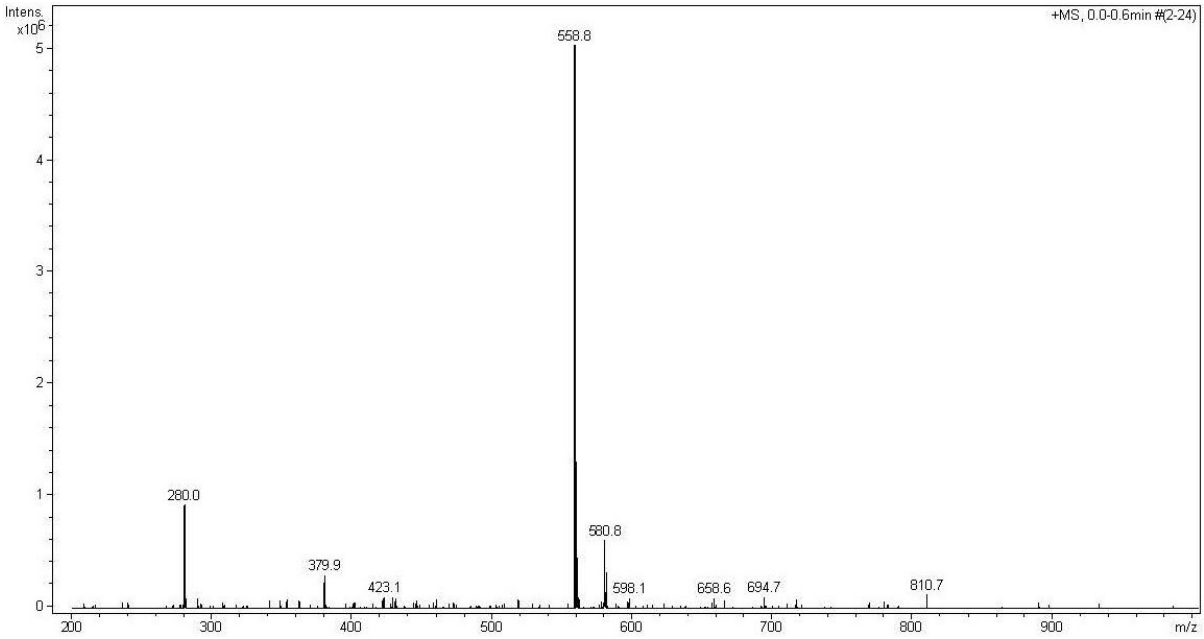

Fig. S91 ESI-MS spectrum of HPQH. $[M+H]^{+}_{calc}$ (m/z) : 559.3 ; $[M+H]^{+}_{exp}$ (m/z) : 558.8 ; $[M+Na]^{+}_{exp}$ (m/z) : 580.8 ; $[M+2H]^{2+}_{exp}$ (m/z) : 280.0

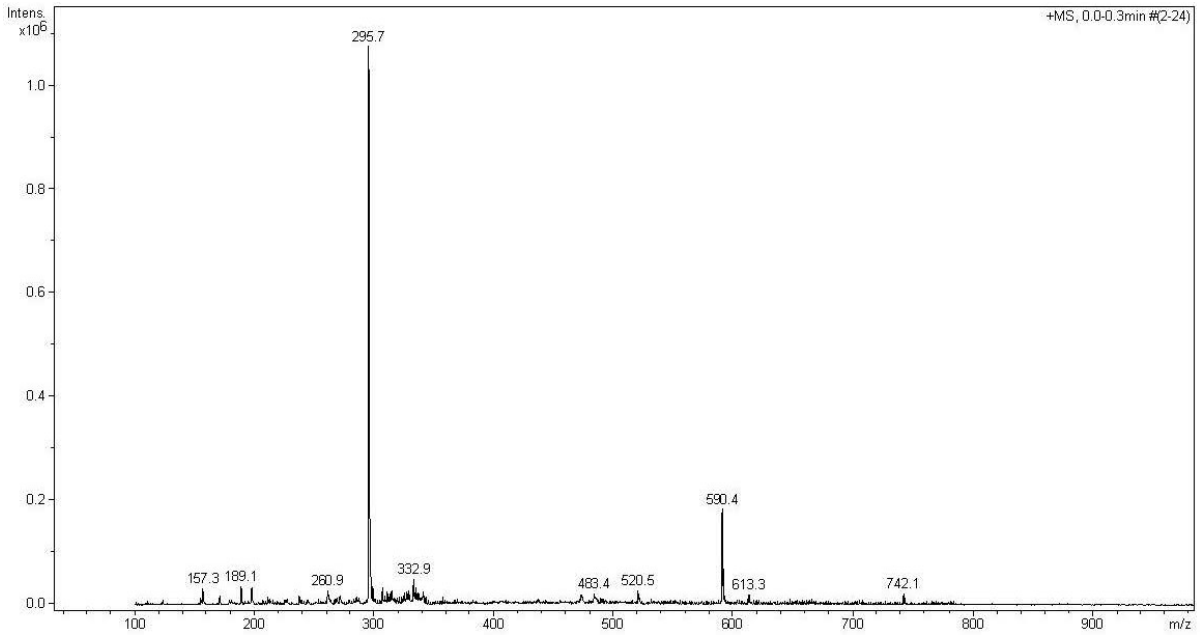

Fig. S92 ESI-MS spectrum of HKKH. $[M+H]^{+}_{calc}$ (m/z) : 590.3 ; $[M+H]^{+}_{exp}$ (m/z) : 590.4 ; $[M+Na]^{+}_{exp}$ (m/z) : 613.3 ; $[M+2H]^{2+}_{exp}$ (m/z) : 295.7

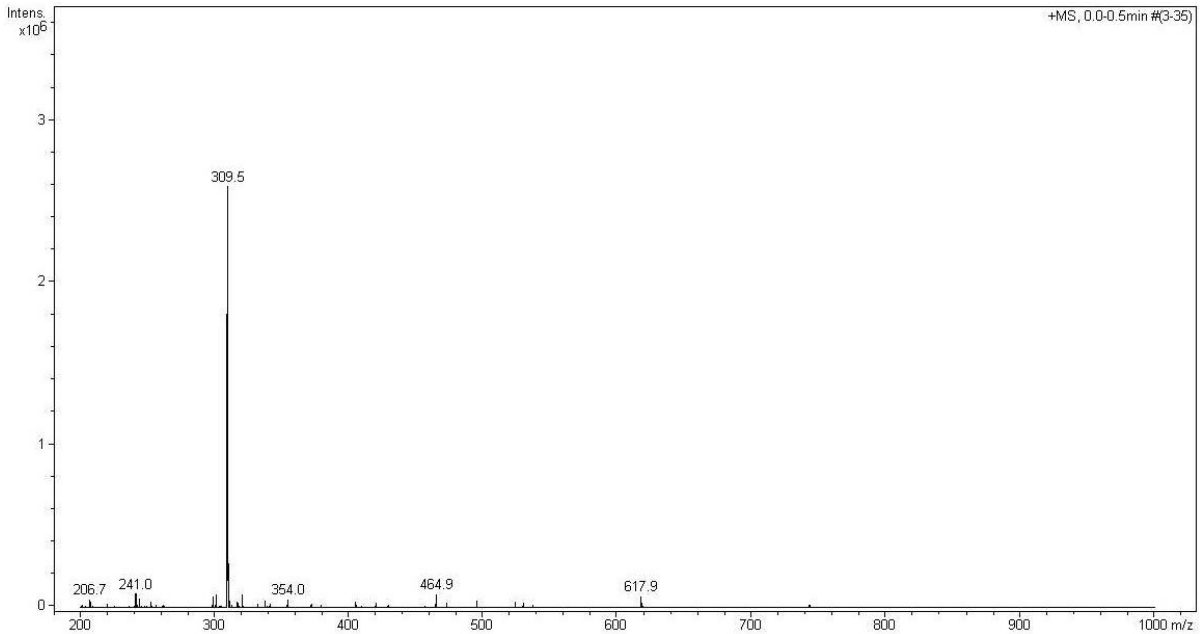

Fig. S93 ESI-MS spectrum of HRKH. $[M+H]^{+}_{calc}$ (m/z) : 618.3 ; $[M+H]^{+}_{exp}$ (m/z) : 617.9 ; $[M+2H]^{2+}_{exp}$ (m/z) : 309.5

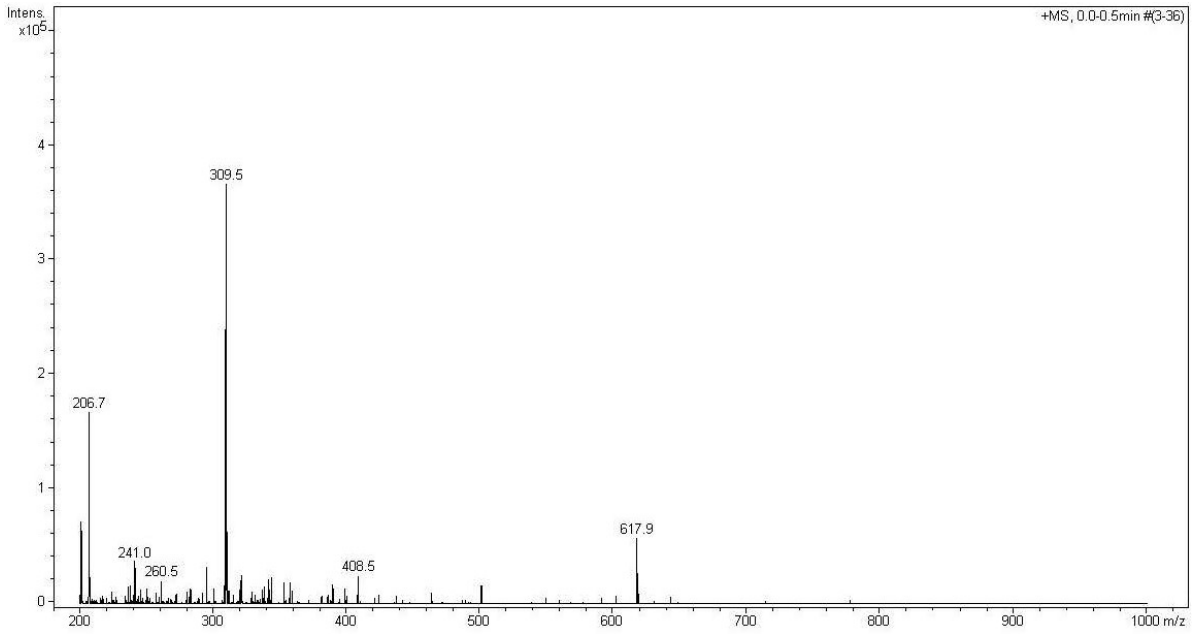

Fig. S94 ESI-MS spectrum of HKRH. $[M+H]^{+}_{calc}$ (m/z) : 618.3 ; $[M+H]^{+}_{exp}$ (m/z) : 617.9 ; $[M+2H]^{2+}_{exp}$ (m/z) : 309.5 ; $[M+3H]^{3+}_{exp}$ (m/z) : 206.7

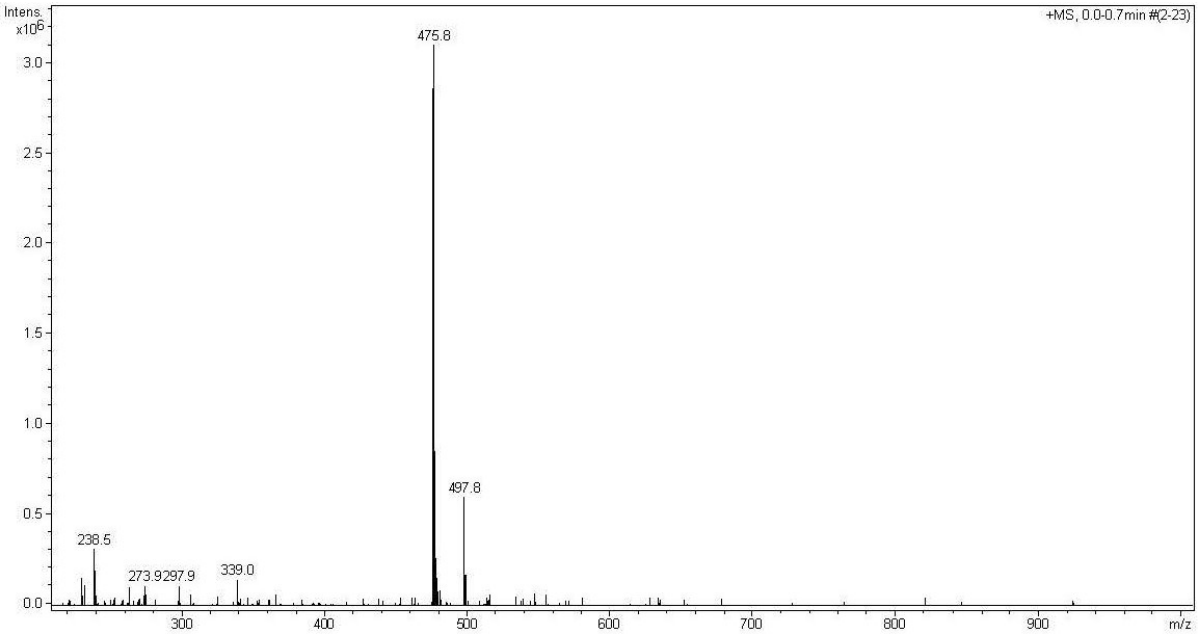

Fig. S95 ESI-MS spectrum of HAAH. $[M+H]^{+}_{calc}$ (m/z) : 476.2 ; $[M+H]^{+}_{exp}$ (m/z) : 475.8 ; $[M+Na]^{+}_{exp}$ (m/z) : 497.8

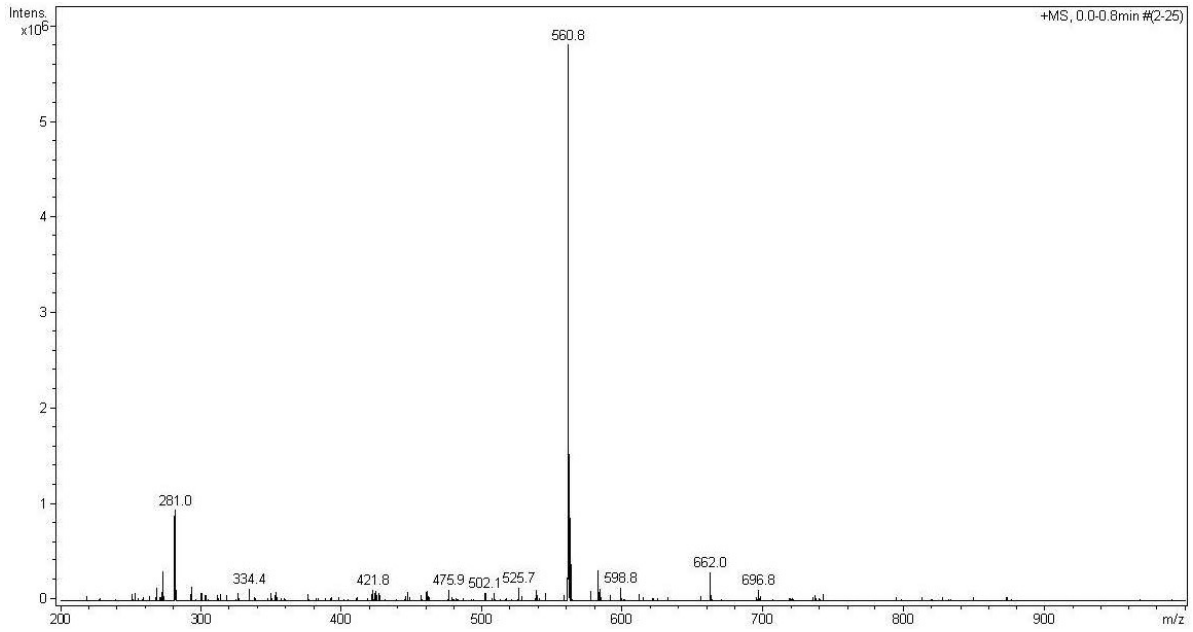

Fig. S96 ESI-MS spectrum of HRAH. $[M+H]^{+}_{calc}$ (m/z) : 561.3 ; $[M+H]^{+}_{exp}$ (m/z) : 560.8 ; $[M+2H]^{2+}_{exp}$ (m/z) : 281.0

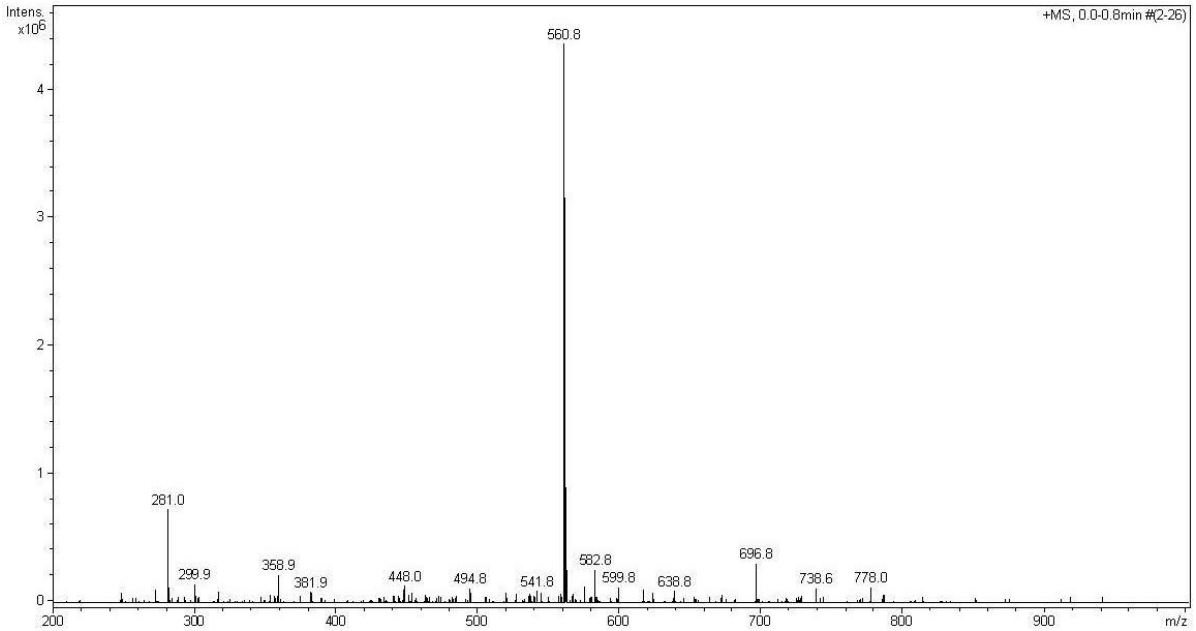

Fig. S97 ESI-MS spectrum of HARH. $[M+H]^{+}_{calc}$ (m/z) : 561.3 ; $[M+H]^{+}_{exp}$ (m/z) : 560.8 ; $[M+Na]^{+}_{exp}$ (m/z) : 582.8 ; $[M+2H]^{2+}_{exp}$ (m/z) : 281.0

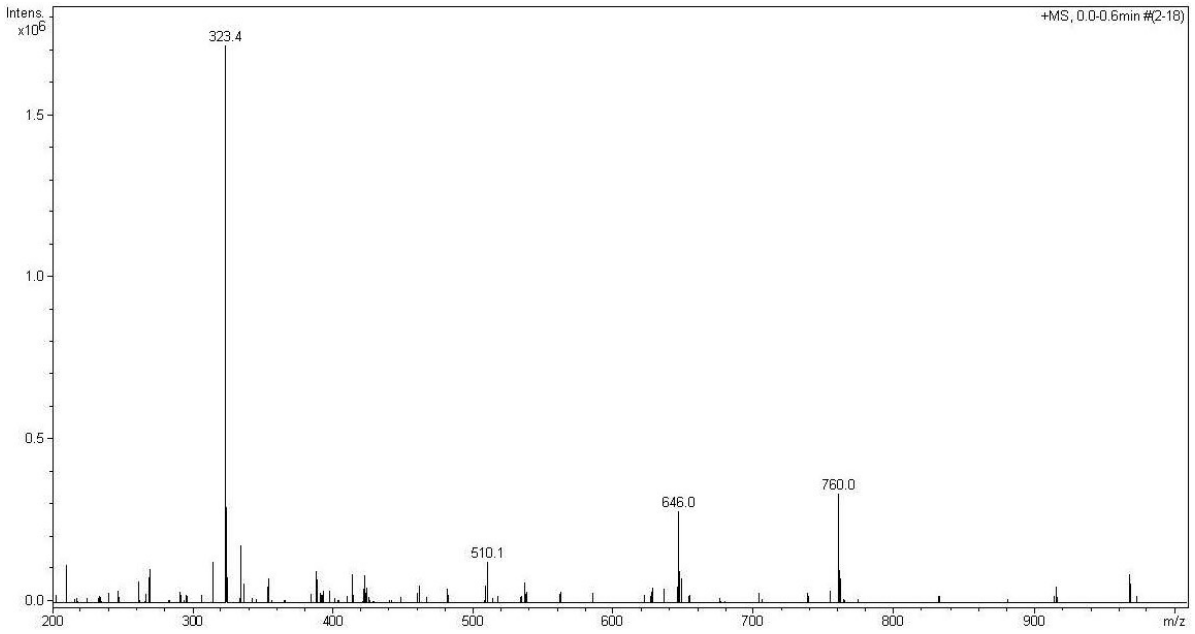

Fig. S98 ESI-MS spectrum of HRRH. $[M+H]^{+}_{calc}$ (m/z) : 646.4 ; $[M+H]^{+}_{exp}$ (m/z) : 646.0 ; $[M+2H]^{2+}_{exp}$ (m/z) : 323.4

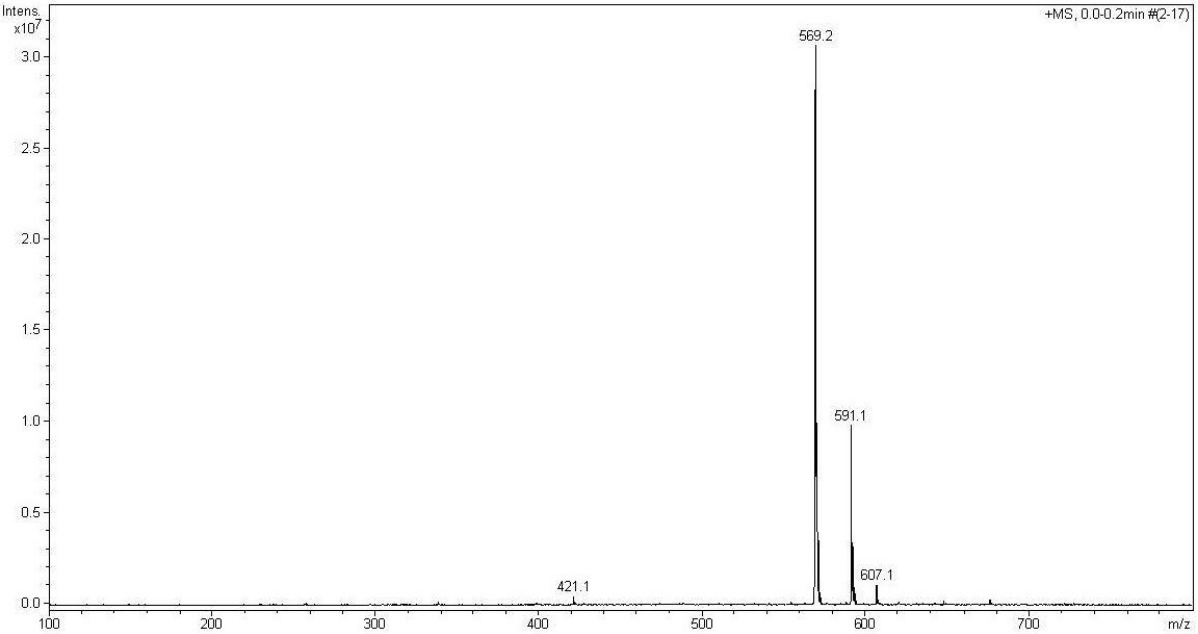

Fig. S99 ESI-MS spectrum of H−Hex−QM. $[M+H]^{+}_{calc}$ (m/z) : 569.3 ; $[M+H]^{+}_{exp}$ (m/z) : 569.2 ; $[M+Na]^{+}_{exp}$ (m/z) : 591.1

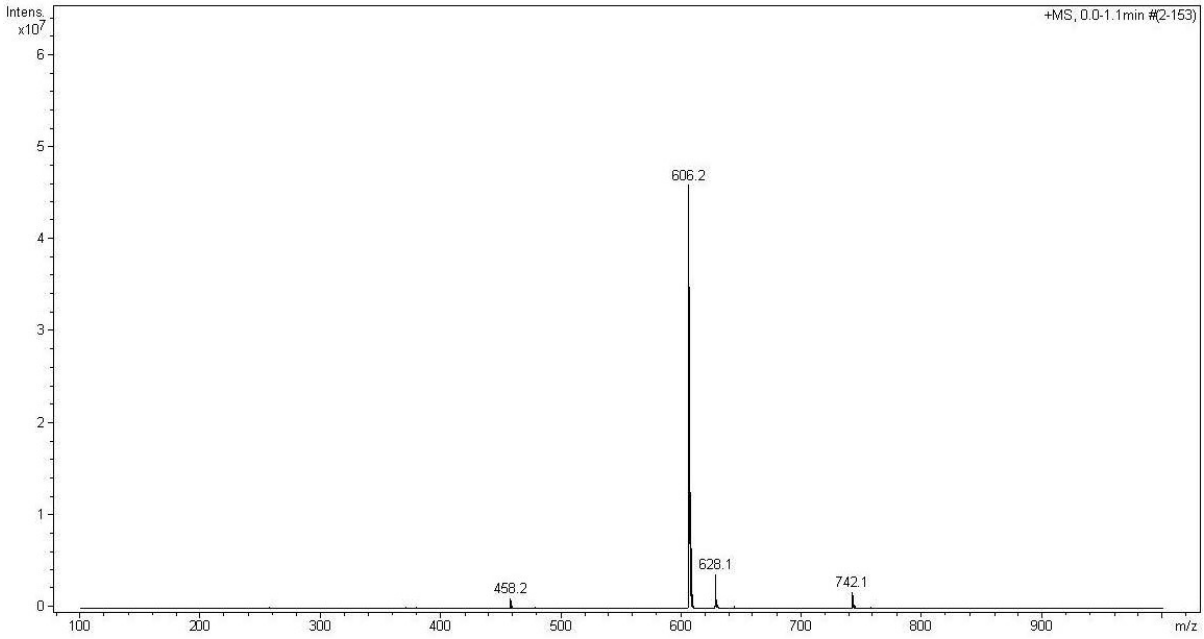

Fig. S100 ESI-MS spectrum of MRQM. $[M+H]^{+}_{calc}$ (m/z) : 606.3 ; $[M+H]^{+}_{exp}$ (m/z) : 606.2 ; $[M+Na]^{+}_{exp}$ (m/z) : 628.1

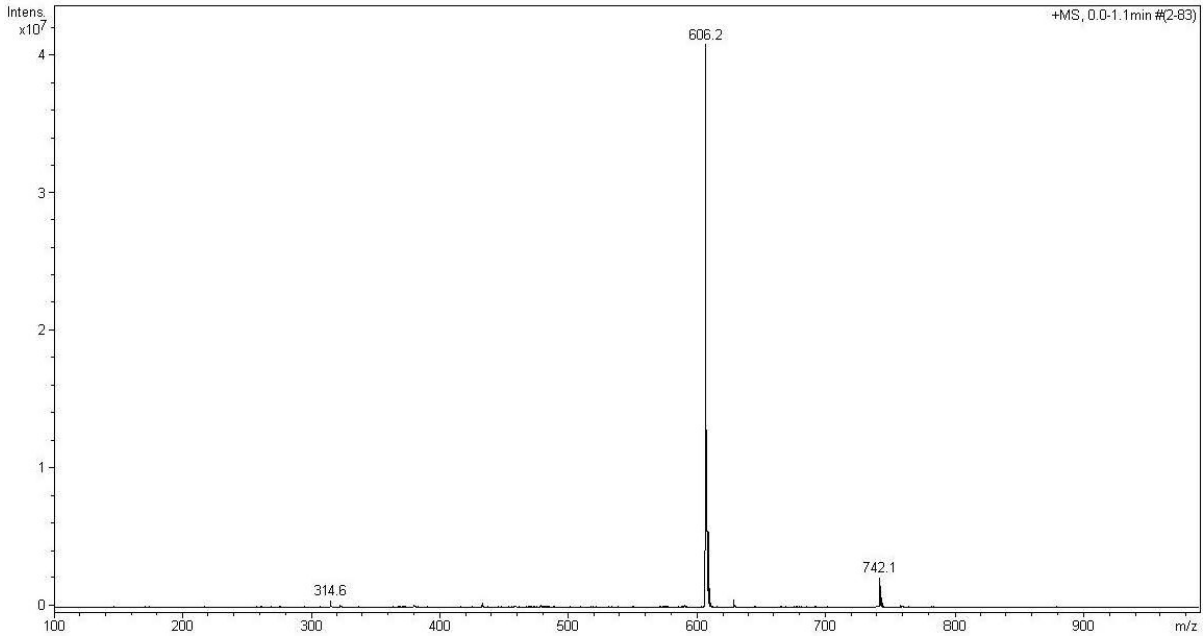

Fig. S101 ESI-MS spectrum of MQRM. $[M+H]^{+}_{calc}$ (m/z) : 606.3 ; $[M+H]^{+}_{exp}$ (m/z) : 606.2 ; $[M+H+Na]^{2+}_{exp}$ (m/z) : 314.6

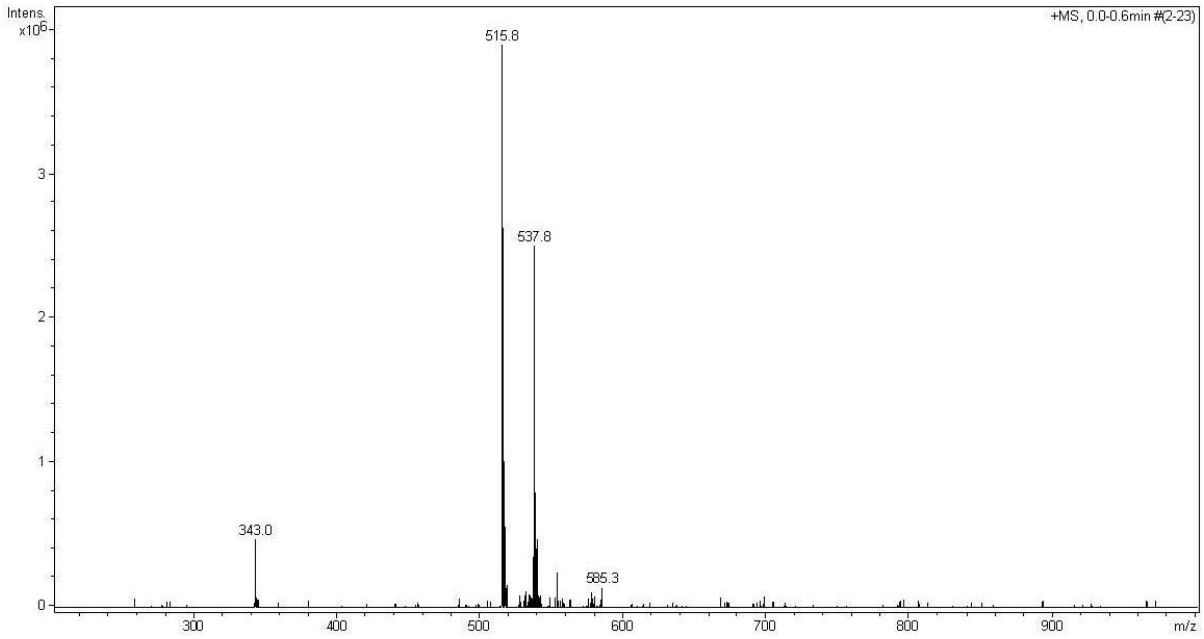

Fig. S102 ESI-MS spectrum of MPPM. $[M+H]^{+}_{calc}$ (m/z) : 516.2 ; $[M+H]^{+}_{exp}$ (m/z) : 515.8 ; $[M+Na]^{+}_{exp}$ (m/z) : 537.8

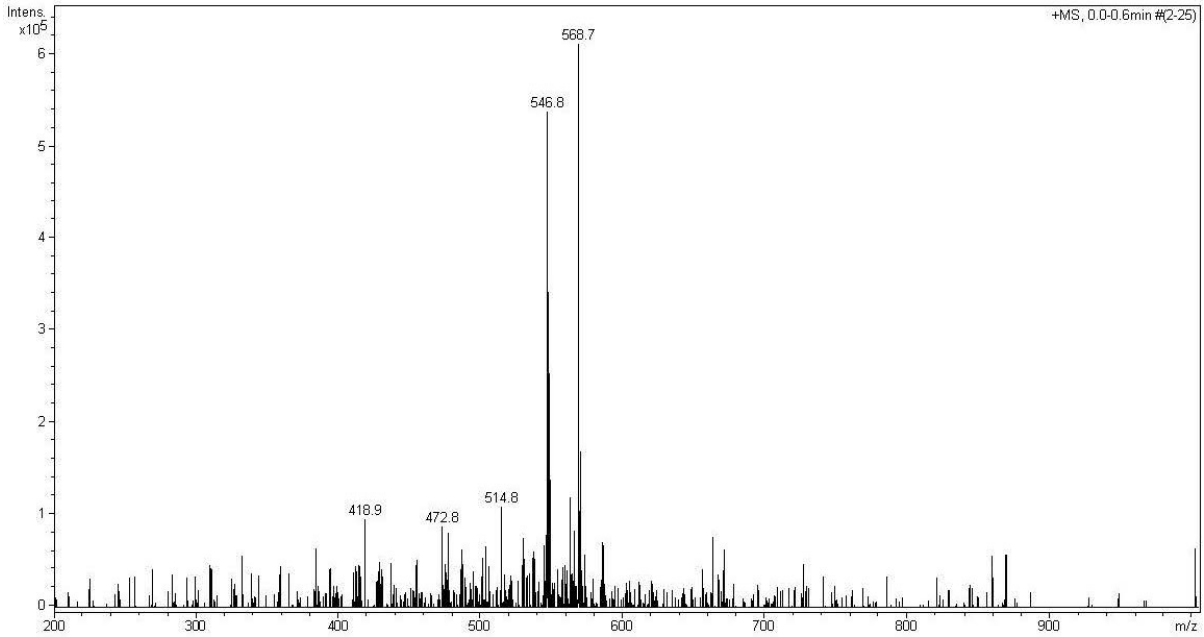

Fig. S103 ESI-MS spectrum of MQPM. $[M+H]^{+}_{calc}$ (m/z) : 547.2 ; $[M+H]^{+}_{exp}$ (m/z) : 546.8 ; $[M+Na]^{+}_{exp}$ (m/z) : 568.7

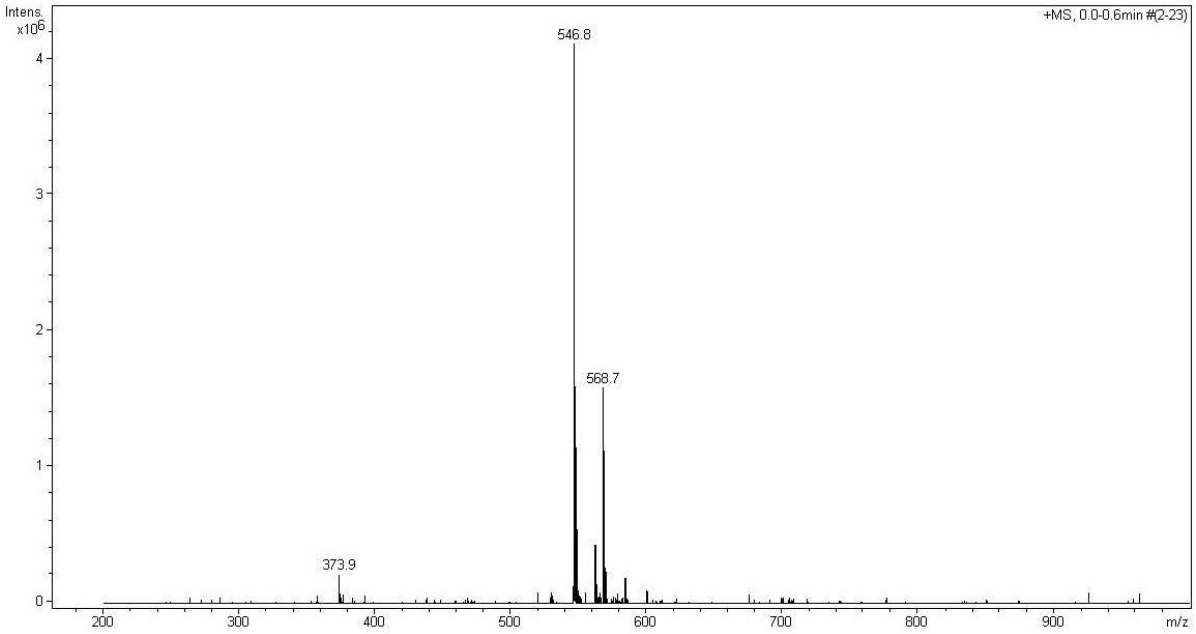

Fig. S104 ESI-MS spectrum of MPQM. $[M+H]^{+}_{calc}$ (m/z) : 547.2 ; $[M+H]^{+}_{exp}$ (m/z) : 546.8 ; $[M+Na]^{+}_{exp}$ (m/z) : 568.7

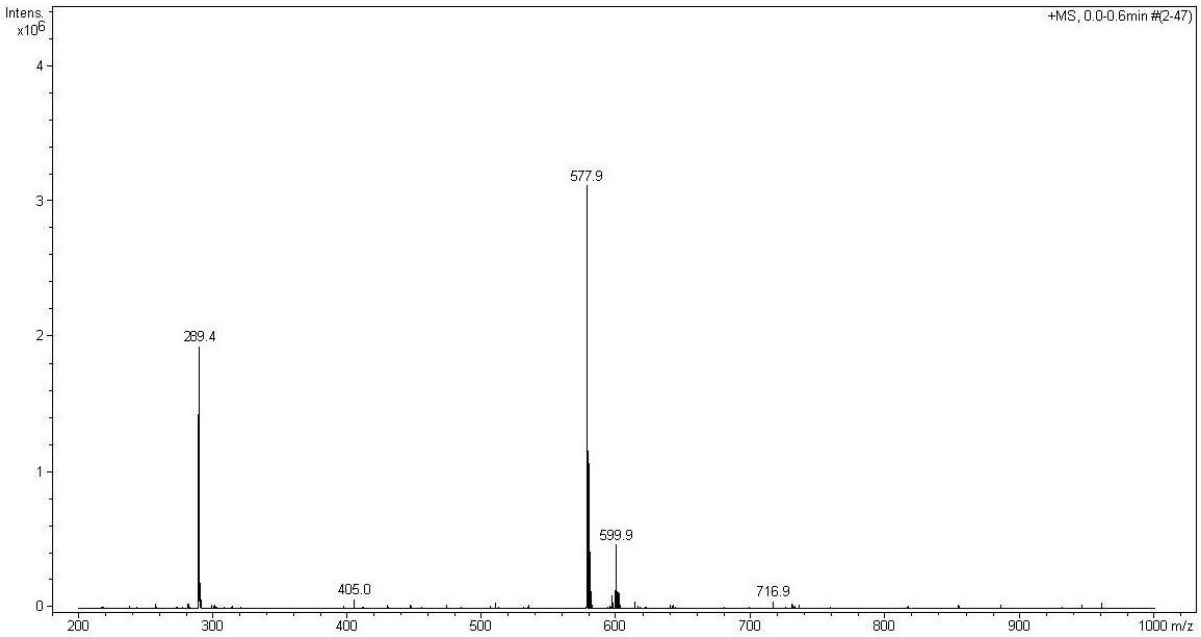

Fig. S105 ESI-MS spectrum of MKKM. $[M+H]^{+}_{calc}$ (m/z) : 578.3 ; $[M+H]^{+}_{exp}$ (m/z) : 577.9 ; $[M+Na]^{+}_{exp}$ (m/z) : 599.9 ; $[M+2H]^{2+}_{exp}$ (m/z) : 289.4

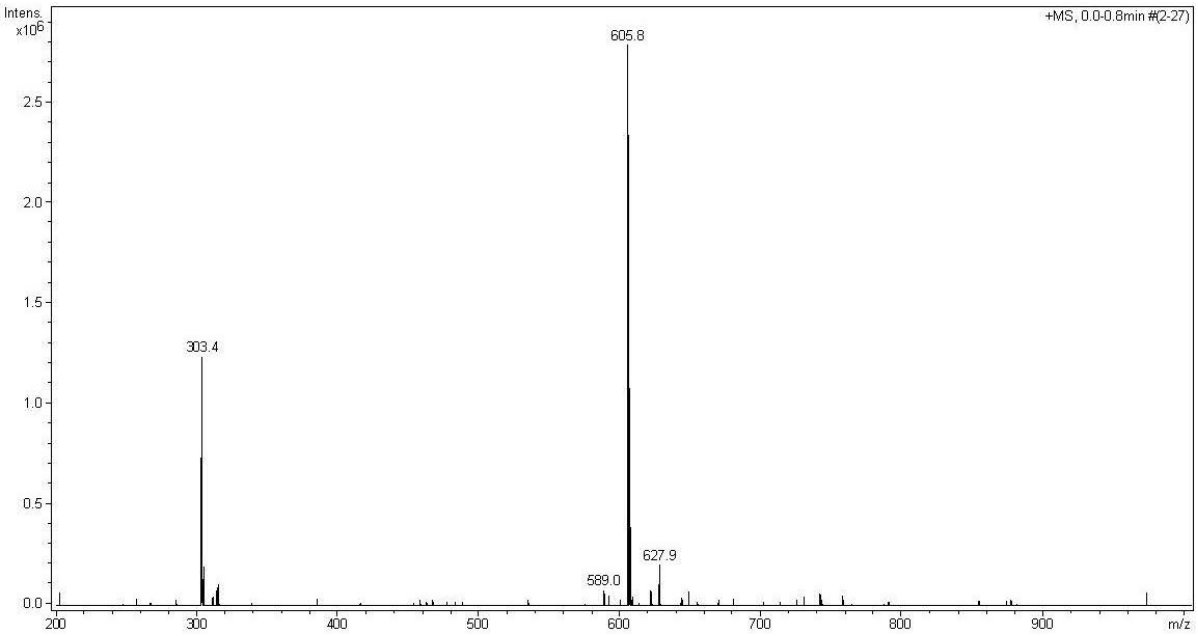

Fig. S106 ESI-MS spectrum of MRKM. $[M+H]^{+}_{calc}$ (m/z) : 606.3 ; $[M+H]^{+}_{exp}$ (m/z) : 605.8 ; $[M+Na]^{+}_{exp}$ (m/z) : 627.9 ; $[M+2H]^{2+}_{exp}$ (m/z) : 303.4

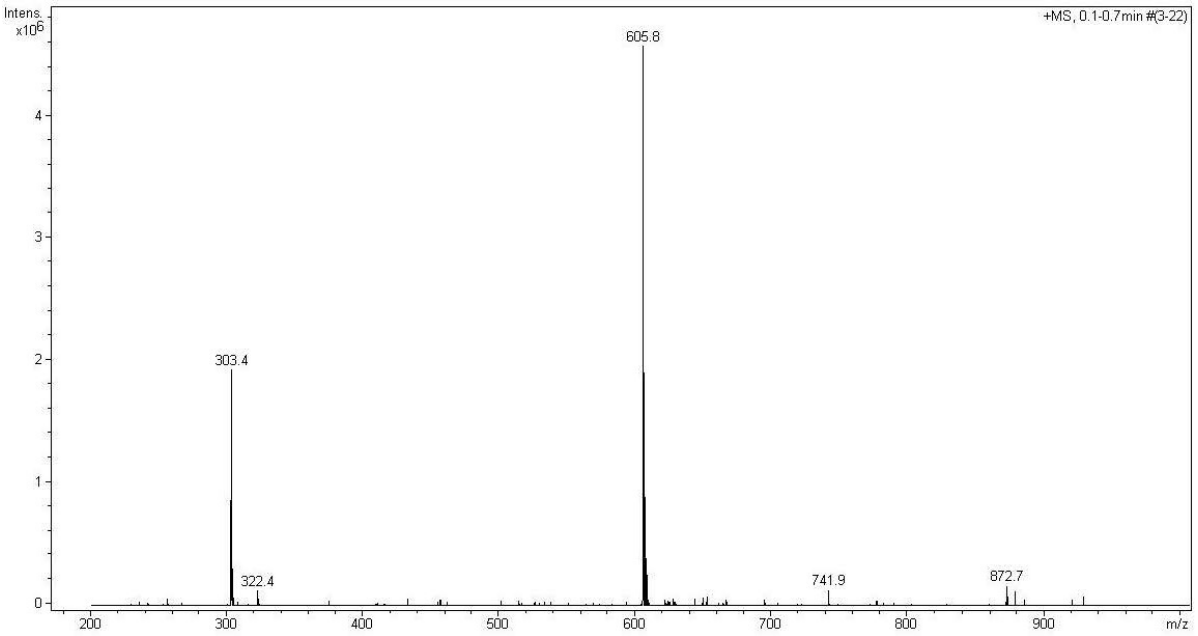

Fig. S107 ESI-MS spectrum of MKRM. $[M+H]^{+}_{calc}$ (m/z) : 606.3 ; $[M+H]^{+}_{exp}$ (m/z) : 605.8 ; $[M+2H]^{2+}_{exp}$ (m/z) : 303.4

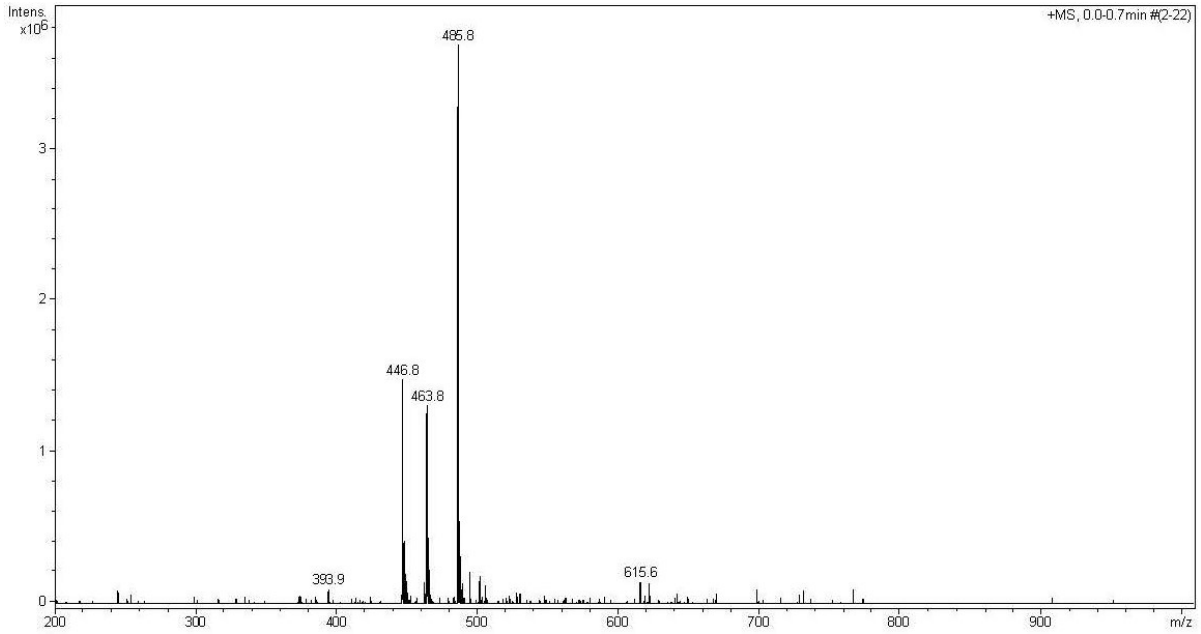

Fig. S108 ESI-MS spectrum of MAAM. $[M+H]^+_{calc}$ (m/z) : 464.2 ; $[M+H]^+_{exp}$ (m/z) : 463.8 ; $[M+Na]^+_{exp}$ (m/z) : 485.8

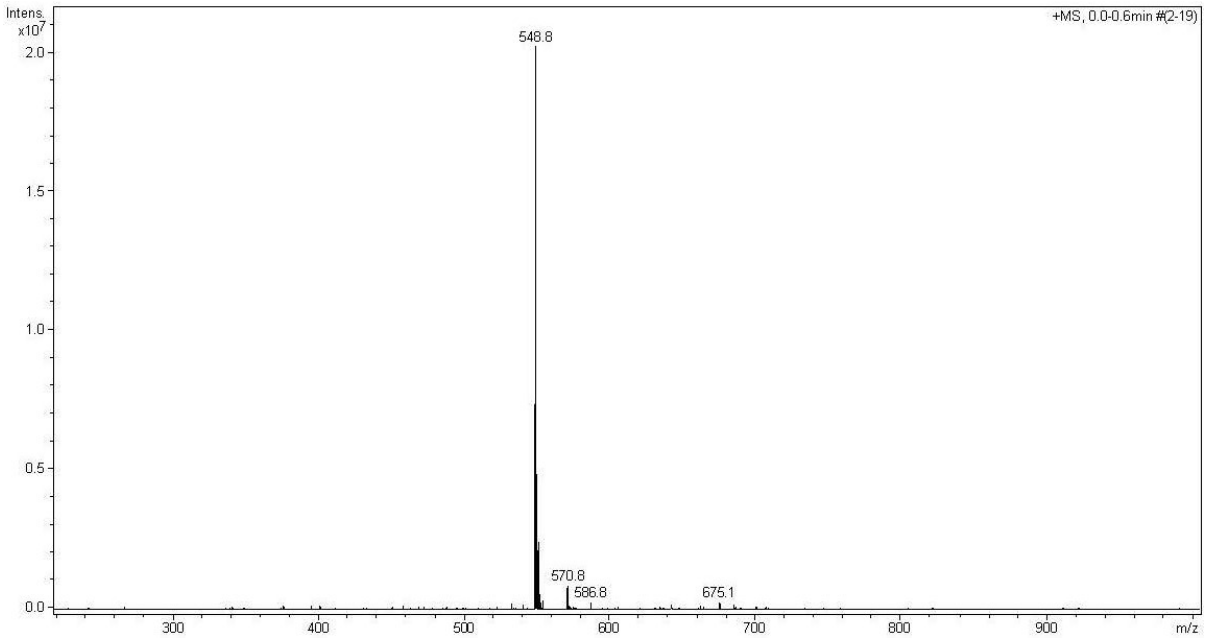

Fig. S109 ESI-MS spectrum of MRAM. $[M+H]^+_{calc}$ (m/z) : 549.3 ; $[M+H]^+_{exp}$ (m/z) : 548.8 ; $[M+Na]^+_{exp}$ (m/z) : 570.8

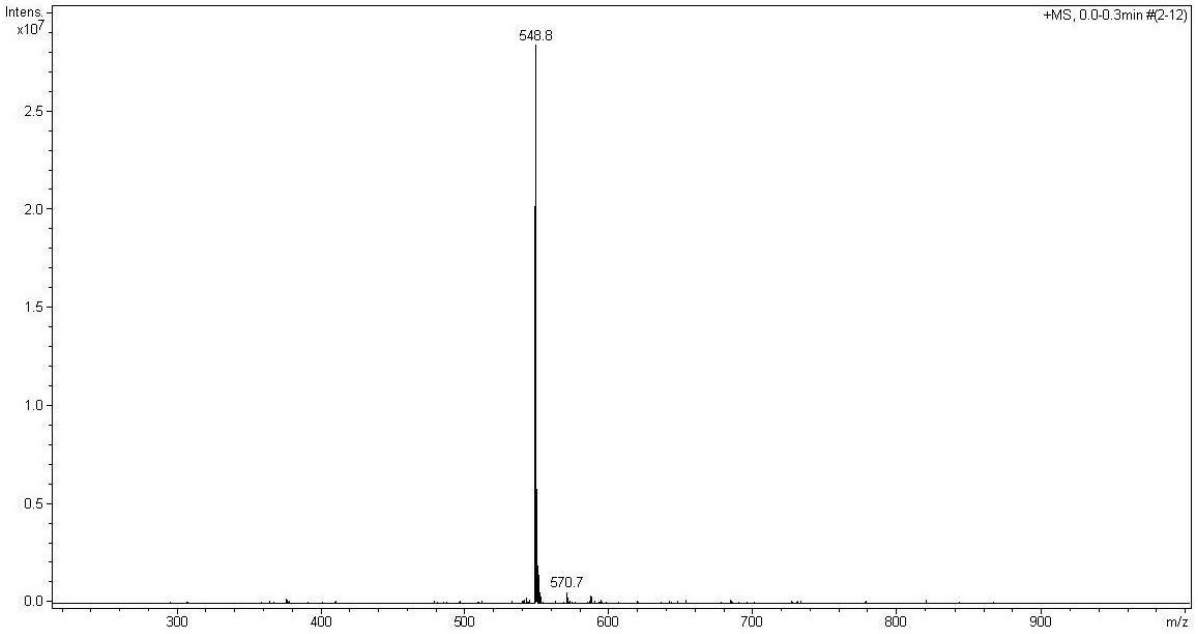

Fig. S110 ESI-MS spectrum of MARM. $[M+H]^{+}_{calc}$ (m/z) : 549.3 ; $[M+H]^{+}_{exp}$ (m/z) : 548.8 ; $[M+Na]^{+}_{exp}$ (m/z) : 570.7

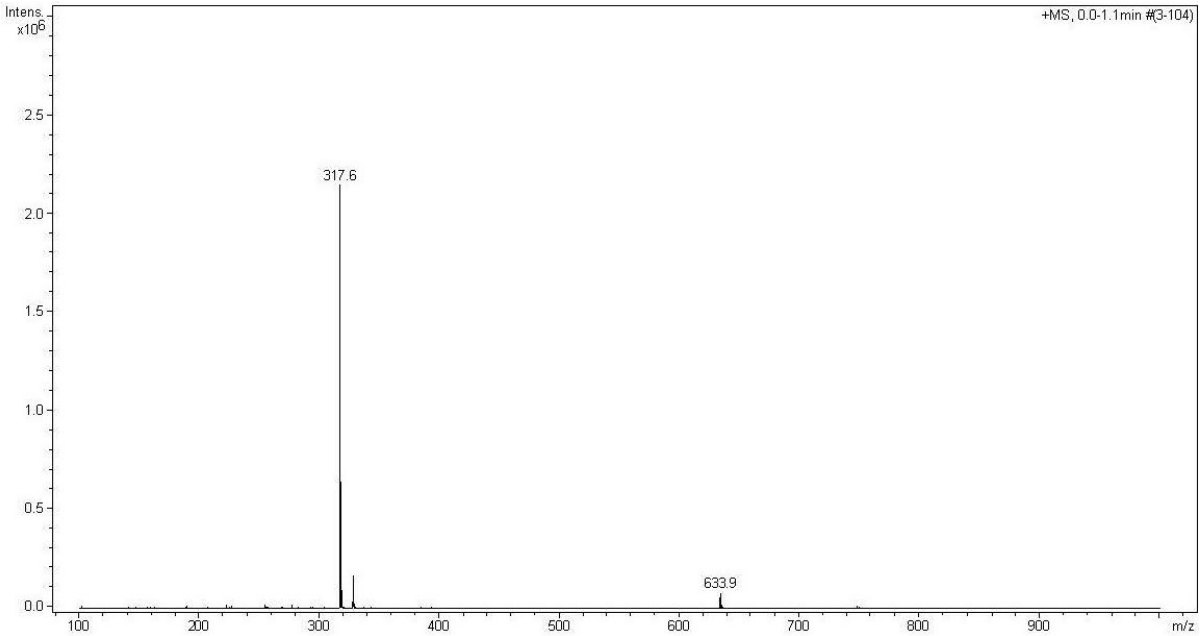

Fig. S111 ESI-MS spectrum of MRRM. $[M+H]^{+}_{calc}$ (m/z) : 634.3 ; $[M+H]^{+}_{exp}$ (m/z) : 633.9 ; $[M+2H]^{2+}_{exp}$ (m/z) : 317.6

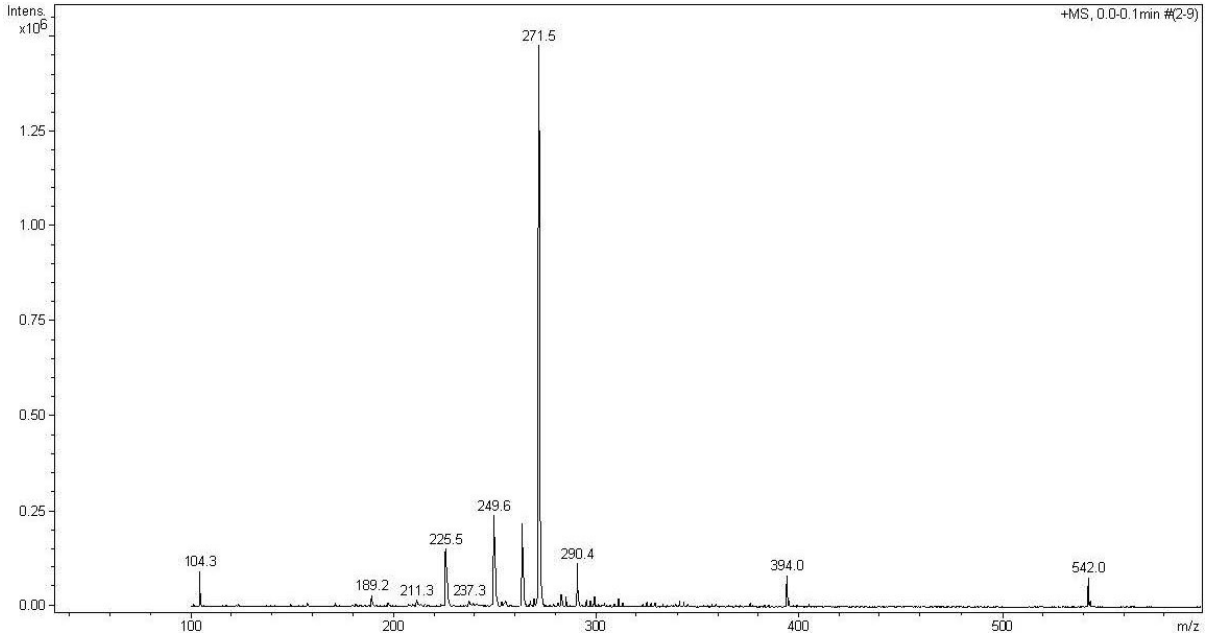

Fig. S112 ESI-MS spectrum of H–Dap–QM. $[M+H]^{+}_{calc}$ (m/z) : 542.6 ; $[M+H]^{+}_{exp}$ (m/z) : 542.0 ; $[M+2H]^{2+}_{exp}$ (m/z) : 271.5

Stability of the complex Ag^{+}-peptide over time

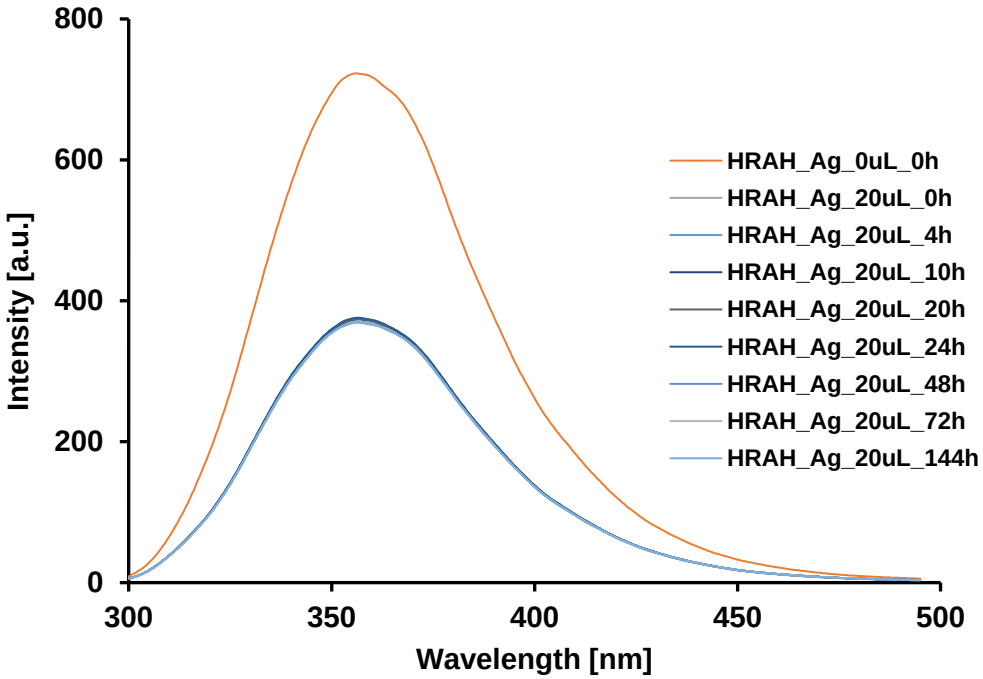

Fig. S113 Stability over time (from 0 to 144 hours) of the Ag^{+}-HRAH / HEWM complex. Quenching of tryptophan fluorescence (λ_{ex}: 280 nm) by addition of $AgNO_3$ (2.2 equivalents) to a solution of HARH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. The cuvette was stored in the dark at room temperature between measurements.

