# The influence of dicationic surfactant on the aggregation process of the IVAGVN peptide from human cystatin C sequence (56-61)

**Julia Ludwiczak[a], Emilia Iłowska[b]*, Michalina Wilkowska[a], Aneta Szymańska[c], Marek Kempka[a], Maria Dobies[a], Kosma Szutkowski[d], Maciej Kozak[a]**

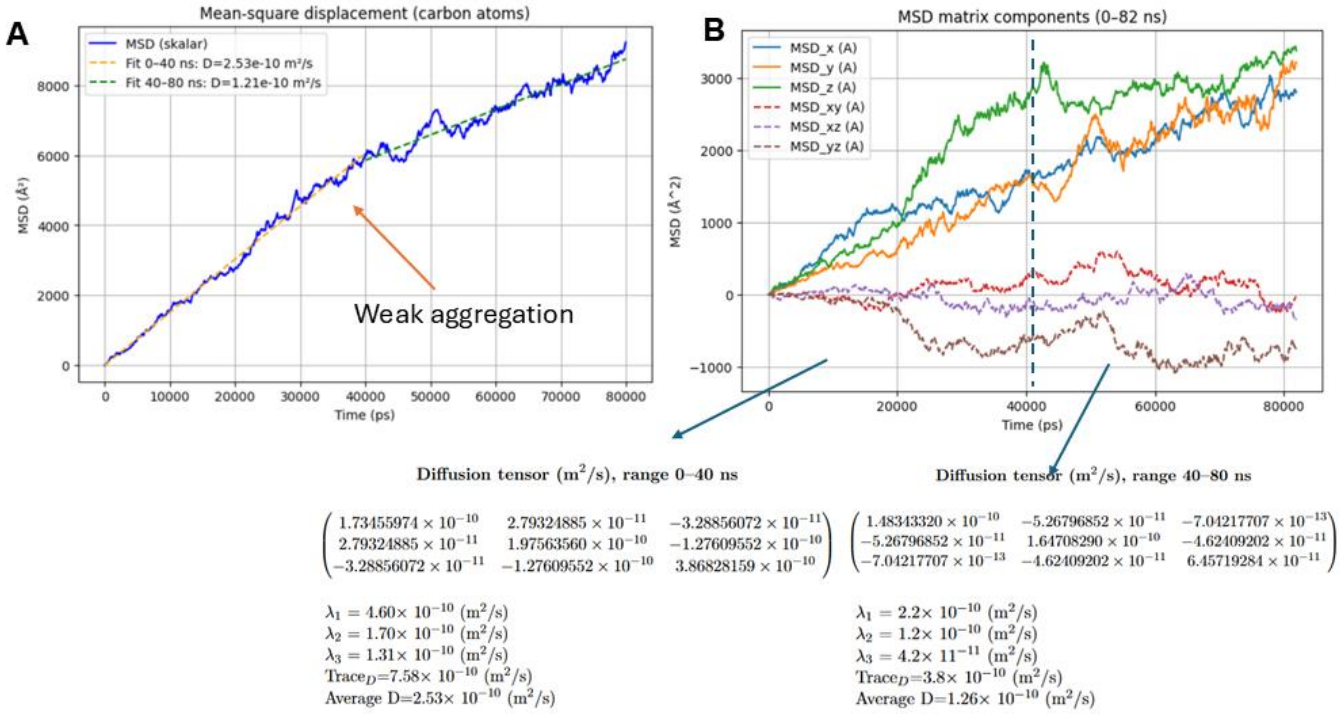
[a] *Department of Biomedical Physics, Adam Mickiewicz University, Poznan, Poland.*
[b] *Department of Organic Chemistry, University of Gdansk, Gdansk, Poland. emilia.ilowska@ug.edu.pl*
[c] *Department of Biomedical Chemistry, University of Gdansk, Gdansk, Poland.*
[d] *NanoBiomedical Centre,, Adam Mickiewicz University, Poznan, Poland.*
* *Corresponding author: emilia.ilowska@ug.edu.pl*

**Table S1**. Contribution [%] of secondary structure elements determined from CD spectra for different peptide concentrations [mM].

| $C_{IVAGVN}$ [mM] | a-helix [%] | b-sheets [%] | Turns [%] | Unordered [%] |
|---|---|---|---|---|
| 0.52 | 7.8 | 23.5 | 16.6 | 52.1 |
| 1.05 | 9.3 | 17.9 | 17.8 | 55 |
| 2.60 | 16.4 | 22.8 | 16.4 | 44.5 |
| 3.50 | 14.9 | 23.2 | 16 | 45.9 |
| 5.25 | 9.4 | 24.3 | 18.3 | 48.1 |

**Table S2**. Contribution [%] of secondary structure elements determined from CD spectra for different peptide concentrations: 0.52 and 5.25 mM and with C6IMIC12 surfactant with various concentrations (0.25, 1.00 and 4.00 mM).

| $C_{IVAGVN}$ [mM] | $C_{surfactanct}$ [mM] | a-helix [%] | β-sheets [%] | Turns [%] | Unordered [%] |
|---|---|---|---|---|---|
| 0.52 | 0 | 7.8 | 23.5 | 16.6 | 52.1 |
| | 0.25 | 4.5 | 29.3 | 19.0 | 47.2 |
| | 1.00 | 7.9 | 27.4 | 16.1 | 48.9 |
| | 4.00 | 0 | 47.2 | 23.2 | 29.3 |
| 5.25 | 0 | 9.4 | 24.3 | 18.3 | 48.1 |
| | 0.25 | 15.2 | 25.8 | 14.6 | 44.4 |
| | 1.00 | 7.5 | 32.8 | 15.3 | 44.4 |
| | 4.00 | 7.1 | 31.0 | 20.7 | 41.2 |



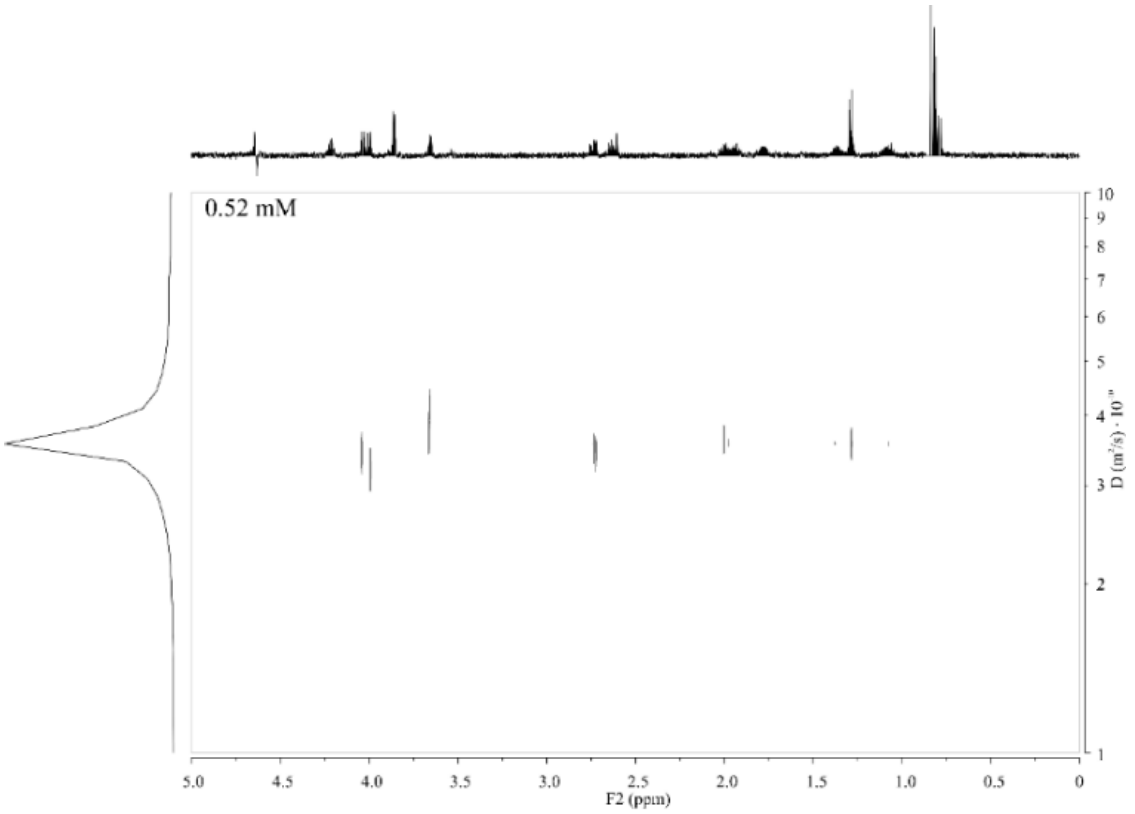

$$\begin{pmatrix} 1.73455974\times10^{-10} & 2.79324885\times10^{-11} & -3.28856072\times10^{-11} \\ 2.79324885\times10^{-11} & 1.97563560\times10^{-10} & -1.27609552\times10^{-10} \\ -3.28856072\times10^{-11} & -1.27609552\times10^{-10} & 3.86828159\times10^{-10} \end{pmatrix}$$