CD titrations

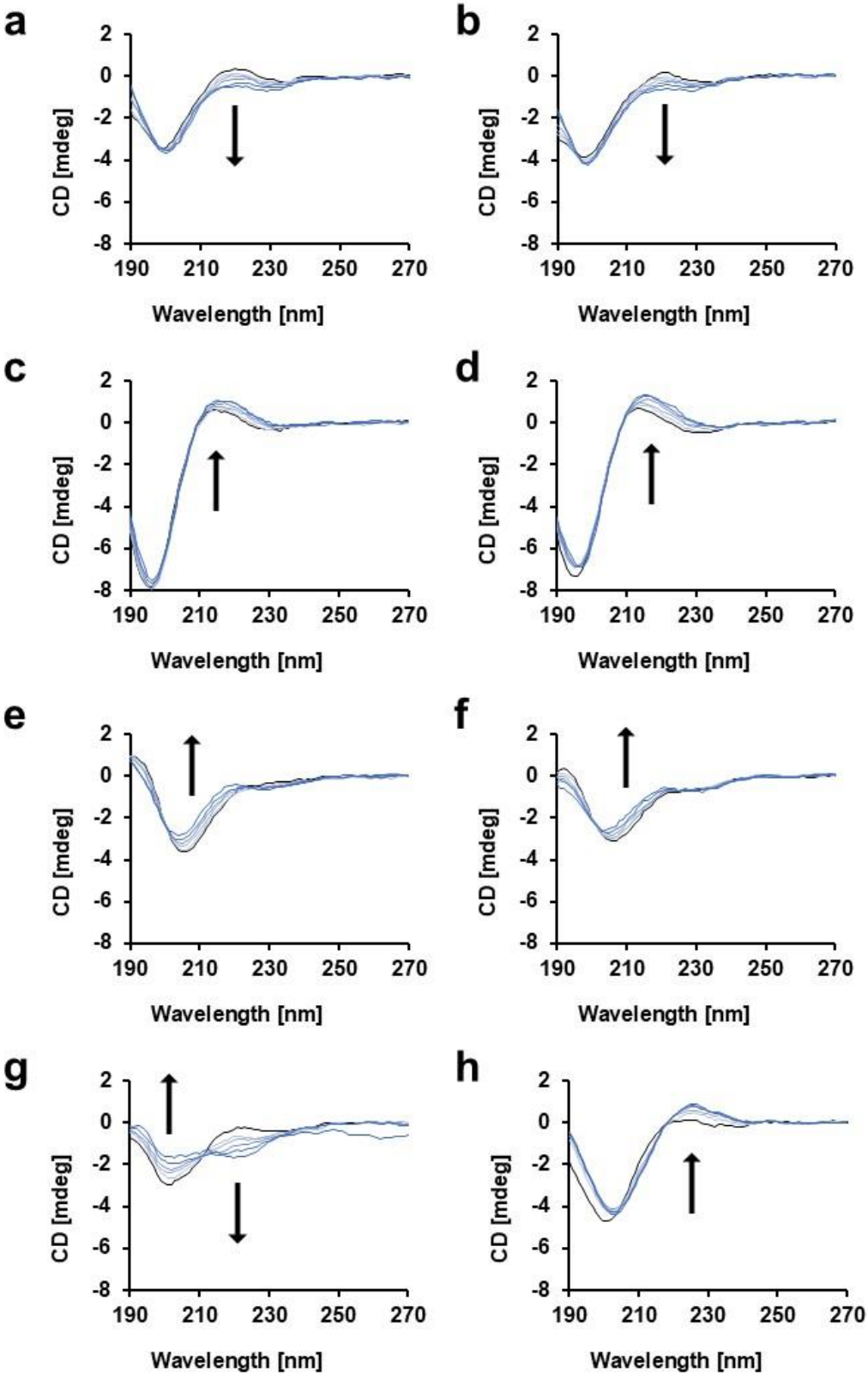

Fig. S114 CD spectra of several tetrapeptides ($1 \cdot 10^{-5}$ M) by addition of $AgNO_3$ (0 to 8 equivalent) at 25°C. (a) HQQH (b) HAAH (c) MKKM (d) MRKM (e) HPPH (f) HPQH (g) HQPH (h) MPPM.

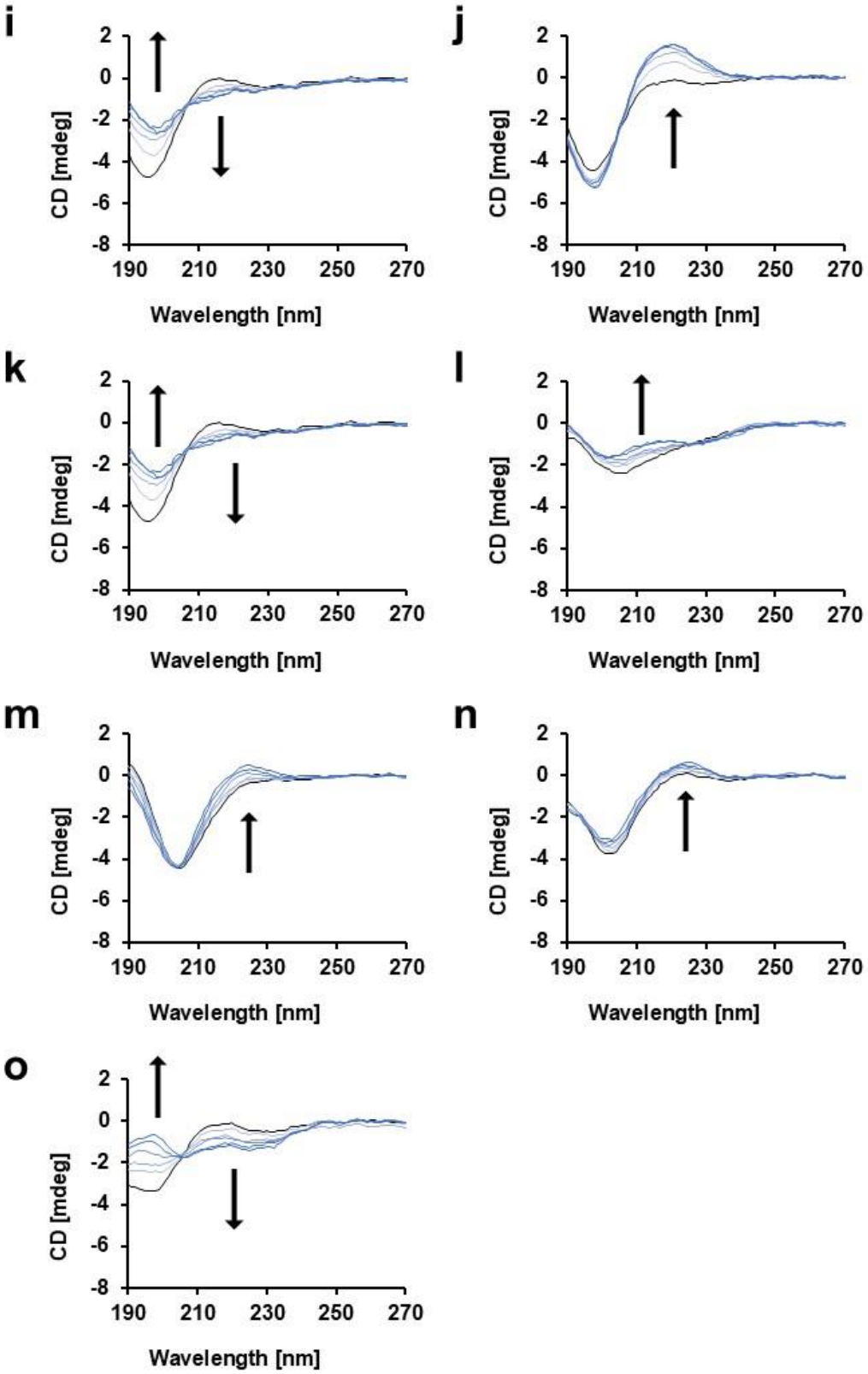

Fig. S115 CD spectra of several tetrapeptides ($1 \cdot 10^{-5}$ M) by addition of $AgNO_3$ (0 to 8 equivalent) at 25°C. (i) MPQM (j) MQPM (k) HPPM (l) HPQM (m) HQPM (n) MPPH (o) MPQH.

Fluorescence titrations

HQQM

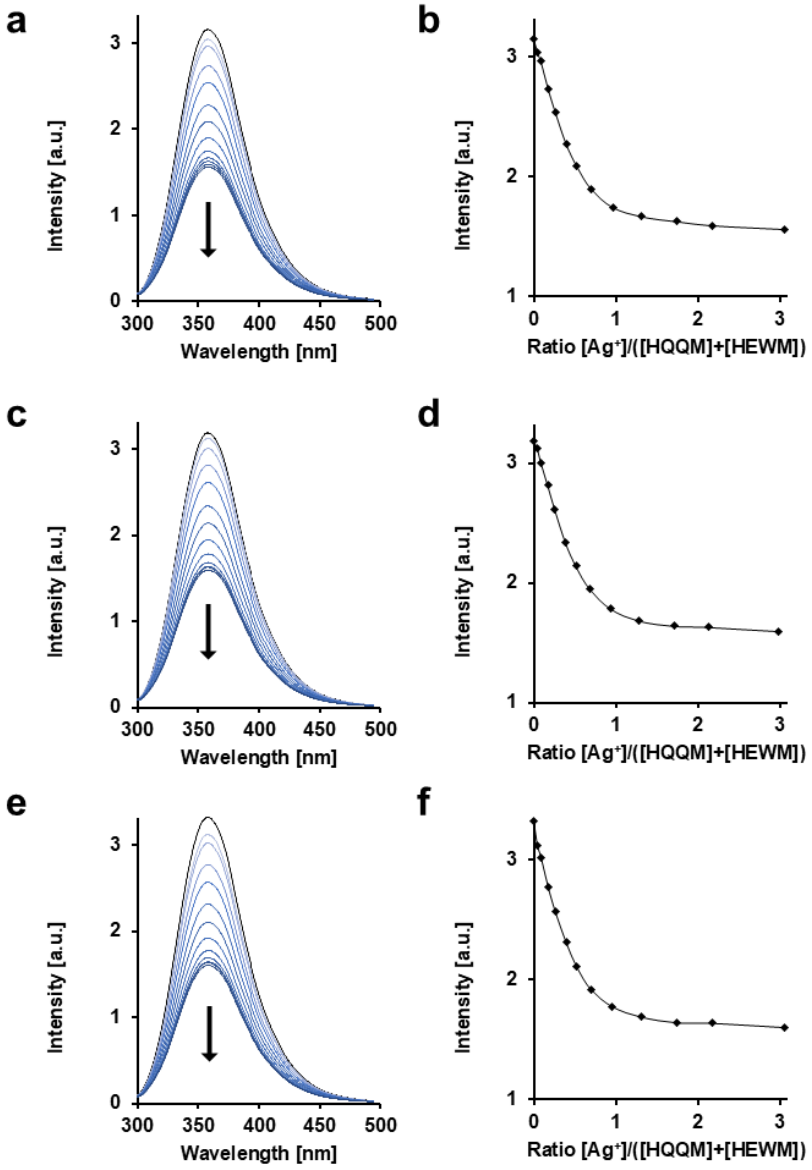

Fig. S116 HQQM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HQQM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

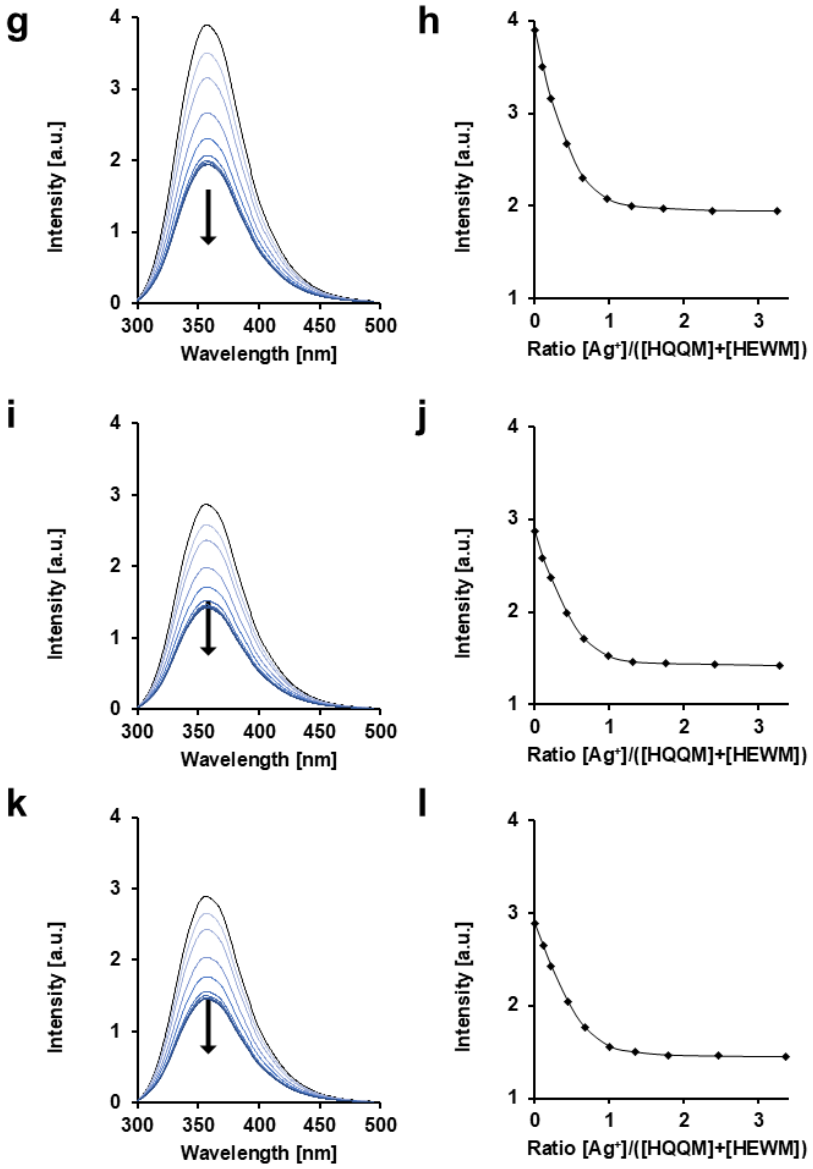

Fig. S117 HQQM / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HQQM ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S3 Determination of the binding constants ($\log(K_{ass})$) of HQQM tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HQQM	$\log(K_{ass-1}) = 5.61 \pm 0.05$	$\log(K_{ass-1}) = 5.55 \pm 0.06$
	$\log(K_{ass-2}) = 5.96 \pm 0.04$	$\log(K_{ass-2}) = 5.68 \pm 0.04$
	$\log(K_{ass-3}) = 5.42 \pm 0.09$	$\log(K_{ass-3}) = 5.79 \pm 0.03$
Average	$\log(K_{ass}) = 5.62 \pm 0.13$	

[a] The values correspond to the peptide and probe concentrations.

HRQM

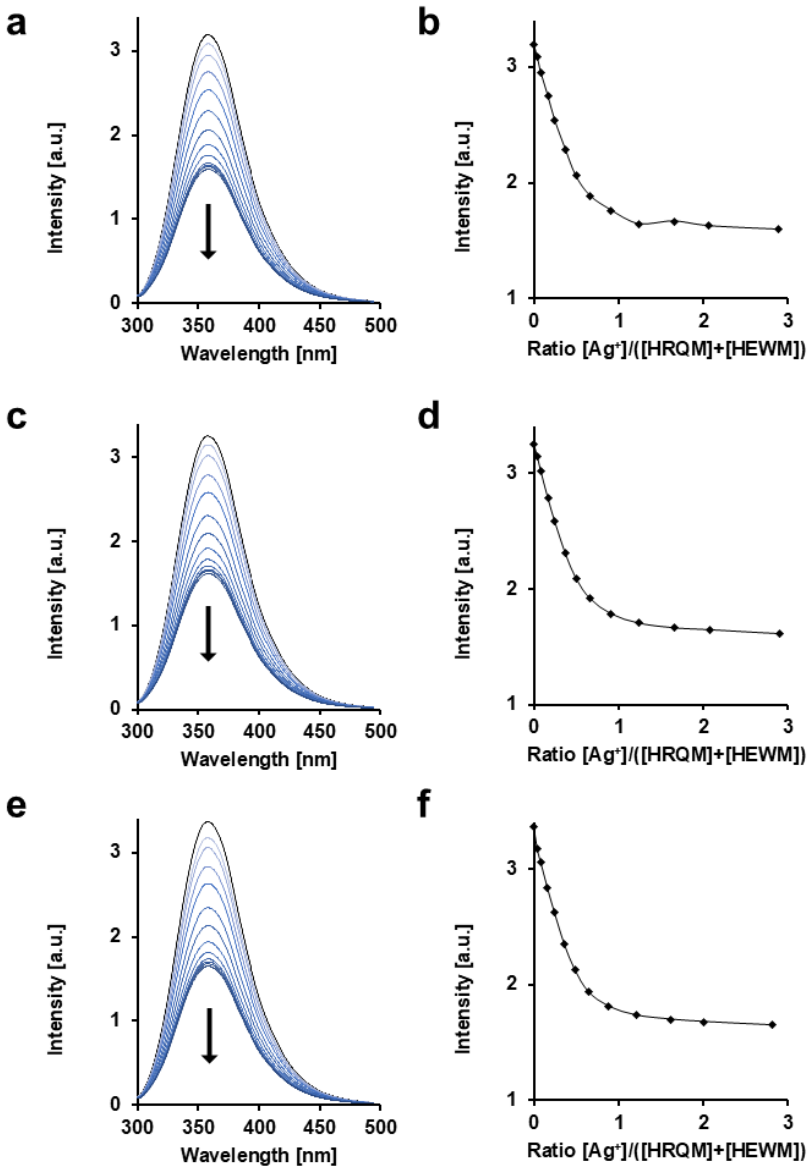

Fig. S118 HRQM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HRQM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

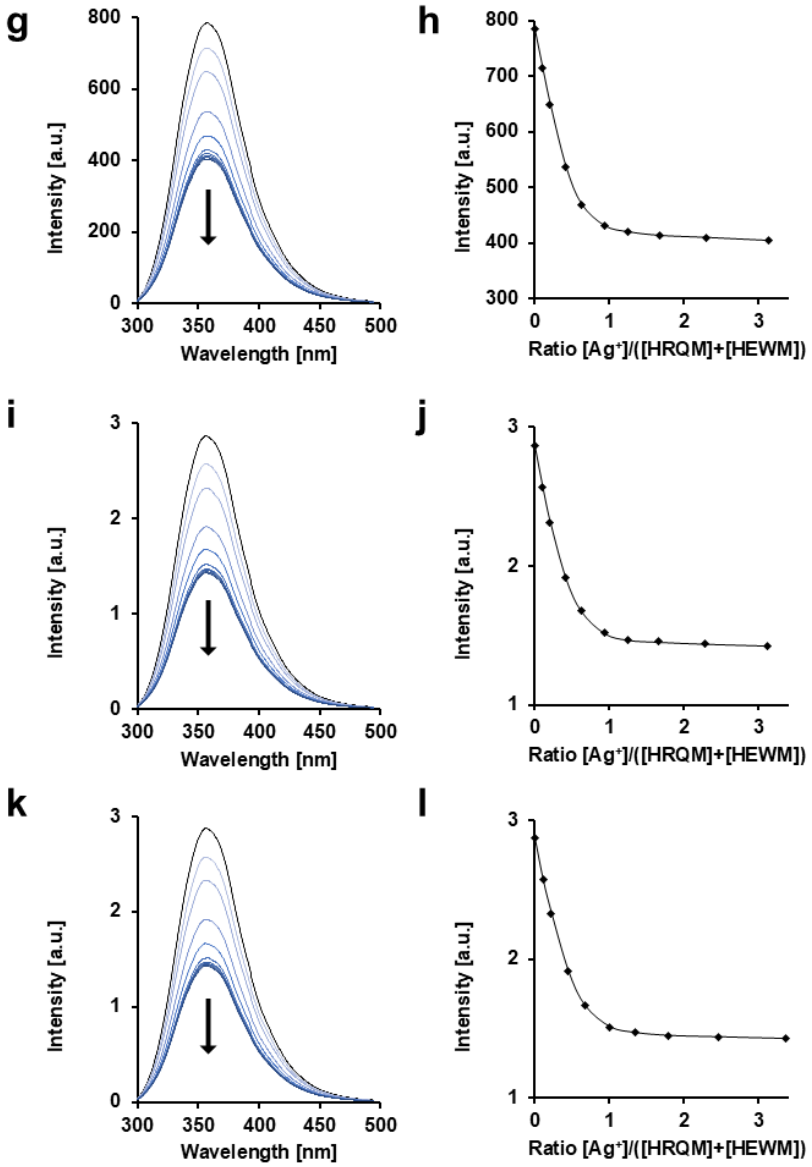

Fig. S119 HRQM / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HRQM ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S4 Determination of the binding constants ($\log(K_{ass})$) of HRQM tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HRQM	$\log(K_{ass-1}) = 5.51 \pm 0.05$	$\log(K_{ass-1}) = 5.28 \pm 0.05$
	$\log(K_{ass-2}) = 5.43 \pm 0.03$	$\log(K_{ass-2}) = 5.36 \pm 0.05$
	$\log(K_{ass-3}) = 5.34 \pm 0.07$	$\log(K_{ass-3}) = 5.43 \pm 0.05$
Average	$\log(K_{ass}) = 5.39 \pm 0.08$	

[a] The values correspond to the peptide and probe concentrations.

HQRM

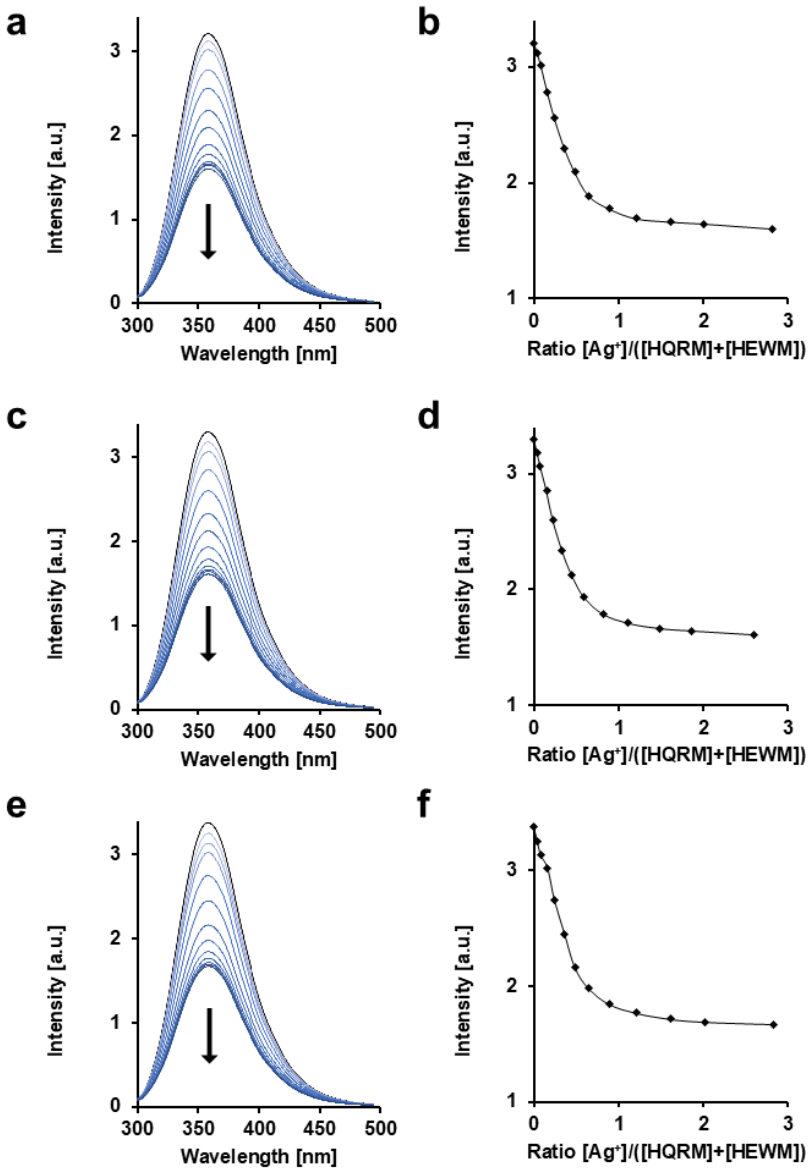

Fig. S120 HQRM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HQRM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

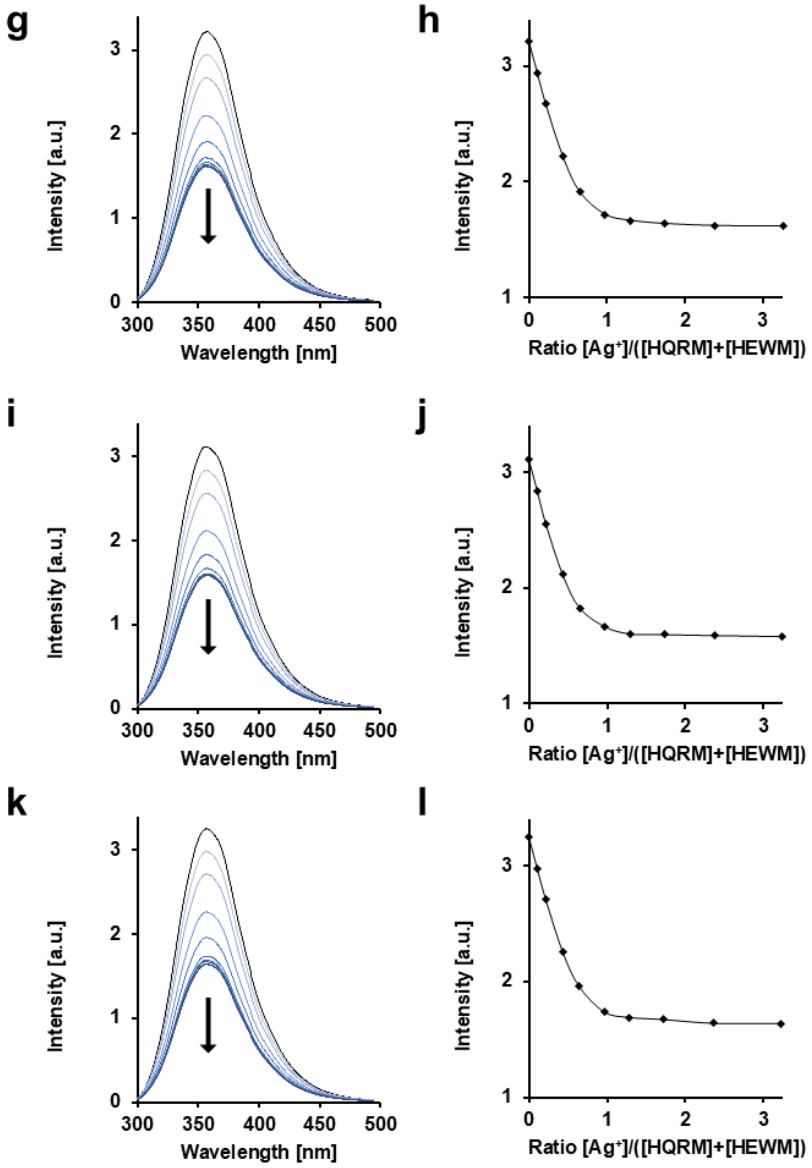

Fig. S121 HQRM / HEWM competition titrations, both at $1{\cdot}10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HQRM ($1{\cdot}10^{-5}$ M) in competition with HEWM probe ($1{\cdot}10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S5 Determination of the binding constants ($\log(K_{ass})$) of HQRM tetrapeptide.

Model	$5{\cdot}10^{-6}$ M[a]	$1{\cdot}10^{-5}$ M[a]
HQRM	$\log(K_{ass\text{-}1}) = 5.41 \pm 0.05$	$\log(K_{ass\text{-}1}) = 5.62 \pm 0.03$
	$\log(K_{ass\text{-}2}) = 5.14 \pm 0.07$	$\log(K_{ass\text{-}2}) = 5.50 \pm 0.02$
	$\log(K_{ass\text{-}3}) = 5.53 \pm 0.10$	$\log(K_{ass\text{-}3}) = 5.64 \pm 0.03$
Average	$\log(K_{ass}) = 5.47 \pm 0.19$	

[a] The values correspond to the peptide and probe concentrations.

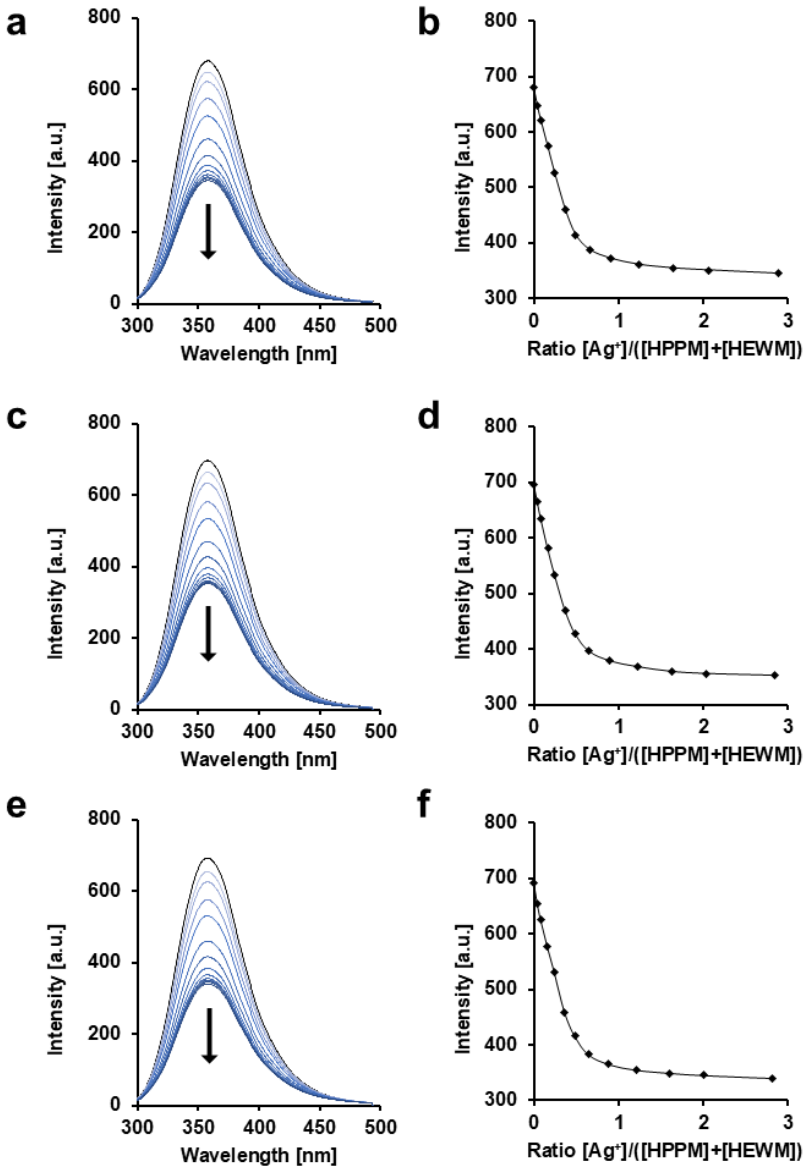

Fig. S122 HPPM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HPPM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

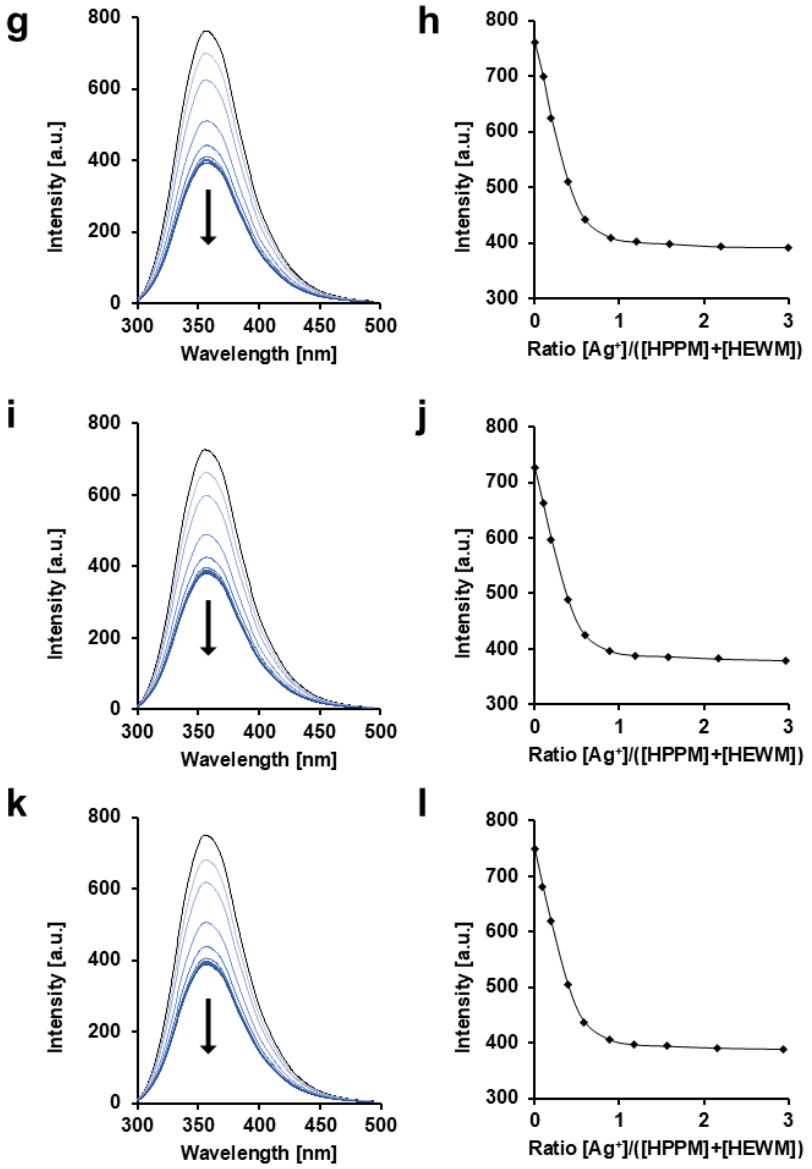

Fig. S123 HPPM / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HPPM ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S6 Determination of the binding constants ($\log(K_{ass})$) of HPPM tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HPPM	$\log(K_{ass\text{-}1}) = 4.88 \pm 0.08$	$\log(K_{ass\text{-}1}) = 5.10 \pm 0.05$
	$\log(K_{ass\text{-}2}) = 4.74 \pm 0.15$	$\log(K_{ass\text{-}2}) = 5.09 \pm 0.03$
	$\log(K_{ass\text{-}3}) = 4.83 \pm 0.14$	$\log(K_{ass\text{-}3}) = 5.11 \pm 0.03$
Average	$\log(K_{ass}) = 4.96 \pm 0.16$	

[a] The values correspond to the peptide and probe concentrations.

HQPM

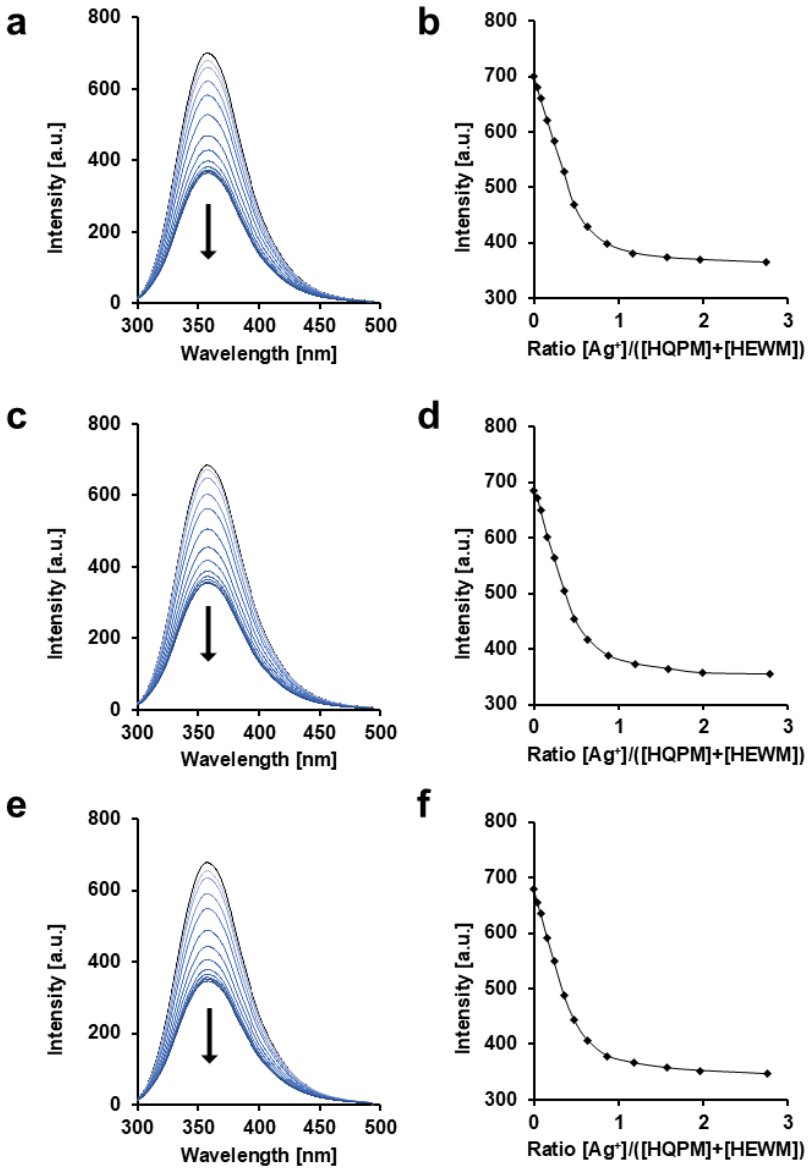

Fig. S124 HQPM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HQPM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

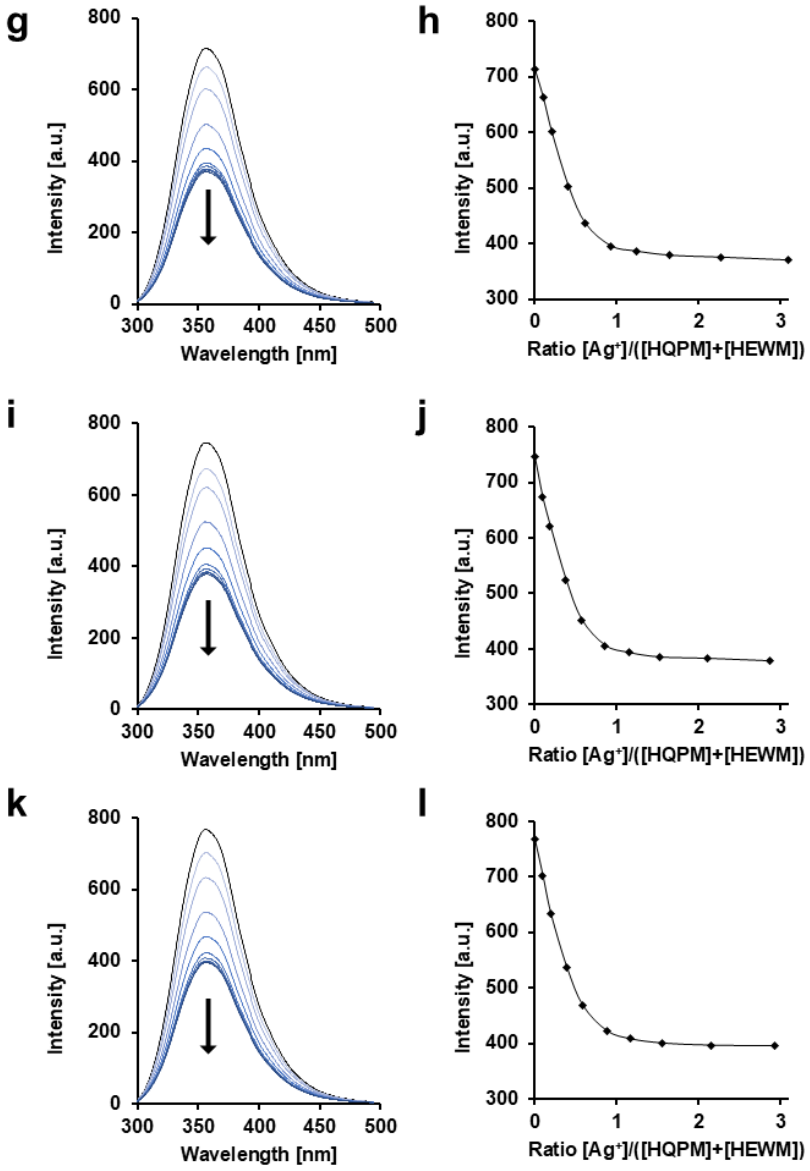

Fig. S125 HQPM / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HQPM ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S7 Determination of the binding constants ($\log(K_{ass})$) of HQPM tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HQPM	$\log(K_{ass\text{-}1}) = 5.56 \pm 0.06$	$\log(K_{ass\text{-}1}) = 5.57 \pm 0.06$
	$\log(K_{ass\text{-}2}) = 5.50 \pm 0.05$	$\log(K_{ass\text{-}2}) = 5.50 \pm 0.05$
	$\log(K_{ass\text{-}3}) = 5.38 \pm 0.04$	$\log(K_{ass\text{-}3}) = 5.45 \pm 0.04$
Average	$\log(K_{ass}) = 5.49 \pm 0.07$	

[a] The values correspond to the peptide and probe concentrations.

HPQM

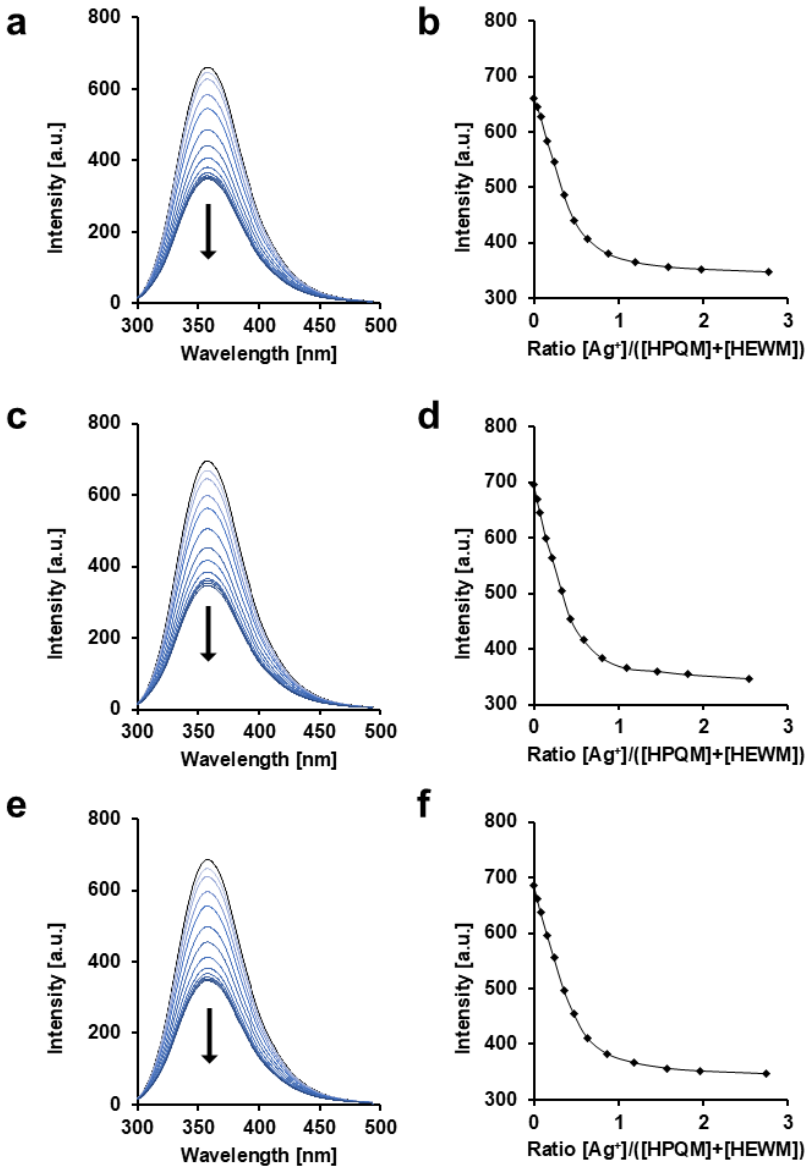

Fig. S126 HPQM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HPQM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

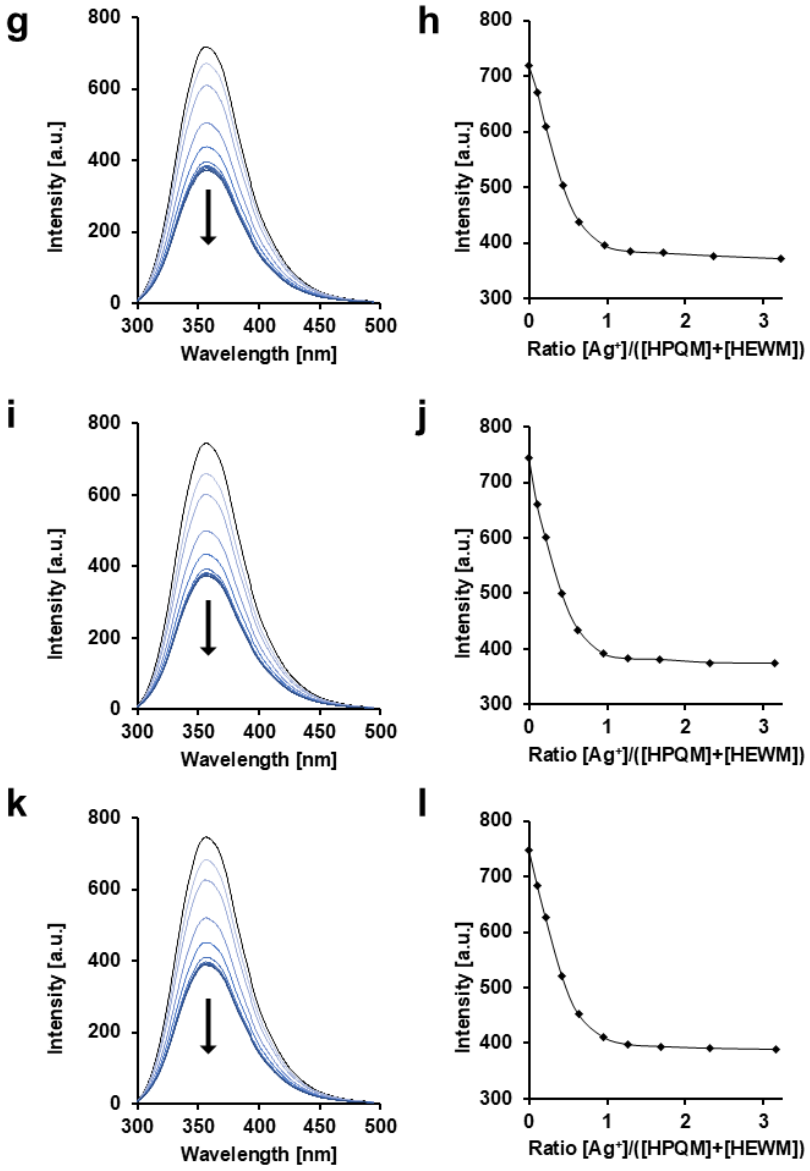

Fig. S127 HPQM / HEWM competition titrations, both at $1{\cdot}10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HPQM ($1{\cdot}10^{-5}$ M) in competition with HEWM probe ($1{\cdot}10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S8 Determination of the binding constants ($\log(K_{ass})$) of HPQM tetrapeptide.