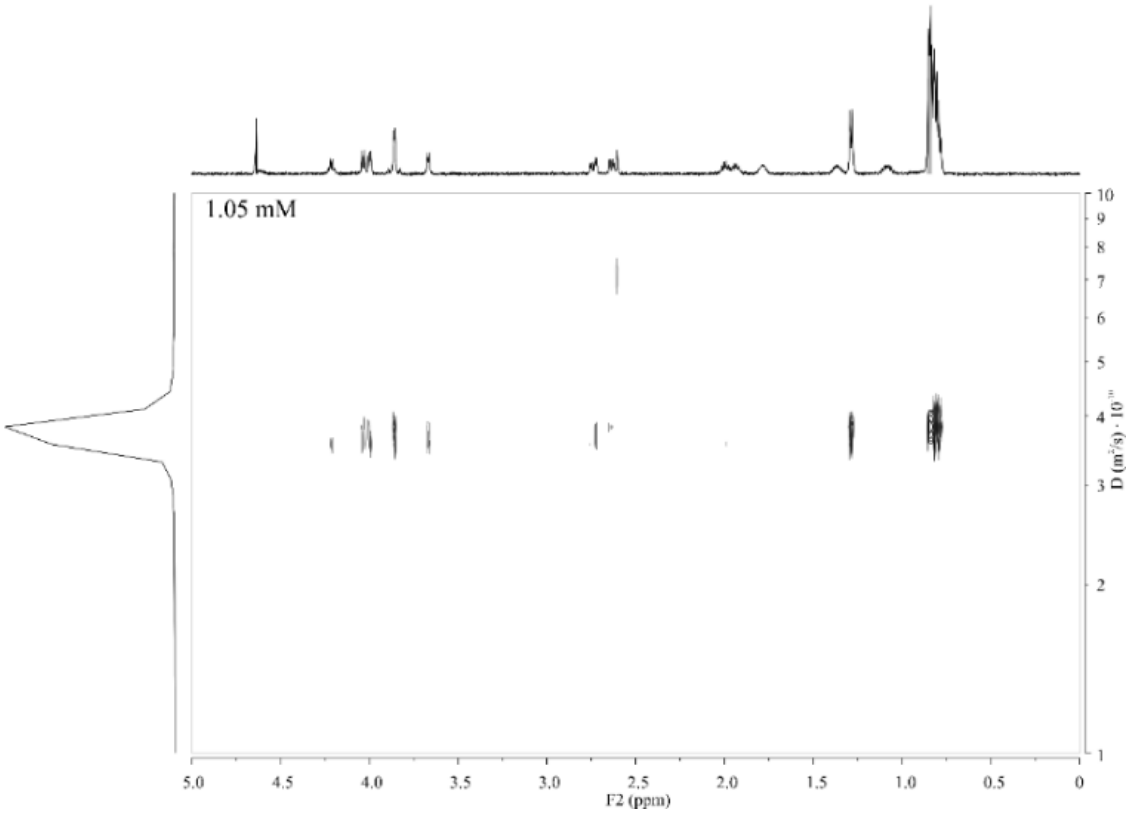
$\lambda_1 = 4.60\times10^{-10}\ (m^2/s)$
$\lambda_2 = 1.70\times10^{-10}\ (m^2/s)$
$\lambda_3 = 1.31\times10^{-10}\ (m^2/s)$
$Trace_D = 7.58\times10^{-10}\ (m^2/s)$
Average $D = 2.53\times10^{-10}\ (m^2/s)$

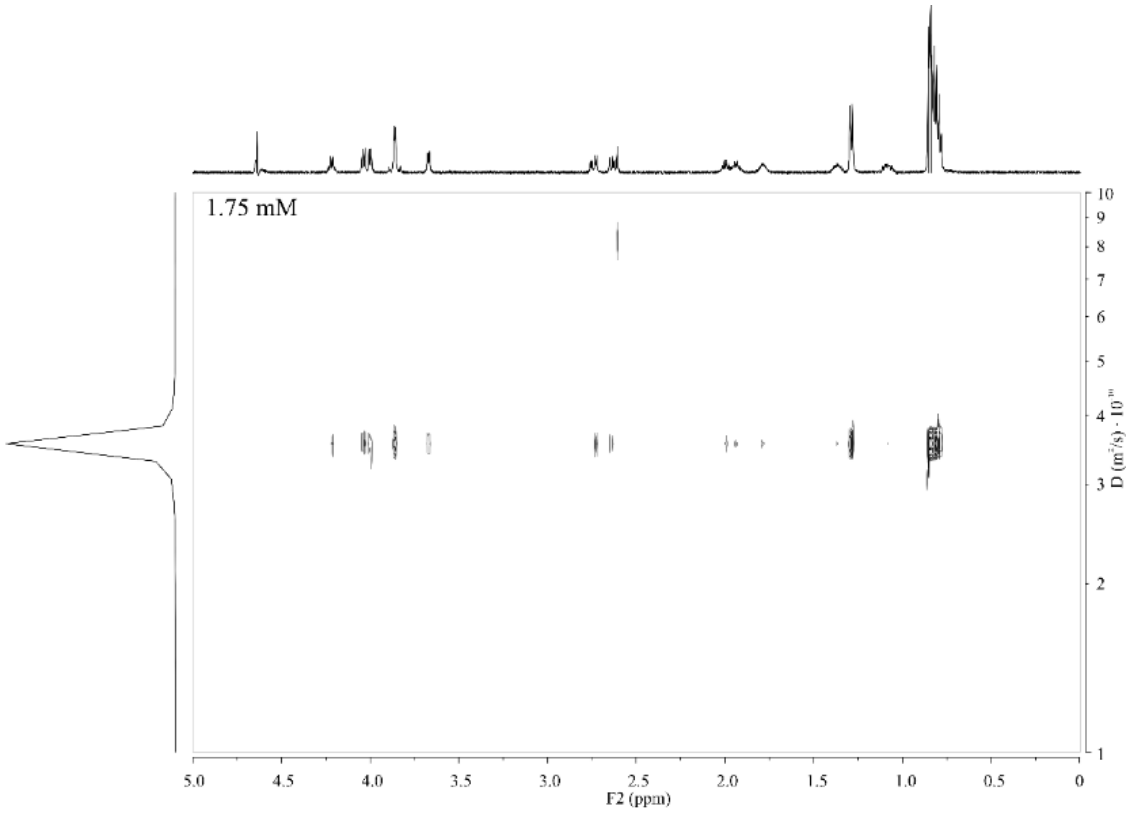
$$\begin{pmatrix} 1.48343320\times10^{-10} & -5.26796852\times10^{-11} & -7.04217707\times10^{-13} \\ -5.26796852\times10^{-11} & 1.64708290\times10^{-10} & -4.62409202\times10^{-11} \\ -7.04217707\times10^{-13} & -4.62409202\times10^{-11} & 6.45719284\times10^{-11} \end{pmatrix}$$