Model	$5{\cdot}10^{-6}$ M[a]	$1{\cdot}10^{-5}$ M[a]
HPQM	$\log(K_{ass\text{-}1}) = 5.45 \pm 0.05$	$\log(K_{ass\text{-}1}) = 5.63 \pm 0.07$
	$\log(K_{ass\text{-}2}) = 5.34 \pm 0.05$	$\log(K_{ass\text{-}2}) = 5.43 \pm 0.08$
	$\log(K_{ass\text{-}3}) = 5.48 \pm 0.03$	$\log(K_{ass\text{-}3}) = 5.53 \pm 0.03$
Average	$\log(K_{ass}) = 5.48 \pm 0.10$	

[a] The values correspond to the peptide and probe concentrations.

HKKM

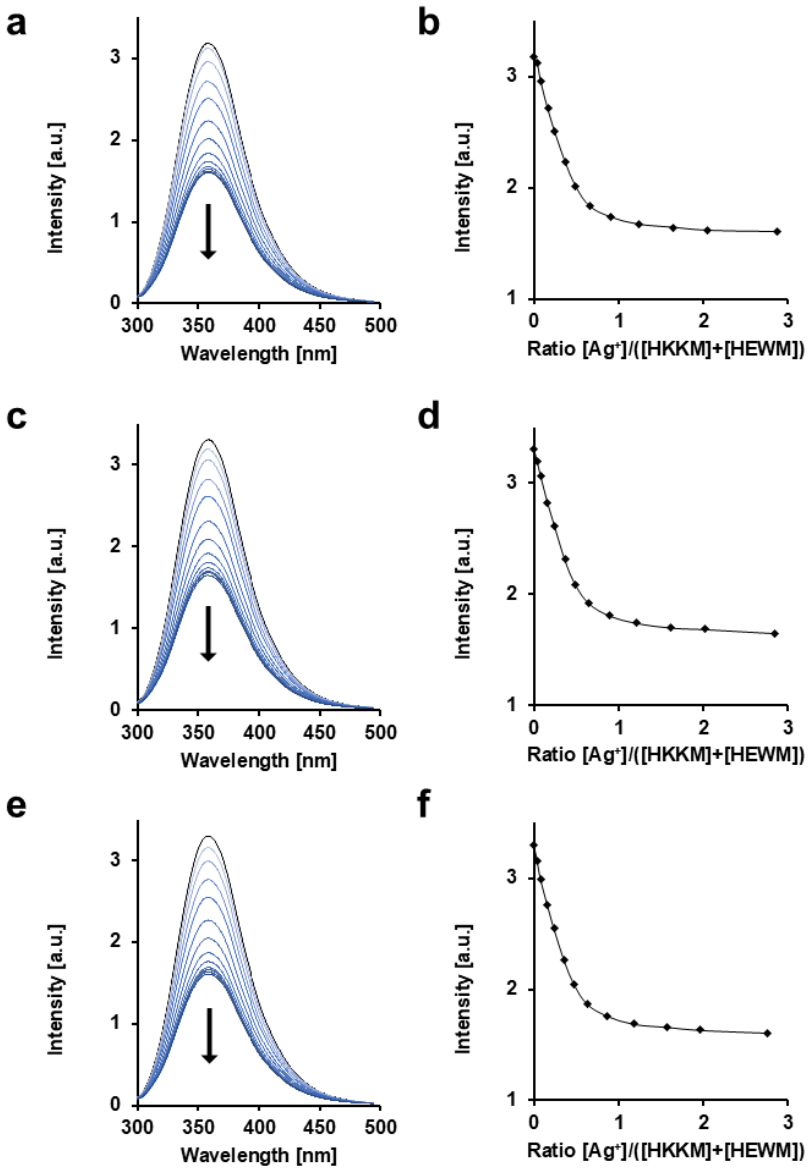

Fig. S128 HKKM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HKKM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

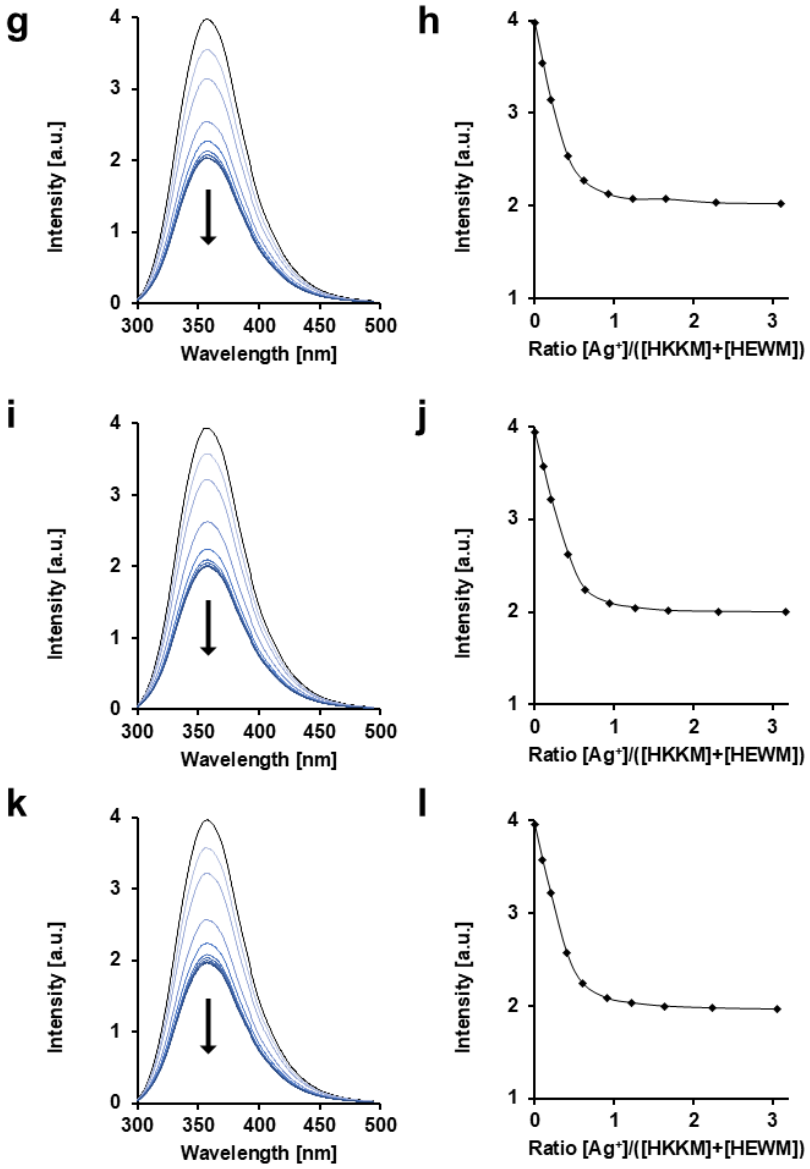

Fig. S129 HKKM / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HKKM ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S9 Determination of the binding constants ($\log(K_{ass})$) of HKKM tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HKKM	$\log(K_{ass-1}) = 5.29 \pm 0.06$	$\log(K_{ass-1}) = 4.78 \pm 0.20$
	$\log(K_{ass-2}) = 5.26 \pm 0.03$	$\log(K_{ass-2}) = 5.29 \pm 0.04$
	$\log(K_{ass-3}) = 5.19 \pm 0.07$	$\log(K_{ass-3}) = 5.09 \pm 0.04$
Average	$\log(K_{ass}) = 5.15 \pm 0.20$	

[a] The values correspond to the peptide and probe concentrations.

HRKM

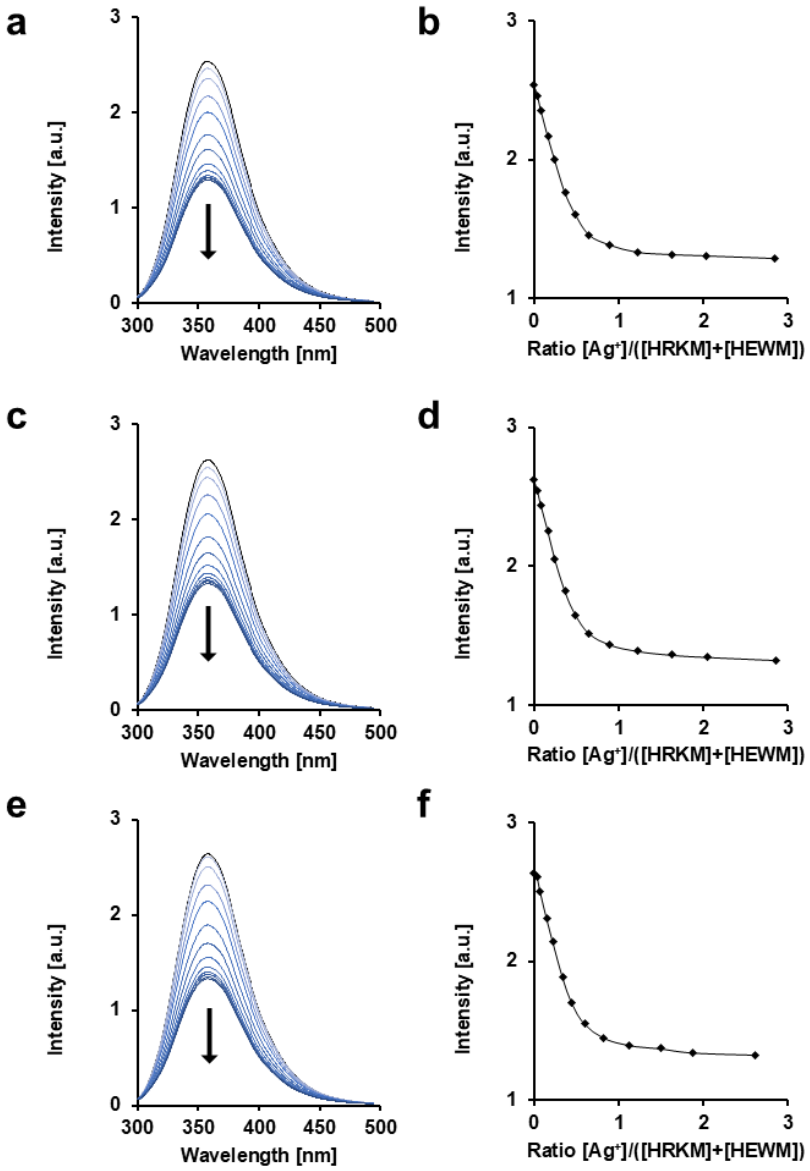

Fig. S130 HRKM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HRKM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

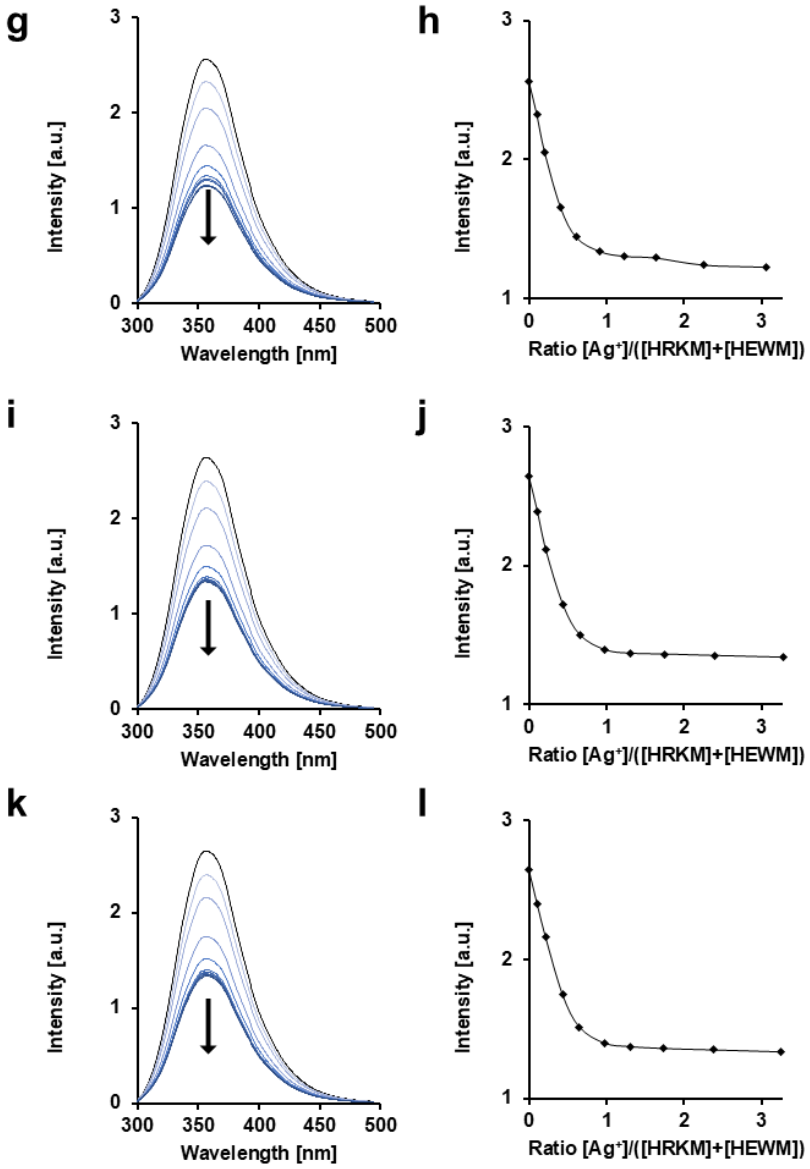

Fig. S131 HRKM / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HRKM ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S10 Determination of the binding constants ($\log(K_{ass})$) of HRKM tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HRKM	$\log(K_{ass-1}) = 5.27 \pm 0.03$	$\log(K_{ass-1}) = 5.08 \pm 0.15$
	$\log(K_{ass-2}) = 5.27 \pm 0.04$	$\log(K_{ass-2}) = 5.13 \pm 0.08$
	$\log(K_{ass-3}) = 5.27 \pm 0.07$	$\log(K_{ass-3}) = 5.33 \pm 0.03$
Average	$\log(K_{ass}) = 5.22 \pm 0.10$	

[a] The values correspond to the peptide and probe concentrations.

HKRM

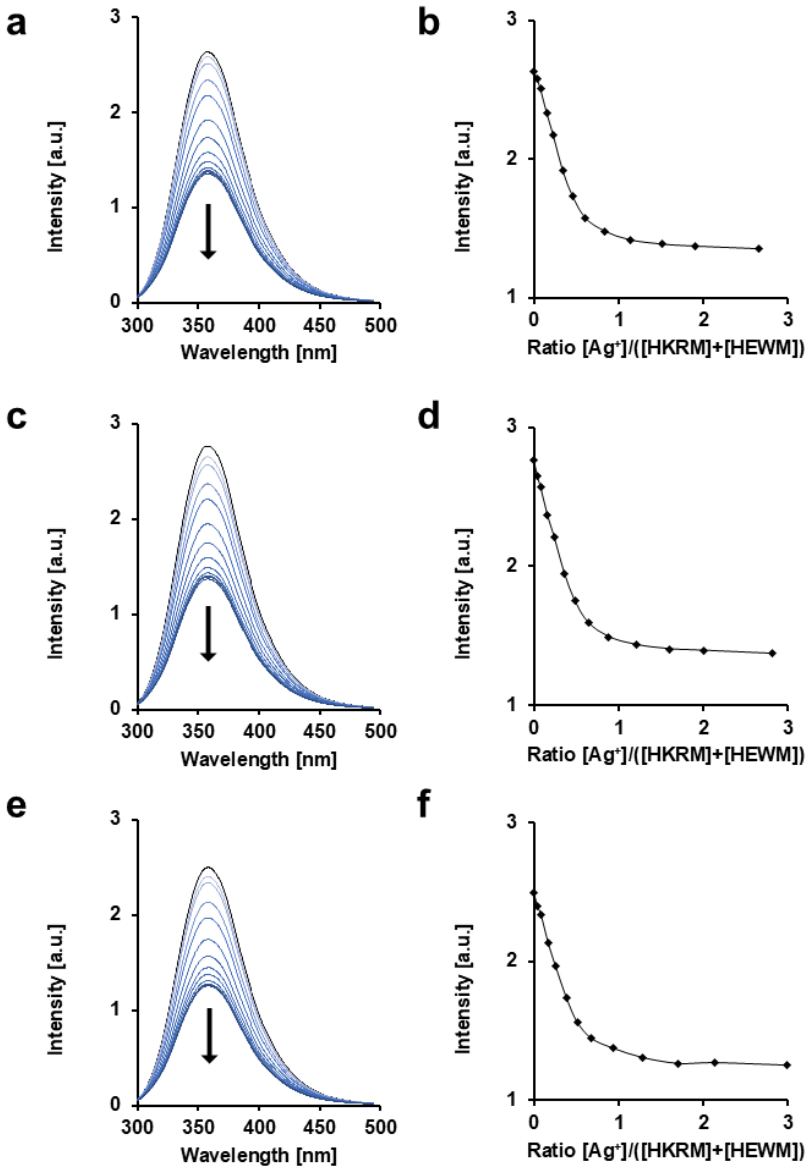

Fig. S132 HKRM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HKRM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

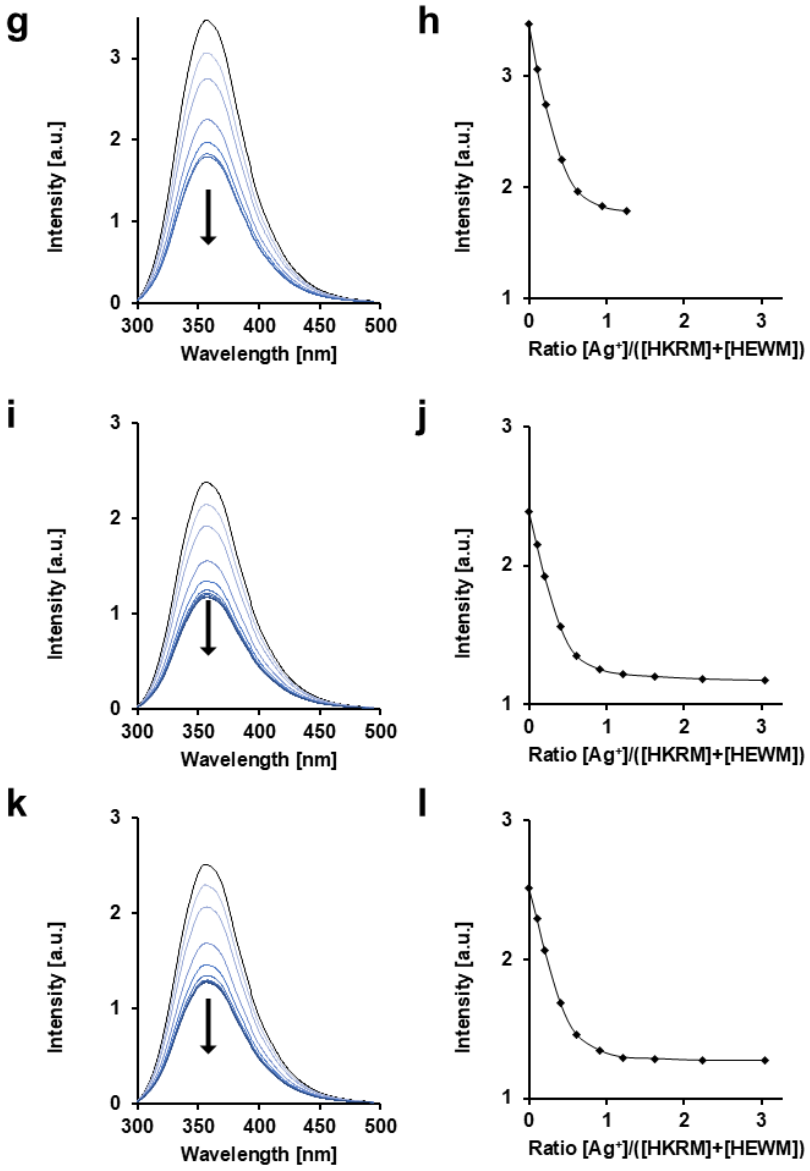

Fig. S133 HKRM / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HKRM ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S11 Determination of the binding constants ($\log(K_{ass})$) of HKRM tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HKRM	$\log(K_{ass-1}) = 5.33 \pm 0.07$	$\log(K_{ass-1}) = 5.00 \pm 0.24$
	$\log(K_{ass-2}) = 5.33 \pm 0.03$	$\log(K_{ass-2}) = 5.20 \pm 0.04$
	$\log(K_{ass-3}) = 5.37 \pm 0.05$	$\log(K_{ass-3}) = 5.33 \pm 0.03$
Average	$\log(K_{ass}) = 5.26 \pm 0.14$	

[a] The values correspond to the peptide and probe concentrations.

HAAM

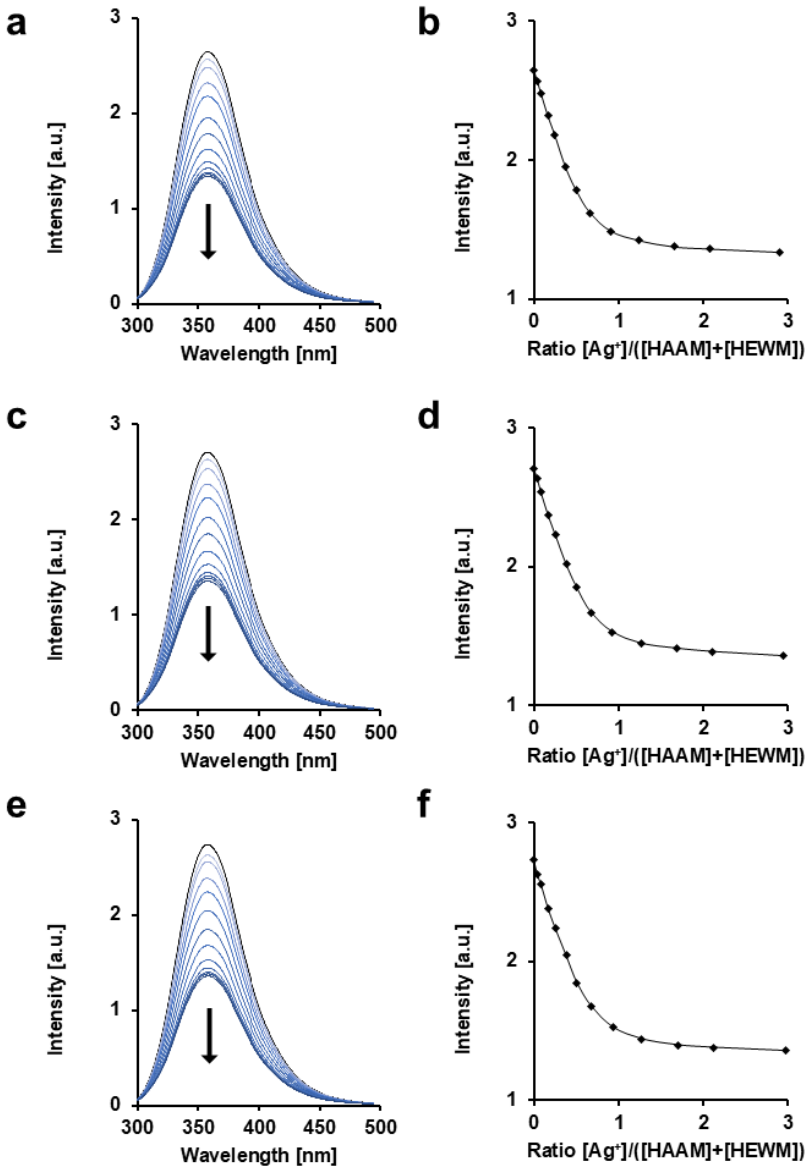

Fig. S134 HAAM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HAAM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

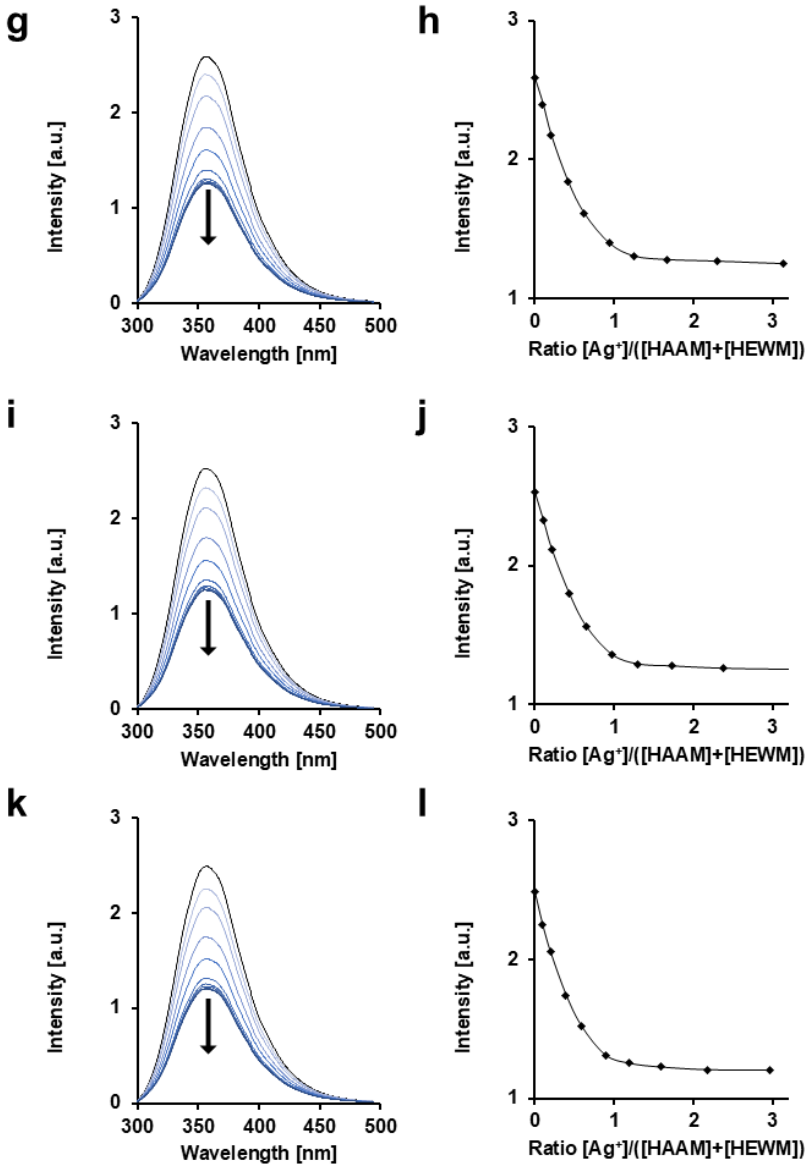

Fig. S135 HAAM / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HAAM ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S12 Determination of the binding constants ($\log(K_{ass})$) of HAAM tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HAAM	$\log(K_{ass-1}) = 5.66 \pm 0.04$	$\log(K_{ass-1}) = 5.79 \pm 0.04$
	$\log(K_{ass-2}) = 5.78 \pm 0.04$	$\log(K_{ass-2}) = 5.81 \pm 0.03$
	$\log(K_{ass-3}) = 5.80 \pm 0.04$	$\log(K_{ass-3}) = 5.62 \pm 0.06$
Average	$\log(K_{ass}) = 5.74 \pm 0.08$	

[a] The values correspond to the peptide and probe concentrations.

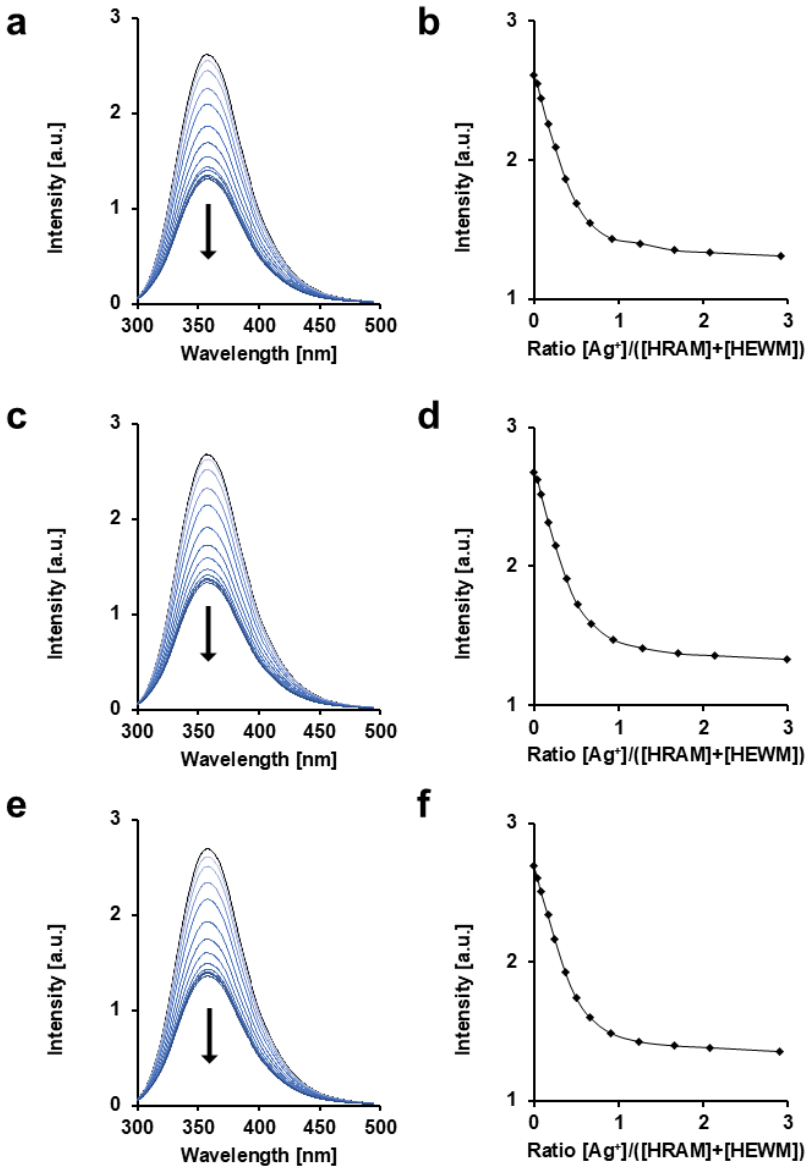

Fig. S136 HRAM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HRAM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

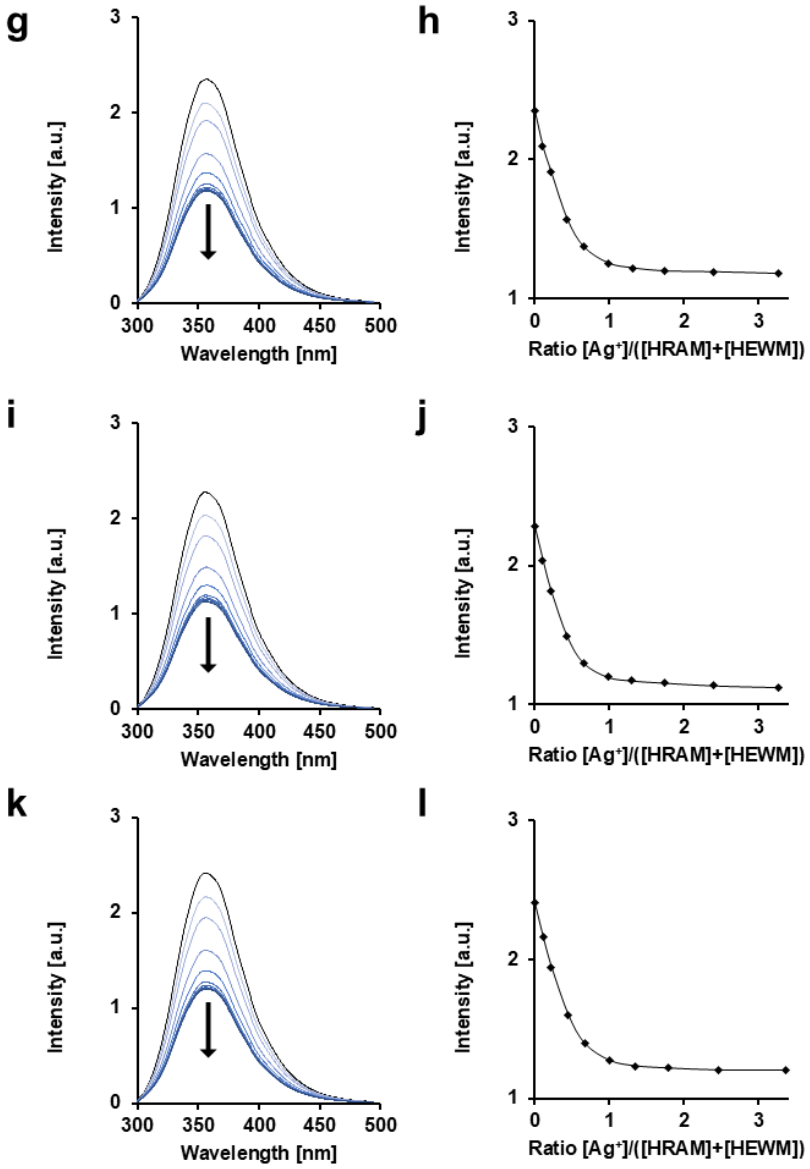

Fig. S137 HRAM / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HRAM ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S13 Determination of the binding constants ($\log(K_{ass})$) of HRAM tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HRAM	$\log(K_{ass-1}) = 5.48 \pm 0.05$	$\log(K_{ass-1}) = 5.42 \pm 0.06$
	$\log(K_{ass-2}) = 5.51 \pm 0.05$	$\log(K_{ass-2}) = 5.31 \pm 0.06$
	$\log(K_{ass-3}) = 5.52 \pm 0.03$	$\log(K_{ass-3}) = 5.49 \pm 0.03$
Average	$\log(K_{ass}) = 5.45 \pm 0.08$	

[a] The values correspond to the peptide and probe concentrations.

HARM

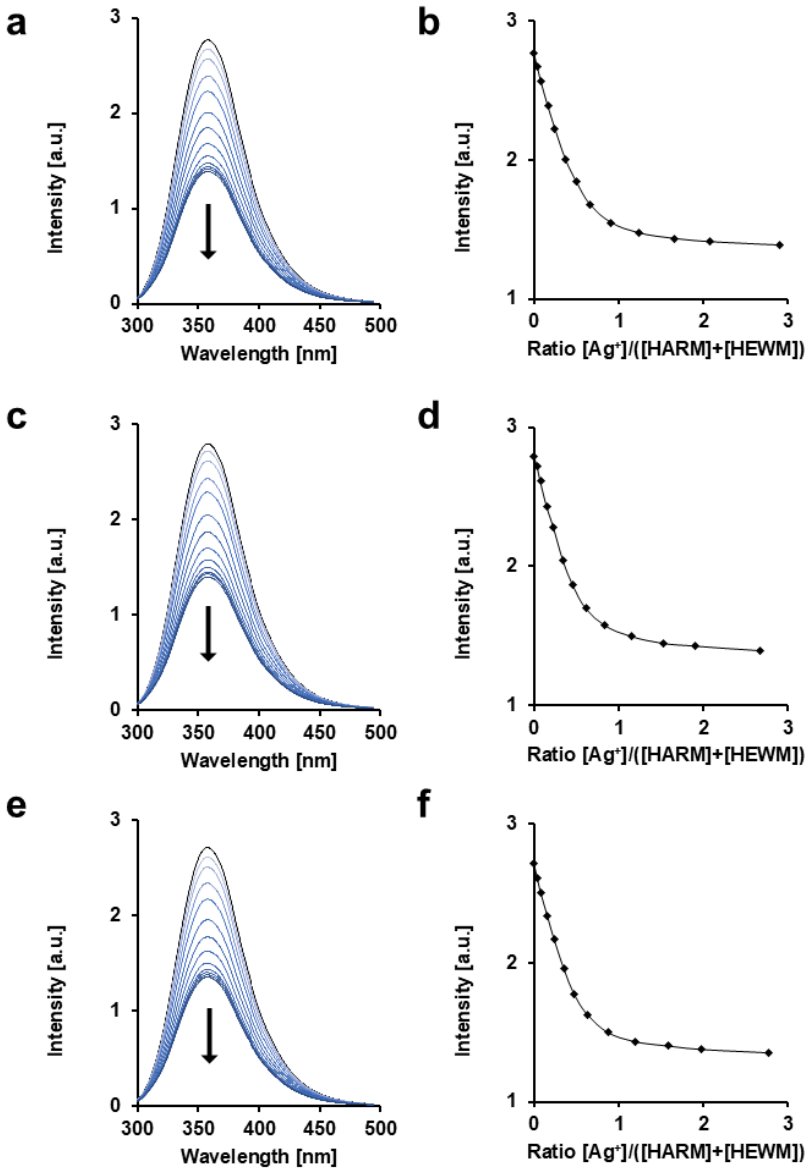

Fig. S138 HARM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HARM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

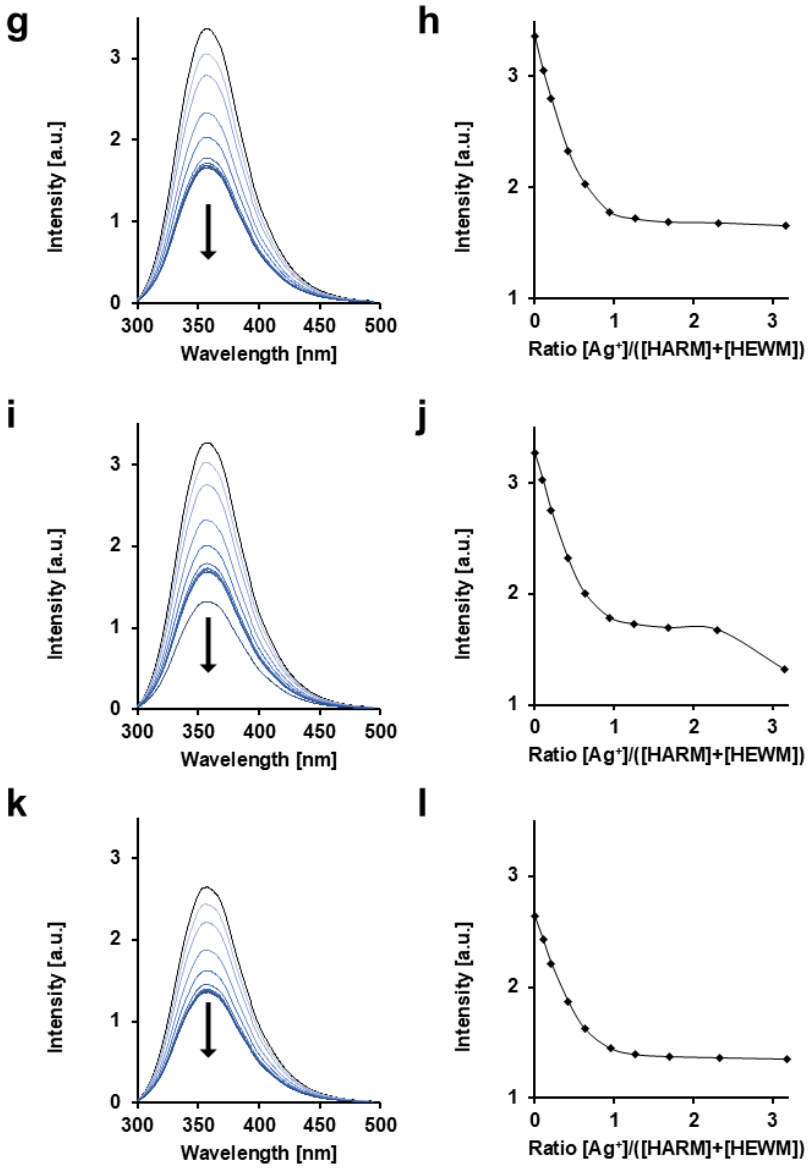

Fig. S139 HARM / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HARM ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S14 Determination of the binding constants ($\log(K_{ass})$) of HARM tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HARM	$\log(K_{ass-1}) = 5.63 \pm 0.03$	$\log(K_{ass-1}) = 5.67 \pm 0.03$
	$\log(K_{ass-2}) = 5.50 \pm 0.04$	$\log(K_{ass-2}) = 5.67 \pm 0.04$
	$\log(K_{ass-3}) = 5.38 \pm 0.04$	$\log(K_{ass-3}) = 5.67 \pm 0.02$
Average	$\log(K_{ass}) = 5.59 \pm 0.12$	

[a] The values correspond to the peptide and probe concentrations.

HRRM

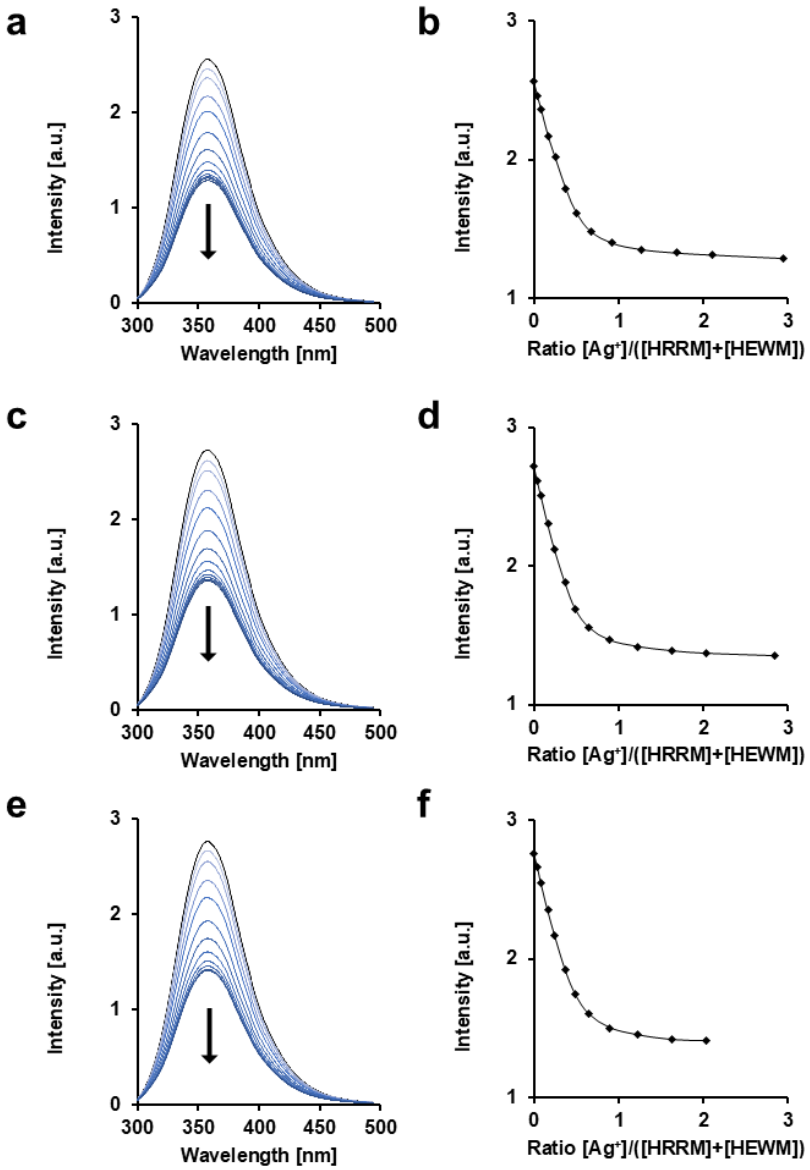

Fig. S140 HRRM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HRRM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

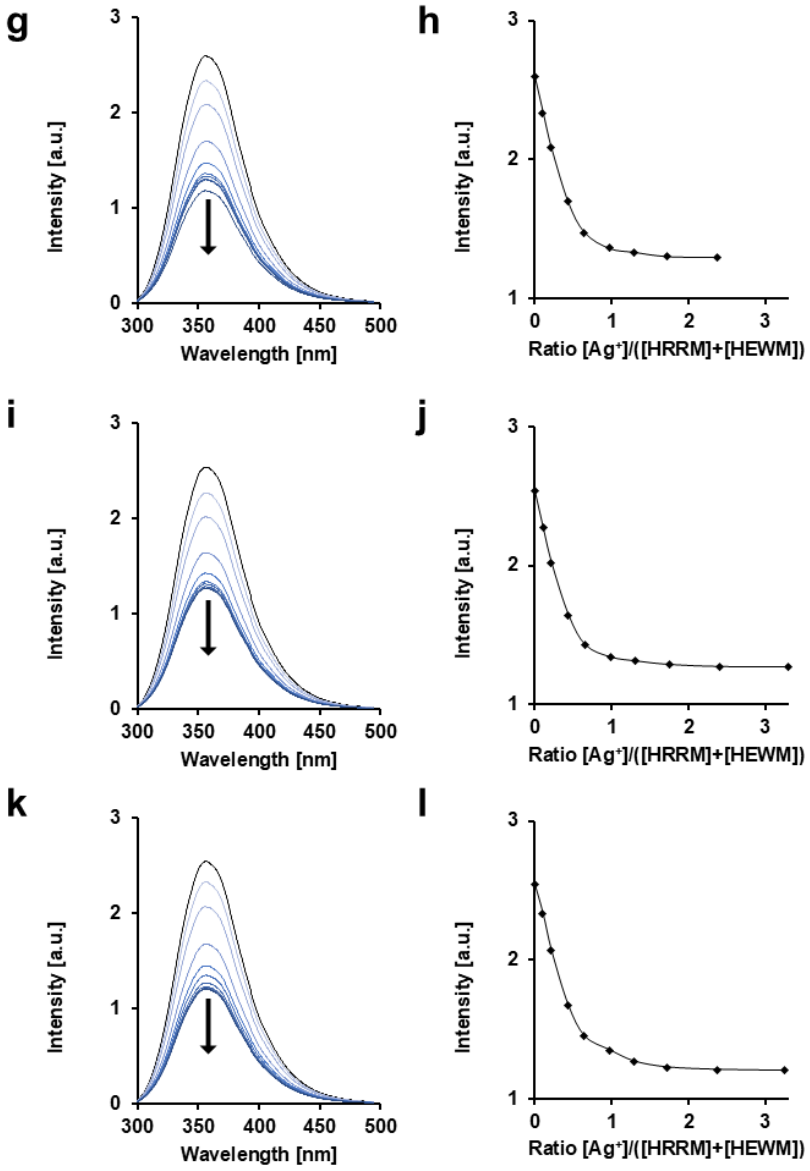

Fig. S141 HRRM / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HRRM ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S15 Determination of the binding constants ($\log(K_{ass})$) of HRRM tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HRRM	$\log(K_{ass-1}) = 5.36 \pm 0.03$	$\log(K_{ass-1}) = 5.28 \pm 0.04$
	$\log(K_{ass-2}) = 5.13 \pm 0.04$	$\log(K_{ass-2}) = 5.20 \pm 0.06$
	$\log(K_{ass-3}) = 5.18 \pm 0.03$	$\log(K_{ass-3}) = 5.41 \pm 0.10$
Average	$\log(K_{ass}) = 5.26 \pm 0.11$	

[a] The values correspond to the peptide and probe concentrations.

HAQM

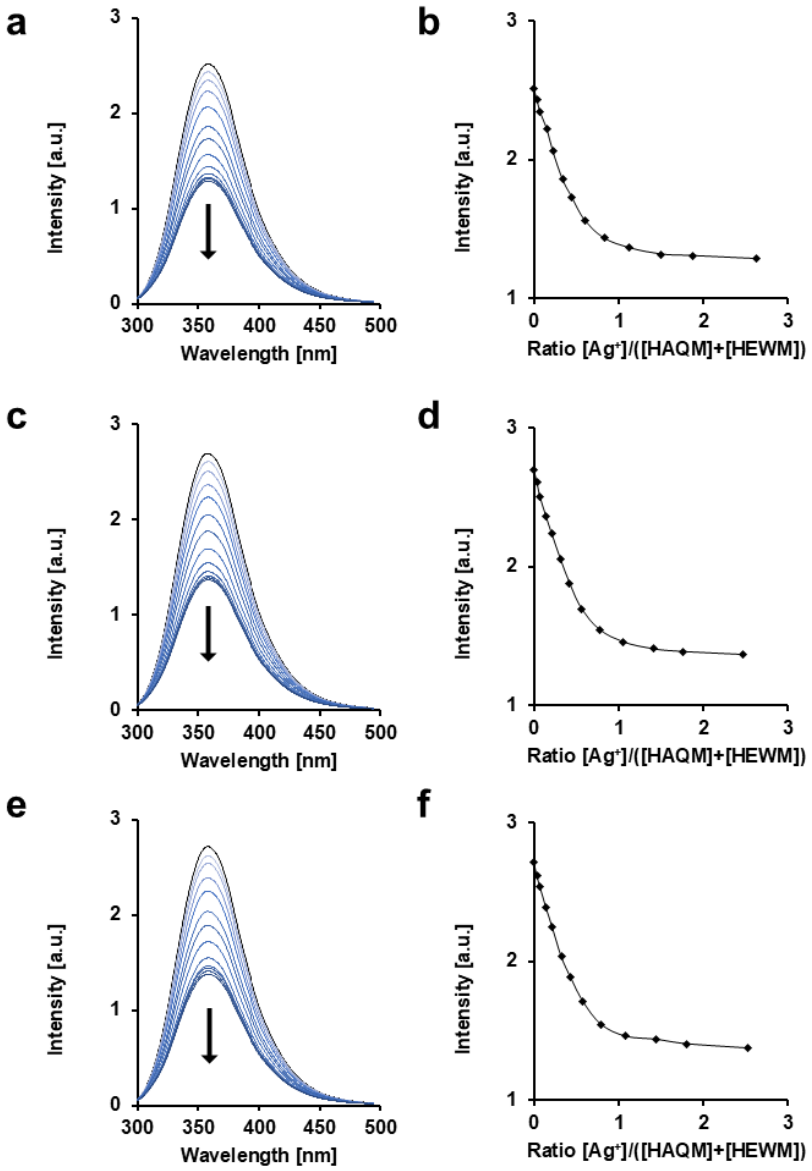

Fig. S142 HAQM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HAQM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

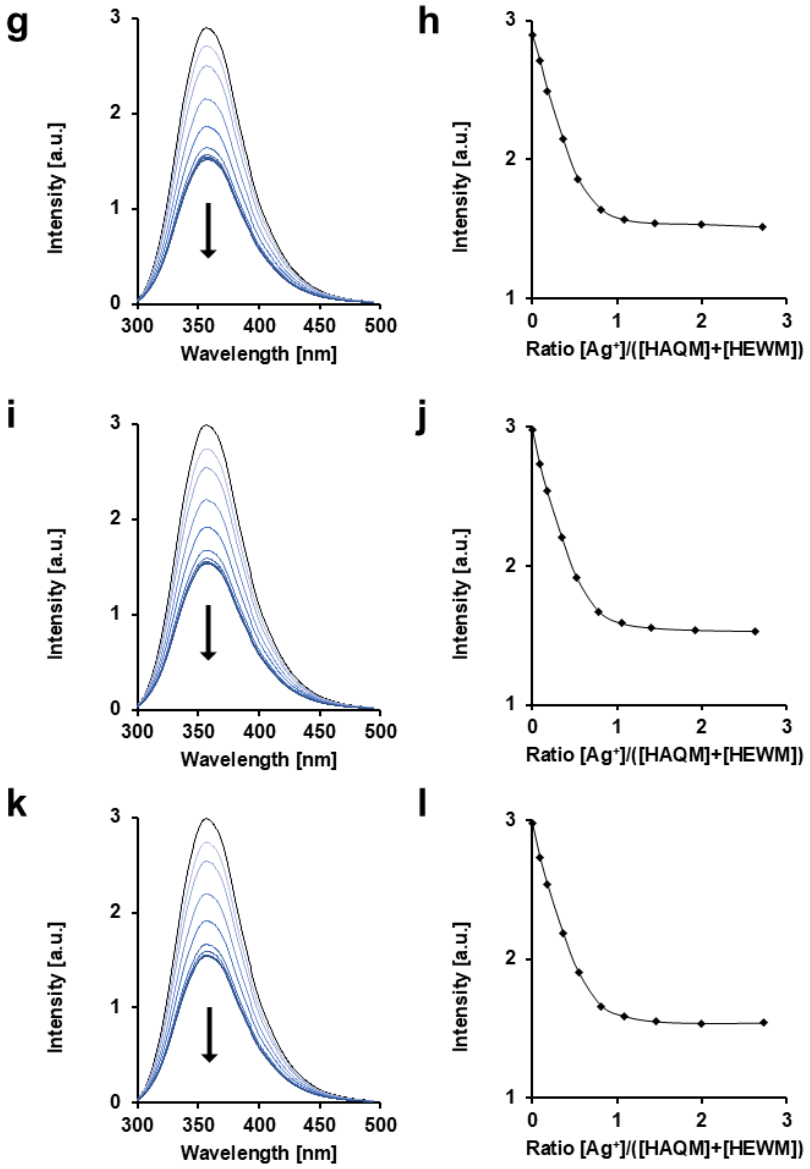

Fig. S143 HAQM / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HAQM ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S16 Determination of the binding constants ($\log(K_{ass})$) of HAQM tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HAQM	$\log(K_{ass\text{-}1}) = 5.57 \pm 0.04$	$\log(K_{ass\text{-}1}) = 5.64 \pm 0.04$
	$\log(K_{ass\text{-}2}) = 5.63 \pm 0.03$	$\log(K_{ass\text{-}2}) = 5.64 \pm 0.03$
	$\log(K_{ass\text{-}3}) = 5.62 \pm 0.04$	$\log(K_{ass\text{-}3}) = 5.67 \pm 0.03$
Average	$\log(K_{ass}) = 5.63 \pm 0.03$	

[a] The values correspond to the peptide and probe concentrations.