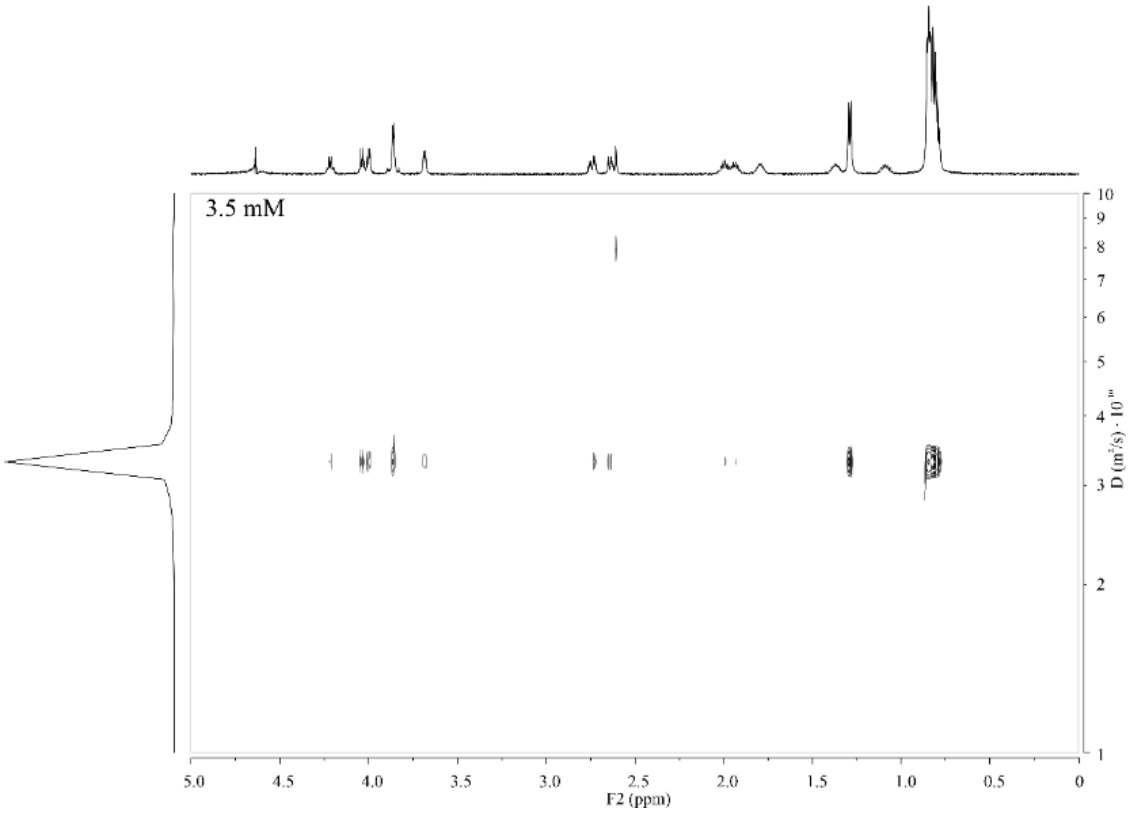
$\lambda_1 = 2.2\times10^{-10}\ (m^2/s)$
$\lambda_2 = 1.2\times10^{-10}\ (m^2/s)$
$\lambda_3 = 4.2\times11^{-11}\ (m^2/s)$
$Trace_D = 3.8\times10^{-10}\ (m^2/s)$
Average $D = 1.26\times10^{-10}\ (m^2/s)$

**Figure S1**. A) The mean-square displacement (MSD) analysis for the 0-80 ns interval and B) the decomposition of MSD into its matrix components ($MSD_{xx}$, $MSD_{yy}$, $MSD_{zz}$, $MSD_{xy}$, $MSD_{xz}$, $MSD_{yz}$), diffusion tensor, diffusion tensor eigenvalues ($l_1$, $l_2$, $l_3$) and resulting mean diffusion coefficients.


0.52 mM
D (m²/s) · 10⁻¹⁰
F2 (ppm)


1.05 mM
D (m²/s) · 10⁻¹⁰
F2 (ppm)


1.75 mM
D (m²/s) · 10⁻¹⁰
F2 (ppm)


3.5 mM
D (m²/s) · 10⁻¹⁰
F2 (ppm)

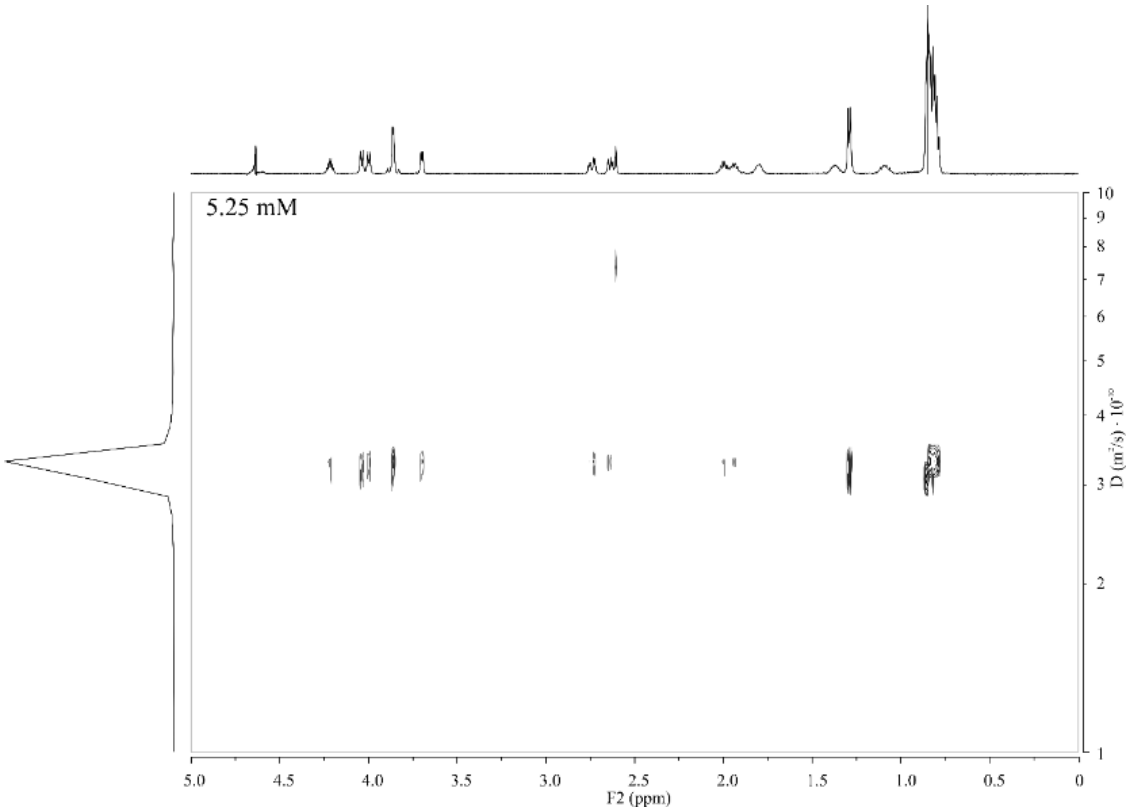
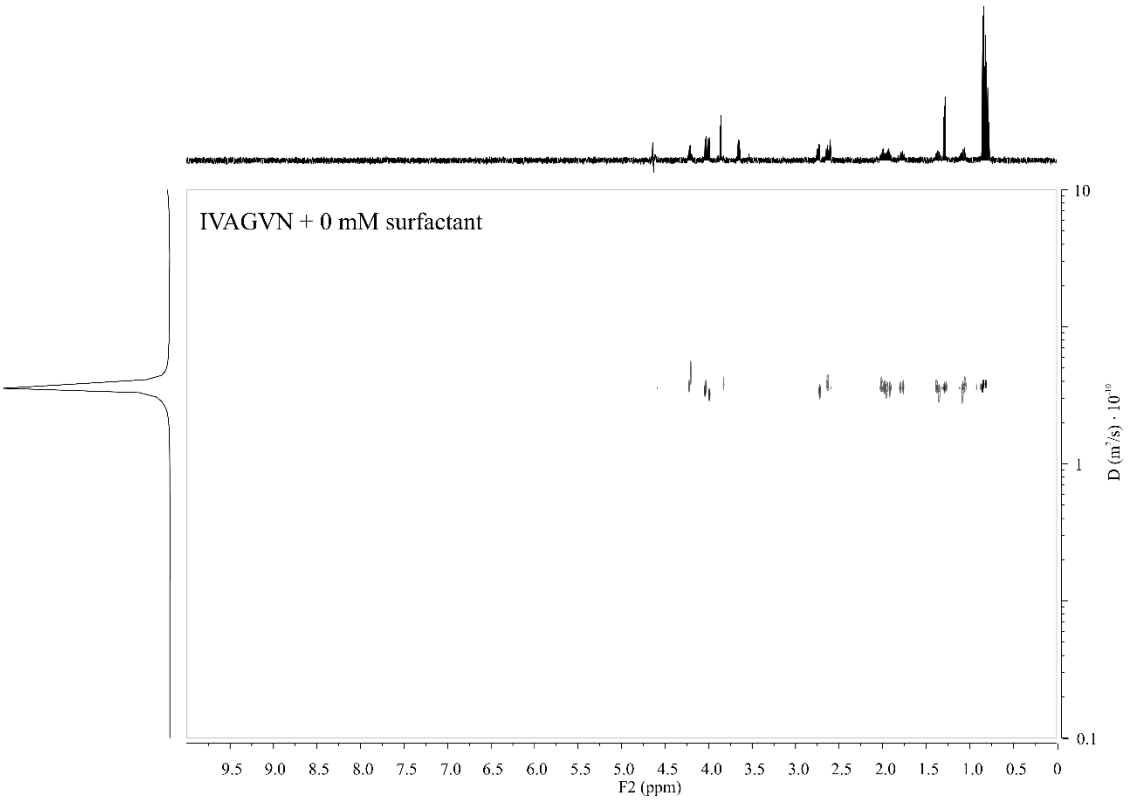