MQQH

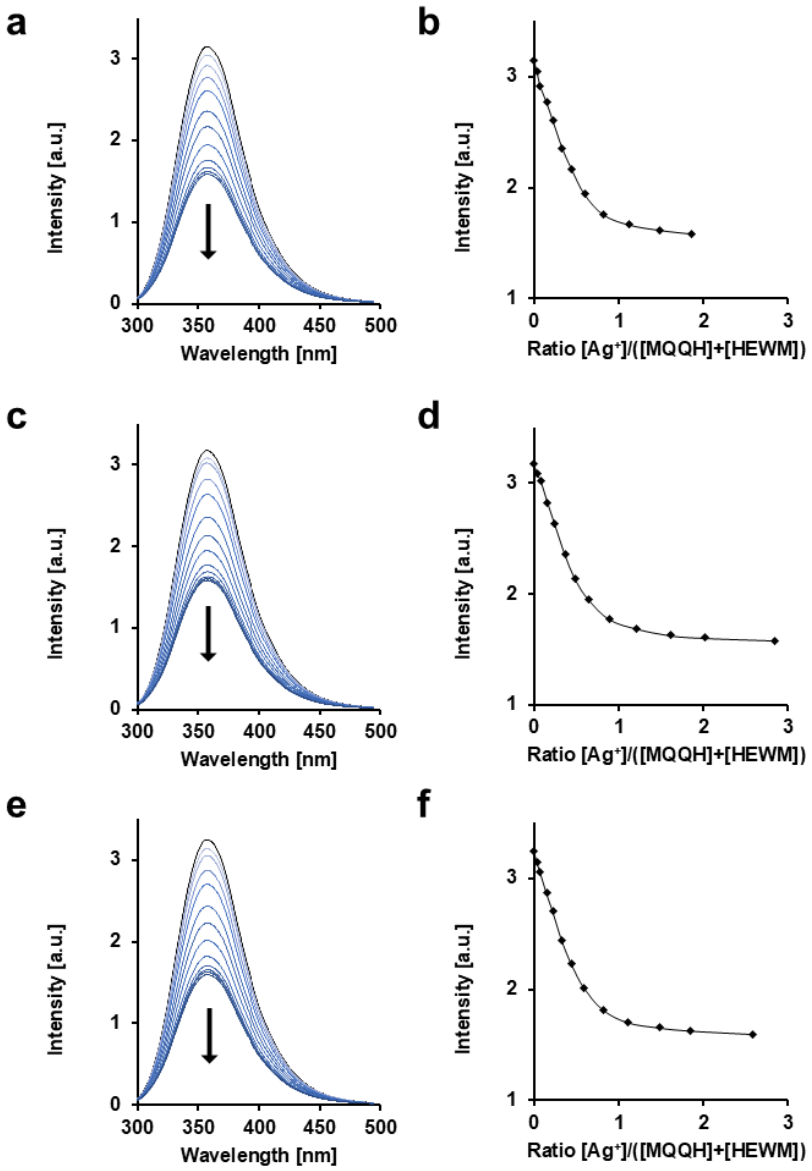

Fig. S144 MQQH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MQQH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

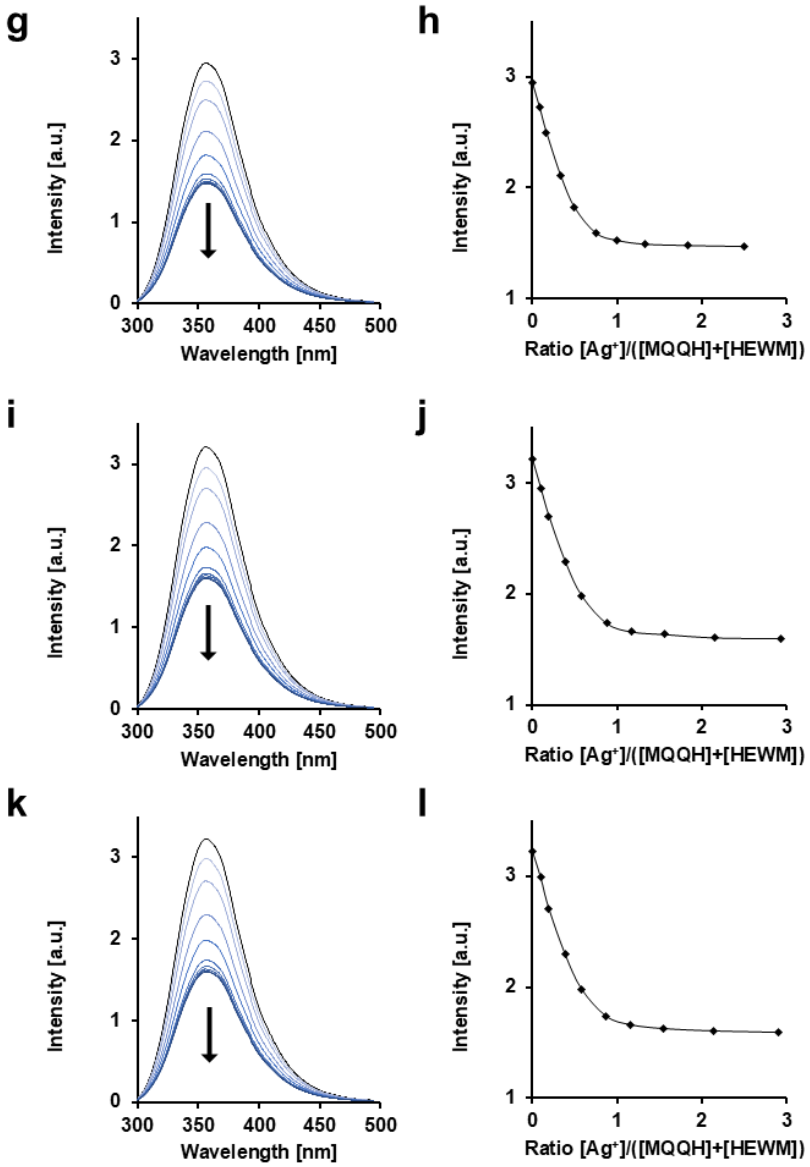

Fig. S145 MQQH / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MQQH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S17 Determination of the binding constants ($\log(K_{ass})$) of MQQH tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
MQQH	$\log(K_{ass-1}) = 5.52 \pm 0.05$	$\log(K_{ass-1}) = 5.37 \pm 0.02$
	$\log(K_{ass-2}) = 5.58 \pm 0.06$	$\log(K_{ass-2}) = 5.51 \pm 0.04$
	$\log(K_{ass-3}) = 5.59 \pm 0.03$	$\log(K_{ass-3}) = 5.48 \pm 0.05$
Average	$\log(K_{ass}) = 5.51 \pm 0.08$	

[a] The values correspond to the peptide and probe concentrations.

MRQH

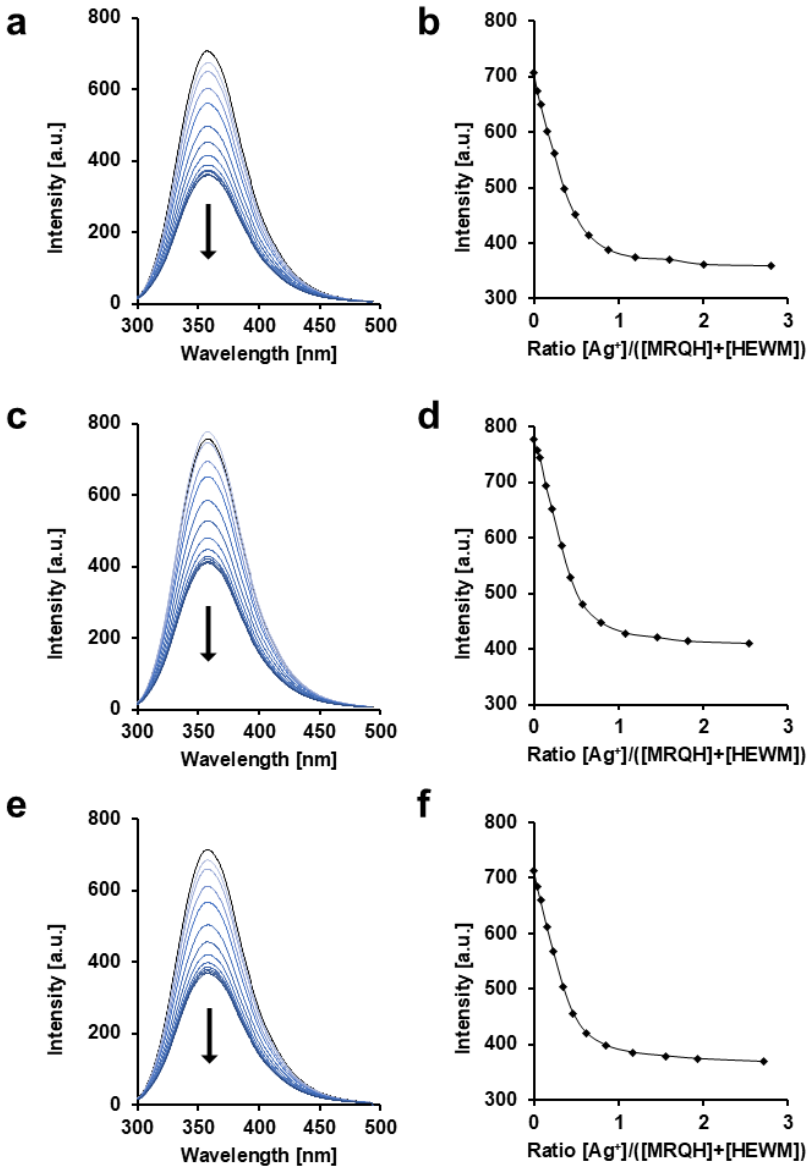

Fig. S146 MRQH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MRQH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

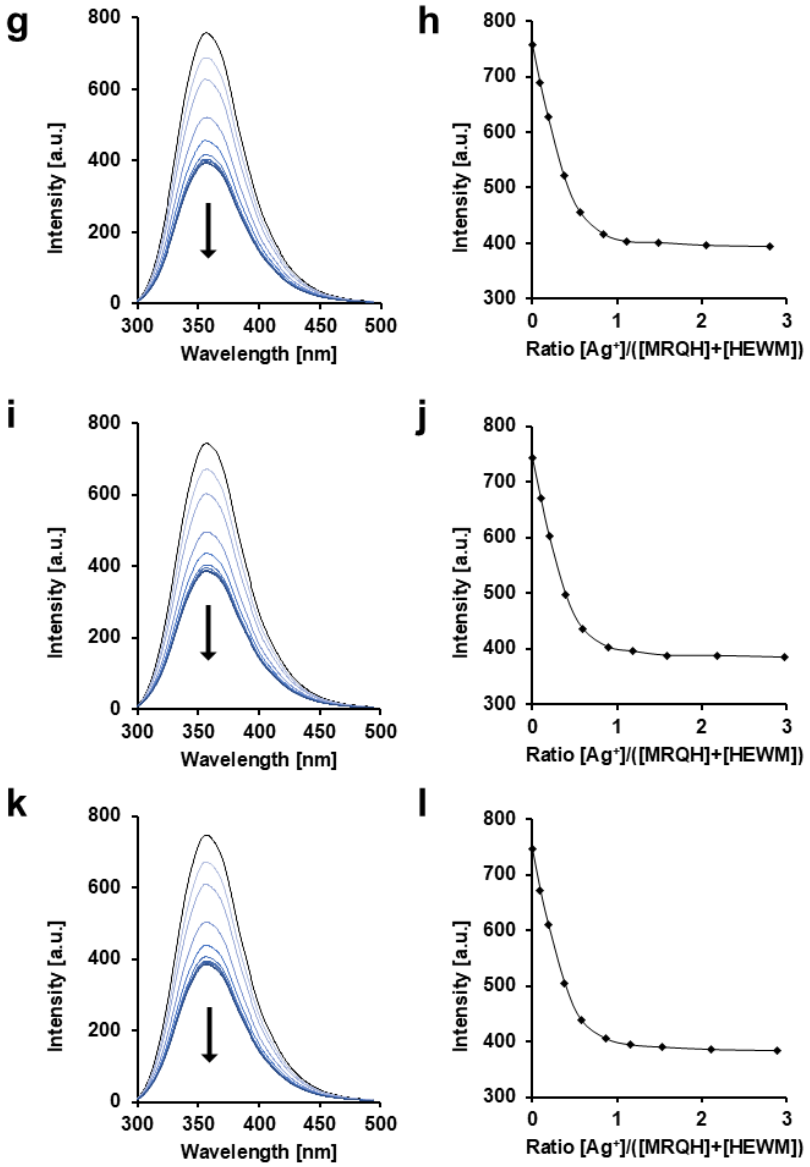

Fig. S147 MRQH / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MRQH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S18 Determination of the binding constants ($\log(K_{ass})$) of MRQH tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
MRQH	$\log(K_{ass-1}) = 5.31 \pm 0.05$	$\log(K_{ass-1}) = 5.23 \pm 0.04$
	$\log(K_{ass-2}) = 5.34 \pm 0.06$	$\log(K_{ass-2}) = 5.05 \pm 0.08$
	$\log(K_{ass-3}) = 5.12 \pm 0.04$	$\log(K_{ass-3}) = 5.09 \pm 0.09$
Average	$\log(K_{ass}) = 5.19 \pm 0.12$	

[a] The values correspond to the peptide and probe concentrations.

MQRH

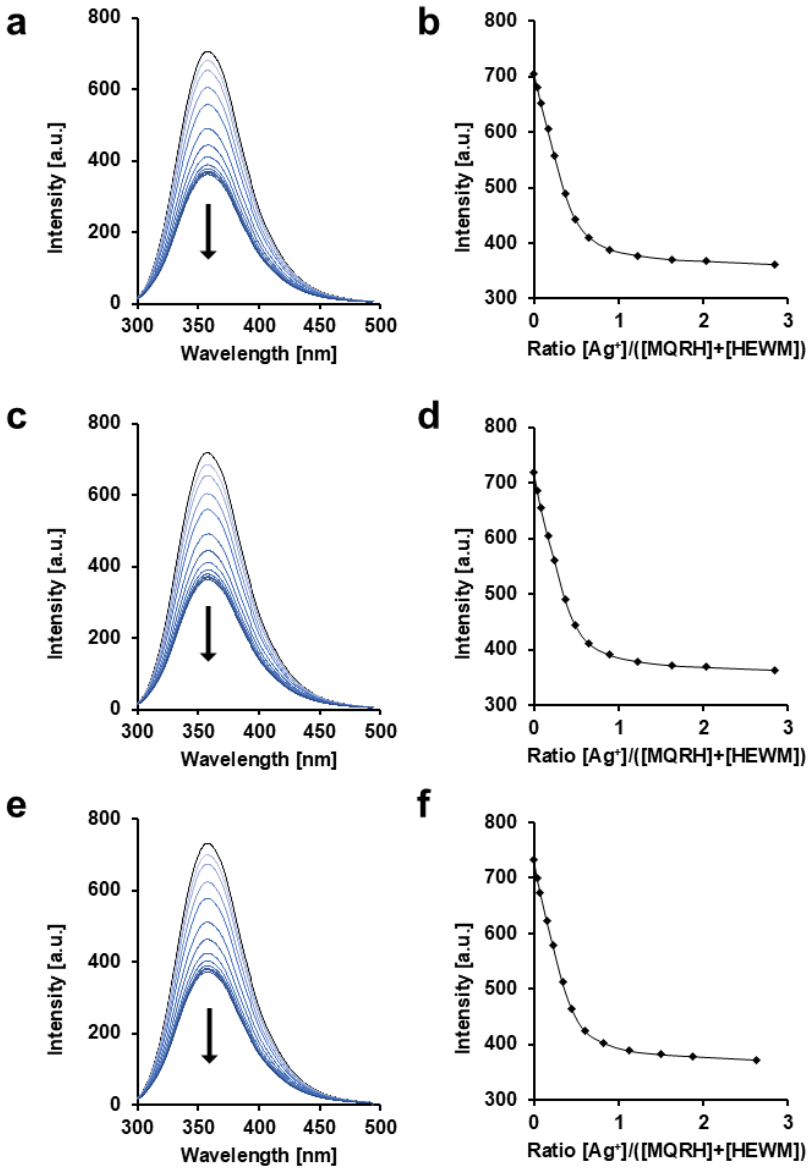

Fig. S148 MQRH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MQRH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

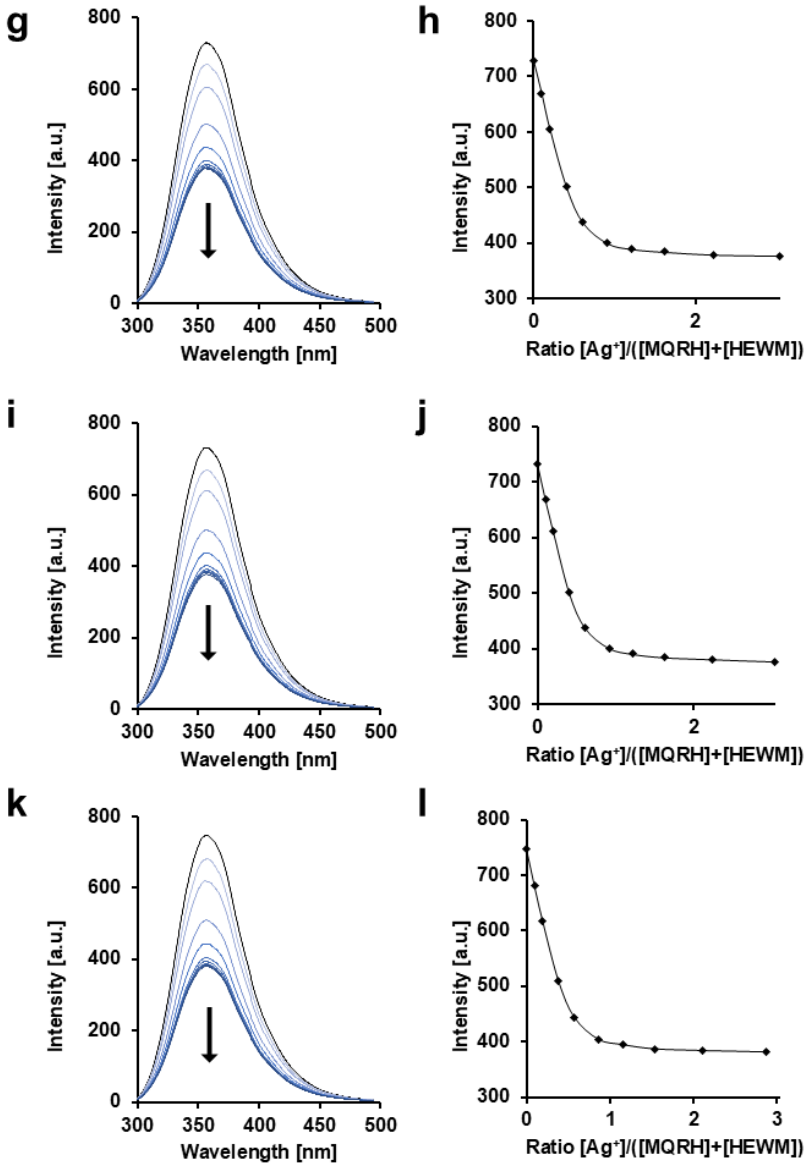

Fig. S149 MQRH / HEWM competition titrations, both at $1{\cdot}10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MQRH ($1{\cdot}10^{-5}$ M) in competition with HEWM probe ($1{\cdot}10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S19 Determination of the binding constants ($\log(K_{ass})$) of MQRH tetrapeptide.

Model	$5{\cdot}10^{-6}$ M[a]	$1{\cdot}10^{-5}$ M[a]
MQRH	$\log(K_{ass\text{-}1}) = 5.03 \pm 0.04$	$\log(K_{ass\text{-}1}) = 5.35 \pm 0.03$
	$\log(K_{ass\text{-}2}) = 4.92 \pm 0.10$	$\log(K_{ass\text{-}2}) = 5.34 \pm 0.04$
	$\log(K_{ass\text{-}3}) = 4.96 \pm 0.07$	$\log(K_{ass\text{-}3}) = 5.16 \pm 0.04$
Average	$\log(K_{ass}) = 5.13 \pm 0.19$	

[a] The values correspond to the peptide and probe concentrations.

MPPH

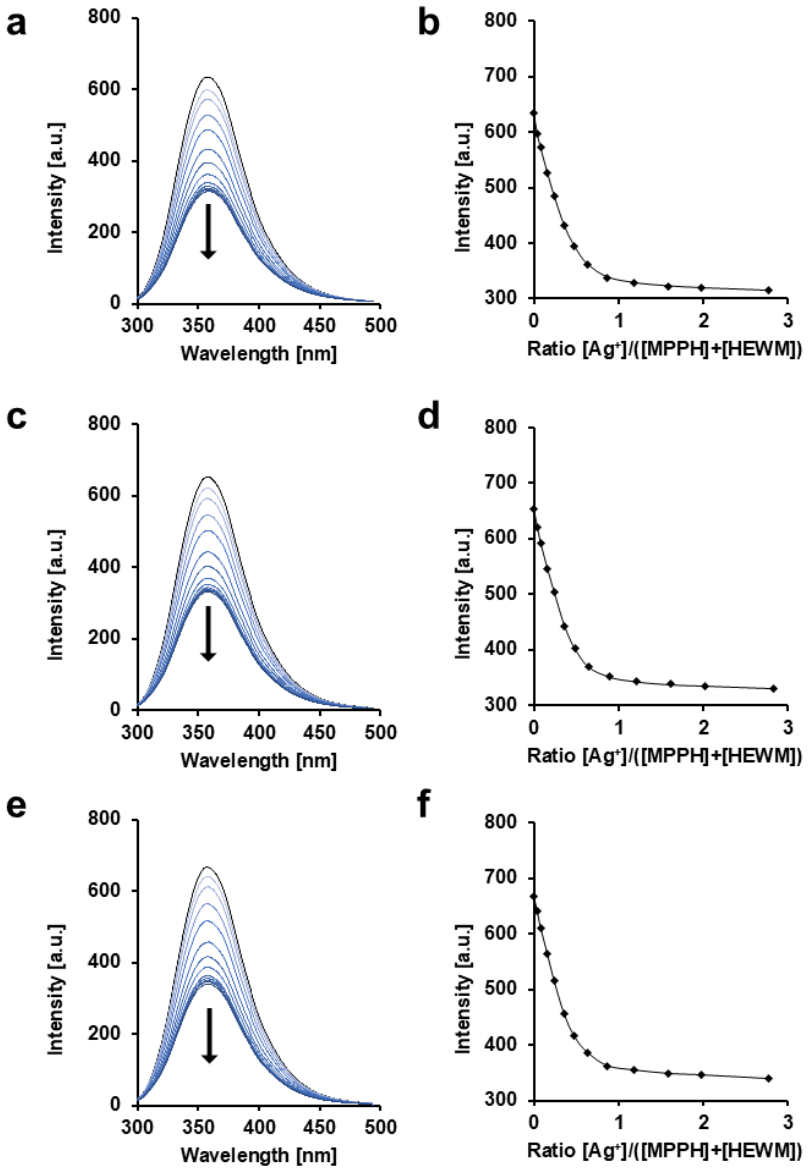

Fig. S150 MPPH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MPPH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

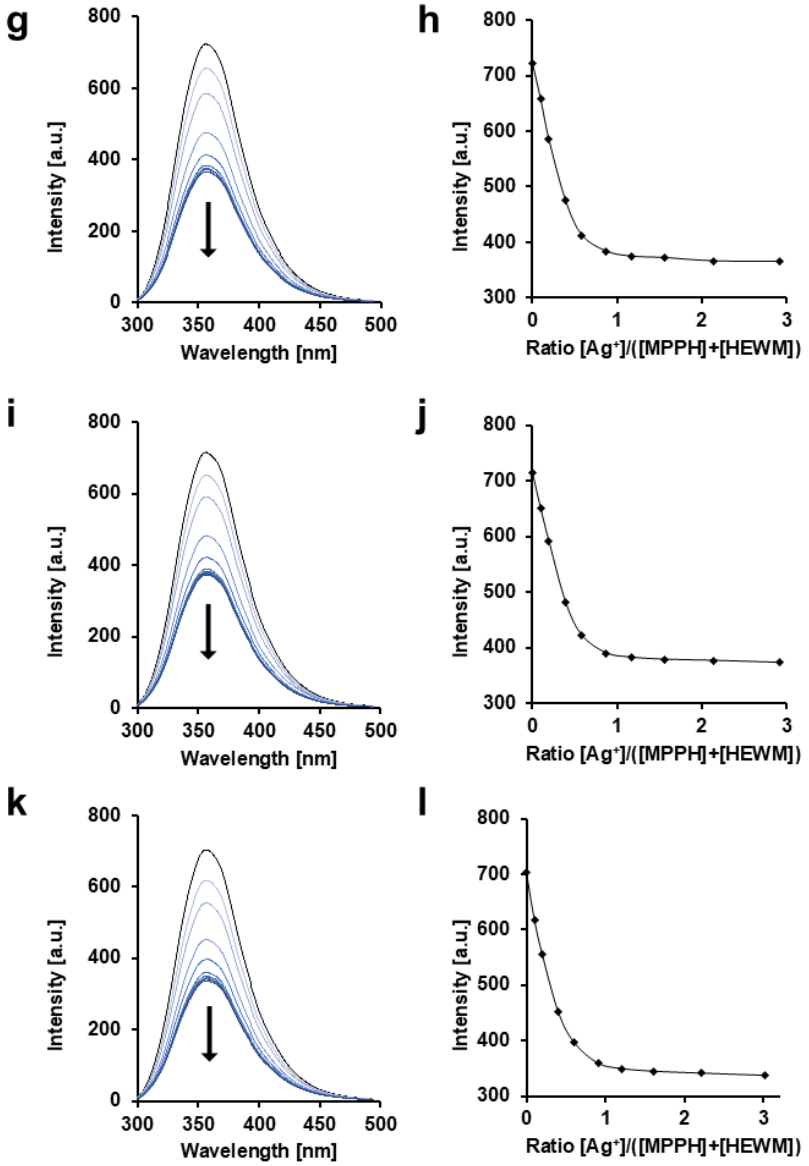

Fig. S151 MPPH / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MPPH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S20 Determination of the binding constants ($\log(K_{ass})$) of MPPH tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
MPPH	$\log(K_{ass\text{-}1}) = 5.17 \pm 0.10$	$\log(K_{ass\text{-}1}) = 4.93 \pm 0.09$
	$\log(K_{ass\text{-}2}) = 5.01 \pm 0.09$	$\log(K_{ass\text{-}2}) = 5.03 \pm 0.05$
	$\log(K_{ass\text{-}3}) = 5.02 \pm 0.07$	$\log(K_{ass\text{-}3}) = 5.10 \pm 0.16$
Average	$\log(K_{ass}) = 5.04 \pm 0.08$	

[a] The values correspond to the peptide and probe concentrations.

MQPH

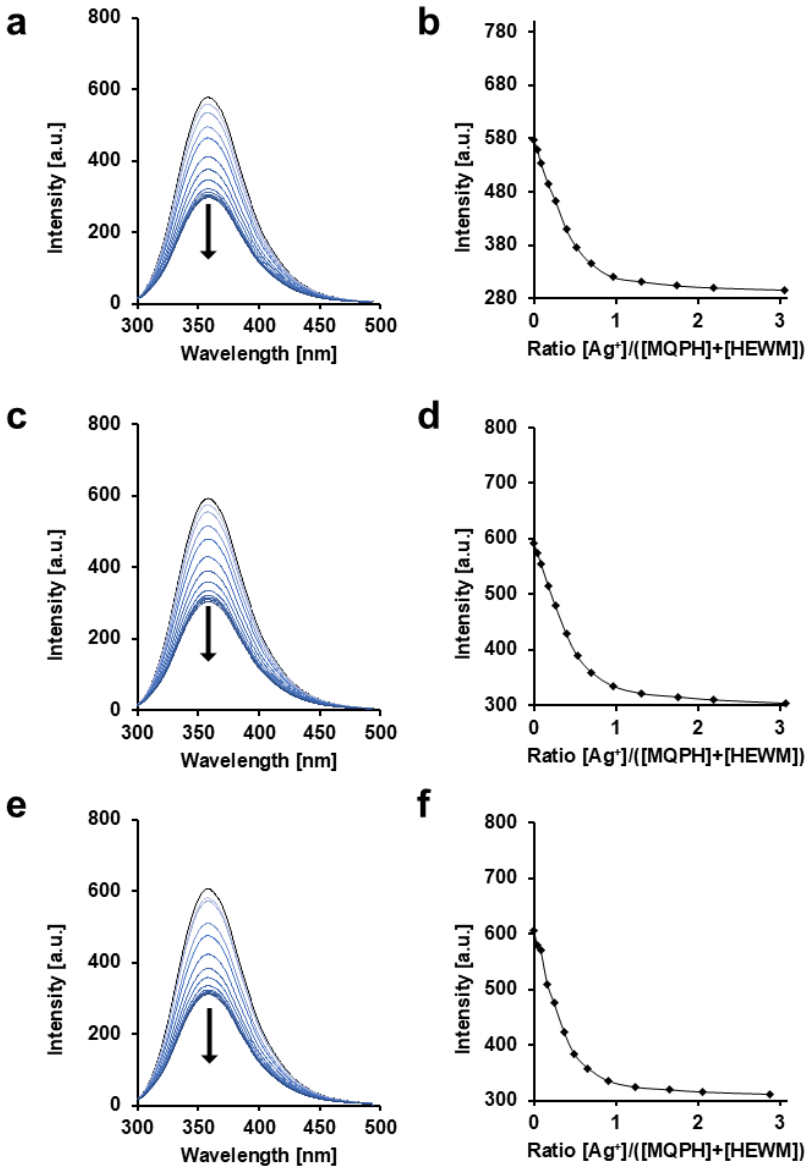

Fig. S152 MQPH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MQPH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

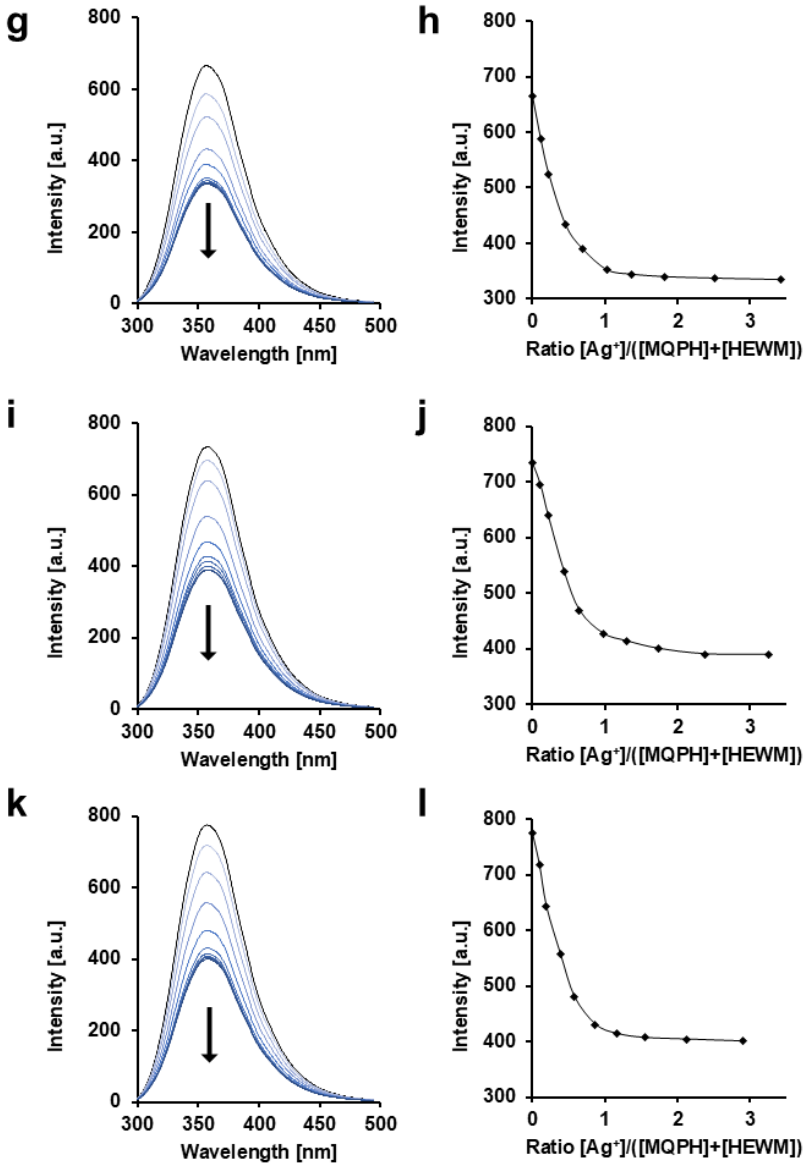

Fig. S153 MQPH / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MQPH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S21 Determination of the binding constants ($\log(K_{ass})$) of MQPH tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
MQPH	$\log(K_{ass-1}) = 5.61 \pm 0.04$	$\log(K_{ass-1}) = 5.30 \pm 0.12$
	$\log(K_{ass-2}) = 5.69 \pm 0.04$	$\log(K_{ass-2}) = 5.80 \pm 0.11$
	$\log(K_{ass-3}) = 5.22 \pm 0.10$	$\log(K_{ass-3}) = 5.52 \pm 0.07$
Average	$\log(K_{ass}) = 5.53 \pm 0.23$	

[a] The values correspond to the peptide and probe concentrations.

MPQH

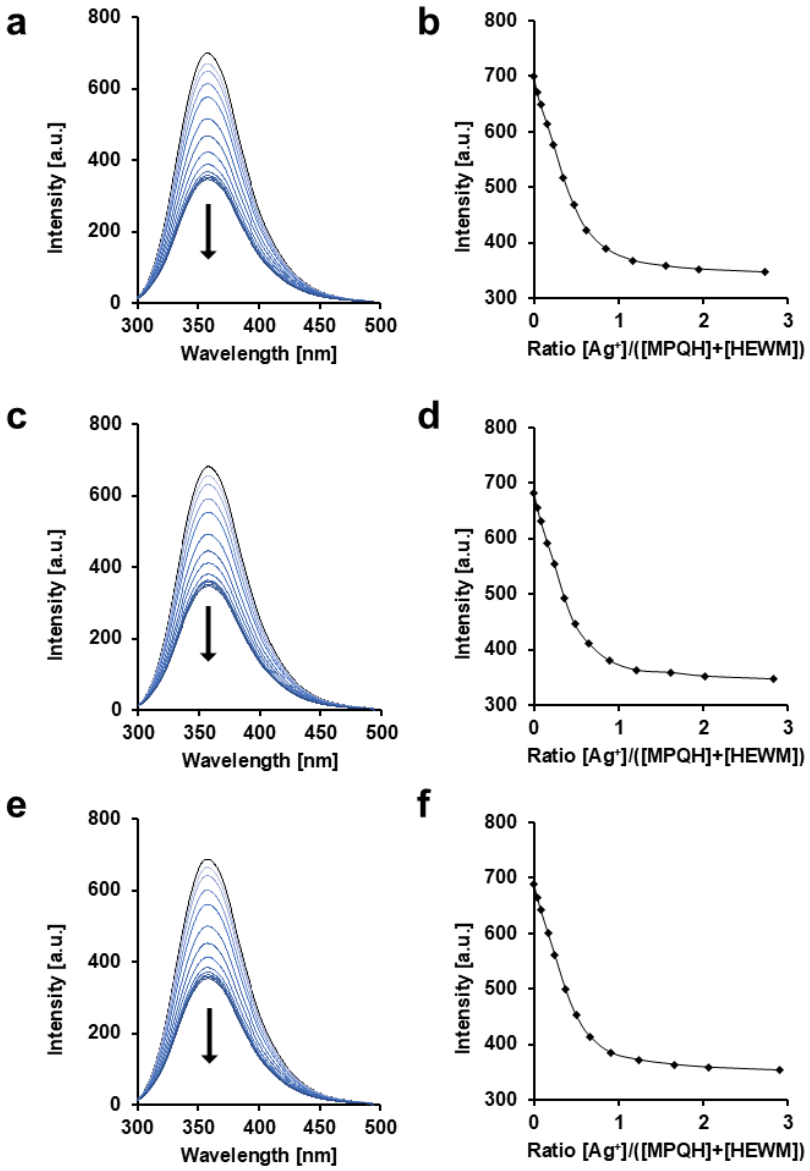

Fig. S154 MPQH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MPQH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

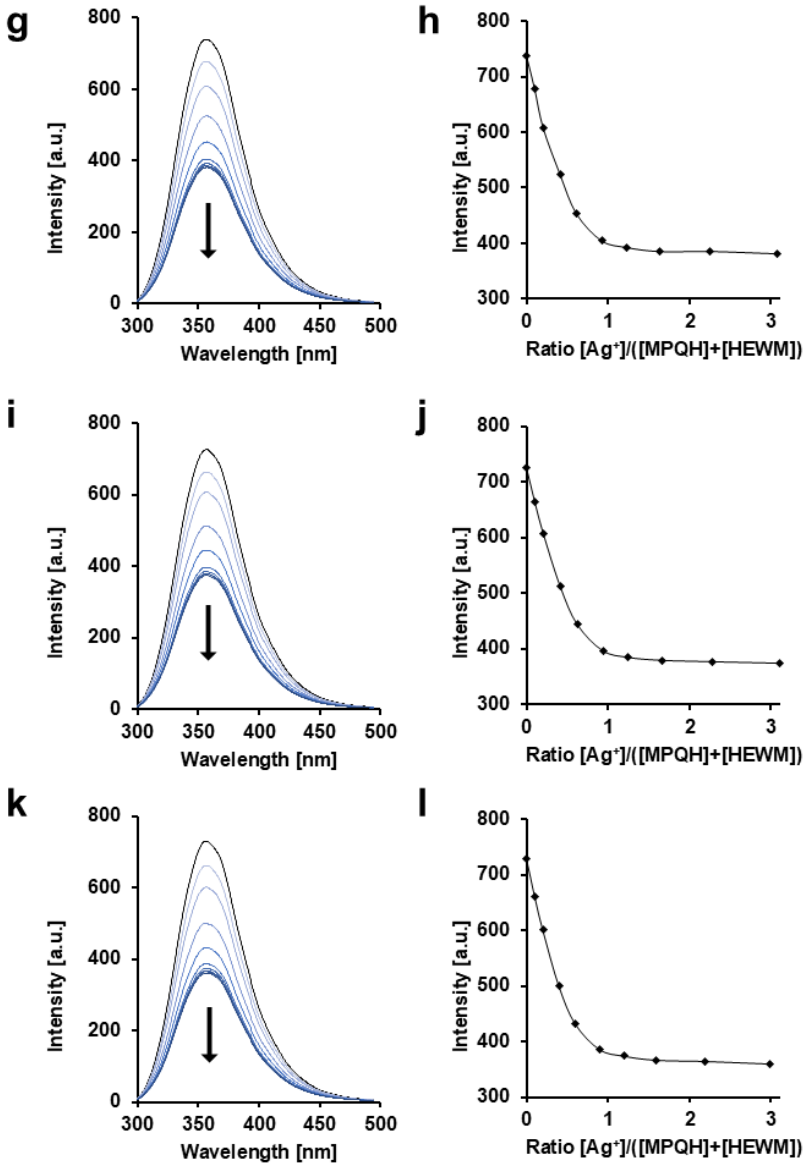

Fig. S155 MPQH / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MPQH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S22 Determination of the binding constants ($\log(K_{ass})$) of MPQH tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
MPQH	$\log(K_{ass-1}) = 5.64 \pm 0.05$	$\log(K_{ass-1}) = 5.59 \pm 0.06$
	$\log(K_{ass-2}) = 5.46 \pm 0.04$	$\log(K_{ass-2}) = 5.62 \pm 0.02$
	$\log(K_{ass-3}) = 5.51 \pm 0.04$	$\log(K_{ass-3}) = 5.47 \pm 0.03$
Average	$\log(K_{ass}) = 5.55 \pm 0.08$	

[a] The values correspond to the peptide and probe concentrations.

MKKH

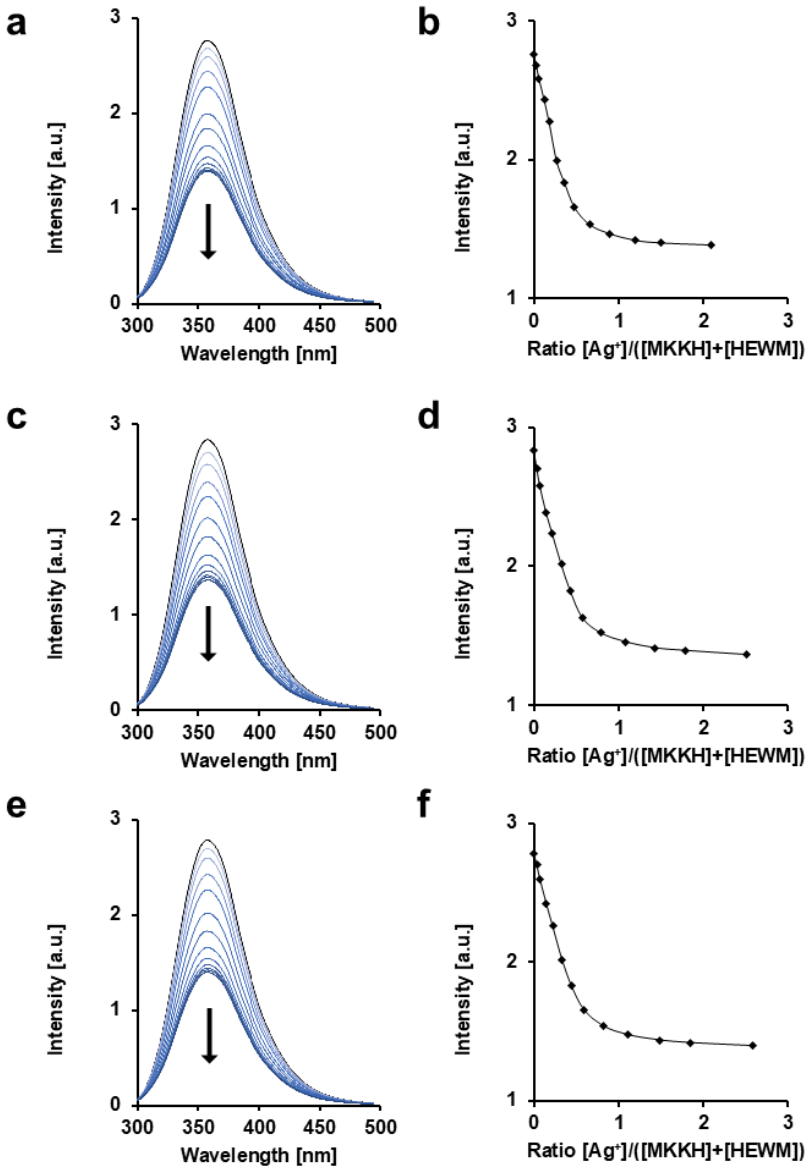

Fig. S156 MKKH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MKKH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

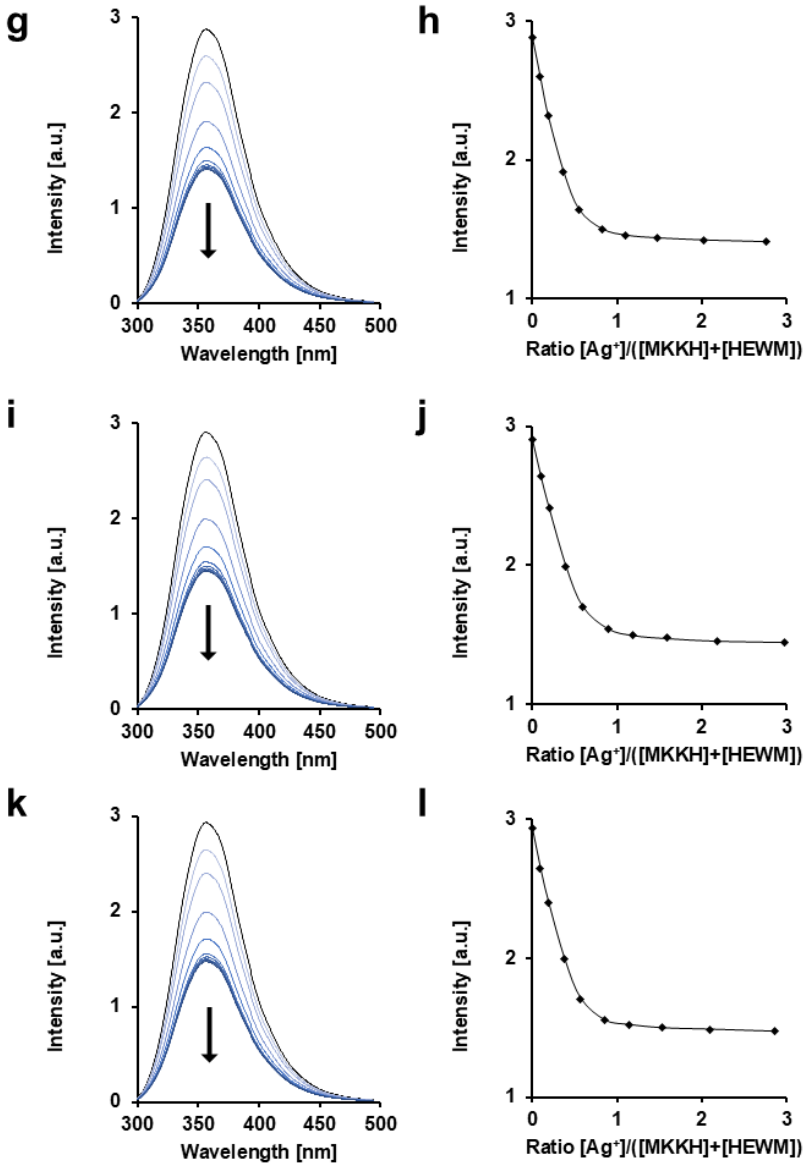

Fig. S157 MKKH / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MKKH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S23 Determination of the binding constants ($\log(K_{ass})$) of MKKH tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
MKKH	$\log(K_{ass-1}) = 5.05 \pm 0.07$	$\log(K_{ass-1}) = 4.80 \pm 0.22$
	$\log(K_{ass-2}) = 5.02 \pm 0.17$	$\log(K_{ass-2}) = 5.26 \pm 0.04$
	$\log(K_{ass-3}) = 5.22 \pm 0.03$	$\log(K_{ass-3}) = 5.09 \pm 0.10$
Average	$\log(K_{ass}) = 5.07 \pm 0.16$	

[a] The values correspond to the peptide and probe concentrations.

MRKH

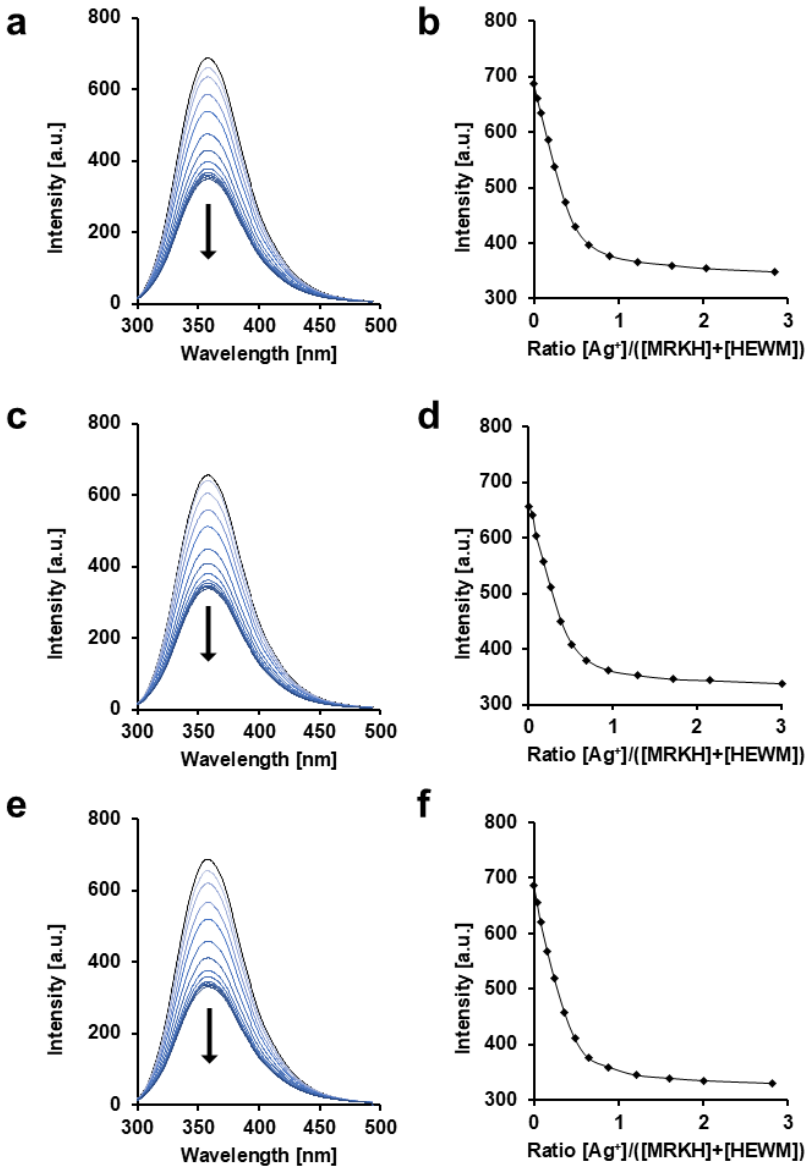

Fig. S158 MRKH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MRKH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

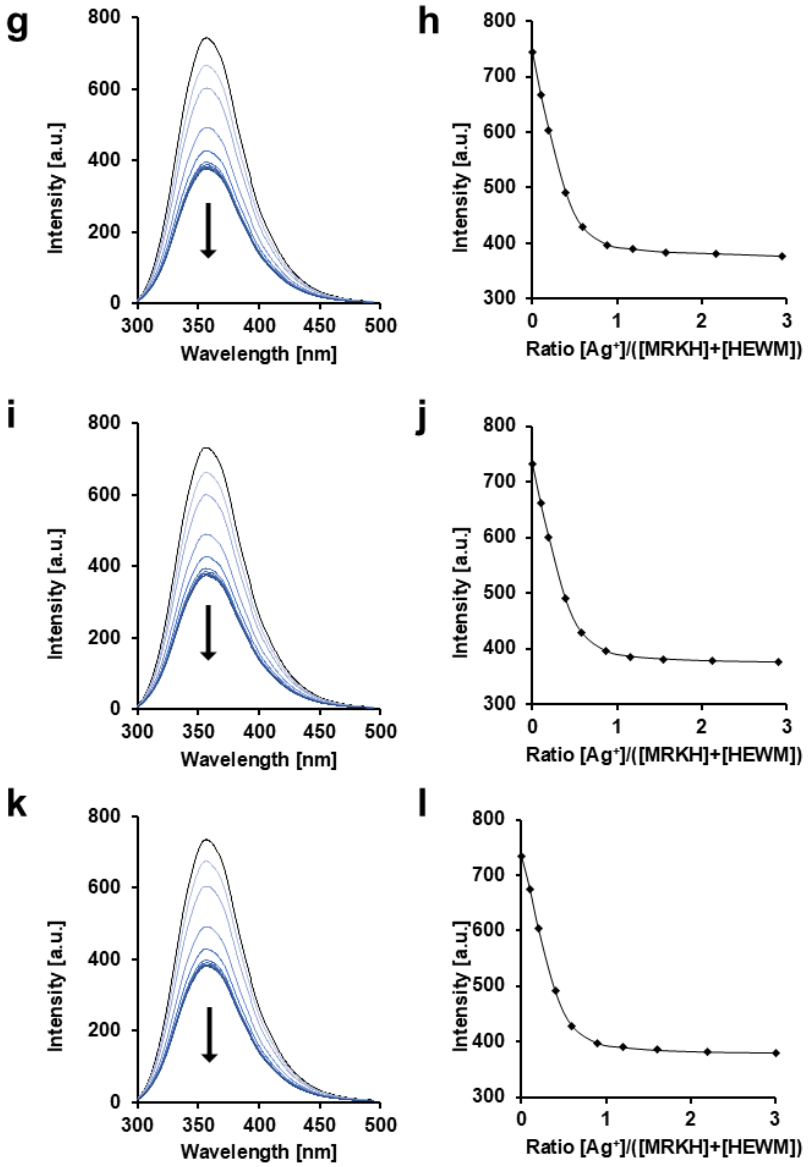

Fig. S159 MRKH / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MRKH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S24 Determination of the binding constants ($\log(K_{ass})$) of MRKH tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
MRKH	$\log(K_{ass-1}) = 4.98 \pm 0.05$	$\log(K_{ass-1}) = 5.09 \pm 0.06$
	$\log(K_{ass-2}) = 5.21 \pm 0.06$	$\log(K_{ass-2}) = 5.06 \pm 0.05$
	$\log(K_{ass-3}) = 5.05 \pm 0.09$	$\log(K_{ass-3}) = 5.20 \pm 0.05$
Average	$\log(K_{ass}) = 5.10 \pm 0.09$	

[a] The values correspond to the peptide and probe concentrations.