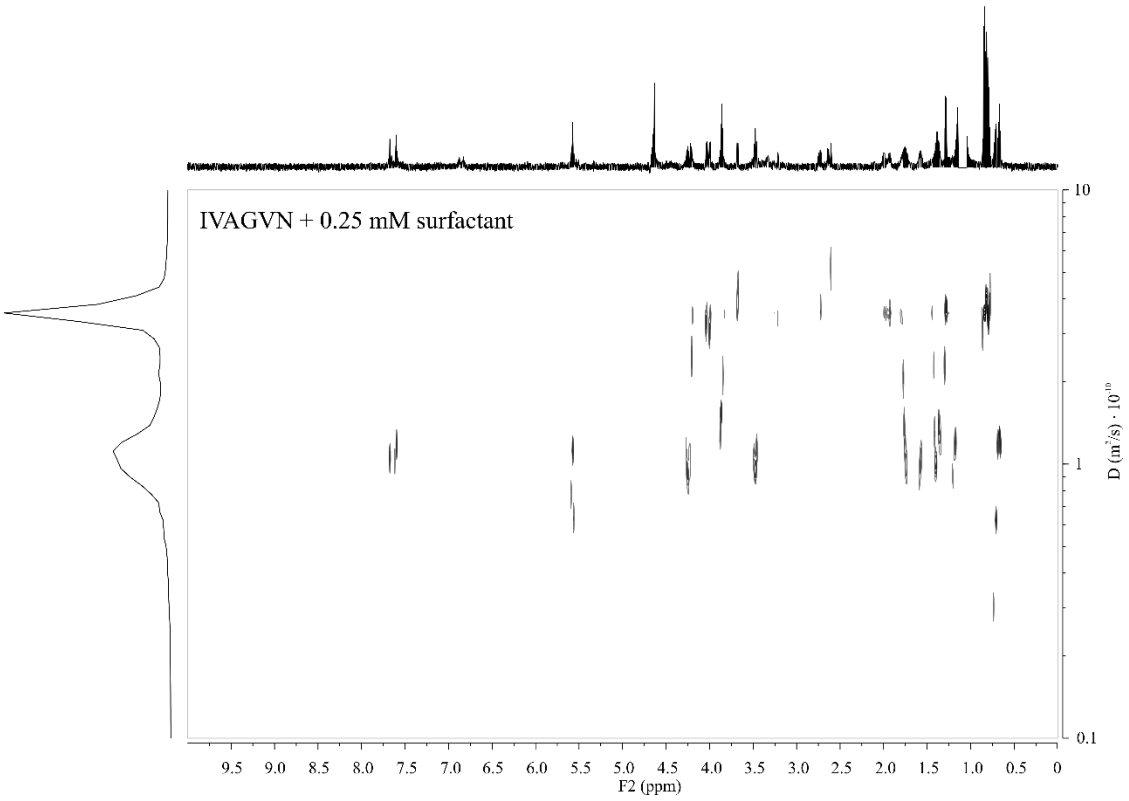
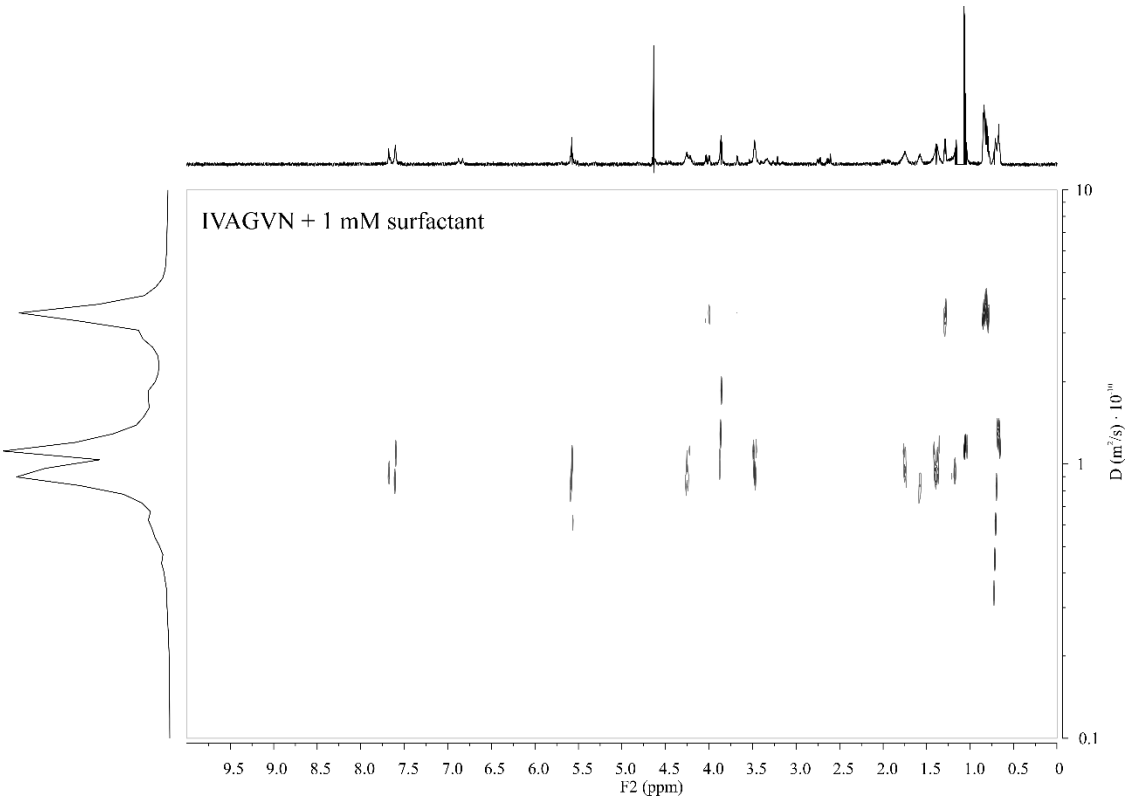
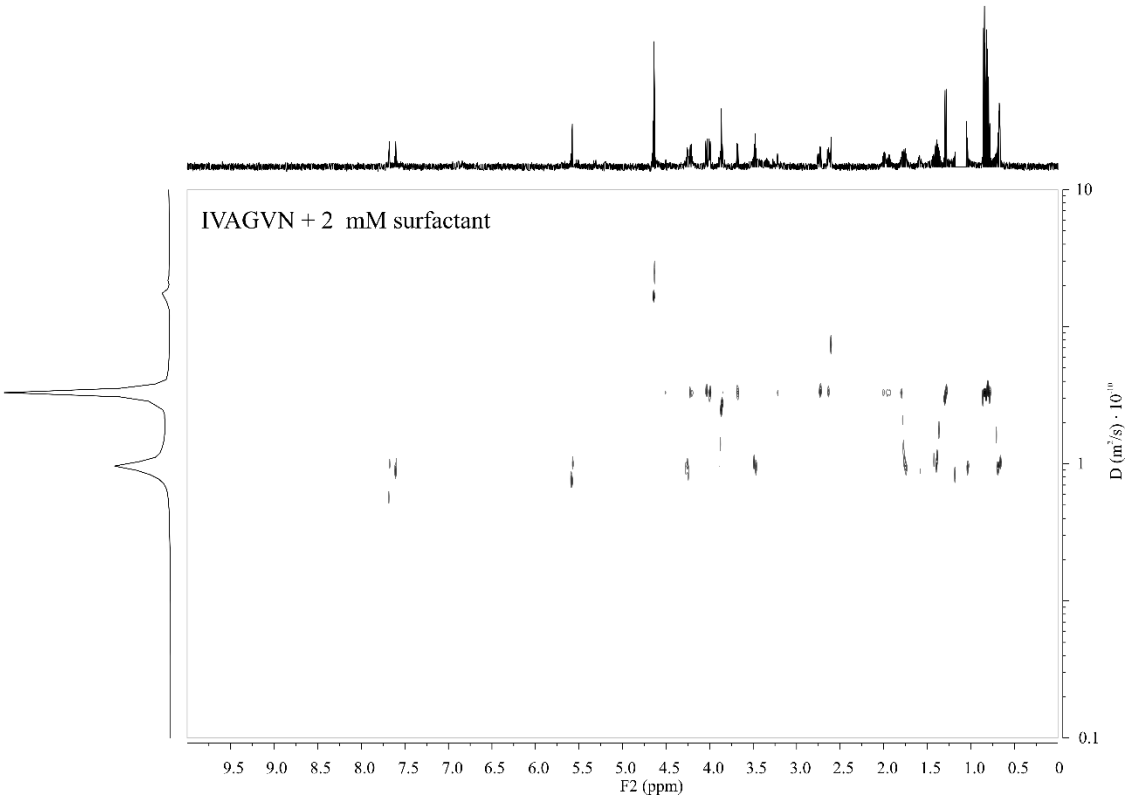