MKRH

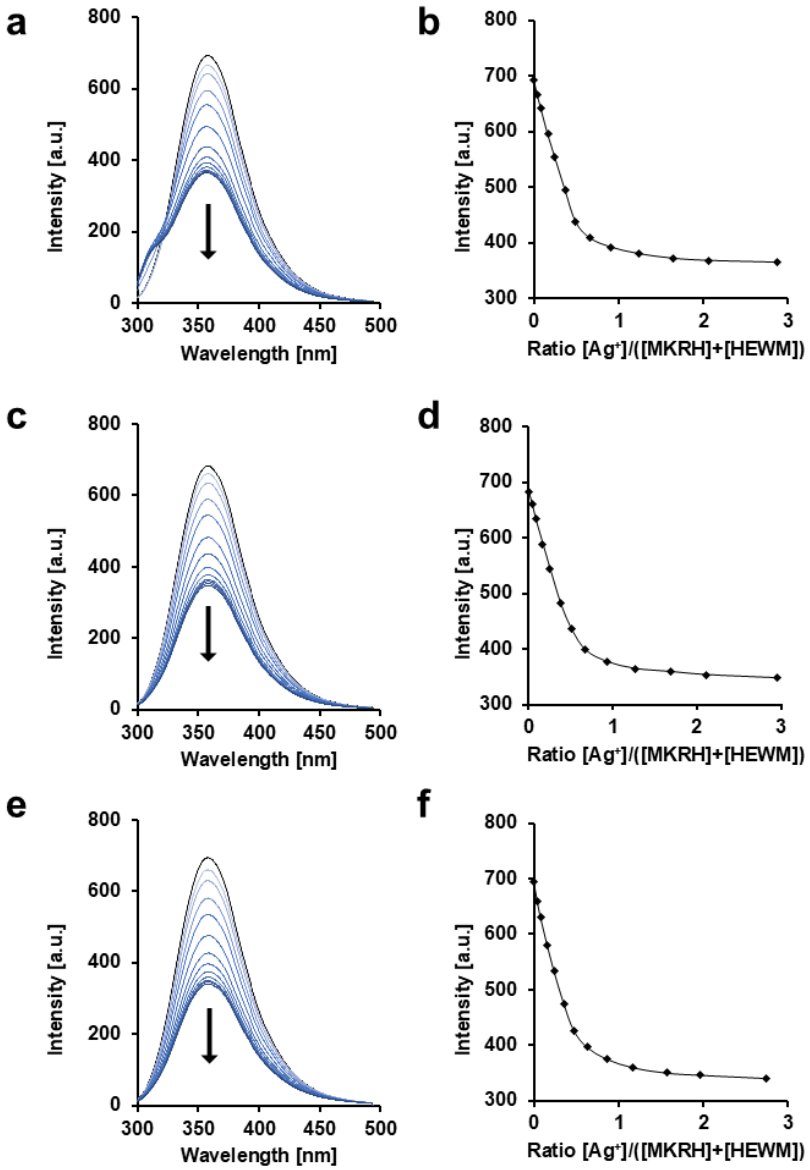

Fig. S160 MKRH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MKRH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

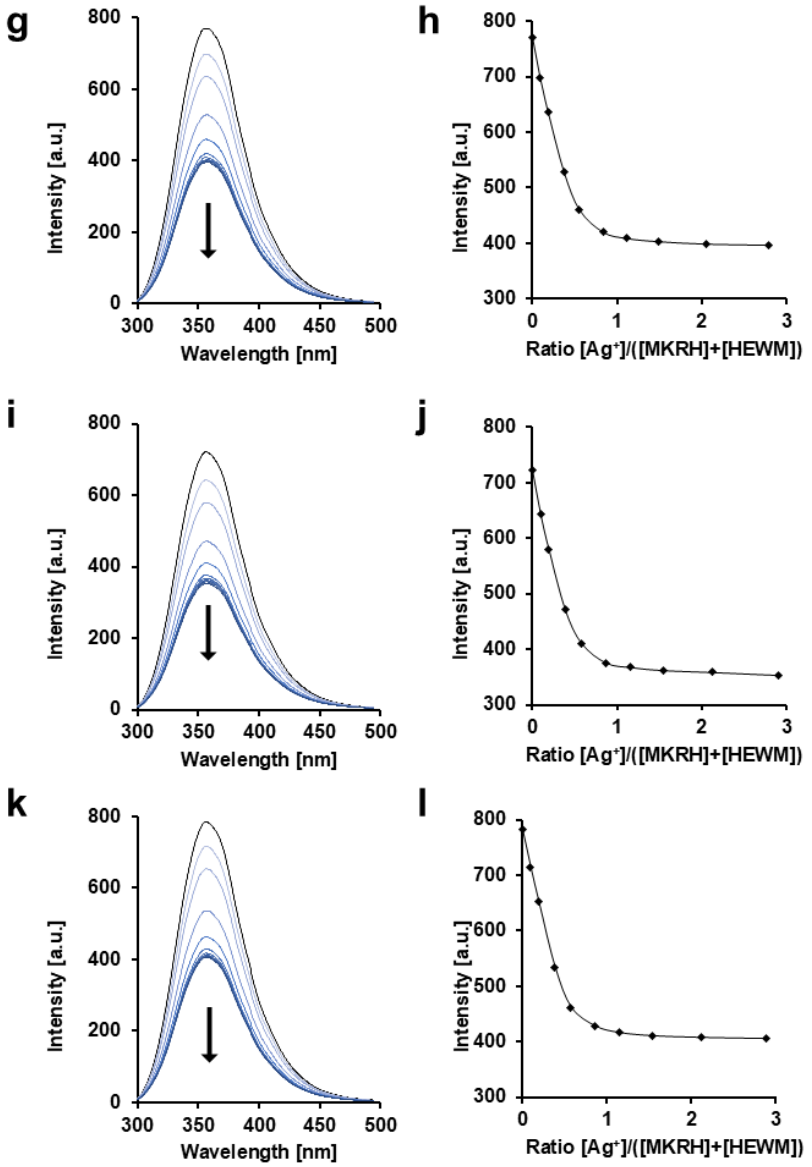

Fig. S161 MKRH / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MKRH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S25 Determination of the binding constants ($\log(K_{ass})$) of MKRH tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
MKRH	$\log(K_{ass-1}) = 5.19 \pm 0.07$	$\log(K_{ass-1}) = 5.17 \pm 0.06$
	$\log(K_{ass-2}) = 5.34 \pm 0.04$	$\log(K_{ass-2}) = 5.03 \pm 0.12$
	$\log(K_{ass-3}) = 4.98 \pm 0.11$	$\log(K_{ass-3}) = 5.19 \pm 0.03$
Average	$\log(K_{ass}) = 5.15 \pm 0.13$	

[a] The values correspond to the peptide and probe concentrations.

MAAH

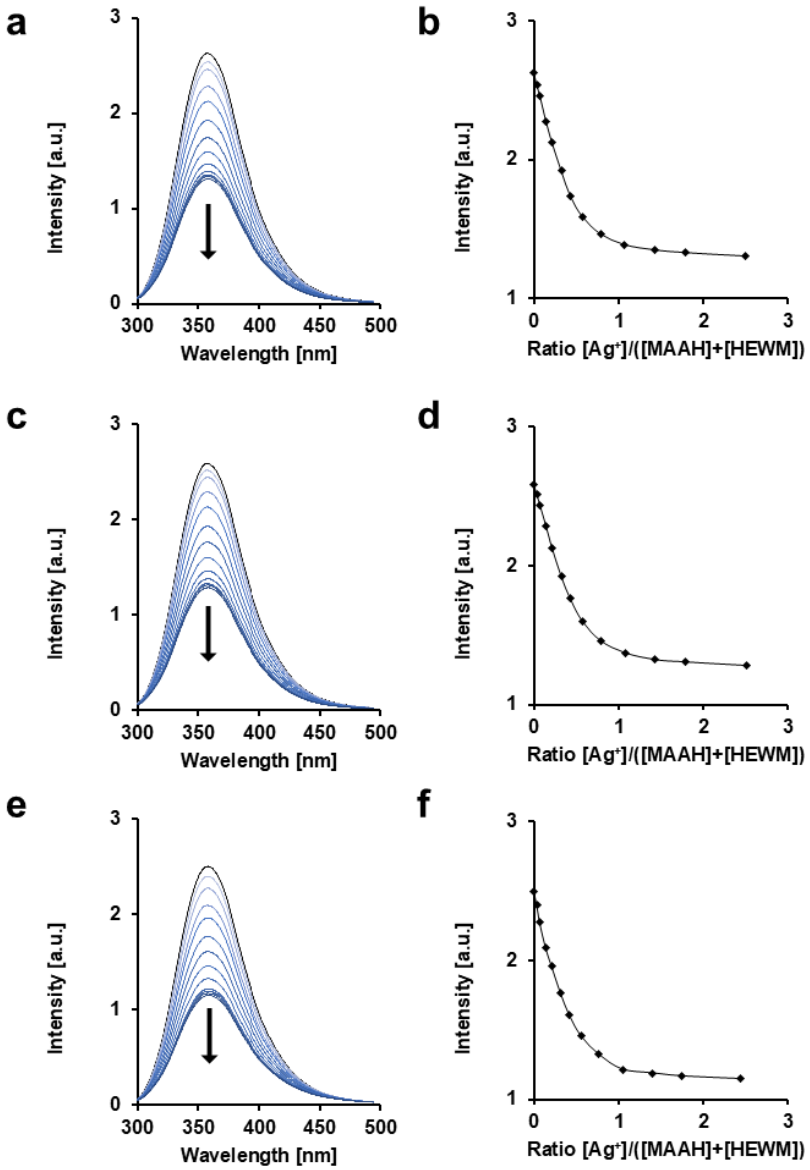

Fig. S162 MAAH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MAAH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

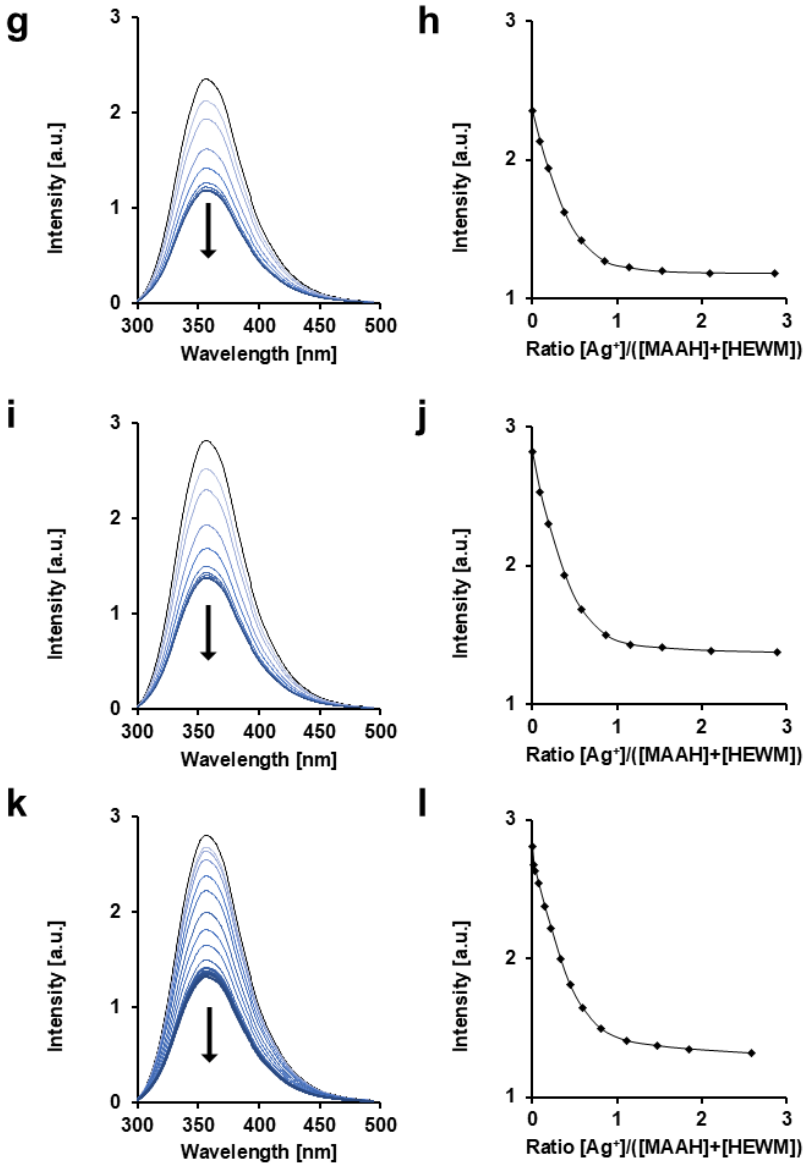

Fig. S163 MAAH / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MAAH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S26 Determination of the binding constants ($\log(K_{ass})$) of MAAH tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
MAAH	$\log(K_{ass-1}) = 5.30 \pm 0.04$	$\log(K_{ass-1}) = 5.38 \pm 0.05$
	$\log(K_{ass-2}) = 5.57 \pm 0.02$	$\log(K_{ass-2}) = 5.40 \pm 0.09$
	$\log(K_{ass-3}) = 5.35 \pm 0.10$	$\log(K_{ass-3}) = 5.48 \pm 0.07$
Average	$\log(K_{ass}) = 5.41 \pm 0.10$	

[a] The values correspond to the peptide and probe concentrations.

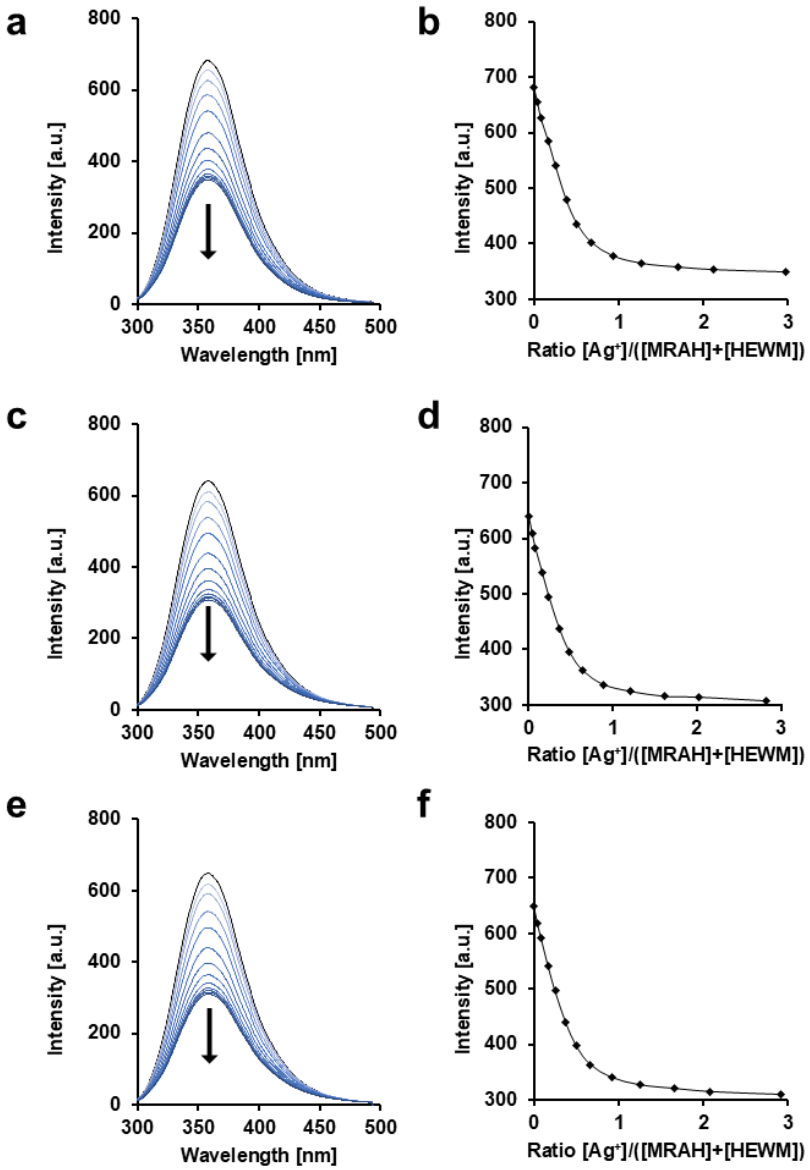

Fig. S164 MRAH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MRAH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

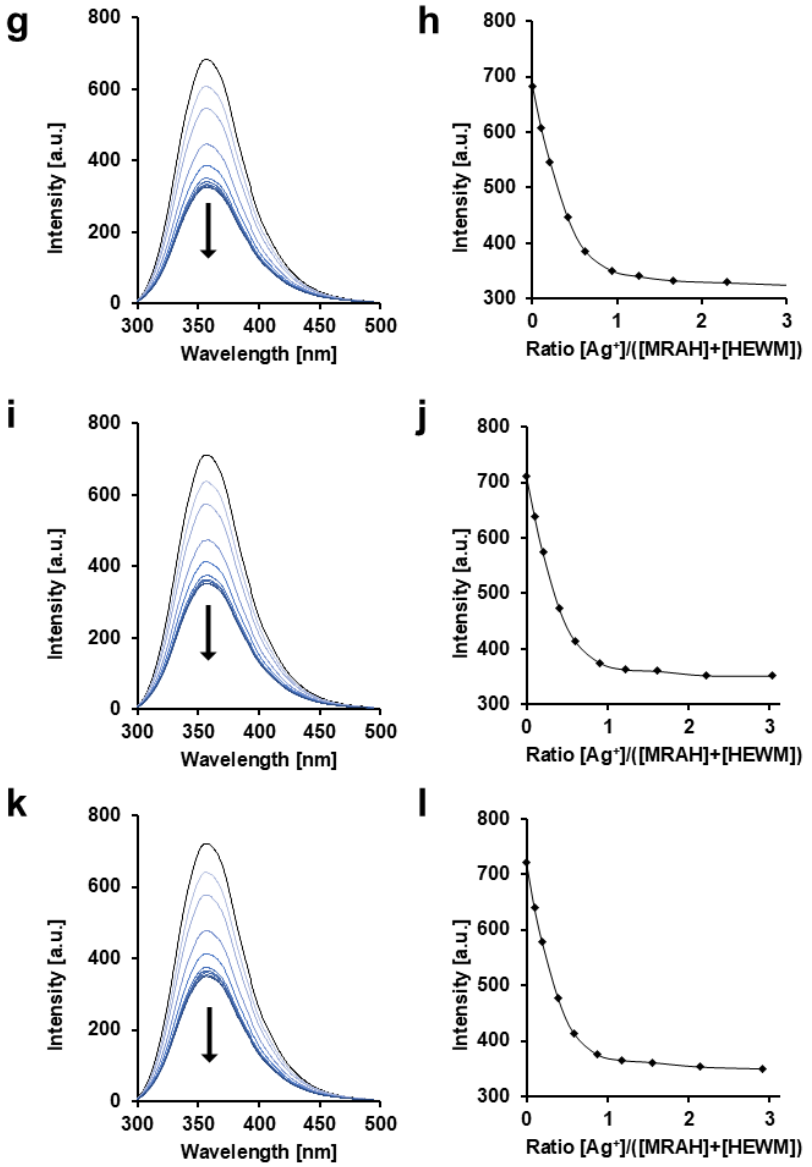

Fig. S165 MRAH / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MRAH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S27 Determination of the binding constants ($\log(K_{ass})$) of MRAH tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
MRAH	$\log(K_{ass-1}) = 5.36 \pm 0.04$	$\log(K_{ass-1}) = 5.29 \pm 0.08$
	$\log(K_{ass-2}) = 5.27 \pm 0.05$	$\log(K_{ass-2}) = 5.11 \pm 0.13$
	$\log(K_{ass-3}) = 5.25 \pm 0.05$	$\log(K_{ass-3}) = 4.92 \pm 0.28$[b]
Average	$\log(K_{ass}) = 5.26 \pm 0.09$	

[a] The values correspond to the peptide and probe concentrations.
[b] The value has not been taken into consideration.

MARH

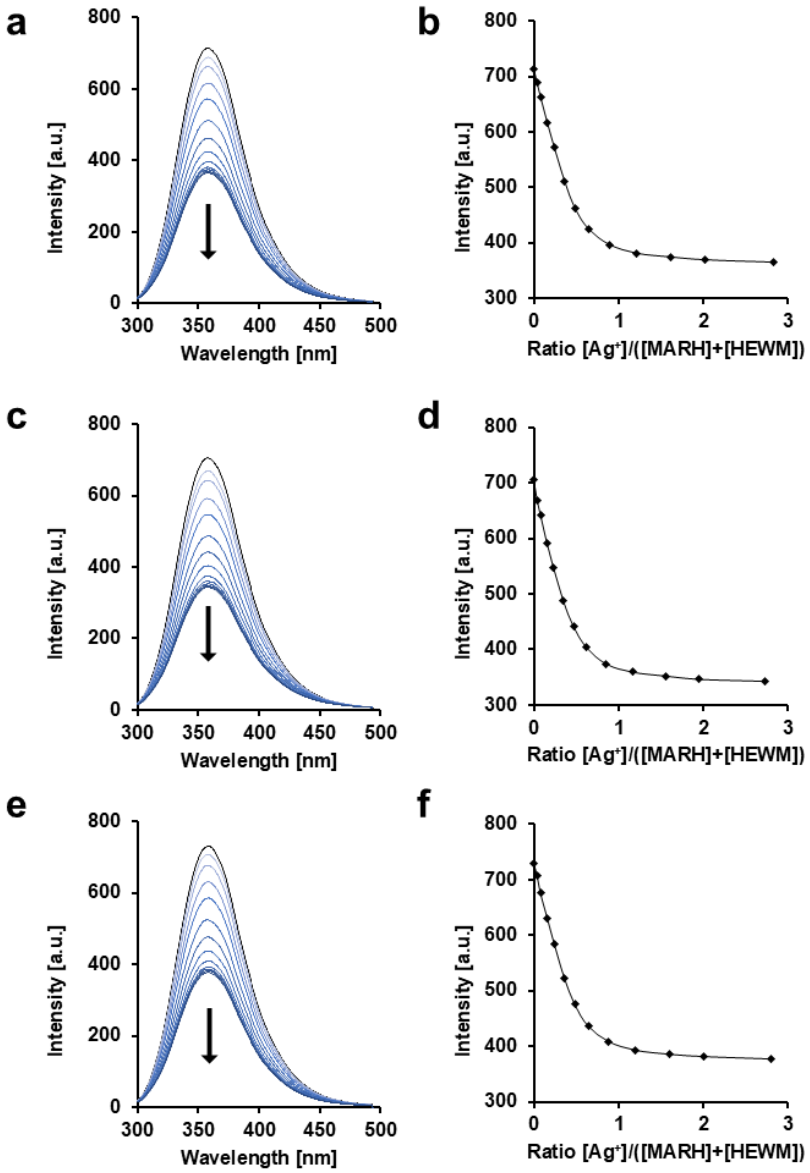

Fig. S166 MARH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MARH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

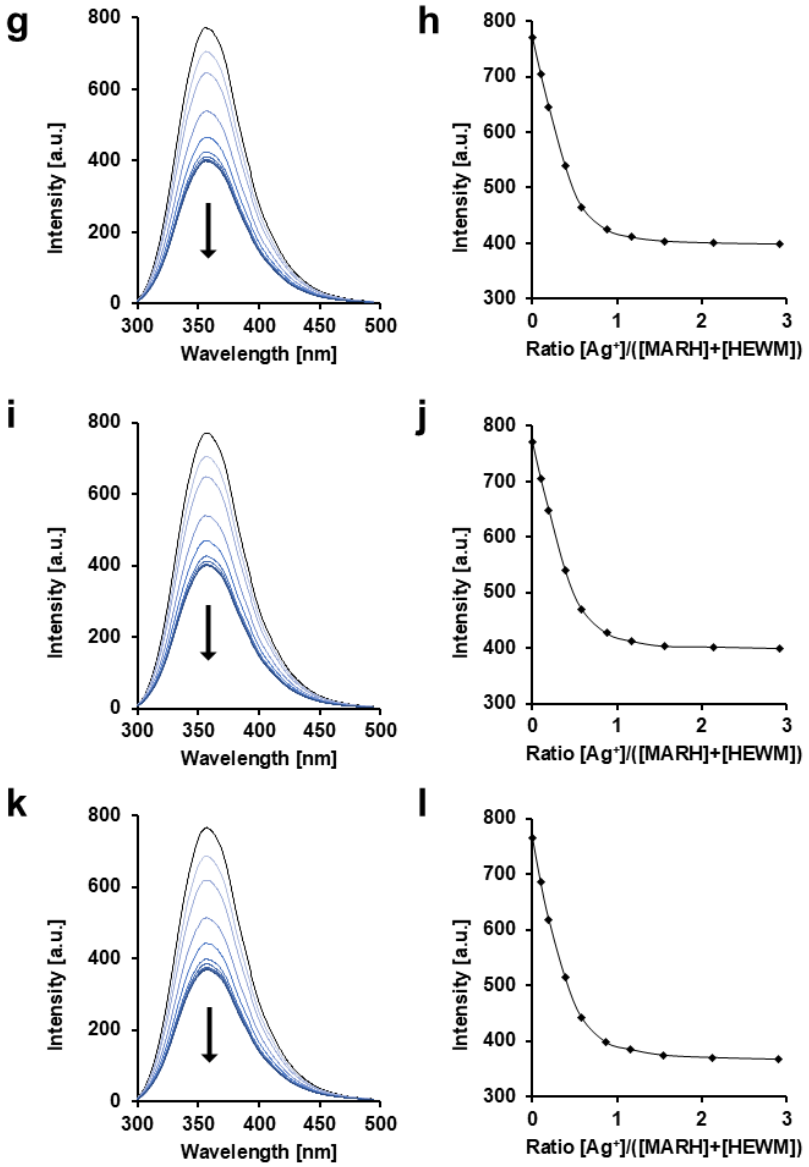

Fig. S167 MARH / HEWM competition titrations, both at $1{\cdot}10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MARH ($1{\cdot}10^{-5}$ M) in competition with HEWM probe ($1{\cdot}10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S28 Determination of the binding constants ($\log(K_{ass})$) of MARH tetrapeptide.

Model	$5{\cdot}10^{-6}$ M[a]	$1{\cdot}10^{-5}$ M[a]
MARH	$\log(K_{ass\text{-}1}) = 5.37 \pm 0.02$	$\log(K_{ass\text{-}1}) = 5.37 \pm 0.02$
	$\log(K_{ass\text{-}2}) = 5.24 \pm 0.07$	$\log(K_{ass\text{-}2}) = 5.39 \pm 0.02$
	$\log(K_{ass\text{-}3}) = 5.32 \pm 0.03$	$\log(K_{ass\text{-}3}) = 5.27 \pm 0.08$
Average	$\log(K_{ass}) = 5.33 \pm 0.06$	

[a] The values correspond to the peptide and probe concentrations.

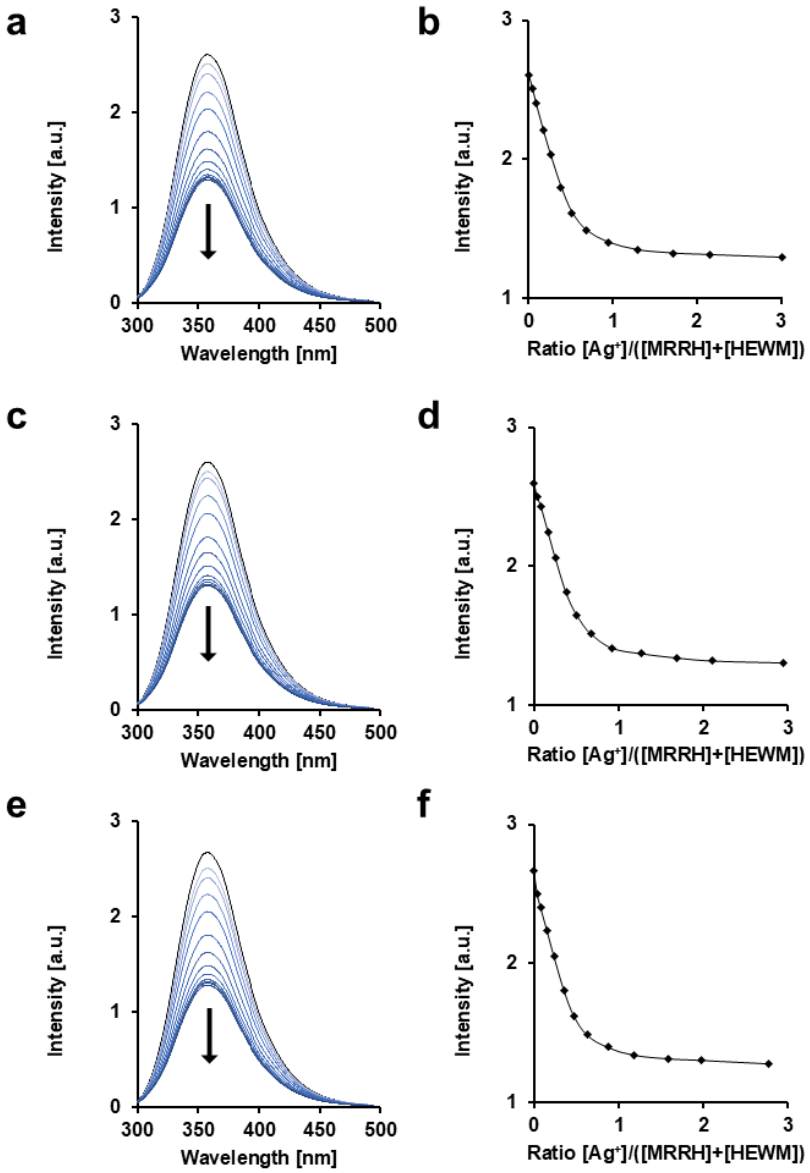

Fig. S168 MRRH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MRRH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

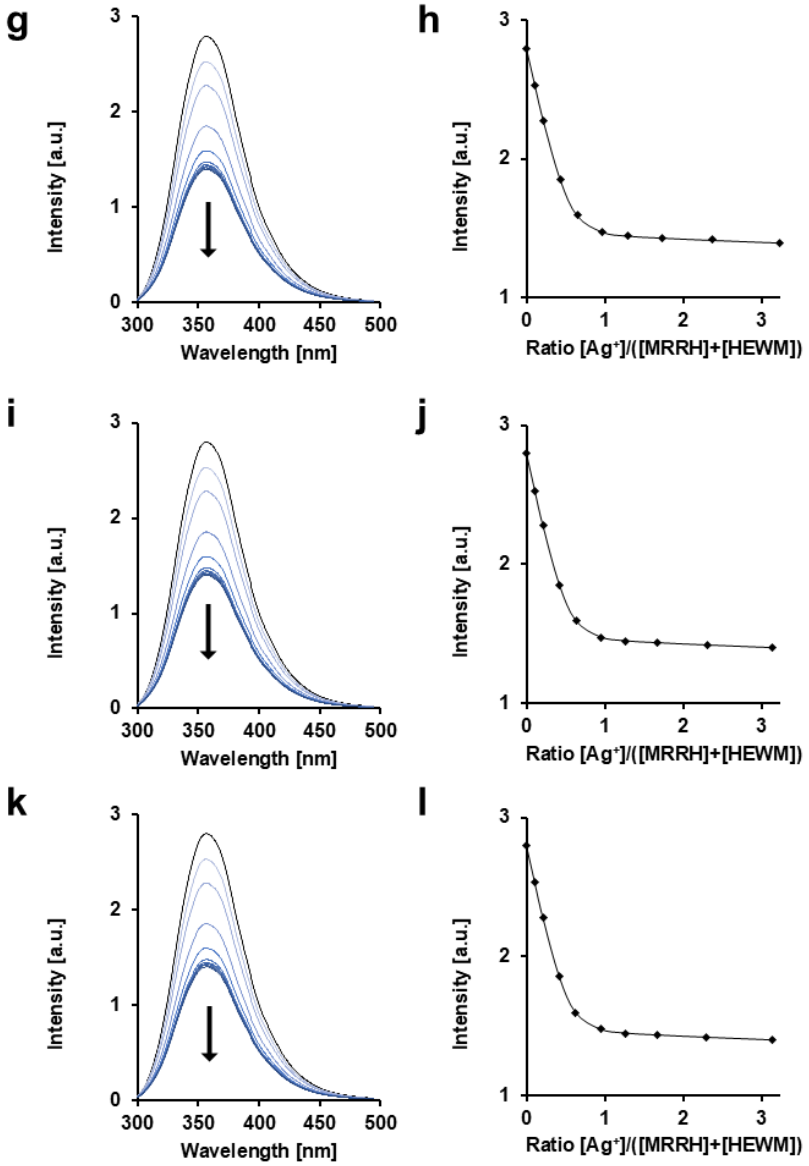

Fig. S169 MRRH / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MRRH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S29 Determination of the binding constants ($\log(K_{ass})$) of MRRH tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
MRRH	$\log(K_{ass\text{-}1}) = 5.30 \pm 0.02$	$\log(K_{ass\text{-}1}) = 5.29 \pm 0.05$
	$\log(K_{ass\text{-}2}) = 5.19 \pm 0.06$	$\log(K_{ass\text{-}2}) = 5.16 \pm 0.05$
	$\log(K_{ass\text{-}3}) = 4.77 \pm 0.26$	$\log(K_{ass\text{-}3}) = 5.16 \pm 0.05$
Average	$\log(K_{ass}) = 5.14 \pm 0.19$	

[a] The values correspond to the peptide and probe concentrations.

HKQM

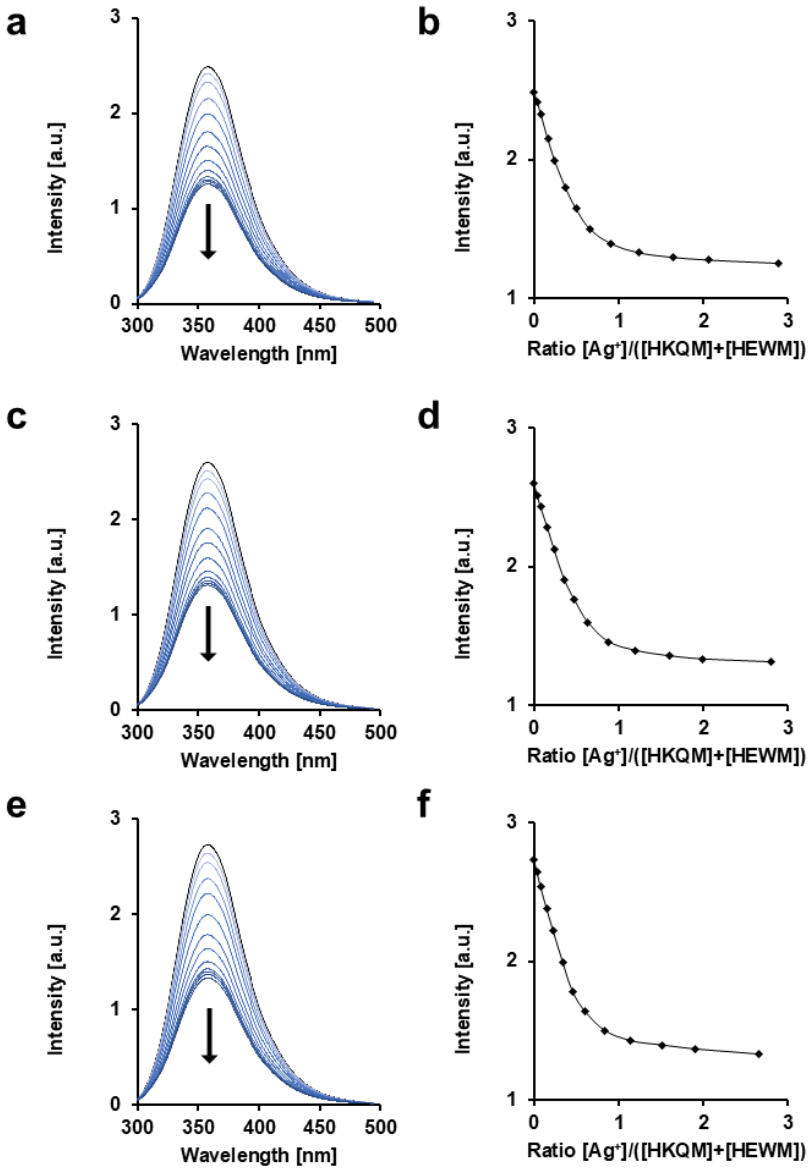

Fig. S170 HKQM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HKQM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

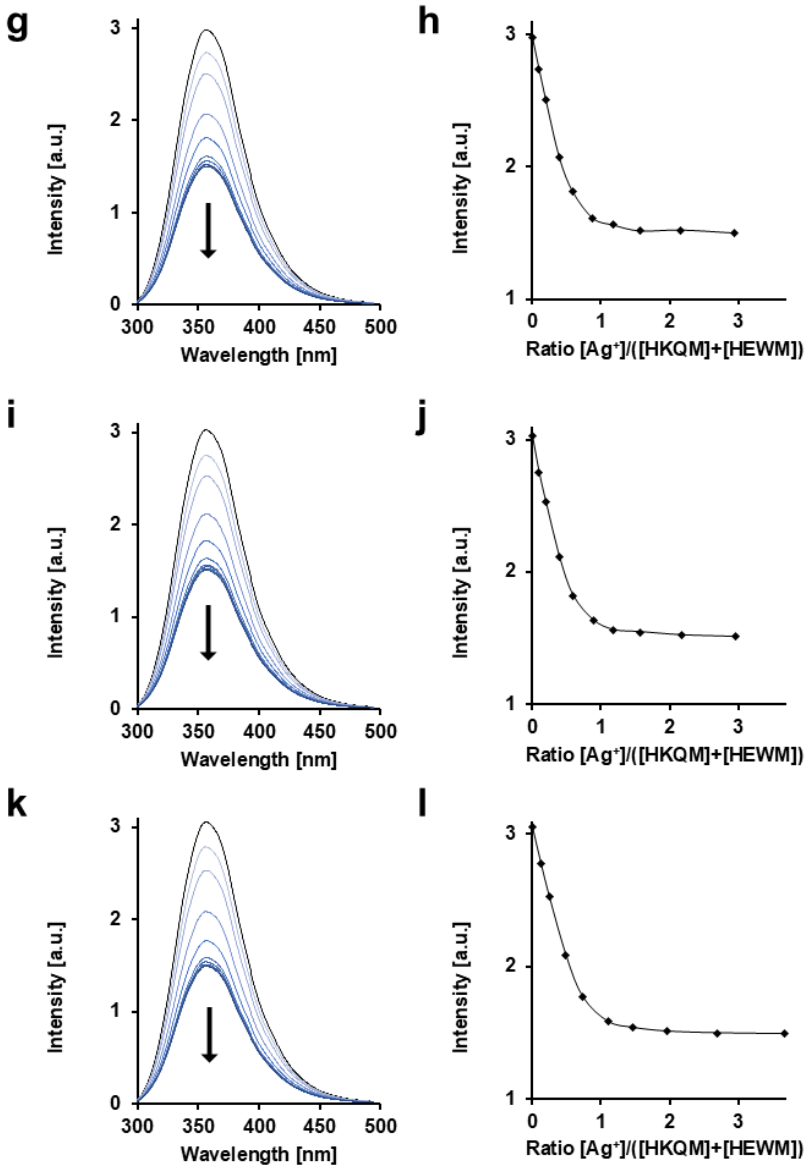

Fig. S171 HKQM / HEWM competition titrations, both at $1{\cdot}10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HKQM ($1{\cdot}10^{-5}$ M) in competition with HEWM probe ($1{\cdot}10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S30 Determination of the binding constants ($\log(K_{ass})$) of HKQM tetrapeptide.

Model	$5{\cdot}10^{-6}$ M[a]	$1{\cdot}10^{-5}$ M[a]
HKQM	$\log(K_{ass\text{-}1}) = 5.40 \pm 0.05$	$\log(K_{ass\text{-}1}) = 5.26 \pm 0.06$
	$\log(K_{ass\text{-}2}) = 5.53 \pm 0.04$	$\log(K_{ass\text{-}2}) = 5.35 \pm 0.06$
	$\log(K_{ass\text{-}3}) = 5.26 \pm 0.07$	$\log(K_{ass\text{-}3}) = 5.28 \pm 0.13$
Average	$\log(K_{ass}) = 5.35 \pm 0.11$	

[a] The values correspond to the peptide and probe concentrations.

HQQH

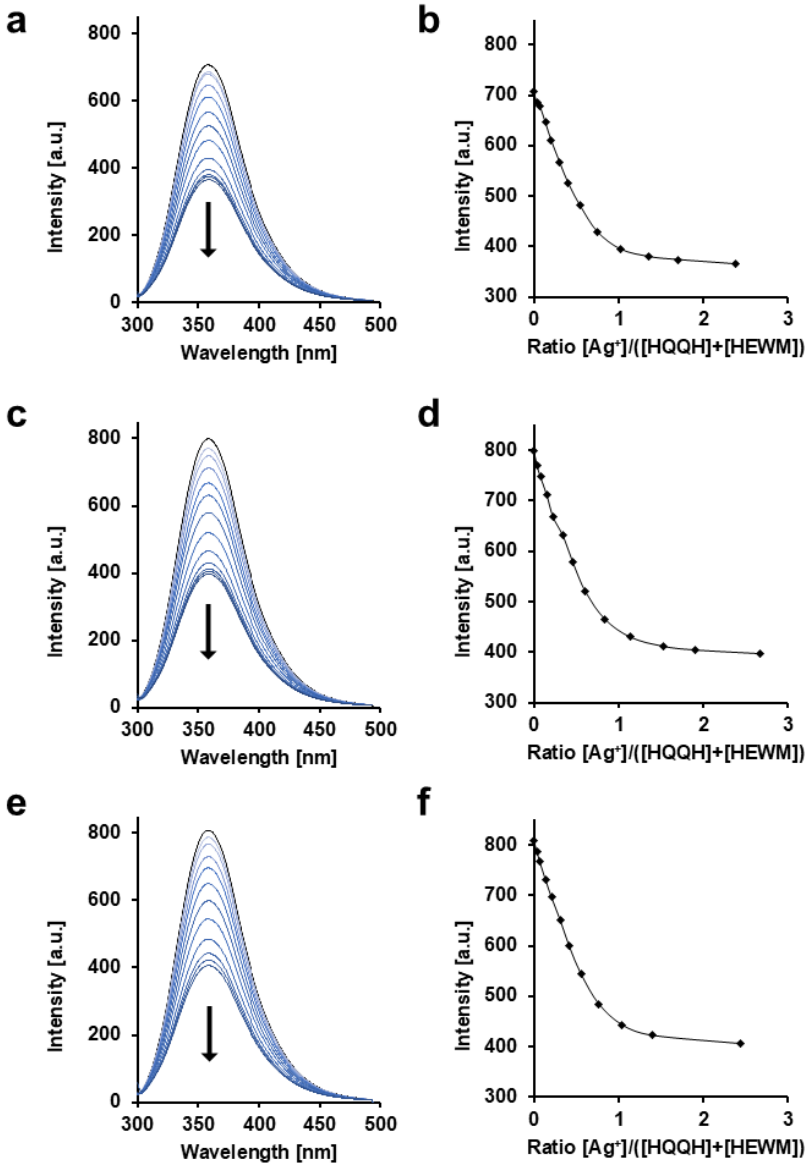

Fig. S172 HQQH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HQQH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

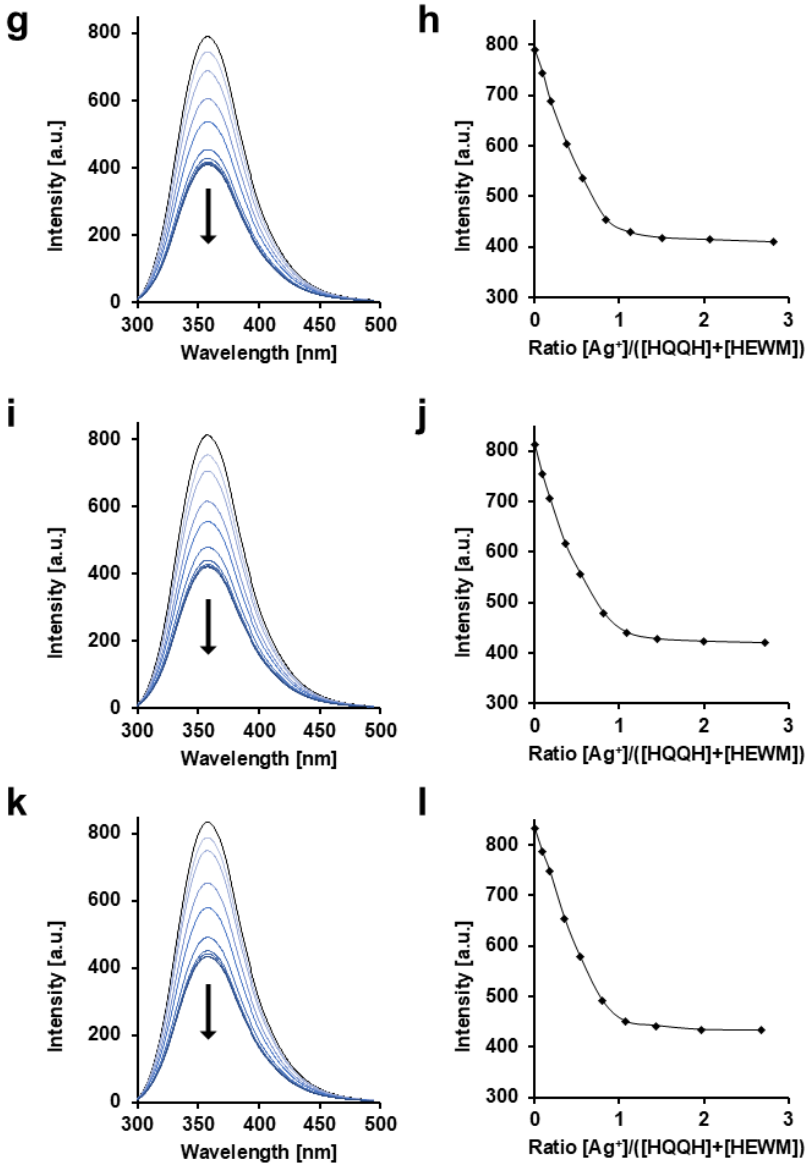

Fig. S173 HQQH / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HQQH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S31 Determination of the binding constants ($\log(K_{ass})$) of HQQH tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HQQH	$\log(K_{ass-1}) = 5.96 \pm 0.03$	$\log(K_{ass-1}) = 5.97 \pm 0.04$
	$\log(K_{ass-2}) = 6.01 \pm 0.04$	$\log(K_{ass-2}) = 5.92 \pm 0.03$
	$\log(K_{ass-3}) = 6.02 \pm 0.03$	$\log(K_{ass-3}) = 6.04 \pm 0.04$
Average	$\log(K_{ass}) = 5.99 \pm 0.05$	

[a] The values correspond to the peptide and probe concentrations.

HRQH

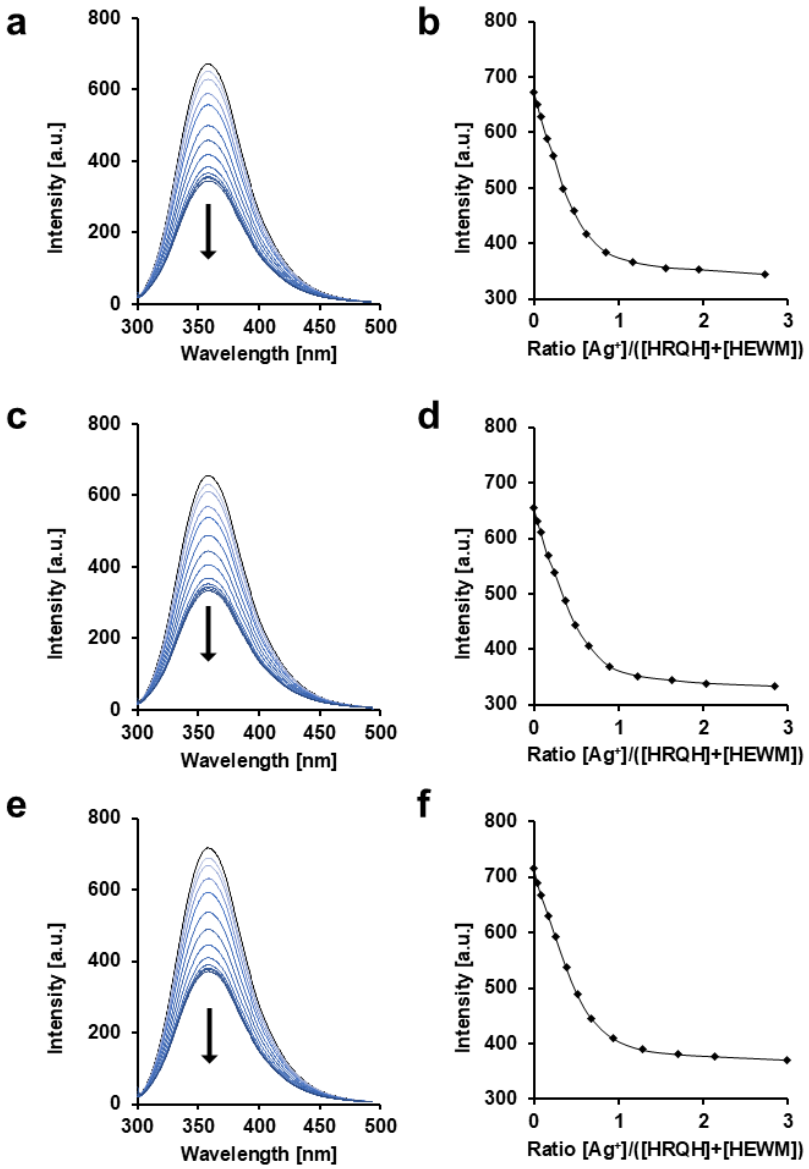

Fig. S174 HRQH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HRQH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

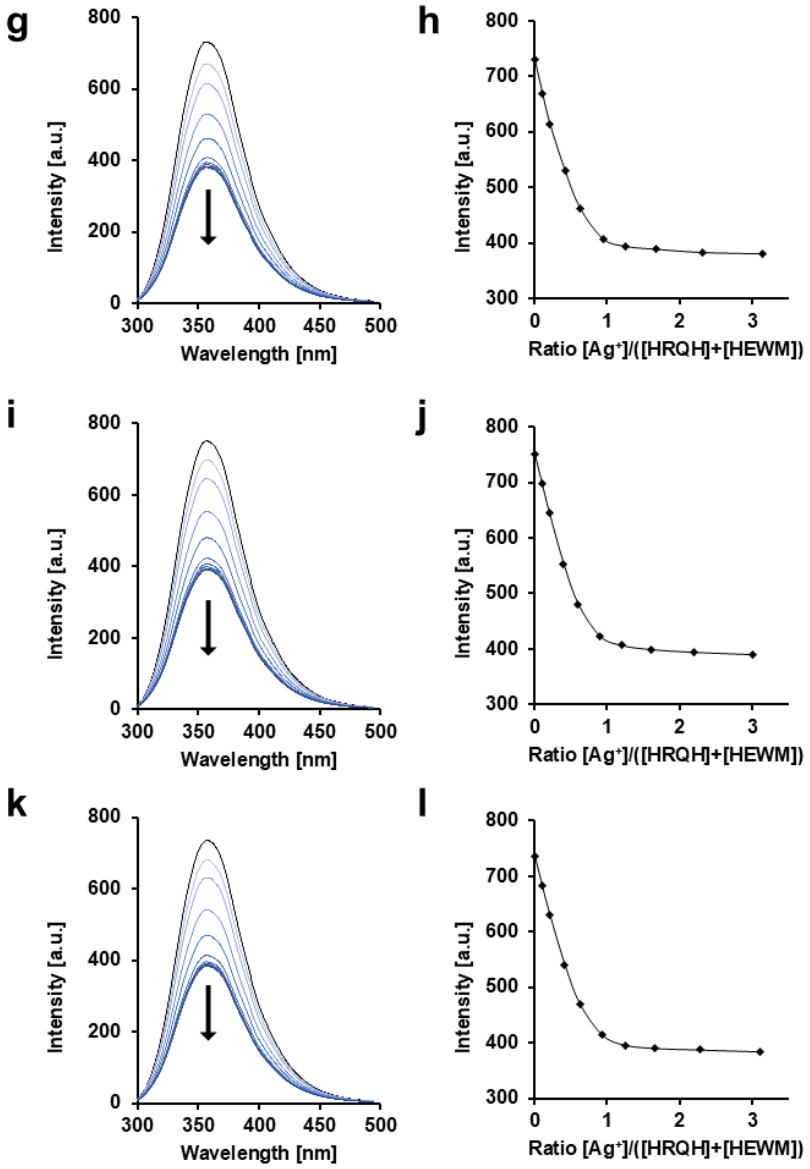

Fig. S175 HRQH / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HRQH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S32 Determination of the binding constants ($\log(K_{ass})$) of HRQH tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HRQH	$\log(K_{ass-1}) = 5.93 \pm 0.04$	$\log(K_{ass-1}) = 5.74 \pm 0.04$
	$\log(K_{ass-2}) = 5.71 \pm 0.03$	$\log(K_{ass-2}) = 5.75 \pm 0.04$
	$\log(K_{ass-3}) = 5.76 \pm 0.03$	$\log(K_{ass-3}) = 5.81 \pm 0.02$
Average	$\log(K_{ass}) = 5.73 \pm 0.06$	

[a] The values correspond to the peptide and probe concentrations.