**Figure S2.** DOSY $^{1}$H NMR spectra for diffusion coefficient measurements of the peptide IVAGVN at various concentrations: 0.52 mM; 1.05 mM, 1.75 mM. 3.50 mM and 5.25 mM.


IVAGVN + 0 mM surfactant
10
1
0.1
D (m²/s) · 10⁻¹⁰
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
F2 (ppm)


IVAGVN + 0.25 mM surfactant
10
1
0.1
D (m²/s) · 10⁻¹⁰
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
F2 (ppm)


IVAGVN + 1 mM surfactant
10
1
0.1
D (m²/s) · 10¹⁰
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
F2 (ppm)


IVAGVN + 2 mM surfactant
10
1
0.1
D (m²/s) · 10¹⁰
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
F2 (ppm)

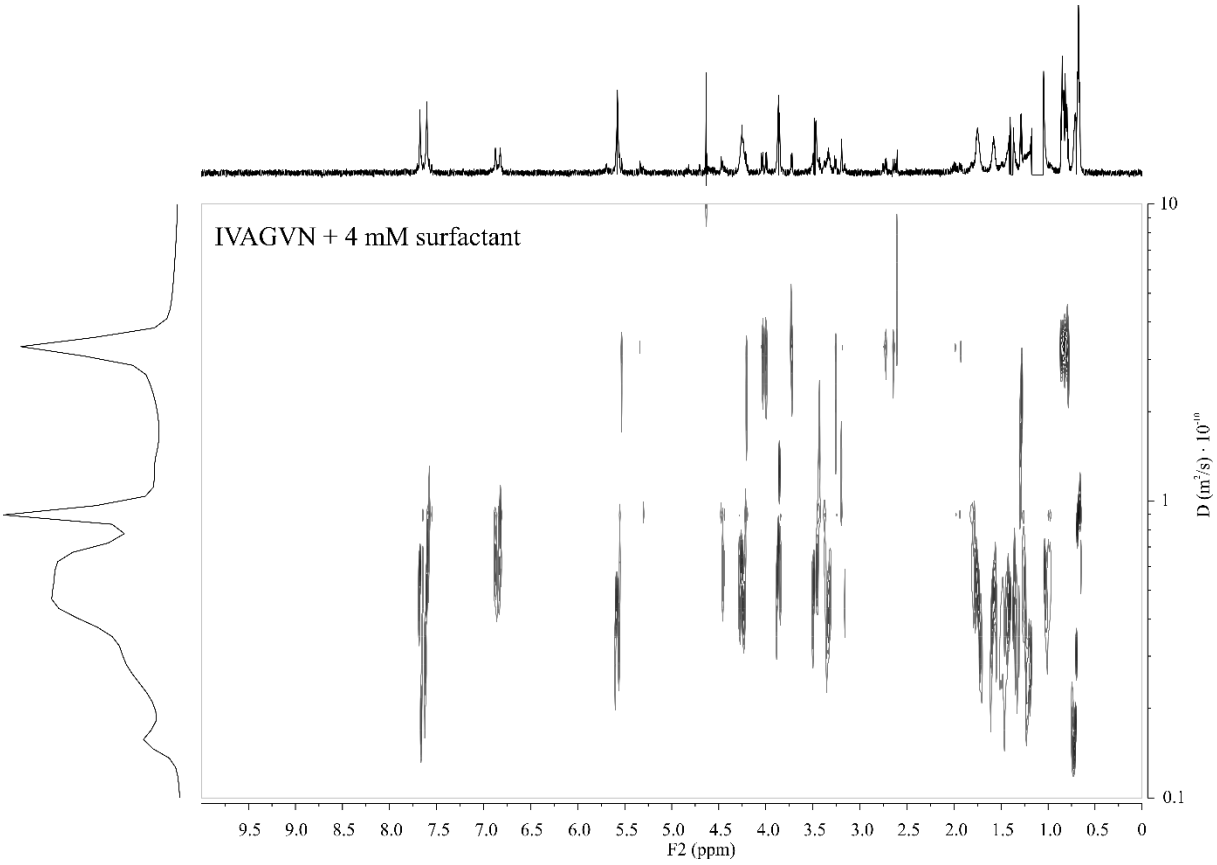



**Figure S3.** DOSY $^{1}$H NMR spectra for diffusion coefficient measurements of the peptide IVAGVN (0.52 mM) with the presence of different surfactant concentrations: 0 mM, 0.25 mM, 1.00 mM, 2.00 mM and 4.00 mM.