HQRH

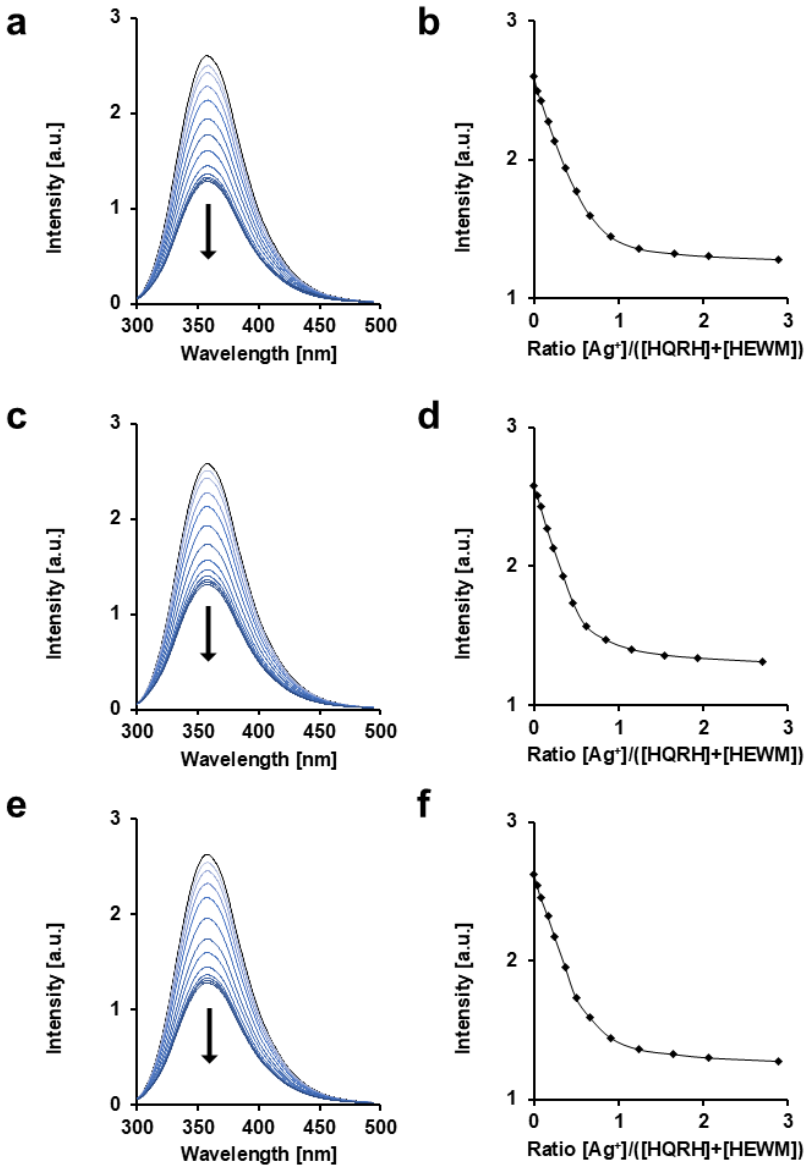

Fig. S176 HQRH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HQRH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

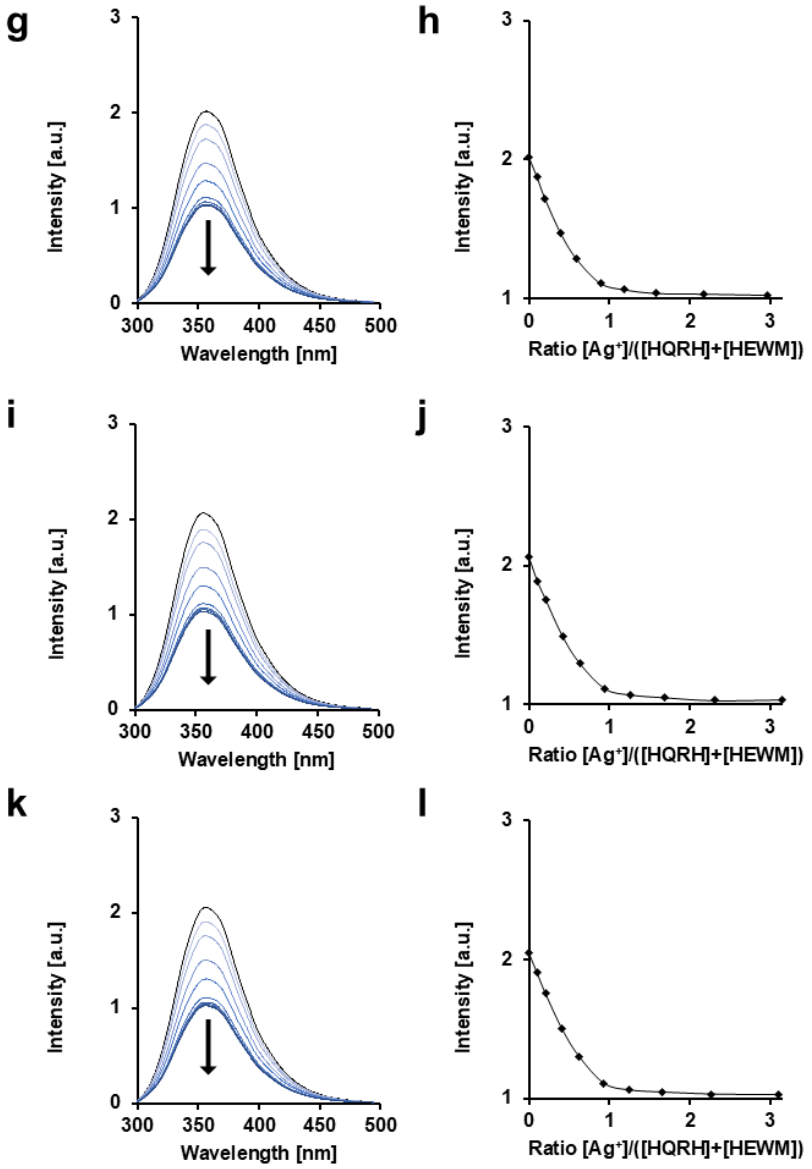

Fig. S177 HQRH / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HQRH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S33 Determination of the binding constants ($\log(K_{ass})$) of HQRH tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HQRH	$\log(K_{ass-1}) = 5.83 \pm 0.03$	$\log(K_{ass-1}) = 5.82 \pm 0.03$
	$\log(K_{ass-2}) = 5.60 \pm 0.05$	$\log(K_{ass-2}) = 5.90 \pm 0.03$
	$\log(K_{ass-3}) = 5.77 \pm 0.05$	$\log(K_{ass-3}) = 5.92 \pm 0.02$
Average	$\log(K_{ass}) = 5.81 \pm 0.12$	

[a] The values correspond to the peptide and probe concentrations.

HPPH

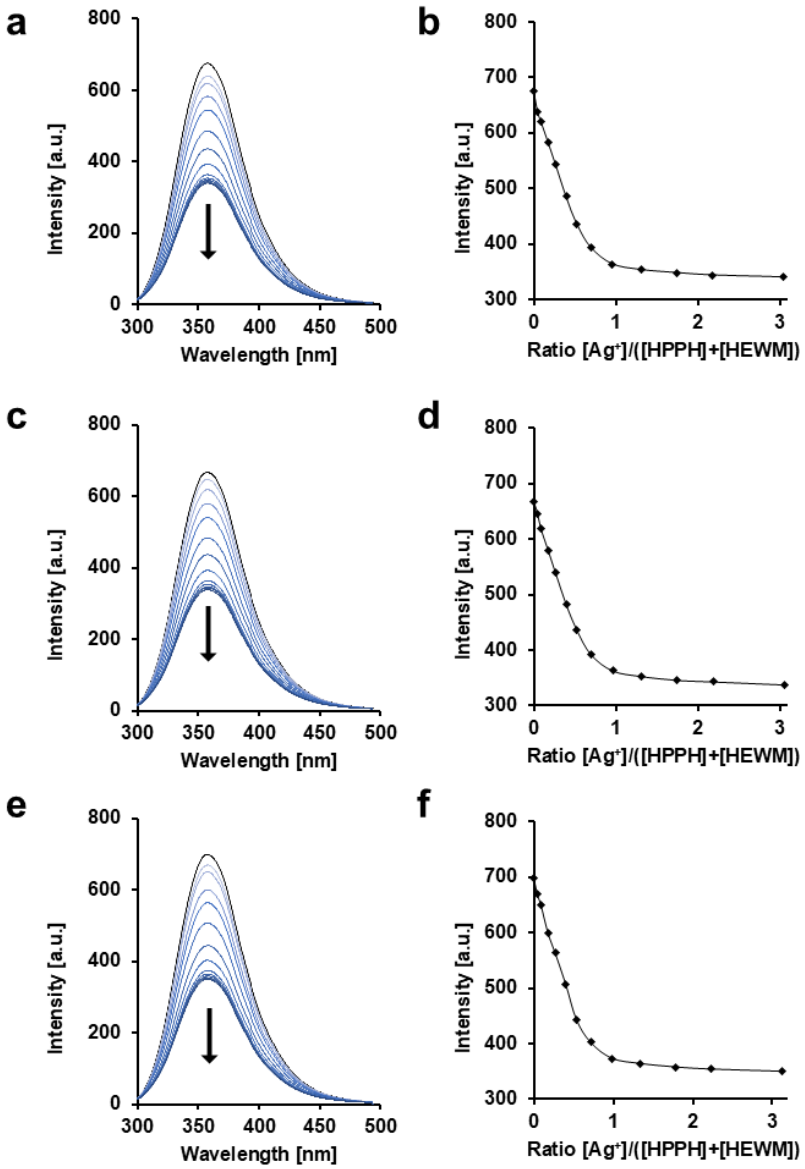

Fig. S178 HPPH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HPPH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

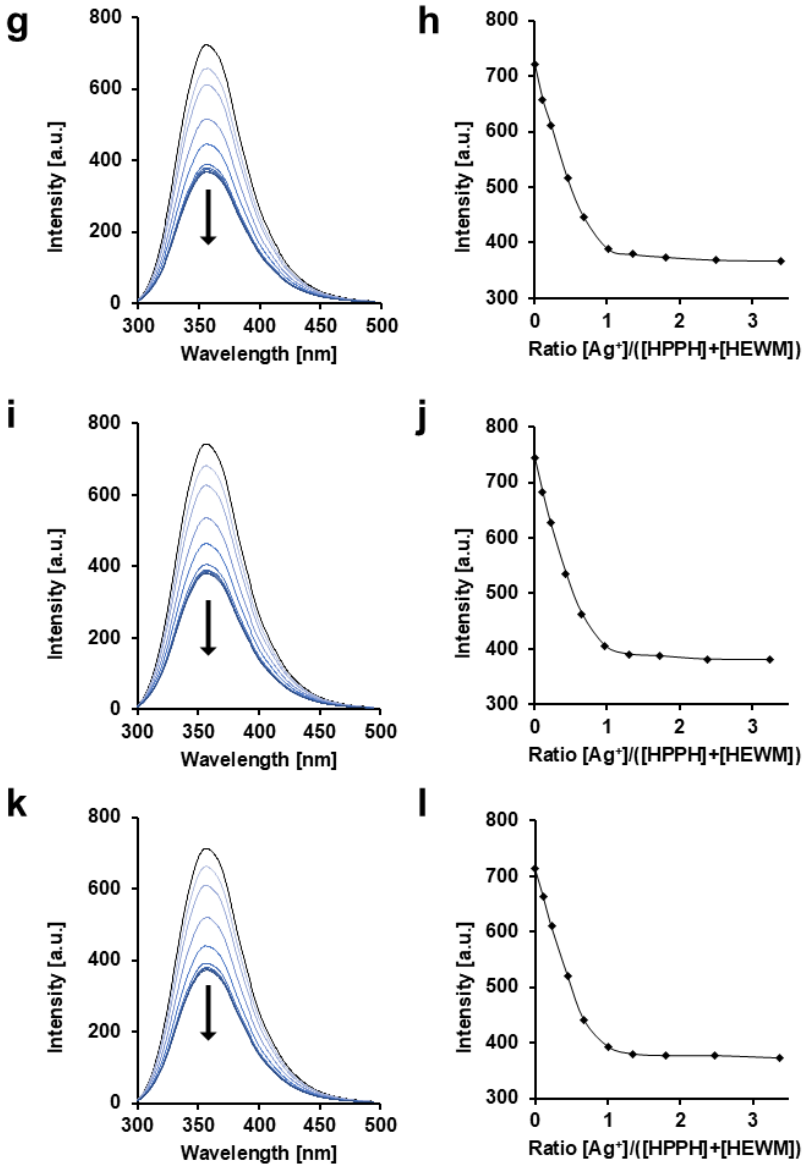

Fig. S179 HPPH / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HPPH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S34 Determination of the binding constants ($\log(K_{ass})$) of HPPH tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HPPH	$\log(K_{ass\text{-}1}) = 5.64 \pm 0.05$	$\log(K_{ass\text{-}1}) = 5.88 \pm 0.04$
	$\log(K_{ass\text{-}2}) = 5.63 \pm 0.03$	$\log(K_{ass\text{-}2}) = 5.83 \pm 0.02$
	$\log(K_{ass\text{-}3}) = 5.66 \pm 0.05$	$\log(K_{ass\text{-}3}) = 5.87 \pm 0.05$
Average	$\log(K_{ass}) = 5.75 \pm 0.12$	

[a] The values correspond to the peptide and probe concentrations.

HQPH

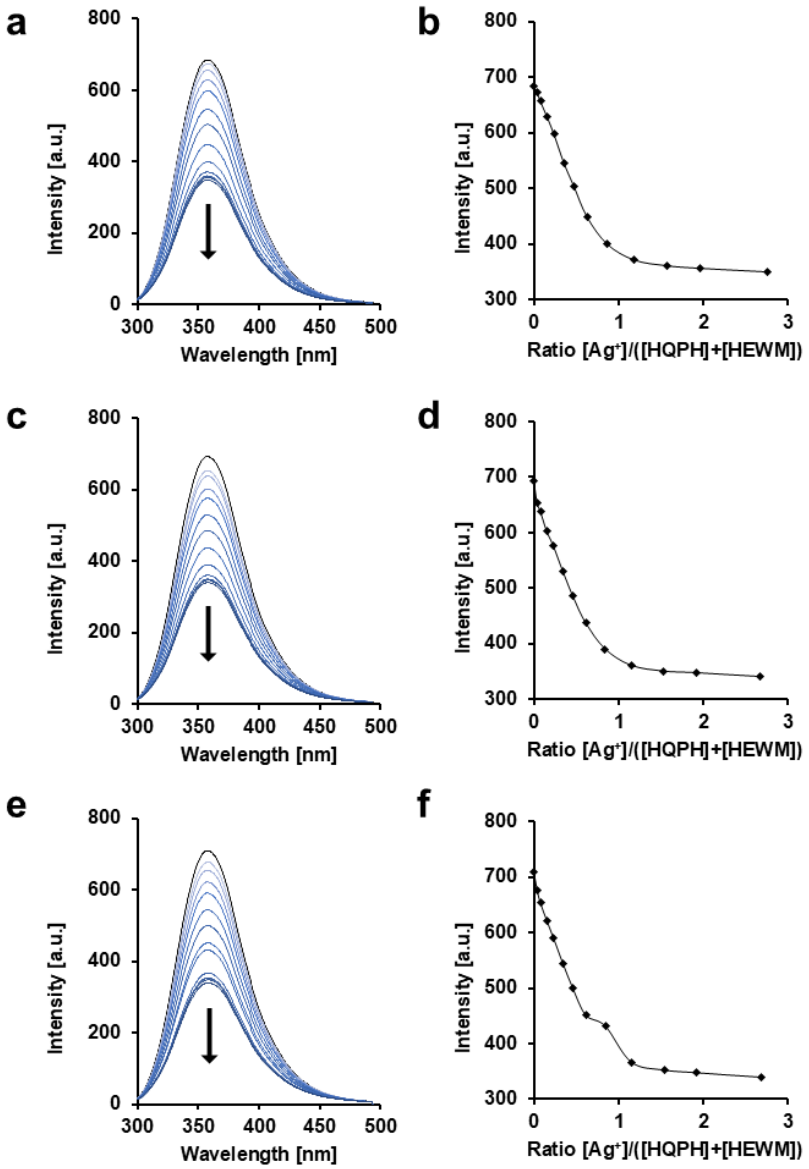

Fig. S180 HQPH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HQPH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

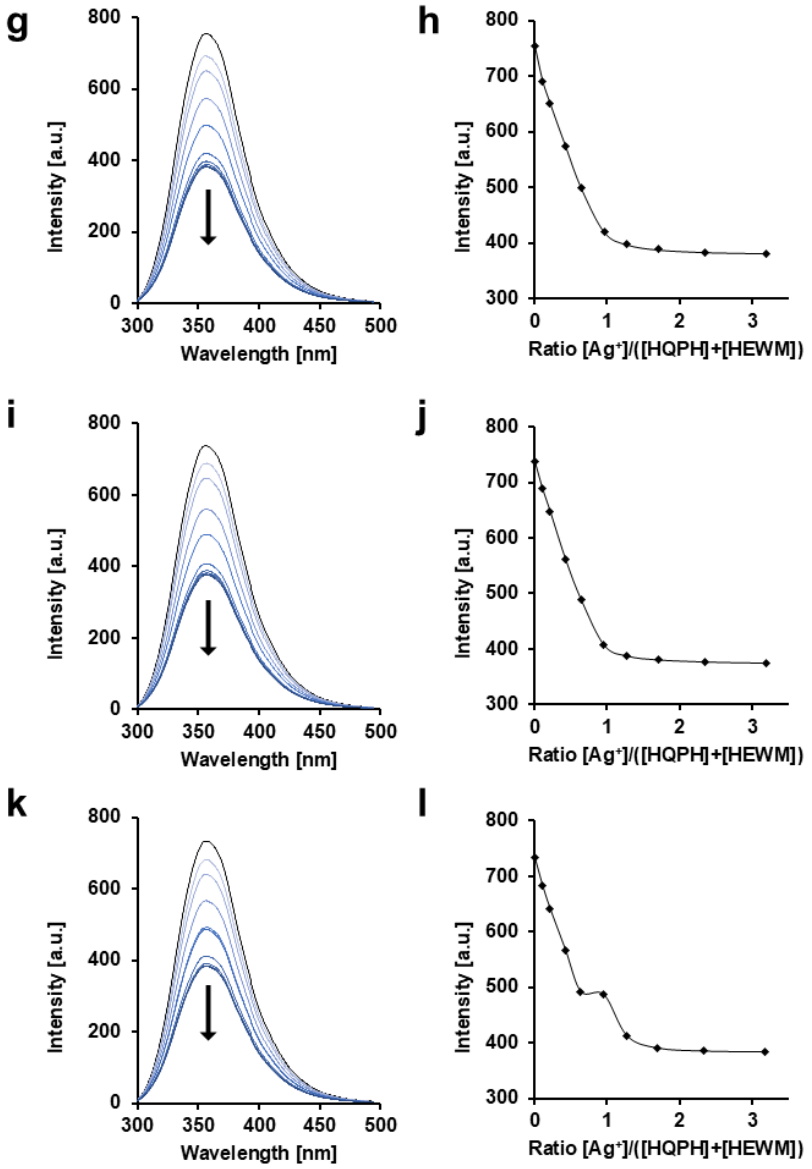

Fig. S181 HQPH / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HQPH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S35 Determination of the binding constants ($\log(K_{ass})$) of HQPH tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HQPH	$\log(K_{ass\text{-}1}) = 6.08 \pm 0.06$	$\log(K_{ass\text{-}1}) = 6.14 \pm 0.05$
	$\log(K_{ass\text{-}2}) = 5.93 \pm 0.06$	$\log(K_{ass\text{-}2}) = 6.17 \pm 0.02$
	$\log(K_{ass\text{-}3}) = 5.94 \pm 0.06$	$\log(K_{ass\text{-}3}) = 5.85 \pm 0.28$
Average	$\log(K_{ass}) = 6.02 \pm 0.13$	

[a] The values correspond to the peptide and probe concentrations.

HPQH

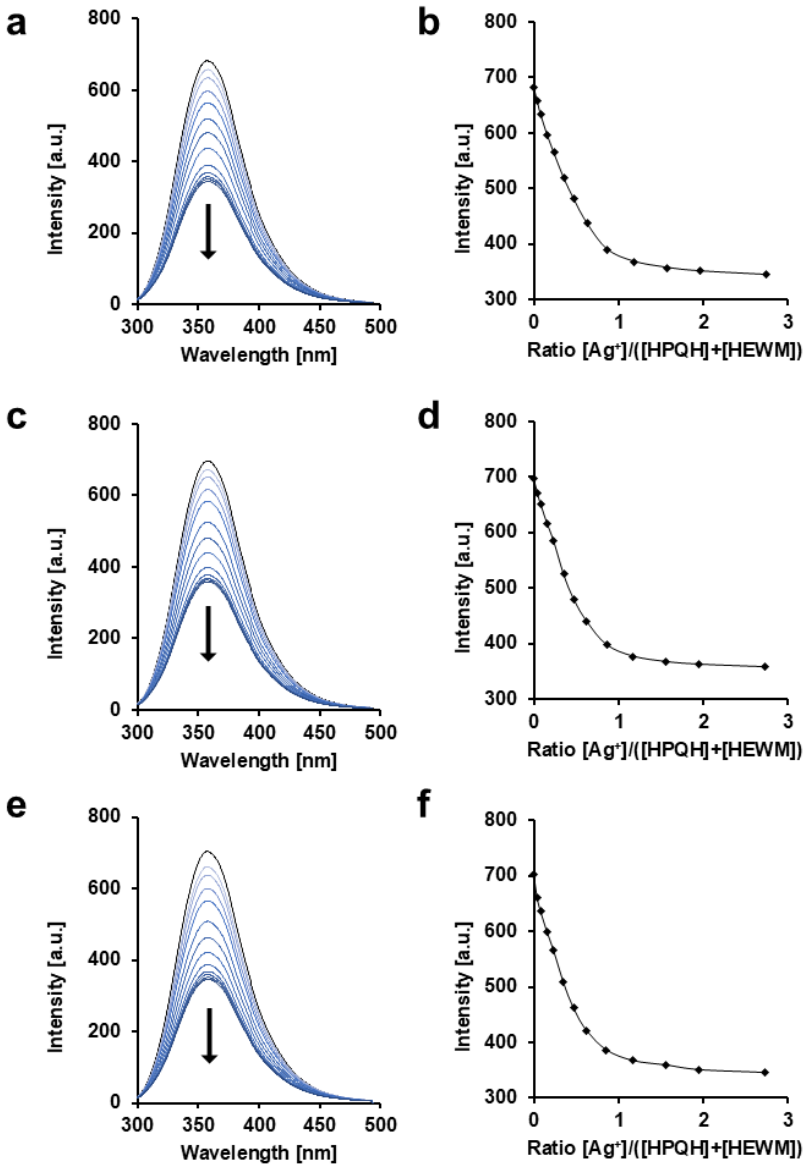

Fig. S182 HPQH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HPQH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

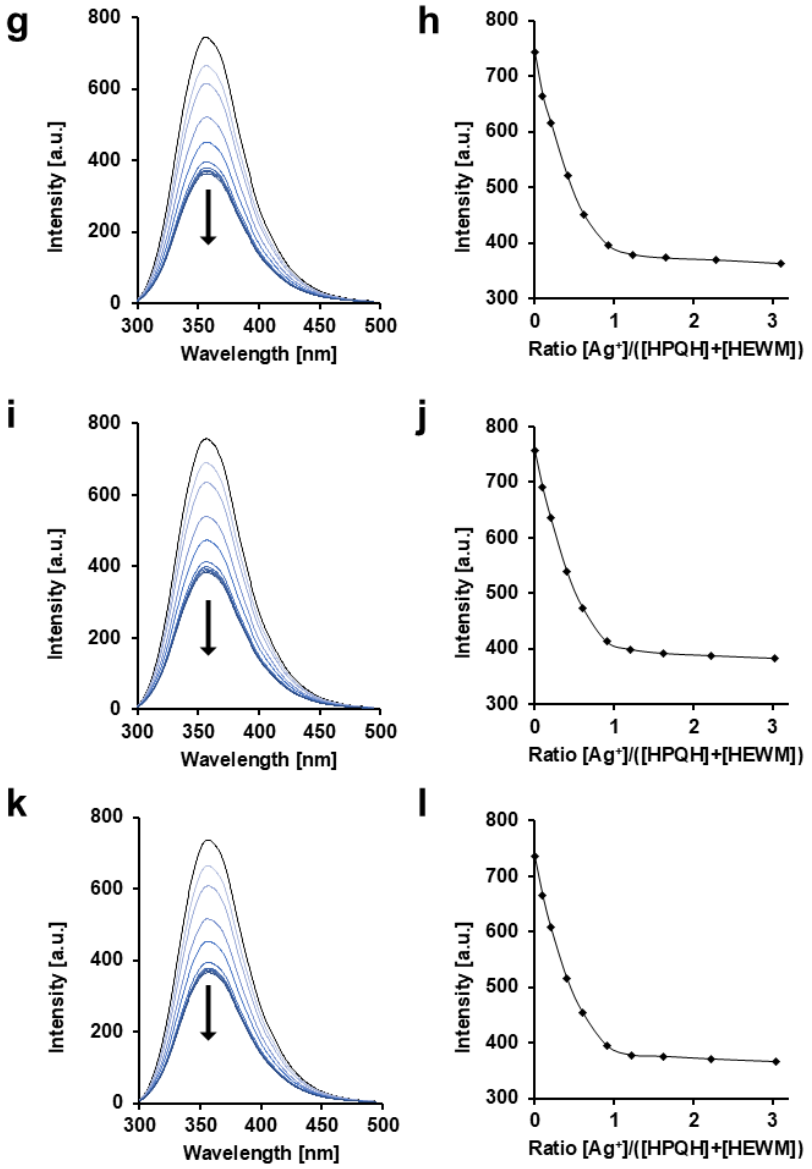

Fig. S183 HPQH / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HPQH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S36 Determination of the binding constants ($\log(K_{ass})$) of HPQH tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HPQH	$\log(K_{ass-1}) = 5.87 \pm 0.05$	$\log(K_{ass-1}) = 5.69 \pm 0.07$
	$\log(K_{ass-2}) = 5.74 \pm 0.05$	$\log(K_{ass-2}) = 5.69 \pm 0.04$
	$\log(K_{ass-3}) = 5.59 \pm 0.08$	$\log(K_{ass-3}) = 5.64 \pm 0.06$
Average	$\log(K_{ass}) = 5.70 \pm 0.10$	

[a] The values correspond to the peptide and probe concentrations.

HKKH

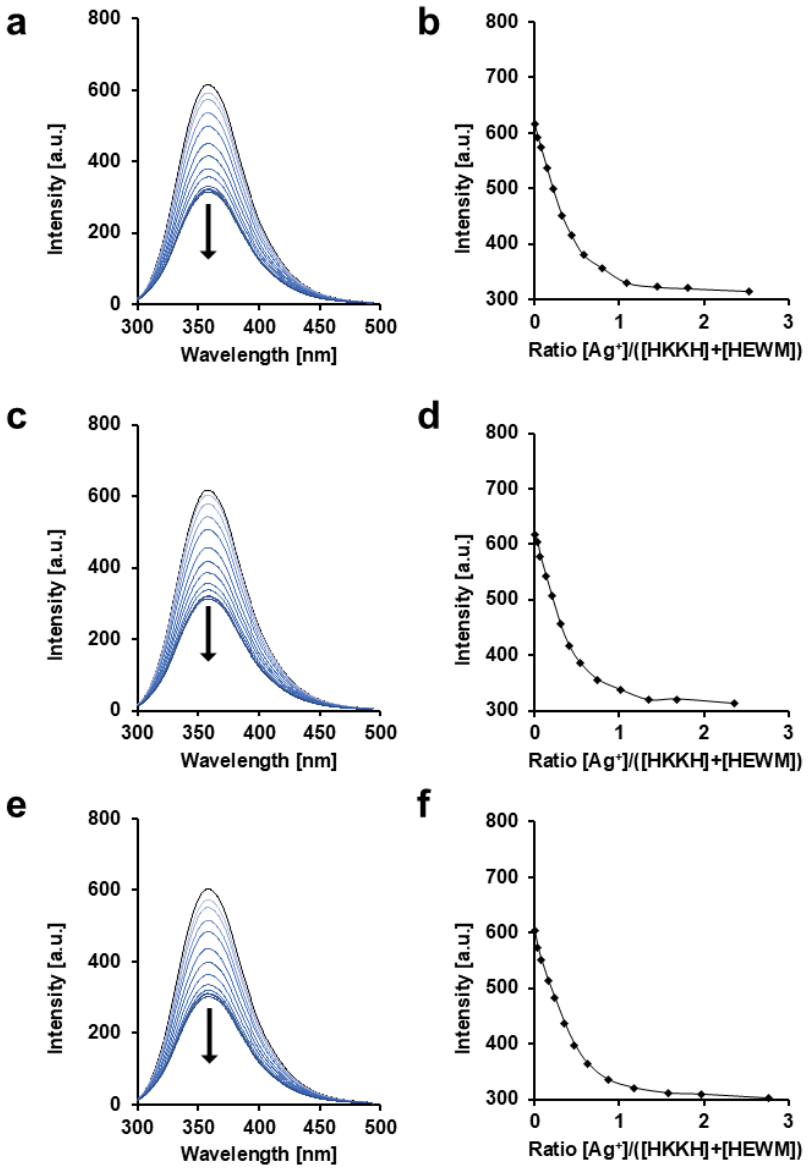

Fig. S184 HKKH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HKKH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

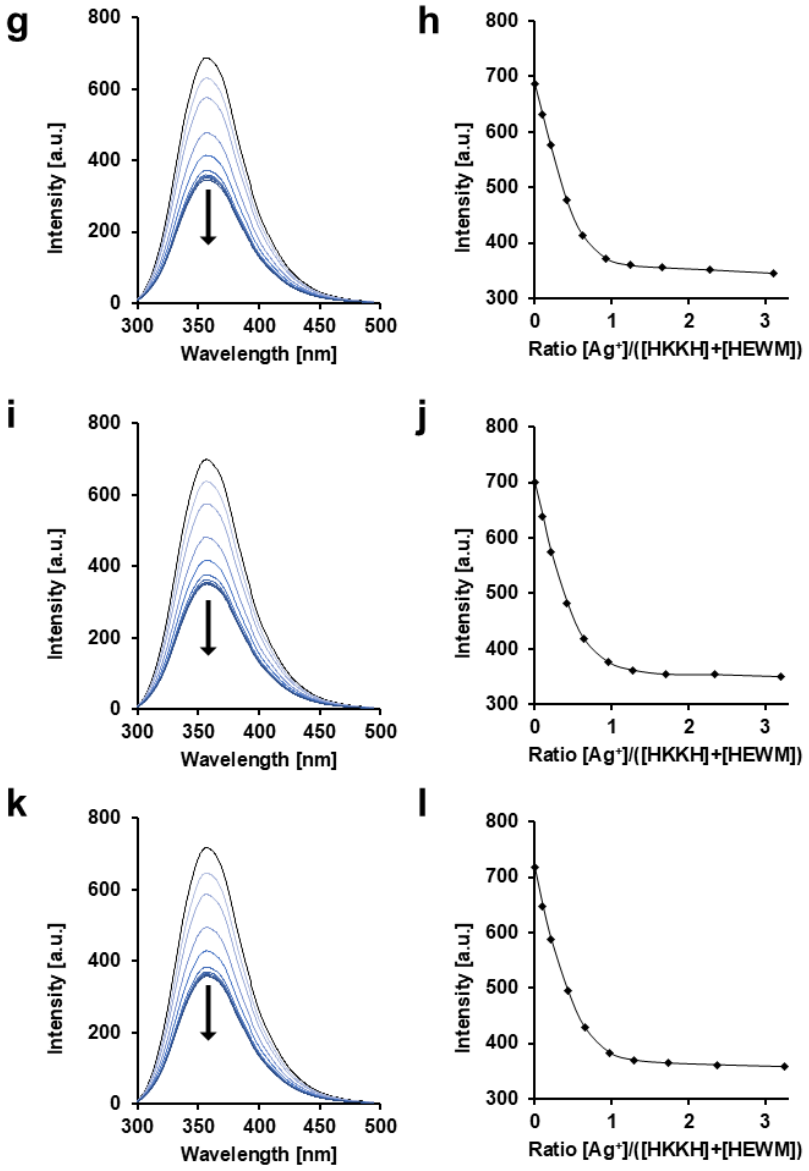

Fig. S185 HKKH / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HKKH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S37 Determination of the binding constants ($\log(K_{ass})$) of HKKH tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HKKH	$\log(K_{ass\text{-}1}) = 5.56 \pm 0.01$	$\log(K_{ass\text{-}1}) = 5.61 \pm 0.04$
	$\log(K_{ass\text{-}2}) = 5.52 \pm 0.04$	$\log(K_{ass\text{-}2}) = 5.57 \pm 0.03$
	$\log(K_{ass\text{-}3}) = 5.61 \pm 0.05$	$\log(K_{ass\text{-}3}) = 5.55 \pm 0.06$
Average	$\log(K_{ass}) = 5.57 \pm 0.04$	

[a] The values correspond to the peptide and probe concentrations.

HRKH

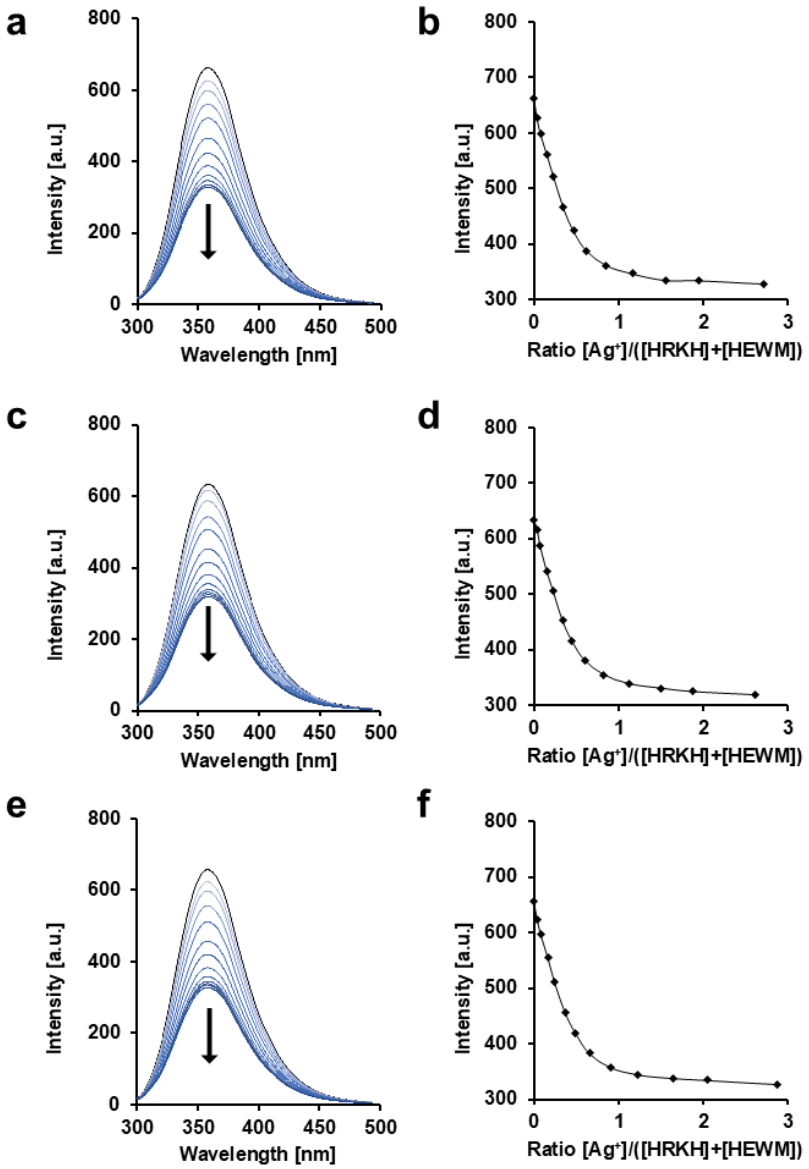

Fig. S186 HRKH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HRKH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

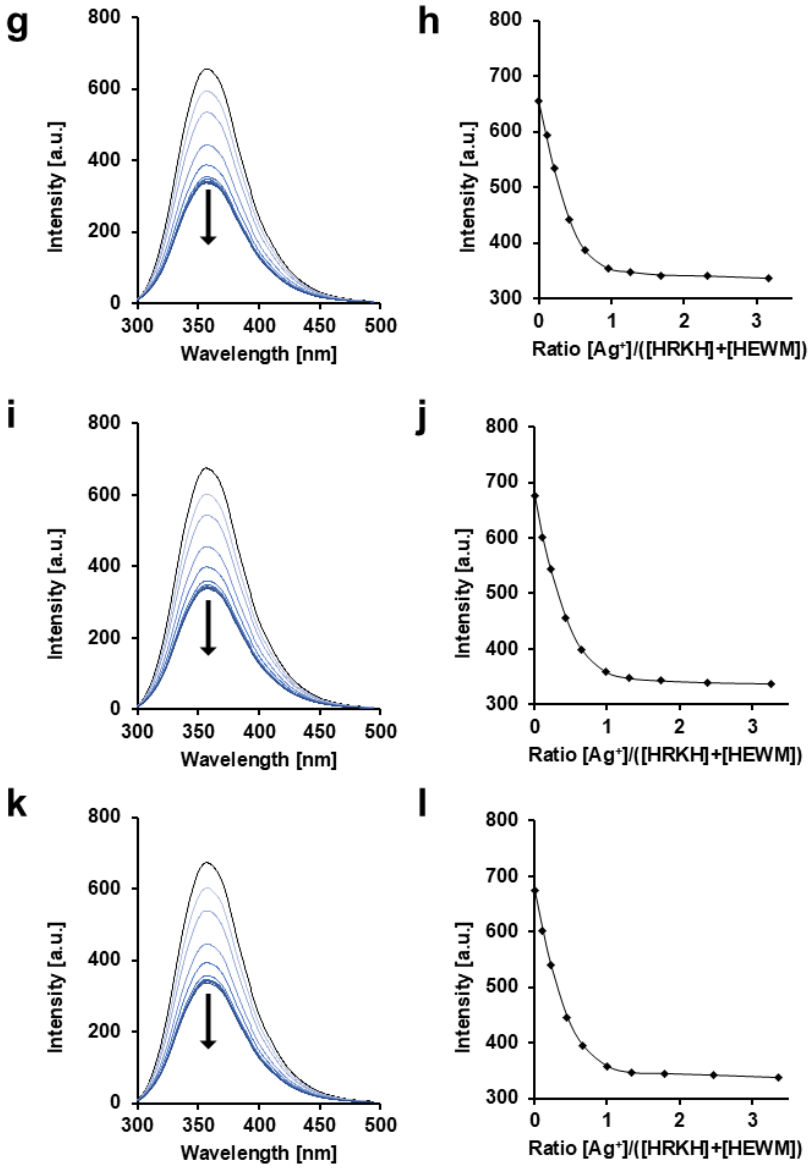

Fig. S187 HRKH / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HRKH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S38 Determination of the binding constants ($\log(K_{ass})$) of HRKH tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HRKH	$\log(K_{ass\text{-}1}) = 5.41 \pm 0.07$	$\log(K_{ass\text{-}1}) = 5.43 \pm 0.03$
	$\log(K_{ass\text{-}2}) = 5.38 \pm 0.05$	$\log(K_{ass\text{-}2}) = 5.55 \pm 0.05$
	$\log(K_{ass\text{-}3}) = 5.39 \pm 0.07$	$\log(K_{ass\text{-}3}) = 5.46 \pm 0.05$
Average	$\log(K_{ass}) = 5.44 \pm 0.06$	

[a] The values correspond to the peptide and probe concentrations.

HKRH

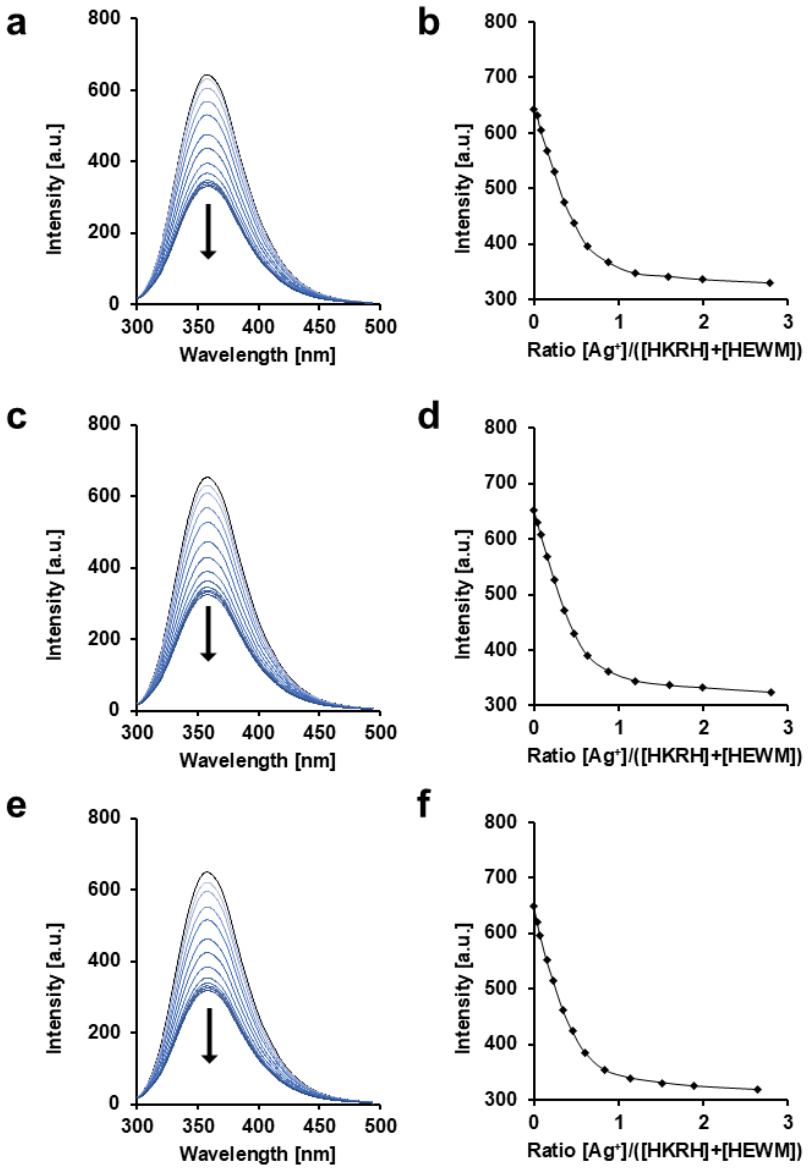

Fig. S188 HKRH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HKRH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

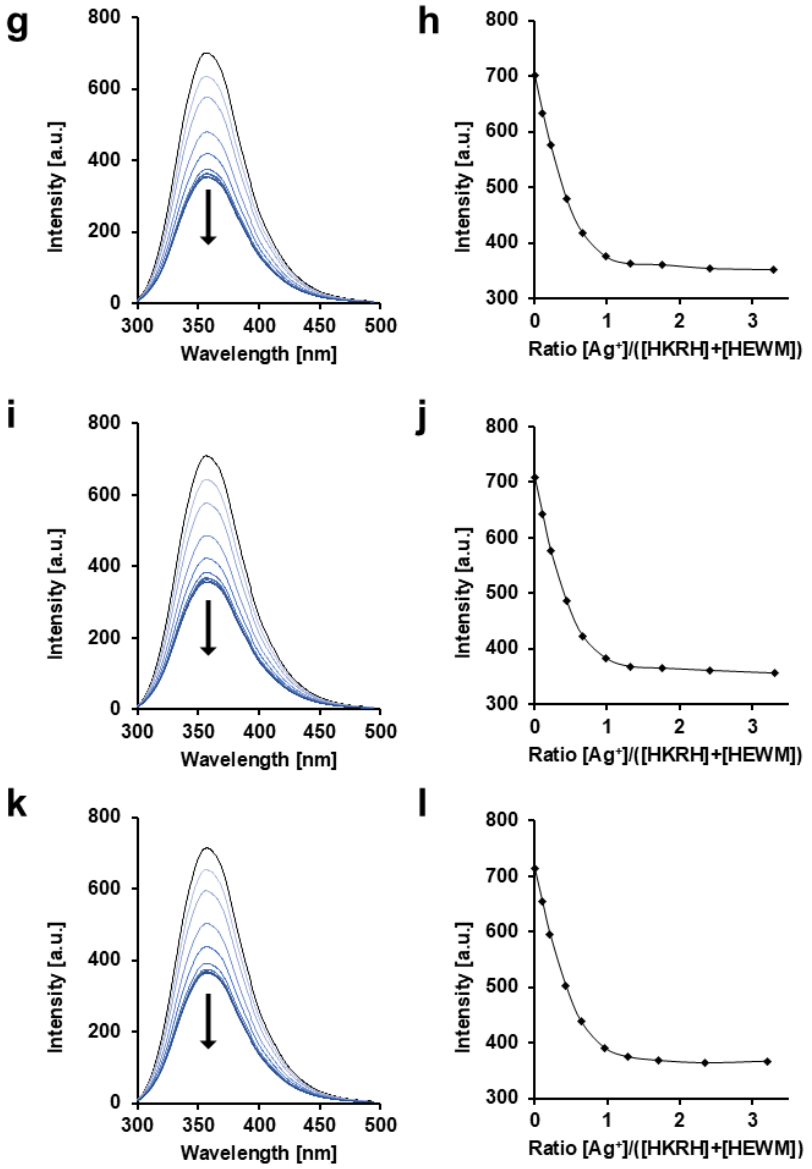

Fig. S189 HKRH / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HKRH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S39 Determination of the binding constants ($\log(K_{ass})$) of HKRH tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HKRH	$\log(K_{ass-1}) = 5.62 \pm 0.04$	$\log(K_{ass-1}) = 5.59 \pm 0.04$
	$\log(K_{ass-2}) = 5.55 \pm 0.04$	$\log(K_{ass-2}) = 5.57 \pm 0.05$
	$\log(K_{ass-3}) = 5.47 \pm 0.06$	$\log(K_{ass-3}) = 5.66 \pm 0.03$
Average	$\log(K_{ass}) = 5.58 \pm 0.07$	

[a] The values correspond to the peptide and probe concentrations.

HAAH

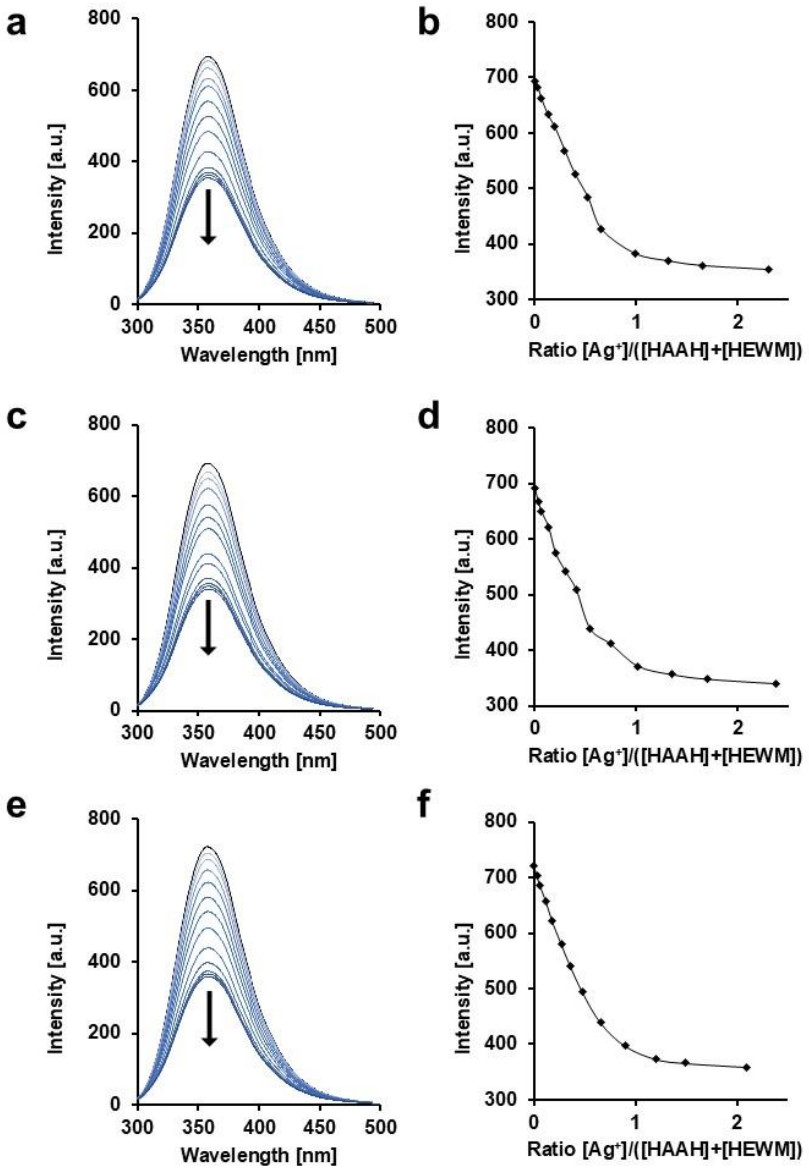

Fig. S190 HAAH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HAAH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

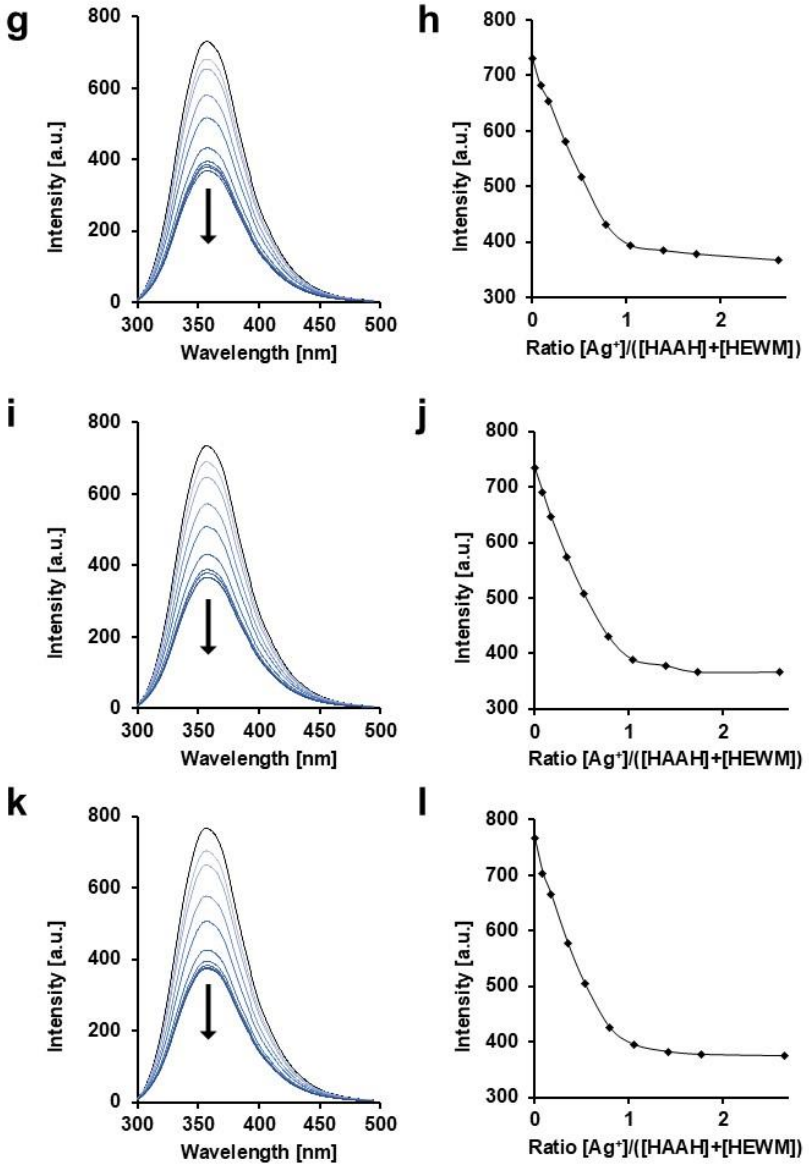

Fig. S191 HAAH / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HAAH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S40 Determination of the binding constants ($\log(K_{ass})$) of HAAH tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HAAH	$\log(K_{ass-1}) = 6.00 \pm 0.06$	$\log(K_{ass-1}) = 6.12 \pm 0.05$
	$\log(K_{ass-2}) = 5.82 \pm 0.07$	$\log(K_{ass-2}) = 6.04 \pm 0.03$
	$\log(K_{ass-3}) = 5.84 \pm 0.05$	$\log(K_{ass-3}) = 5.92 \pm 0.04$
Average	$\log(K_{ass}) = 5.96 \pm 0.12$	

[a] The values correspond to the peptide and probe concentrations.

HRAH

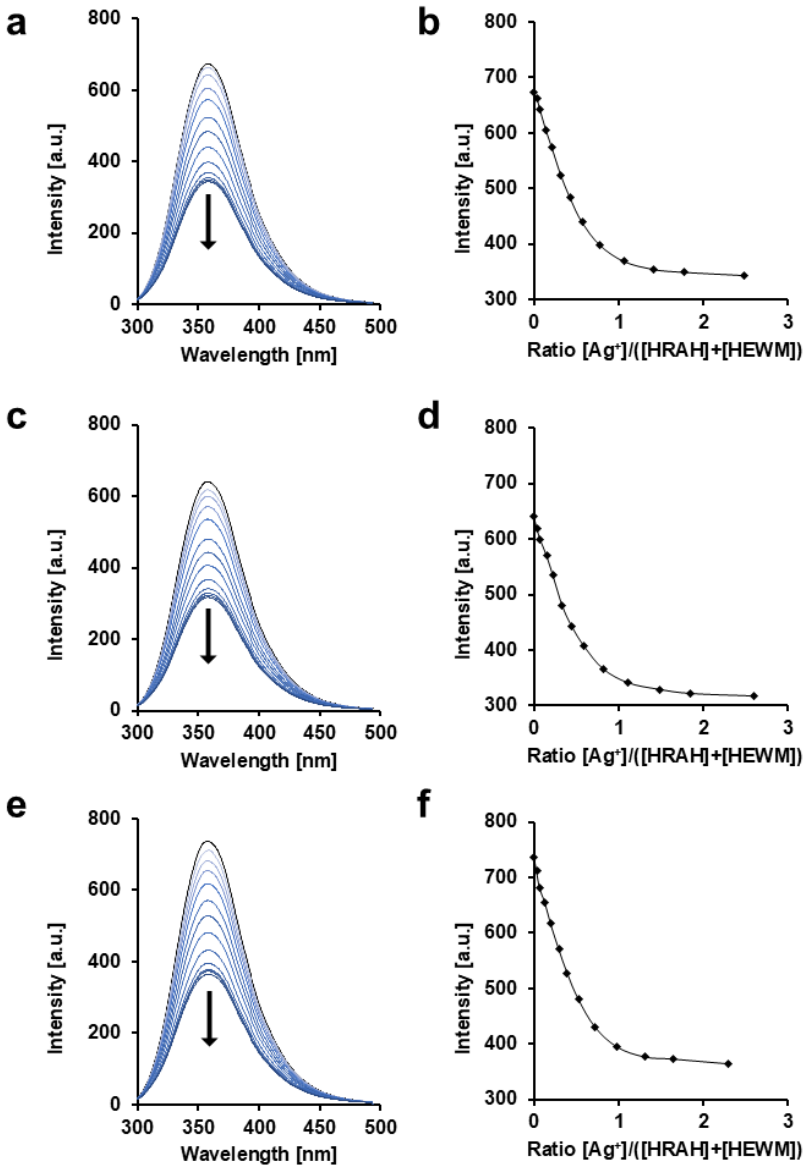

Fig. S192 HRAH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HRAH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

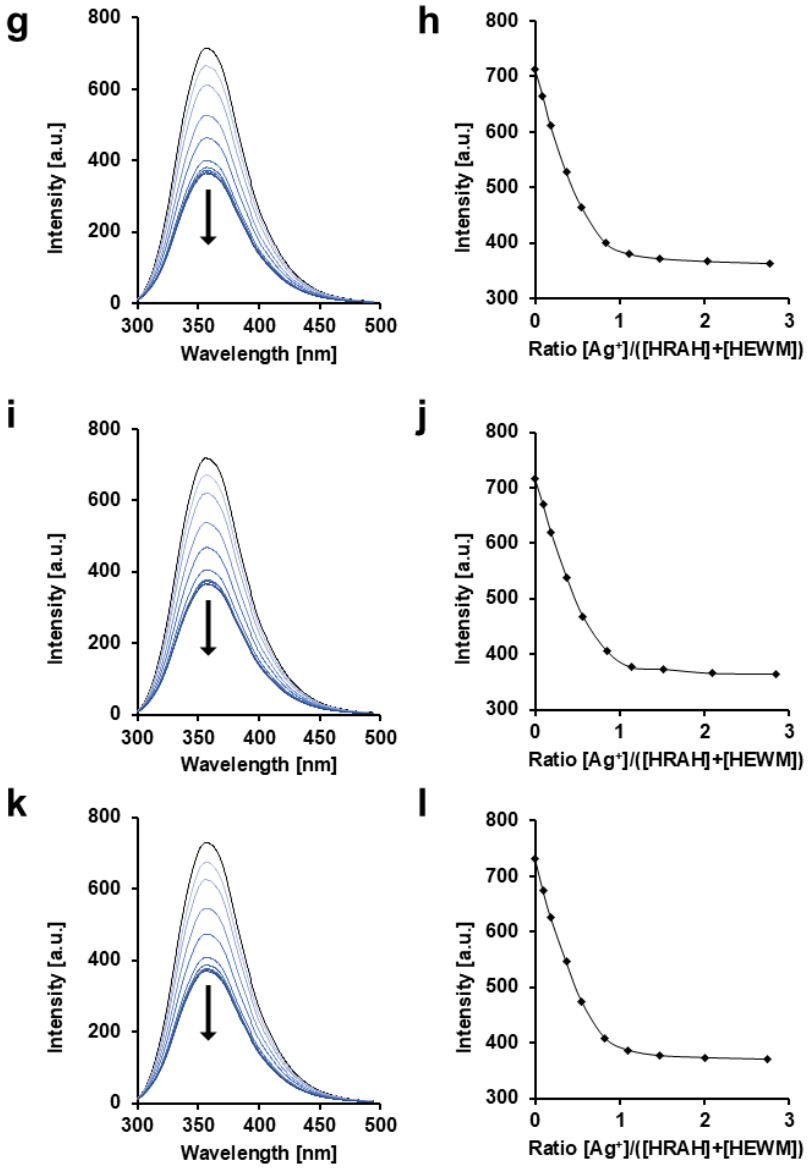

Fig. S193 HRAH / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HRAH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S41 Determination of the binding constants ($\log(K_{ass})$) of HRAH tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HRAH	$\log(K_{ass-1}) = 5.76 \pm 0.04$	$\log(K_{ass-1}) = 5.73 \pm 0.03$
	$\log(K_{ass-2}) = 5.77 \pm 0.05$	$\log(K_{ass-2}) = 5.88 \pm 0.03$
	$\log(K_{ass-3}) = 5.70 \pm 0.05$	$\log(K_{ass-3}) = 5.80 \pm 0.03$
Average	$\log(K_{ass}) = 5.77 \pm 0.06$	

[a] The values correspond to the peptide and probe concentrations.

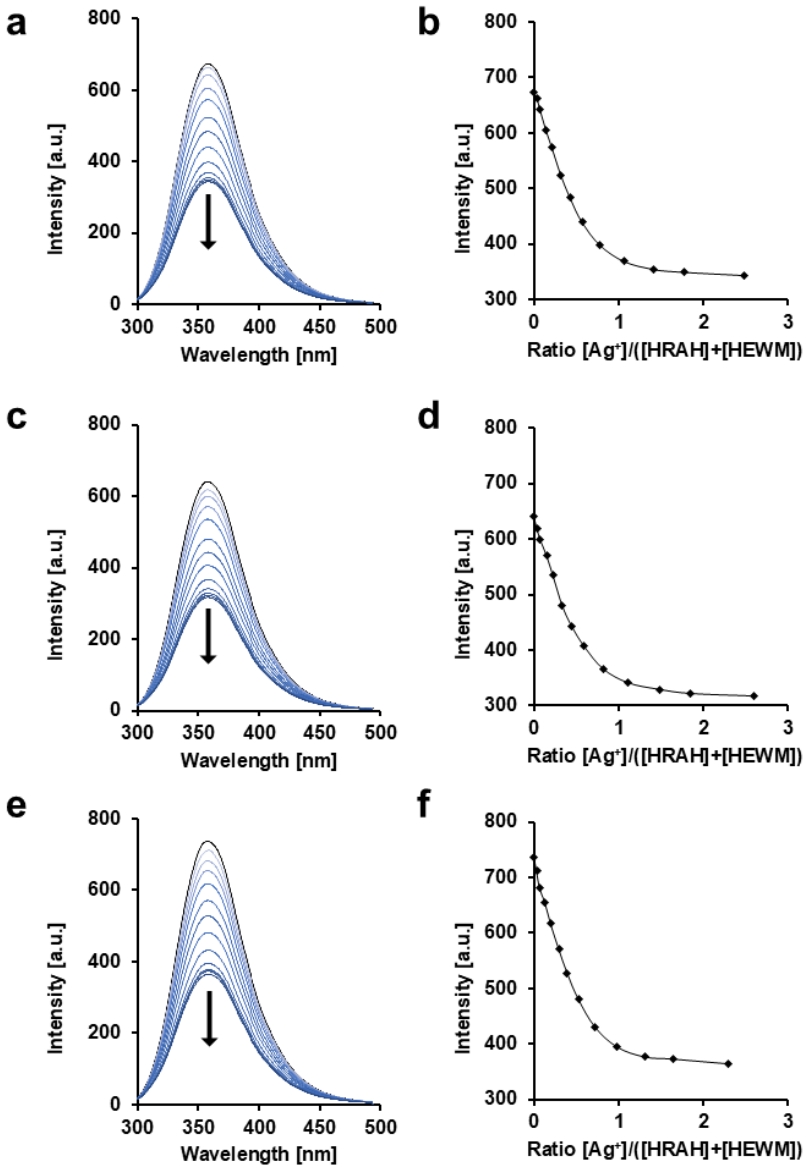

Fig. S194 HARH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HARH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

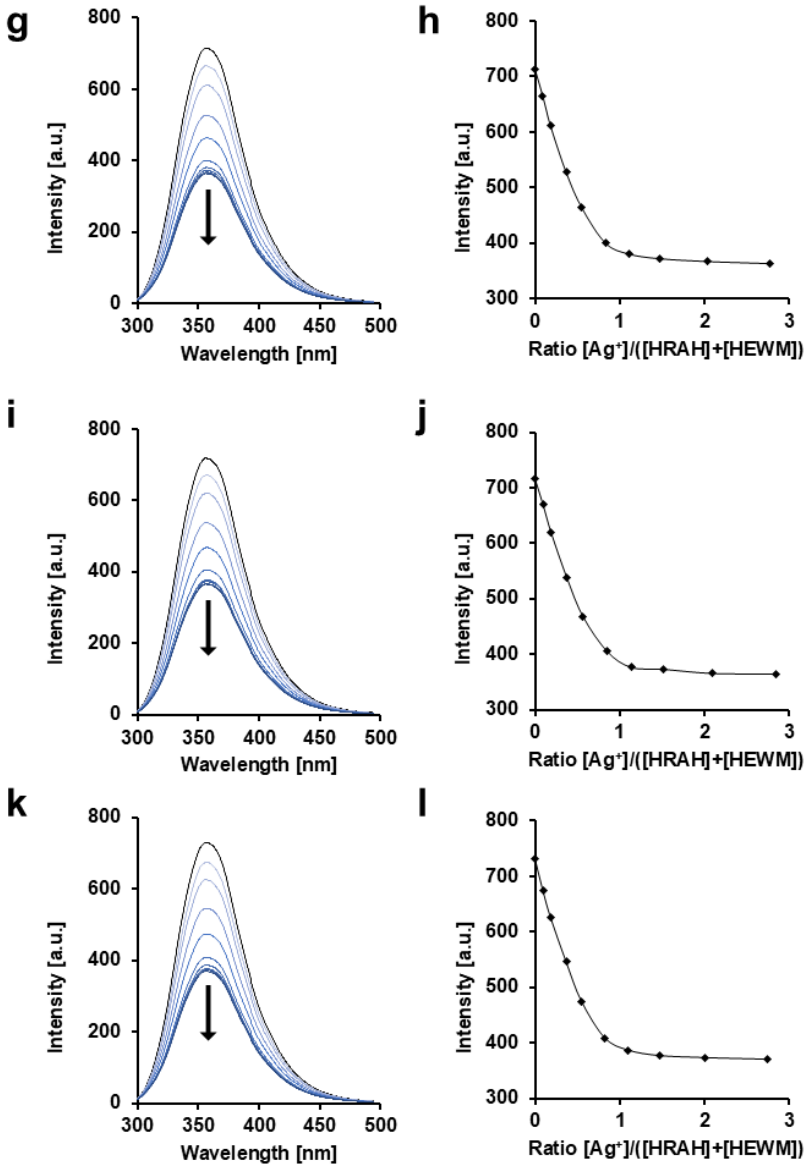

Fig. S195 HARH / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HARH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S42 Determination of the binding constants ($\log(K_{ass})$) of HARH tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HARH	$\log(K_{ass-1}) = 5.84 \pm 0.05$	$\log(K_{ass-1}) = 5.91 \pm 0.07$
	$\log(K_{ass-2}) = 5.76 \pm 0.04$	$\log(K_{ass-2}) = 5.88 \pm 0.06$
	$\log(K_{ass-3}) = 5.55 \pm 0.06$	$\log(K_{ass-3}) = 5.66 \pm 0.09$
Average	$\log(K_{ass}) = 5.77 \pm 0.14$	

[a] The values correspond to the peptide and probe concentrations.

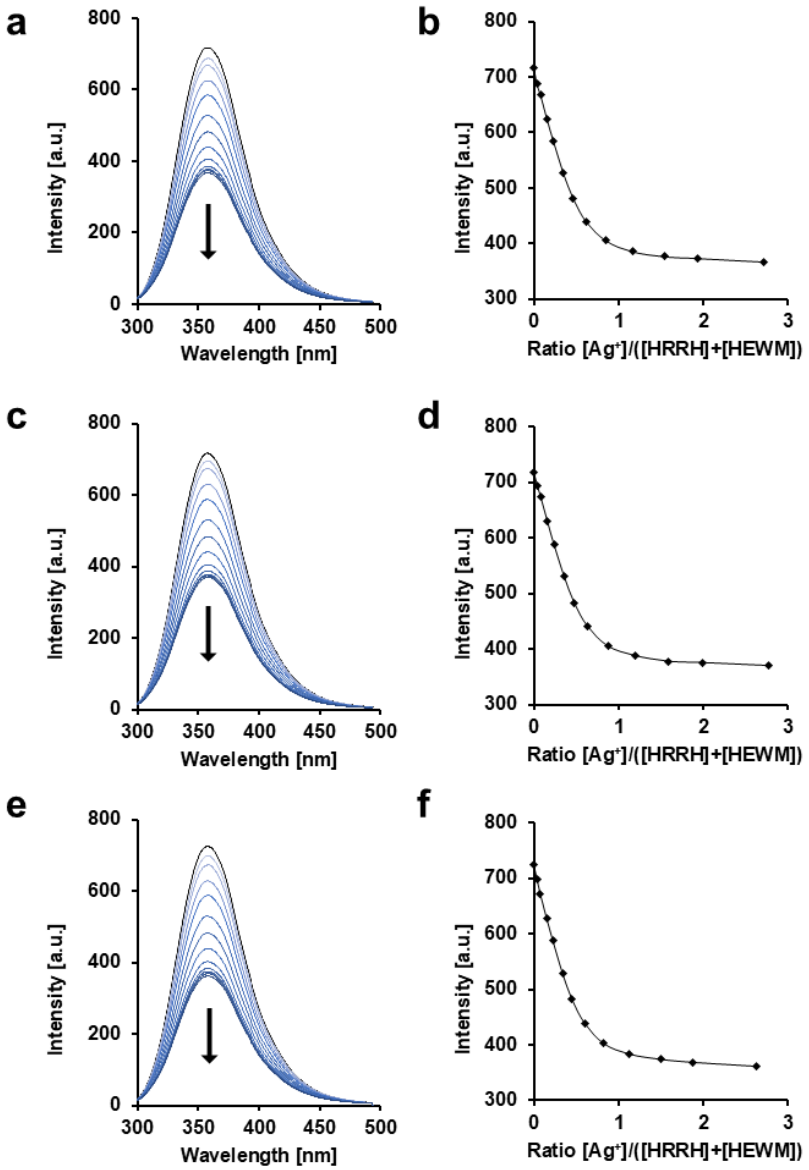

Fig. S196 HRRH / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HRRH ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

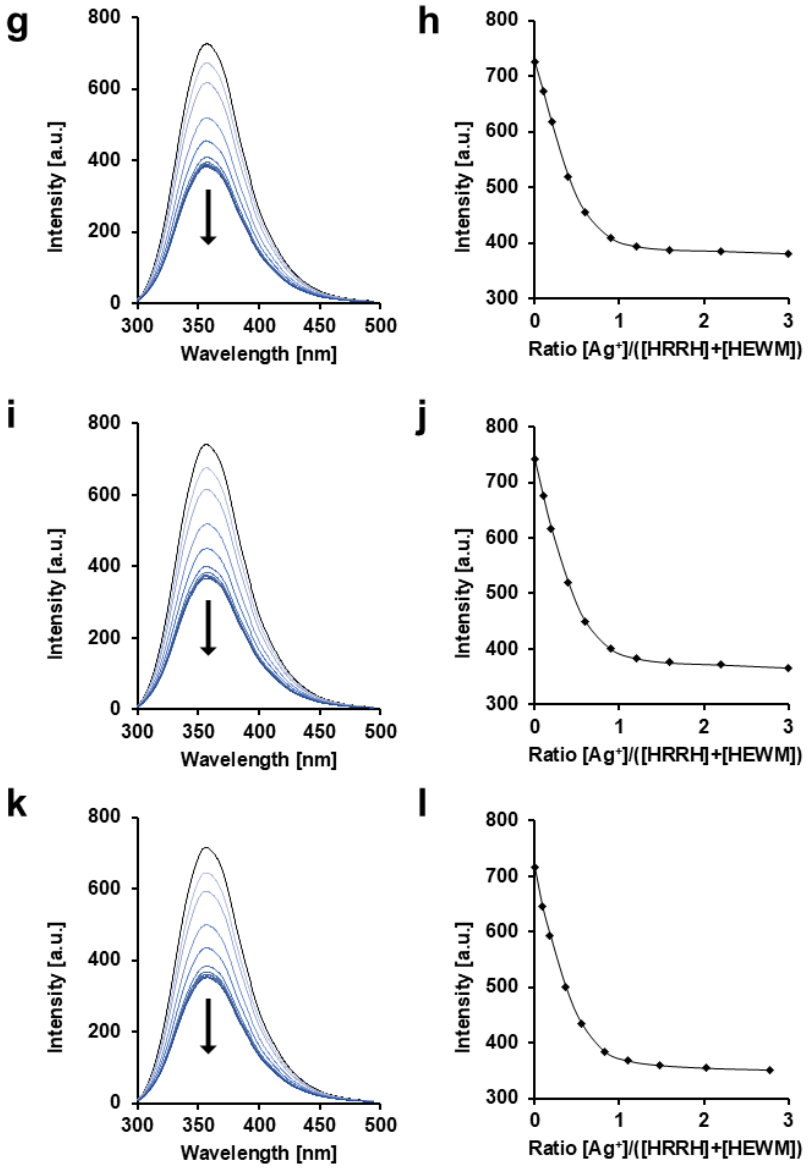

Fig. S197 HRRH / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of HRRH ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S43 Determination of the binding constants ($\log(K_{ass})$) of HRRH tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
HRRH	$\log(K_{ass-1}) = 5.54 \pm 0.03$	$\log(K_{ass-1}) = 5.59 \pm 0.03$
	$\log(K_{ass-2}) = 5.57 \pm 0.02$	$\log(K_{ass-2}) = 5.57 \pm 0.03$
	$\log(K_{ass-3}) = 5.44 \pm 0.03$	$\log(K_{ass-3}) = 5.35 \pm 0.09$
Average	$\log(K_{ass}) = 5.51 \pm 0.10$	

[a] The values correspond to the peptide and probe concentrations.

H−Hex−QM

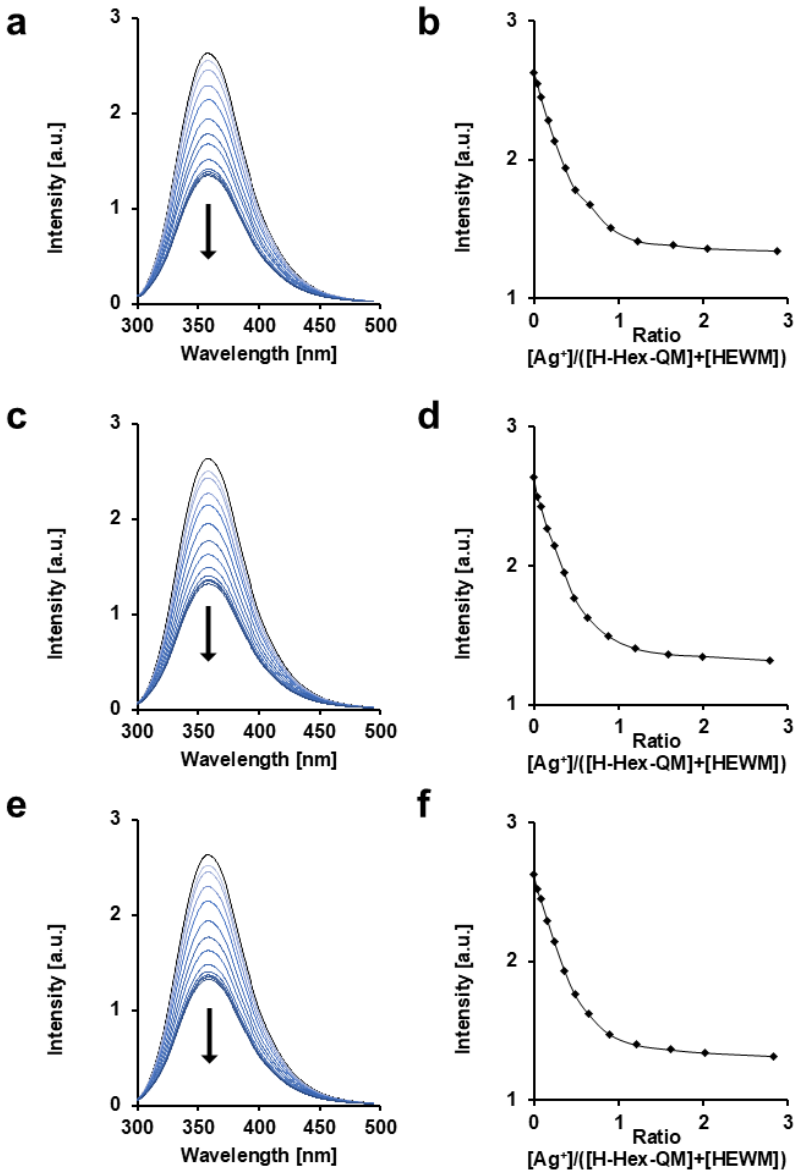

Fig. S198 H−Hex−QM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of H−Hex−QM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

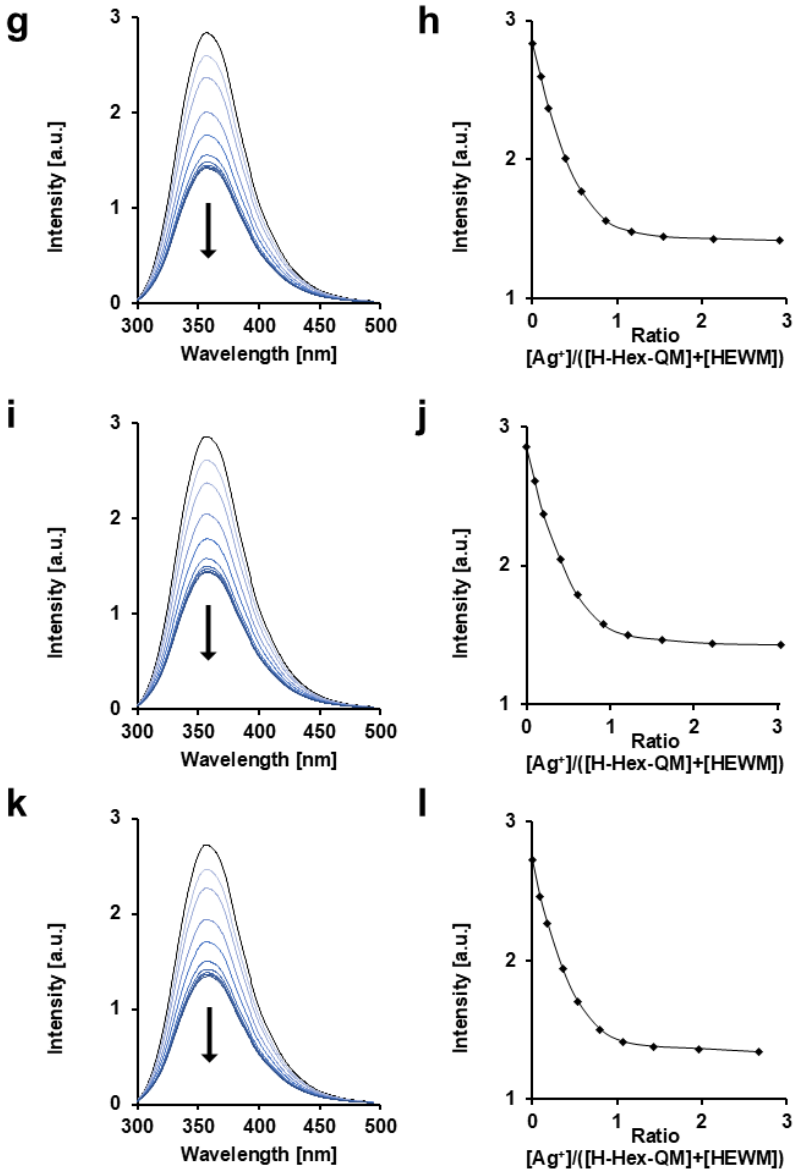

Fig. S199 H−Hex−QM / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of H−Hex−QM ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S44 Determination of the binding constants ($\log(K_{ass})$) of H−Hex−QM tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
H−Hex−QM	$\log(K_{ass-1}) = 5.65 \pm 0.05$	$\log(K_{ass-1}) = 5.63 \pm 0.03$
	$\log(K_{ass-2}) = 5.70 \pm 0.05$	$\log(K_{ass-2}) = 5.71 \pm 0.05$
	$\log(K_{ass-3}) = 5.73 \pm 0.03$	$\log(K_{ass-3}) = 5.43 \pm 0.10$
Average	$\log(K_{ass}) = 5.64 \pm 0.11$	

[a] The values correspond to the peptide and probe concentrations.

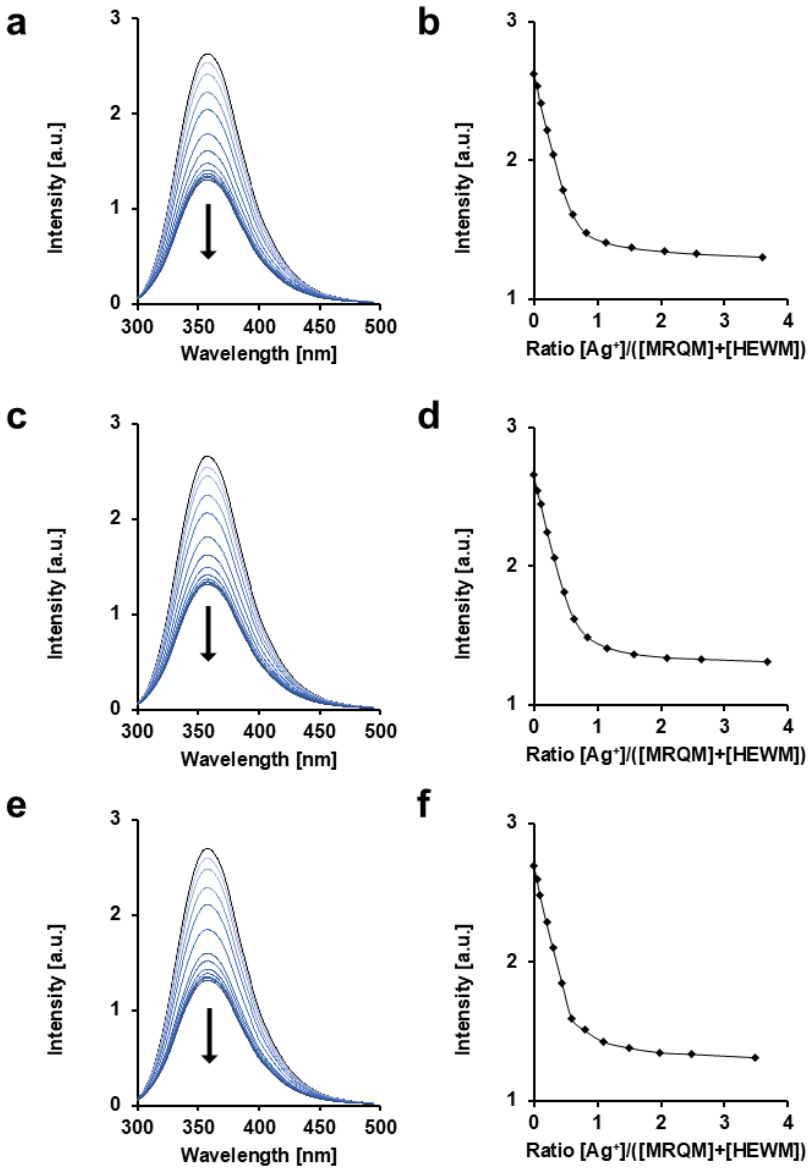

Fig. S200 MRQM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MRQM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

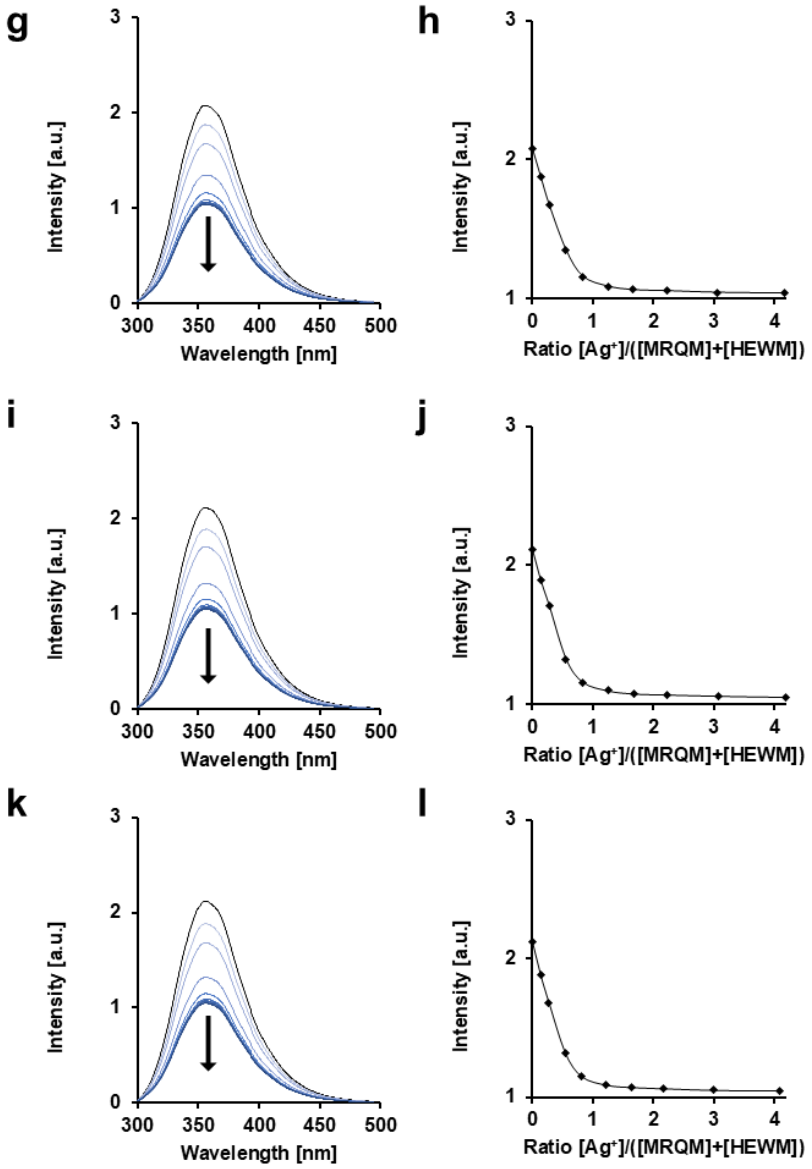

Fig. S201 MRQM / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MRQM ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S45 Determination of the binding constants ($\log(K_{ass})$) of MRQM tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
MRQM	$\log(K_{ass-1}) = 5.12 \pm 0.13$	$\log(K_{ass-1}) = 5.33 \pm 0.12$
	$\log(K_{ass-2}) = 5.11 \pm 0.11$	$\log(K_{ass-2}) = 5.10 \pm 0.17$
	$\log(K_{ass-3}) = 5.05 \pm 0.20$	$\log(K_{ass-3}) = 4.96 \pm 0.17$
Average	$\log(K_{ass}) = 5.11 \pm 0.12$	

[a] The values correspond to the peptide and probe concentrations.

MQRM

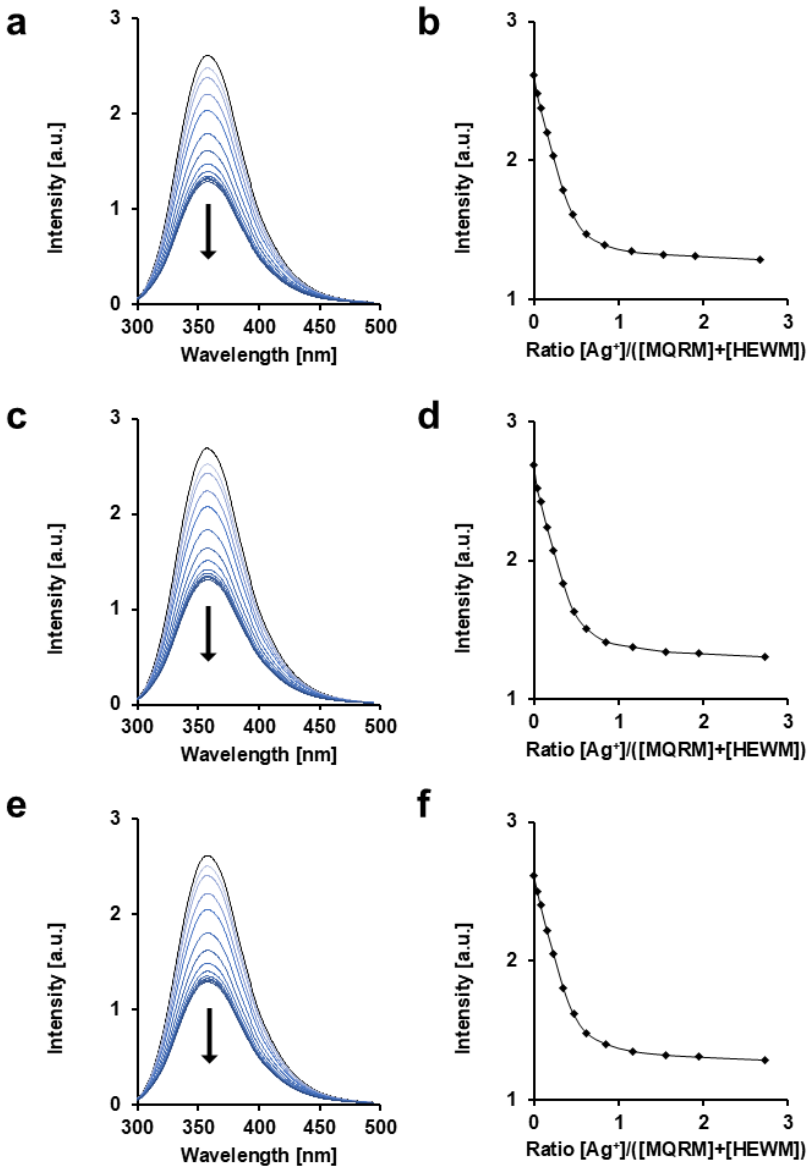

Fig. S202 MQRM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MQRM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

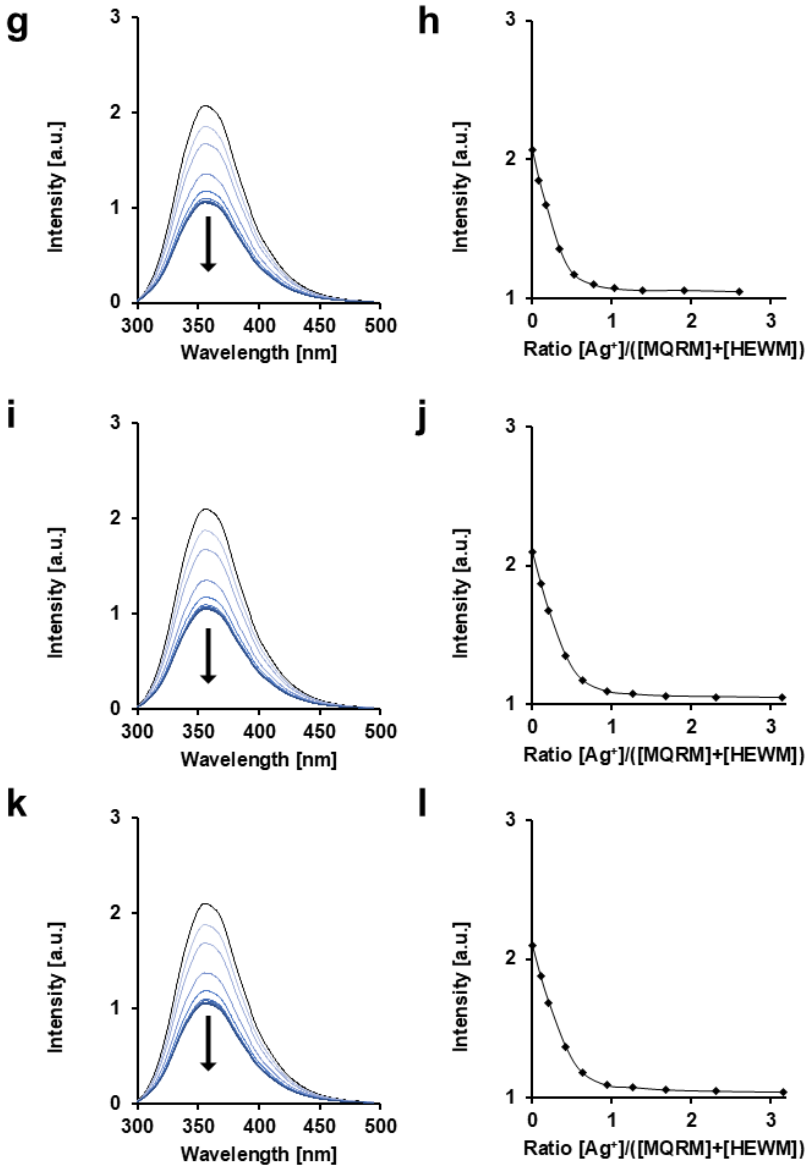

Fig. S203 MQRM / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MQRM ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S46 Determination of the binding constants ($\log(K_{ass})$) of MQRM tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
MQRM	$\log(K_{ass-1}) = 5.15 \pm 0.05$	$\log(K_{ass-1}) = 5.02 \pm 0.04$
	$\log(K_{ass-2}) = 5.02 \pm 0.13$	$\log(K_{ass-2}) = 5.08 \pm 0.07$
	$\log(K_{ass-3}) = 5.15 \pm 0.03$	$\log(K_{ass-3}) = 5.23 \pm 0.05$
Average	$\log(K_{ass}) = 5.11 \pm 0.08$	

[a] The values correspond to the peptide and probe concentrations.

MPPM

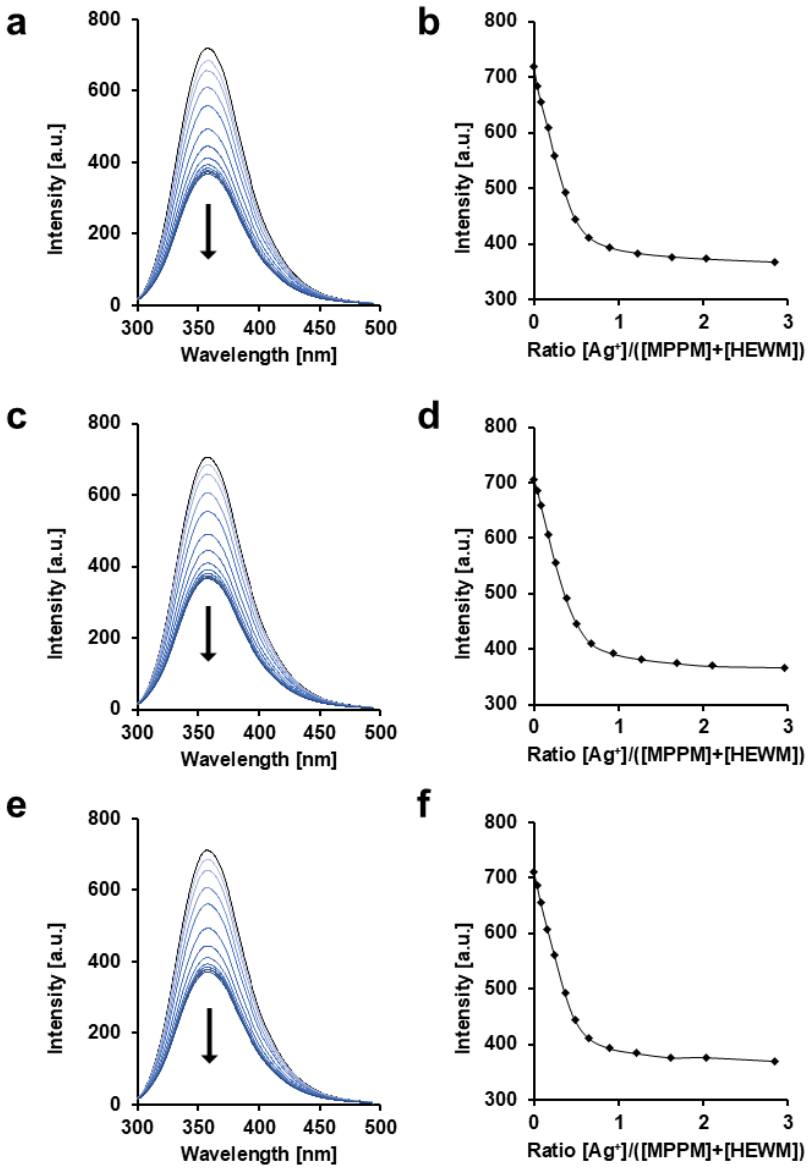

Fig. S204 MPPM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MPPM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

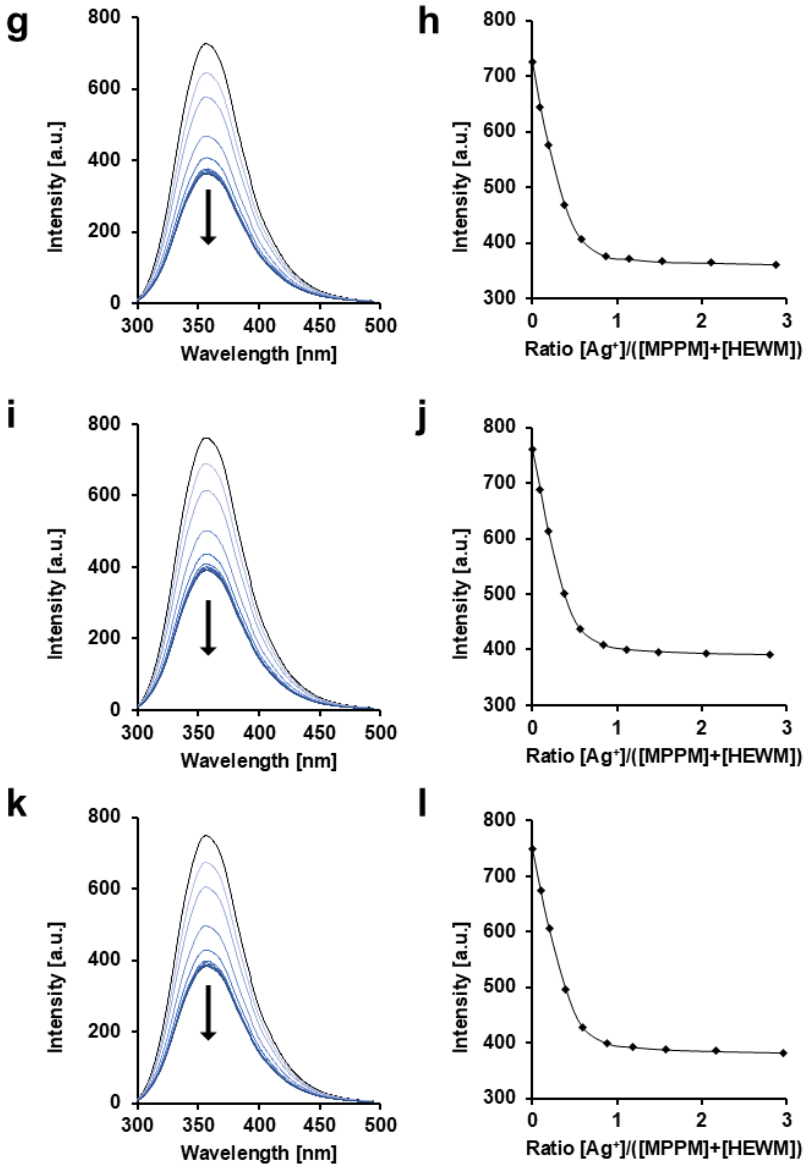

Fig. S205 MPPM / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MPPM ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S47 Determination of the binding constants ($\log(K_{ass})$) of MPPM tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
MPPM	$\log(K_{ass-1}) = 4.93 \pm 0.08$	$\log(K_{ass-1}) = 4.80 \pm 0.21$
	$\log(K_{ass-2}) = 5.10 \pm 0.05$	$\log(K_{ass-2}) = 4.76 \pm 0.14$
	$\log(K_{ass-3}) = 4.95 \pm 0.04$	$\log(K_{ass-3}) = 4.98 \pm 0.10$
Average	$\log(K_{ass}) = 4.92 \pm 0.12$	

[a] The values correspond to the peptide and probe concentrations.

MQPM

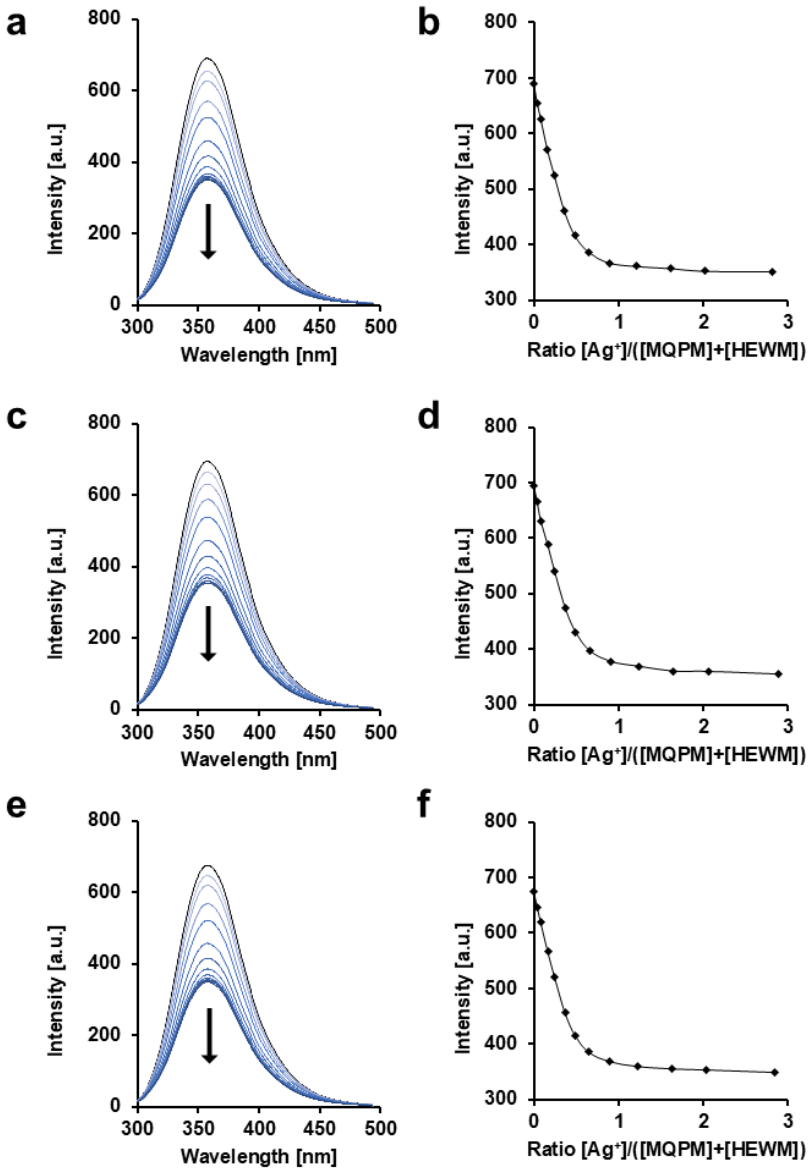

Fig. S206 MQPM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MQPM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

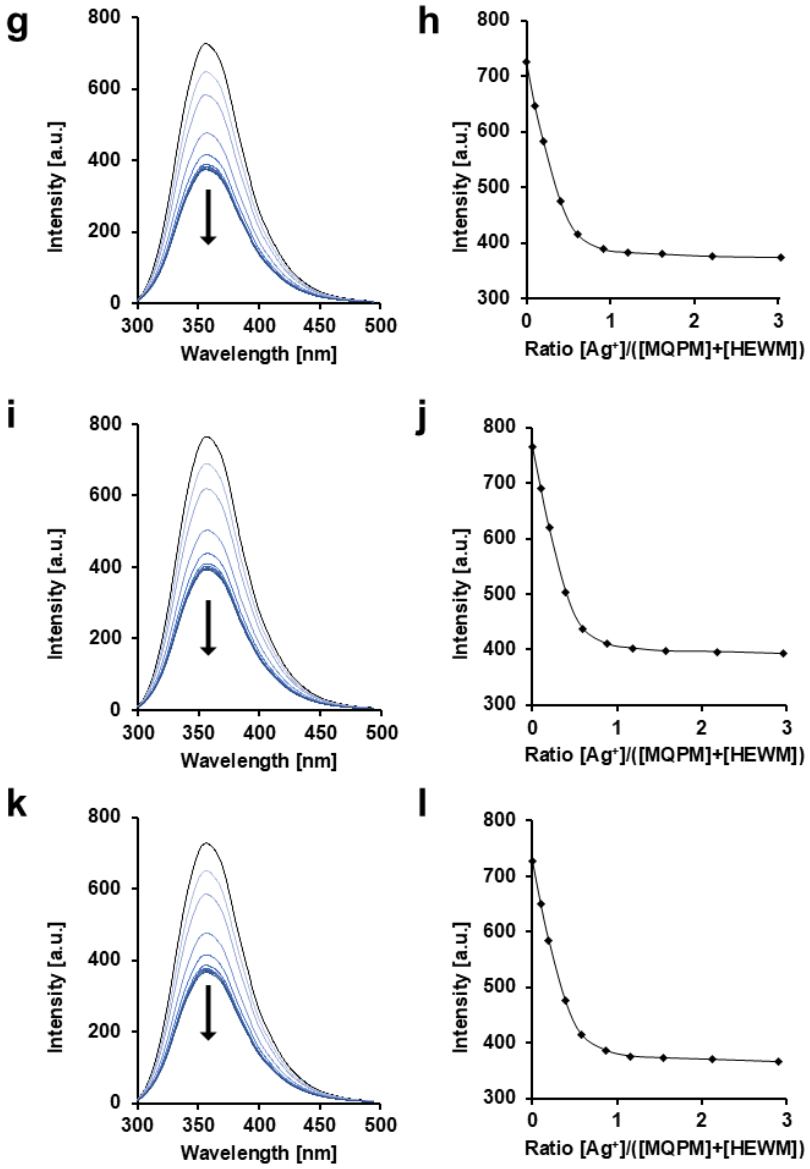

Fig. S207 MQPM / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MQPM ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S48 Determination of the binding constants ($\log(K_{ass})$) of MQPM tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
MQPM	$\log(K_{ass-1}) = 4.69 \pm 0.21$	$\log(K_{ass-1}) = 4.92 \pm 0.14$
	$\log(K_{ass-2}) = 4.97 \pm 0.09$	$\log(K_{ass-2}) = 4.97 \pm 0.06$
	$\log(K_{ass-3}) = 4.89 \pm 0.07$	$\log(K_{ass-3}) = 5.02 \pm 0.09$
Average	$\log(K_{ass}) = 4.91 \pm 0.12$	

[a] The values correspond to the peptide and probe concentrations.

MPQM

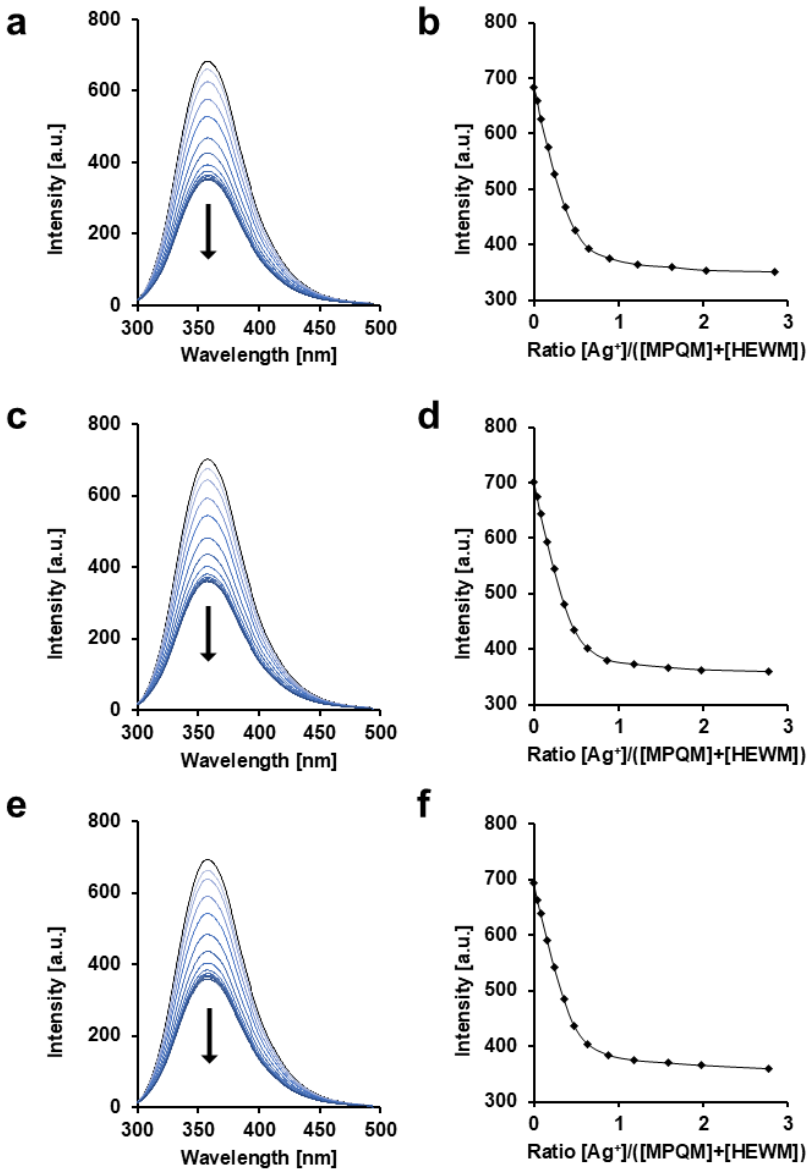

Fig. S208 MPQM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MPQM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

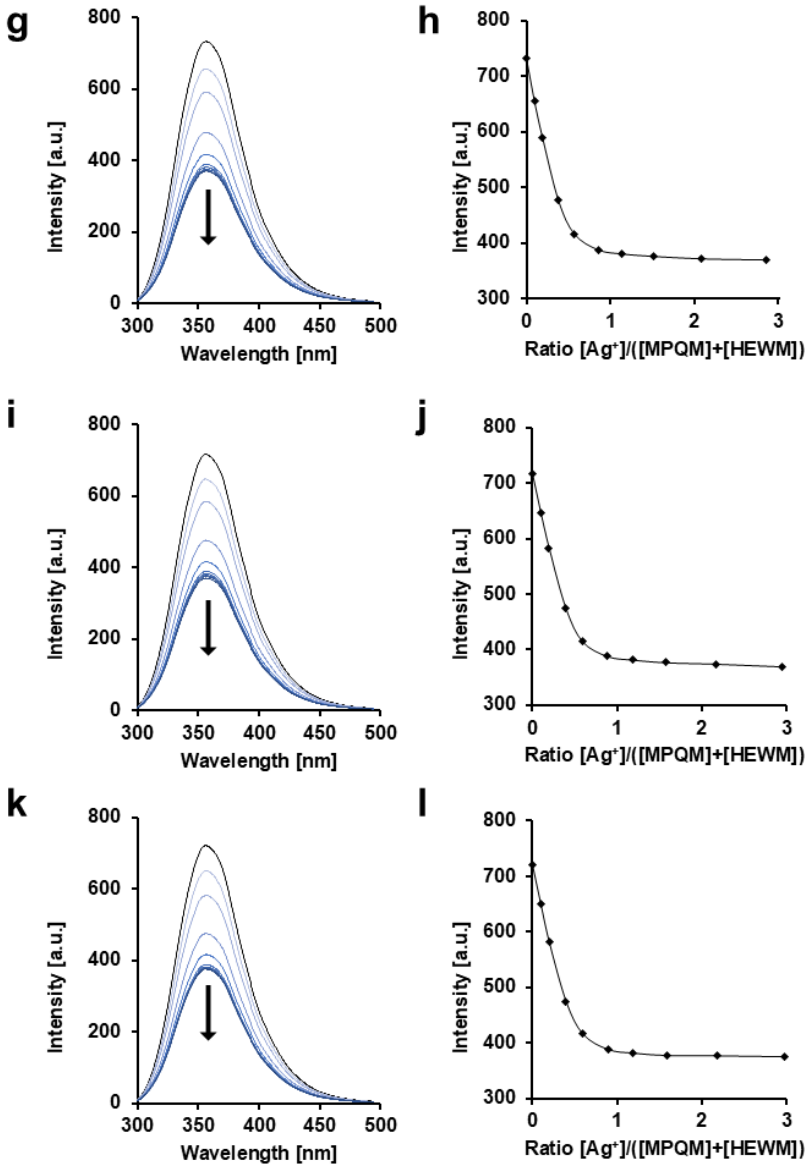

Fig. S209 MPQM / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MPQM ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S49 Determination of the binding constants ($\log(K_{ass})$) of MPQM tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
MPQM	$\log(K_{ass-1}) = 4.97 \pm 0.09$	$\log(K_{ass-1}) = 5.03 \pm 0.06$
	$\log(K_{ass-2}) = 4.87 \pm 0.11$	$\log(K_{ass-2}) = 5.01 \pm 0.06$
	$\log(K_{ass-3}) = 5.03 \pm 0.06$	$\log(K_{ass-3}) = 4.94 \pm 0.09$
Average	$\log(K_{ass}) = 4.97 \pm 0.06$	

[a] The values correspond to the peptide and probe concentrations.

MKKM

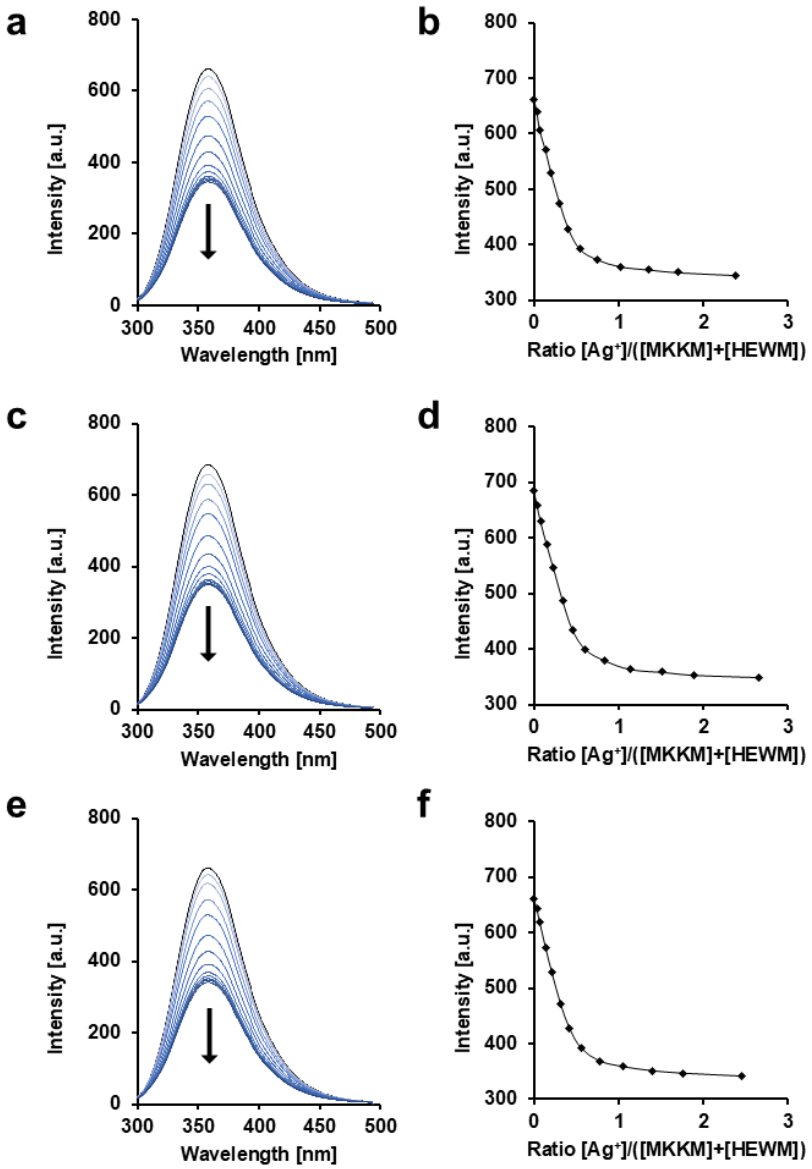

Fig. S210 MKKM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MKKM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

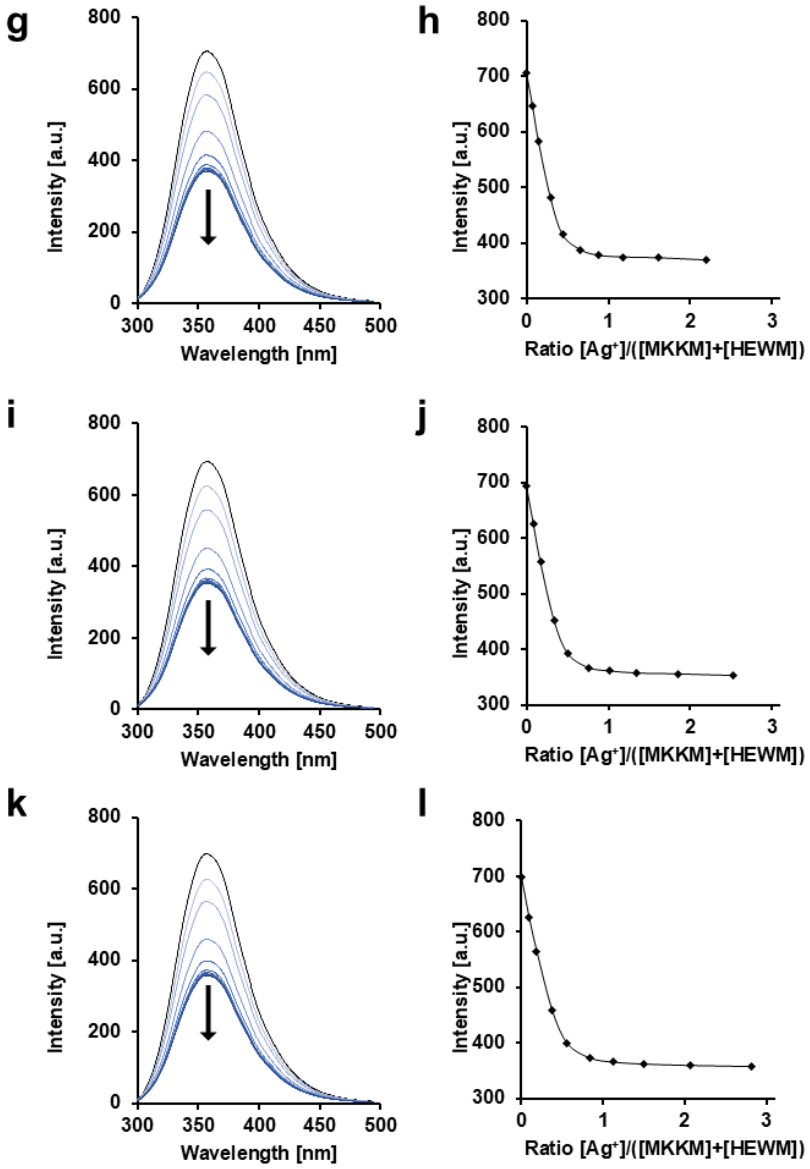

Fig. S211 MKKM / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MKKM ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S50 Determination of the binding constants ($\log(K_{ass})$) of MKKM tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
MKKM	$\log(K_{ass-1}) = 4.85 \pm 0.11$	$\log(K_{ass-1}) = 4.47 \pm 0.19$
	$\log(K_{ass-2}) = 4.86 \pm 0.10$	$\log(K_{ass-2}) = 4.64 \pm 0.14$
	$\log(K_{ass-3}) = 5.02 \pm 0.03$	$\log(K_{ass-3}) = 4.78 \pm 0.14$
Average	$\log(K_{ass}) = 4.77 \pm 0.19$	

[a] The values correspond to the peptide and probe concentrations.

MRKM

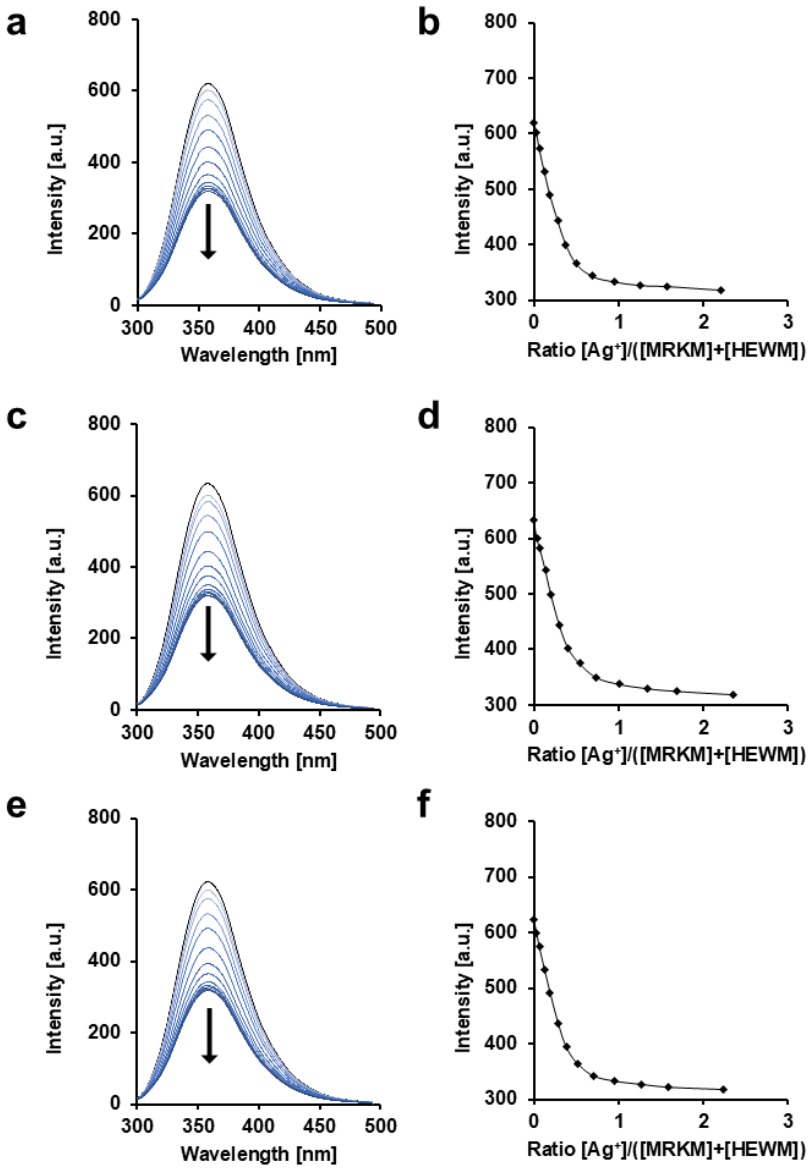

Fig. S212 MRKM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MRKM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

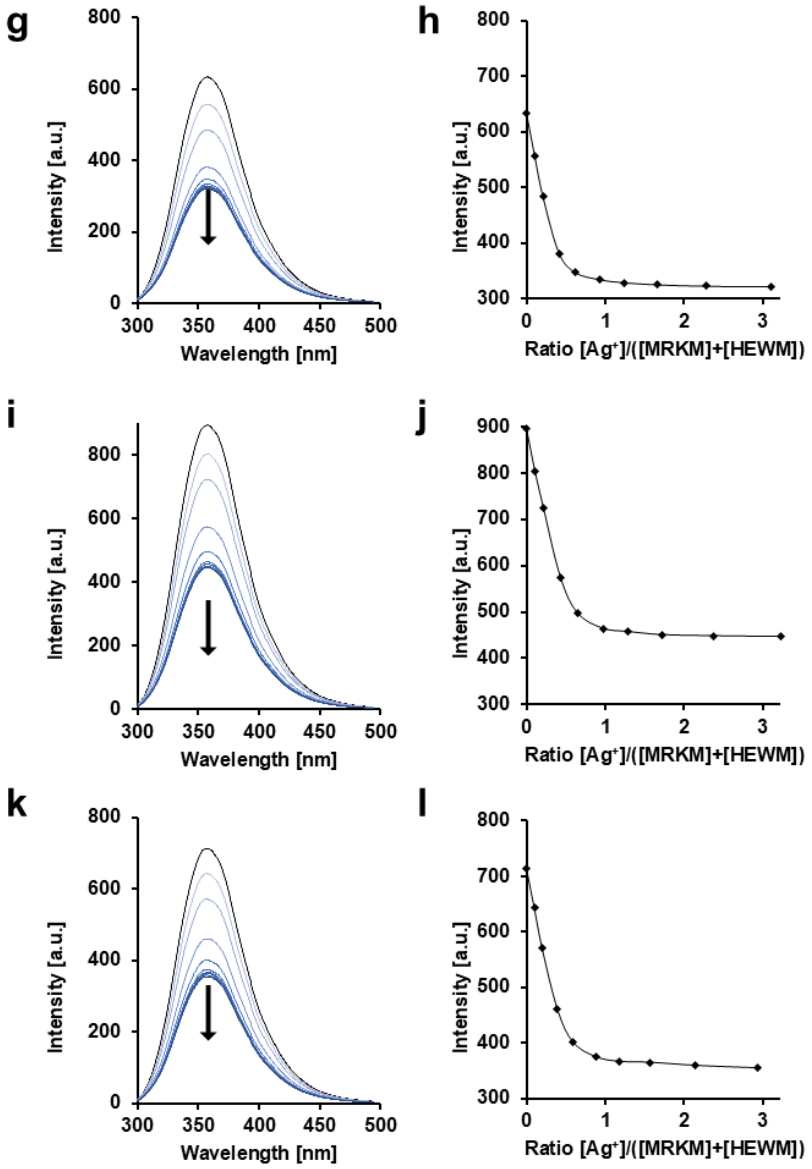

Fig. S213 MRKM / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MRKM ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S51 Determination of the binding constants ($\log(K_{ass})$) of MRKM tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
MRKM	$\log(K_{ass-1}) = 4.91 \pm 0.08$	$\log(K_{ass-1}) = 4.98 \pm 0.02$
	$\log(K_{ass-2}) = 5.07 \pm 0.07$	$\log(K_{ass-2}) = 4.81 \pm 0.09$
	$\log(K_{ass-3}) = 4.80 \pm 0.06$	$\log(K_{ass-3}) = 4.66 \pm 0.22$
Average	$\log(K_{ass}) = 4.87 \pm 0.15$	

[a] The values correspond to the peptide and probe concentrations.

MKRM

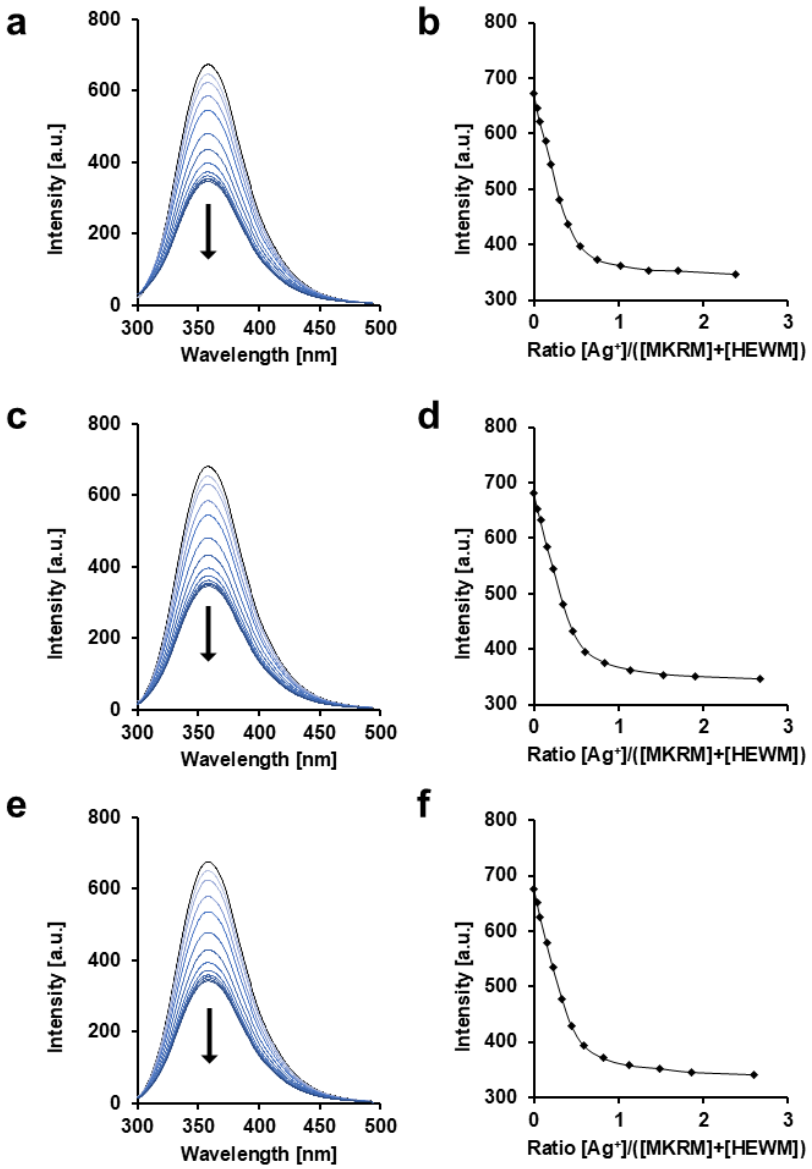

Fig. S214 MKRM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MKRM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

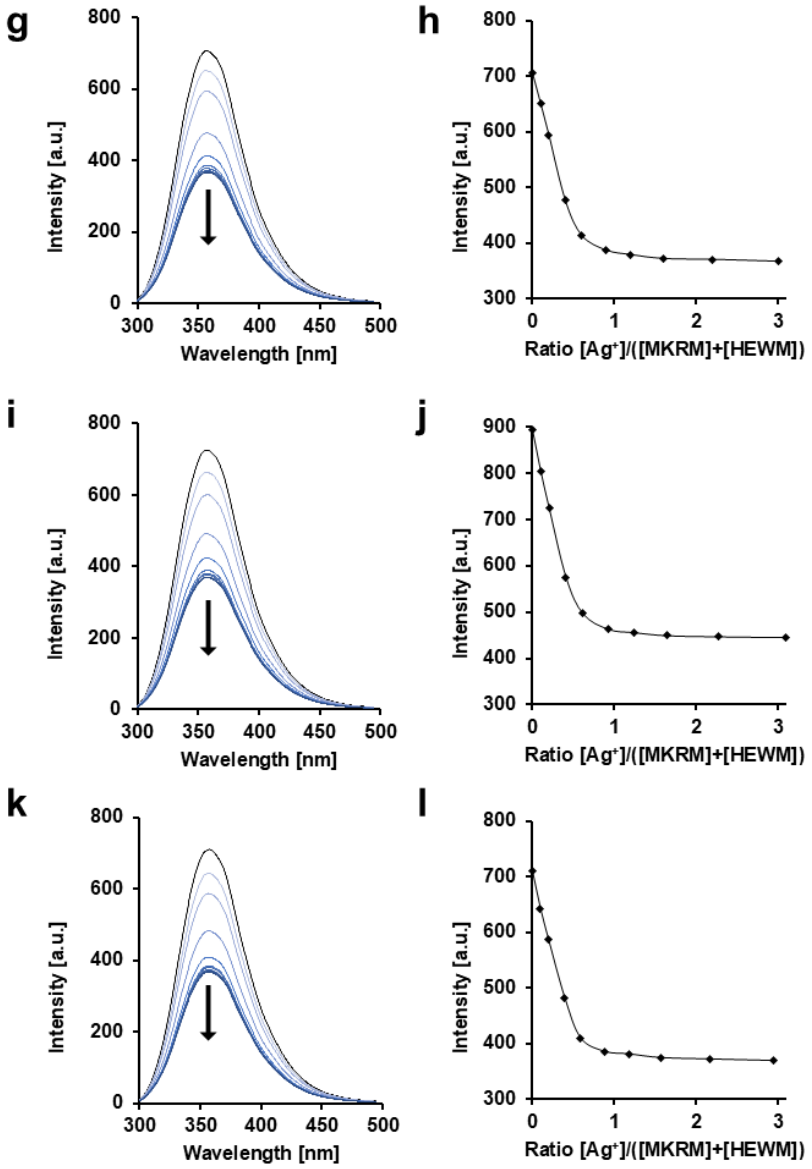

Fig. S215 MKRM / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MKRM ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S52 Determination of the binding constants ($\log(K_{ass})$) of MKRM tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
MKRM	$\log(K_{ass-1}) = 4.81 \pm 0.10$	$\log(K_{ass-1}) = 4.96 \pm 0.10$
	$\log(K_{ass-2}) = 4.89 \pm 0.06$	$\log(K_{ass-2}) = 4.57 \pm 0.18$
	$\log(K_{ass-3}) = 4.76 \pm 0.12$	$\log(K_{ass-3}) = 4.98 \pm 0.08$
Average	$\log(K_{ass}) = 4.83 \pm 0.15$	

[a] The values correspond to the peptide and probe concentrations.

MAAM

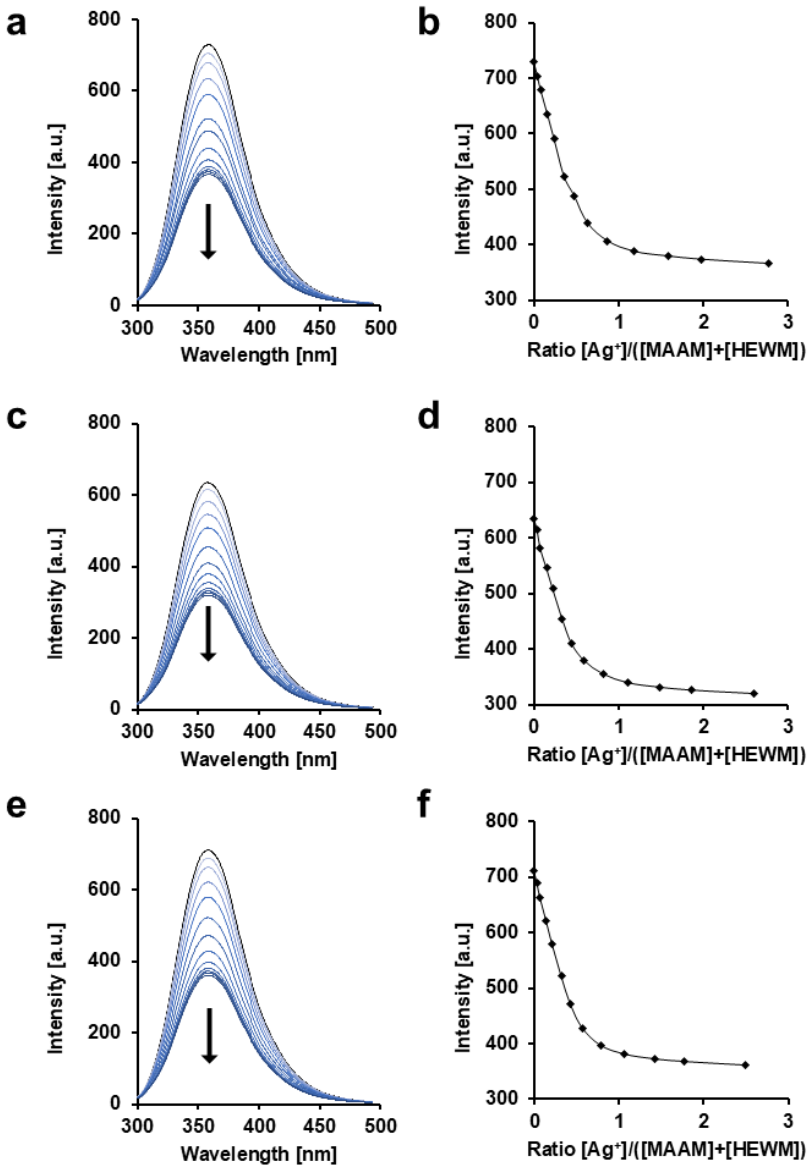

Fig. S216 MAAM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MAAM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

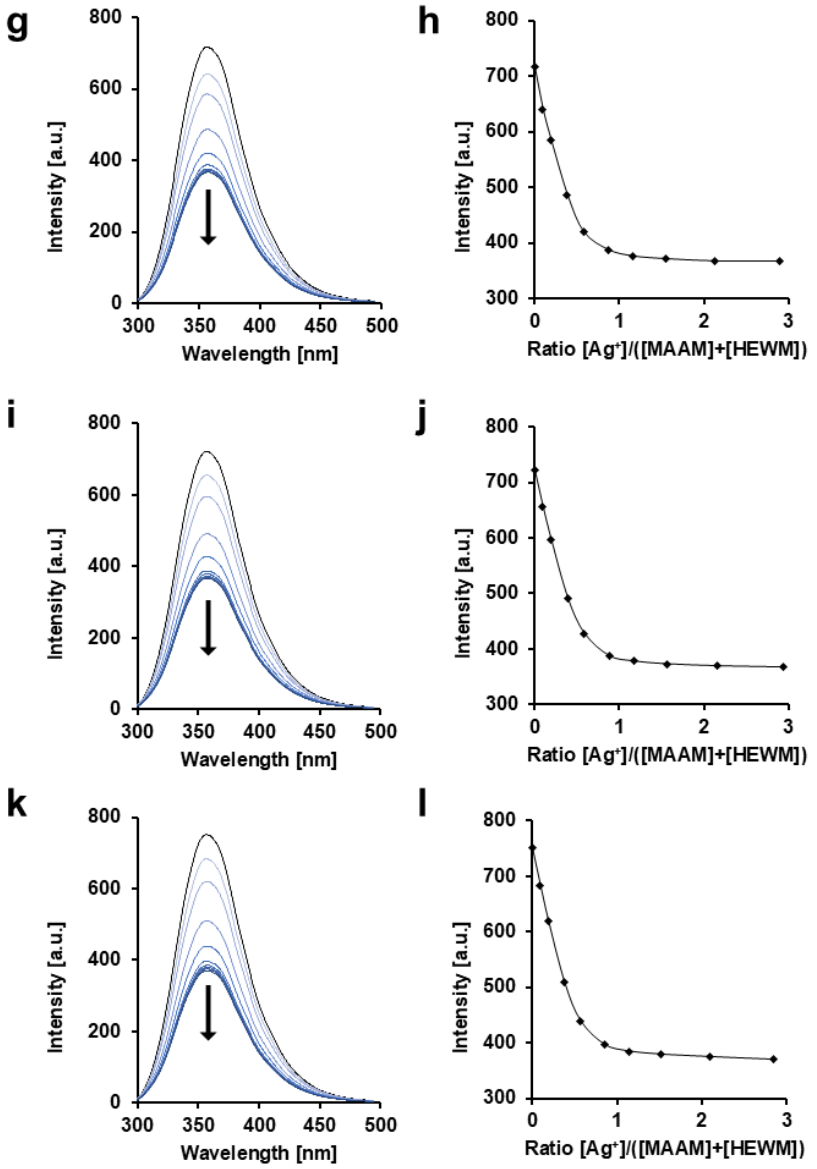

Fig. S217 MAAM / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MAAM ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S53 Determination of the binding constants ($\log(K_{ass})$) of MAAM tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
MAAM	$\log(K_{ass-1}) = 5.03 \pm 0.17$	$\log(K_{ass-1}) = 5.17 \pm 0.09$
	$\log(K_{ass-2}) = 5.14 \pm 0.09$	$\log(K_{ass-2}) = 5.25 \pm 0.04$
	$\log(K_{ass-3}) = 5.24 \pm 0.03$	$\log(K_{ass-3}) = 5.29 \pm 0.03$
Average	$\log(K_{ass}) = 5.19 \pm 0.09$	

[a] The values correspond to the peptide and probe concentrations.

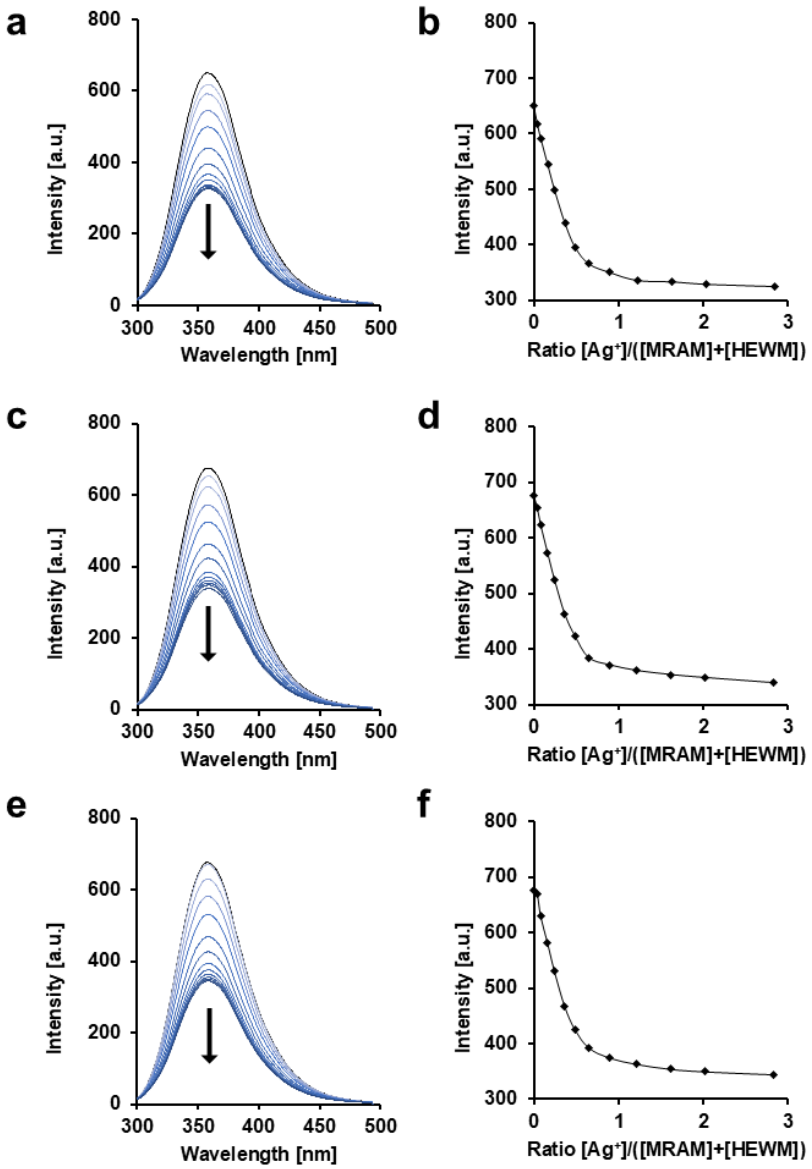

Fig. S218 MRAM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MRAM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

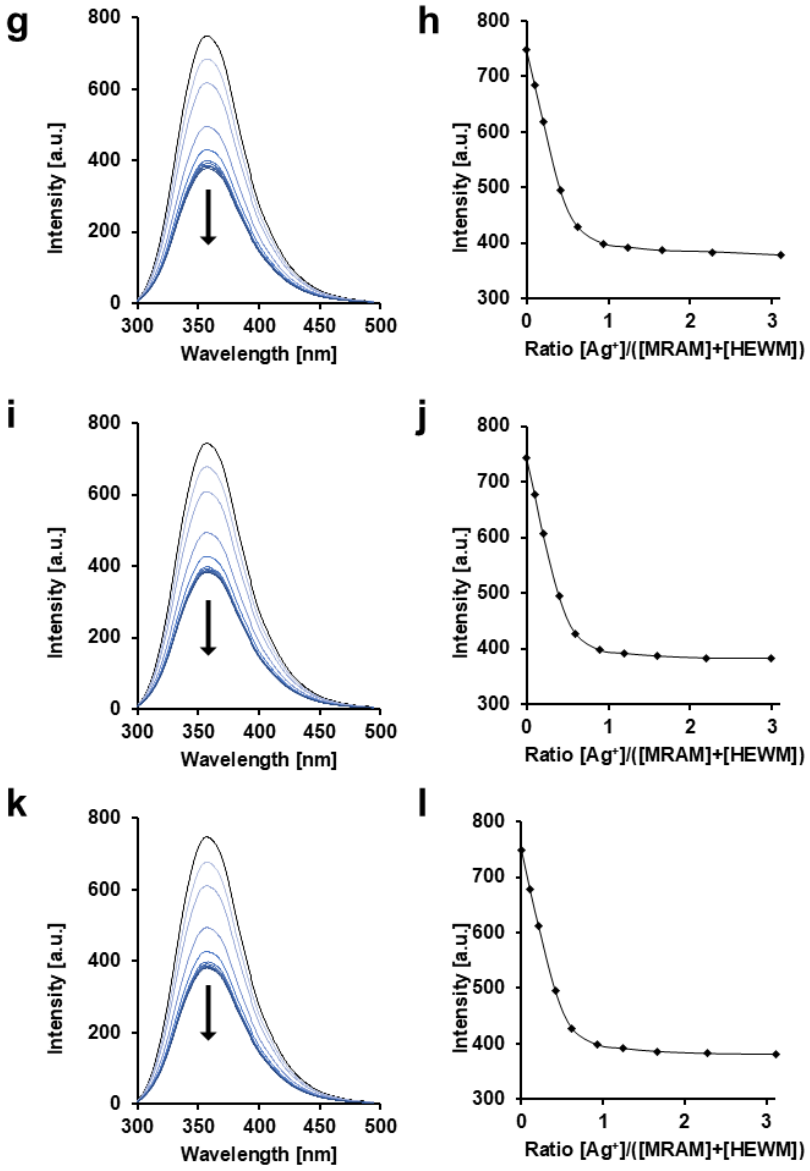

Fig. S219 MRAM / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MRAM ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S54 Determination of the binding constants ($\log(K_{ass})$) of MRAM tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
MRAM	$\log(K_{ass-1}) = 4.94 \pm 0.09$	$\log(K_{ass-1}) = 4.69 \pm 0.14$
	$\log(K_{ass-2}) = 4.95 \pm 0.11$	$\log(K_{ass-2}) = 4.90 \pm 0.07$
	$\log(K_{ass-3}) = 4.89 \pm 0.19$	$\log(K_{ass-3}) = 5.02 \pm 0.04$
Average	$\log(K_{ass}) = 4.90 \pm 0.11$	

[a] The values correspond to the peptide and probe concentrations.

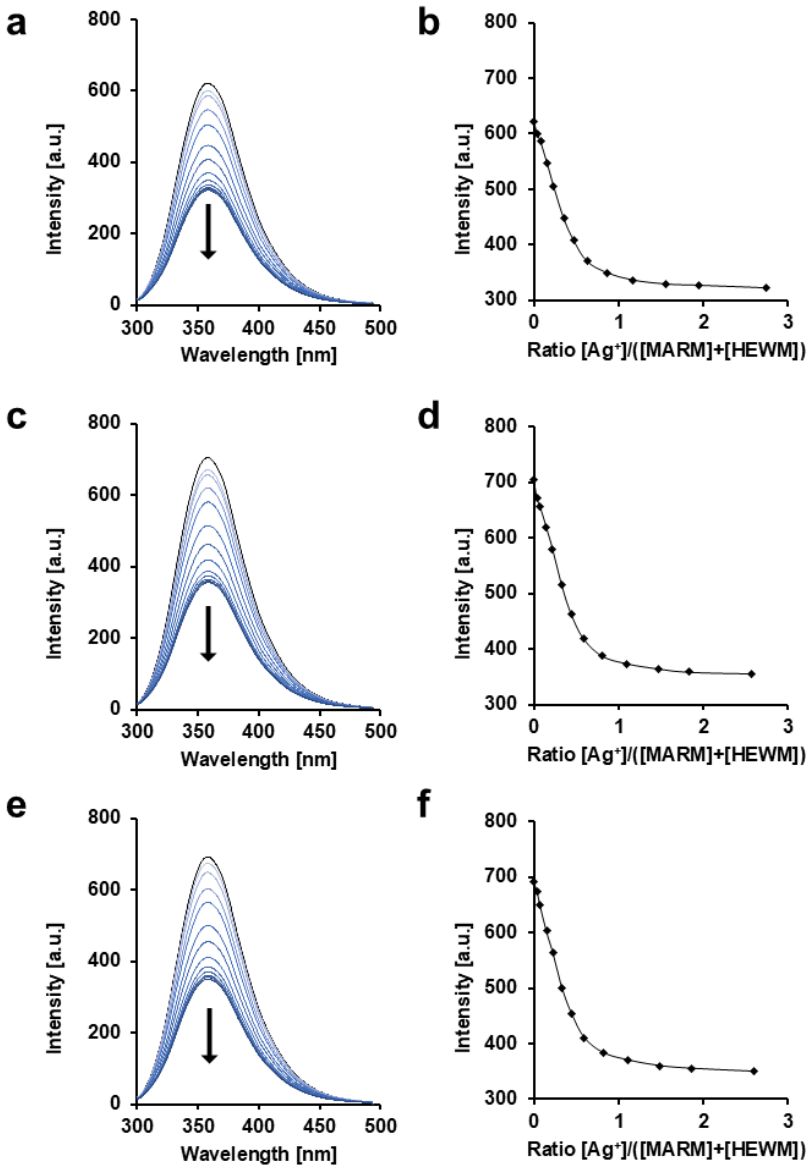

Fig. S220 MARM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MARM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

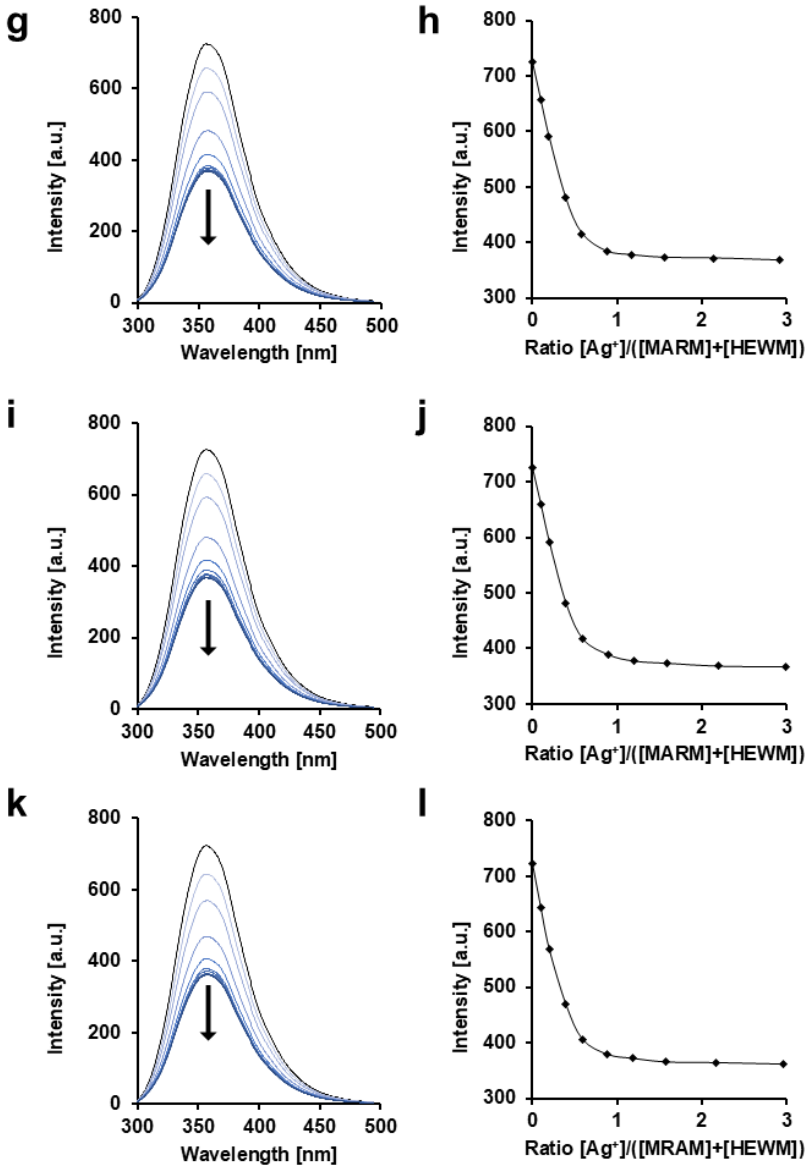

Fig. S221 MARM / HEWM competition titrations, both at $1 \cdot 10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MARM ($1 \cdot 10^{-5}$ M) in competition with HEWM probe ($1 \cdot 10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S55 Determination of the binding constants ($\log(K_{ass})$) of MARM tetrapeptide.

Model	$5 \cdot 10^{-6}$ M[a]	$1 \cdot 10^{-5}$ M[a]
MARM	$\log(K_{ass-1}) = 5.30 \pm 0.05$	$\log(K_{ass-1}) = 4.88 \pm 0.10$
	$\log(K_{ass-2}) = 5.24 \pm 0.08$	$\log(K_{ass-2}) = 5.09 \pm 0.04$
	$\log(K_{ass-3}) = 5.18 \pm 0.05$	$\log(K_{ass-3}) = 4.92 \pm 0.19$
Average	$\log(K_{ass}) = 5.10 \pm 0.17$	

[a] The values correspond to the peptide and probe concentrations.

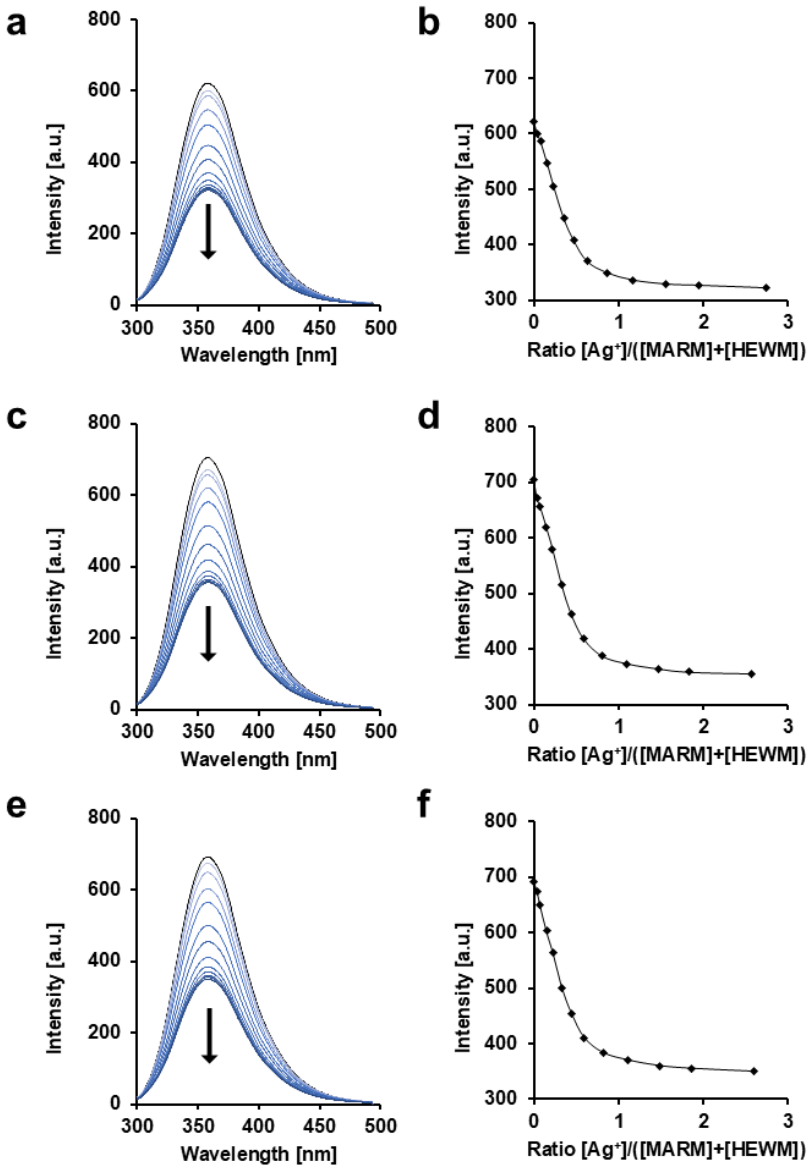

Fig. S222 MRRM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MRRM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

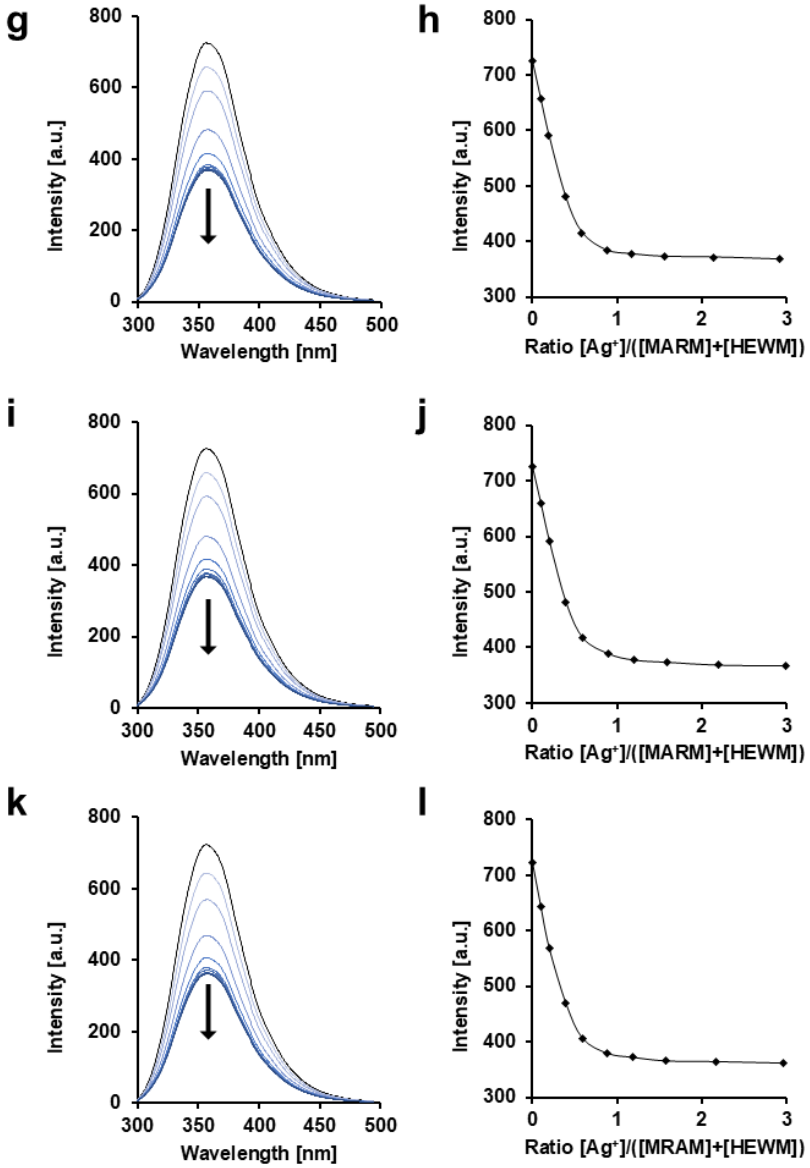

Fig. S223 MRRM / HEWM competition titrations, both at $1{\cdot}10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of MRRM ($1{\cdot}10^{-5}$ M) in competition with HEWM probe ($1{\cdot}10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S56 Determination of the binding constants ($\log(K_{ass})$) of MRRM tetrapeptide.

Model	$5{\cdot}10^{-6}$ M[a]	$1{\cdot}10^{-5}$ M[a]
MRRM	$\log(K_{ass\text{-}1}) = 5.10 \pm 0.08$	$\log(K_{ass\text{-}1}) = 4.92 \pm 0.10$
	$\log(K_{ass\text{-}2}) = 5.11 \pm 0.07$	$\log(K_{ass\text{-}2}) = 5.06 \pm 0.08$
	$\log(K_{ass\text{-}3}) = 4.97 \pm 0.02$	$\log(K_{ass\text{-}3}) = 4.70 \pm 0.24$
Average	$\log(K_{ass}) = 4.98 \pm 0.16$	

[a] The values correspond to the peptide and probe concentrations.

H−Dap−QM

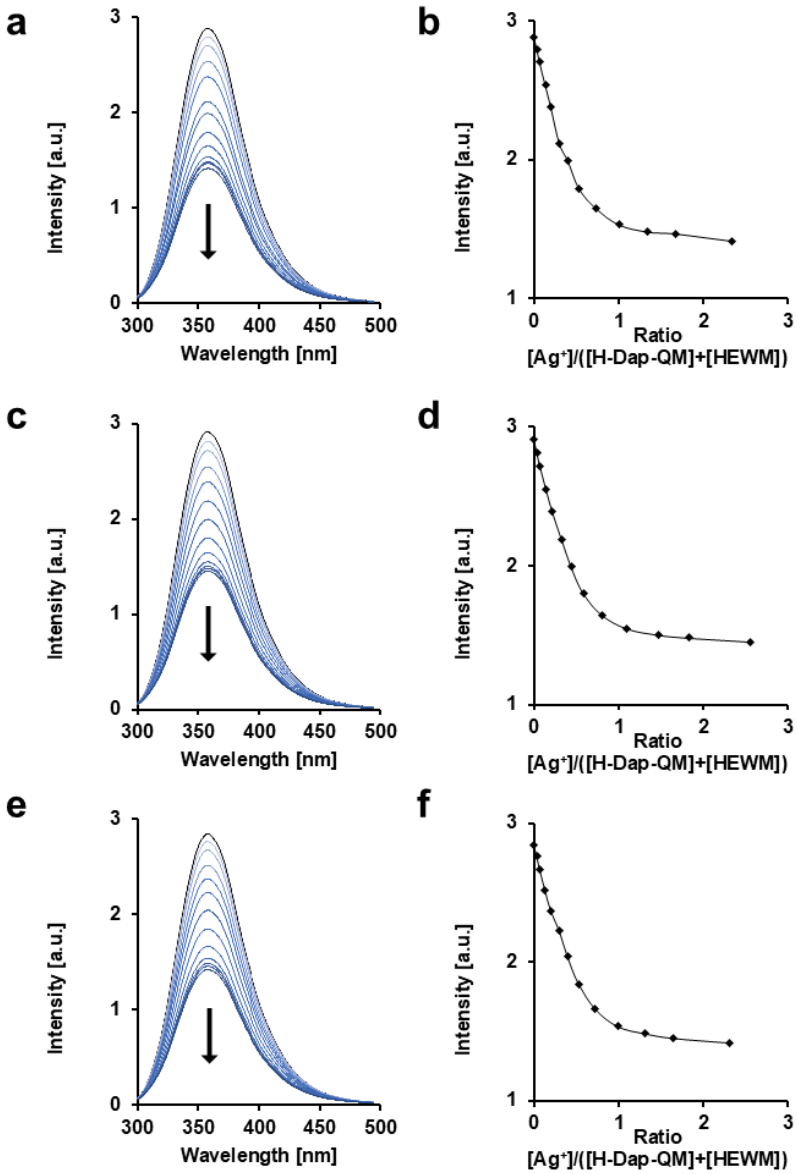

Fig. S224 H−Dap−QM / HEWM competition titrations, both at $5 \cdot 10^{-6}$ M. (a, c & e) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of H−Dap−QM ($5 \cdot 10^{-6}$ M) in competition with HEWM probe ($5 \cdot 10^{-6}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (b, d & f) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

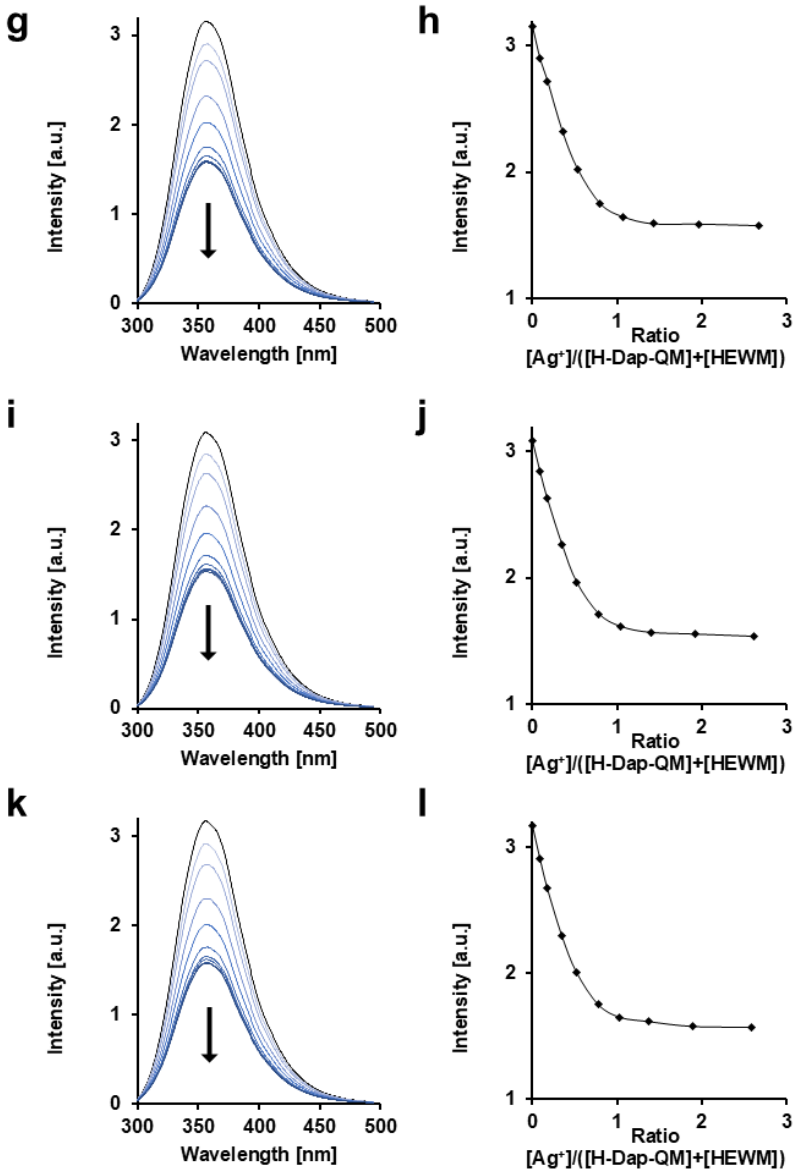

Fig. S225 H−Dap−QM / HEWM competition titrations, both at $1{\cdot}10^{-5}$ M. (g, I & k) Tryptophan fluorescence (λ_{ex}:280 nm) quench by addition of $AgNO_3$ (0 to 2.6 equivalents) to a solution of H−Dap−QM ($1{\cdot}10^{-5}$ M) in competition with HEWM probe ($1{\cdot}10^{-5}$ M), in MOPS buffer (20 equivalents, pH 7.4-7.5) at 25°C. (h, j & l) Plot of the maxima of fluorescence intensities. The solid line corresponds to the fit obtained using *DynaFit* software.[9,10]

Table S57 Determination of the binding constants ($\log(K_{ass})$) of H−Dap−QM tetrapeptide.

Model	$5{\cdot}10^{-6}$ M[a]	$1{\cdot}10^{-5}$ M[a]
H−Dap−QM	$\log(K_{ass\text{-}1}) = 5.37 \pm 0.07$	$\log(K_{ass\text{-}1}) = 5.64 \pm 0.03$
	$\log(K_{ass\text{-}2}) = 5.43 \pm 0.05$	$\log(K_{ass\text{-}2}) = 5.54 \pm 0.03$
	$\log(K_{ass\text{-}3}) = 5.65 \pm 0.05$	$\log(K_{ass\text{-}3}) = 5.48 \pm 0.05$
Average	$\log(K_{ass}) = 5.52 \pm 0.11$	

[a] The values correspond to the peptide and probe concentrations.

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