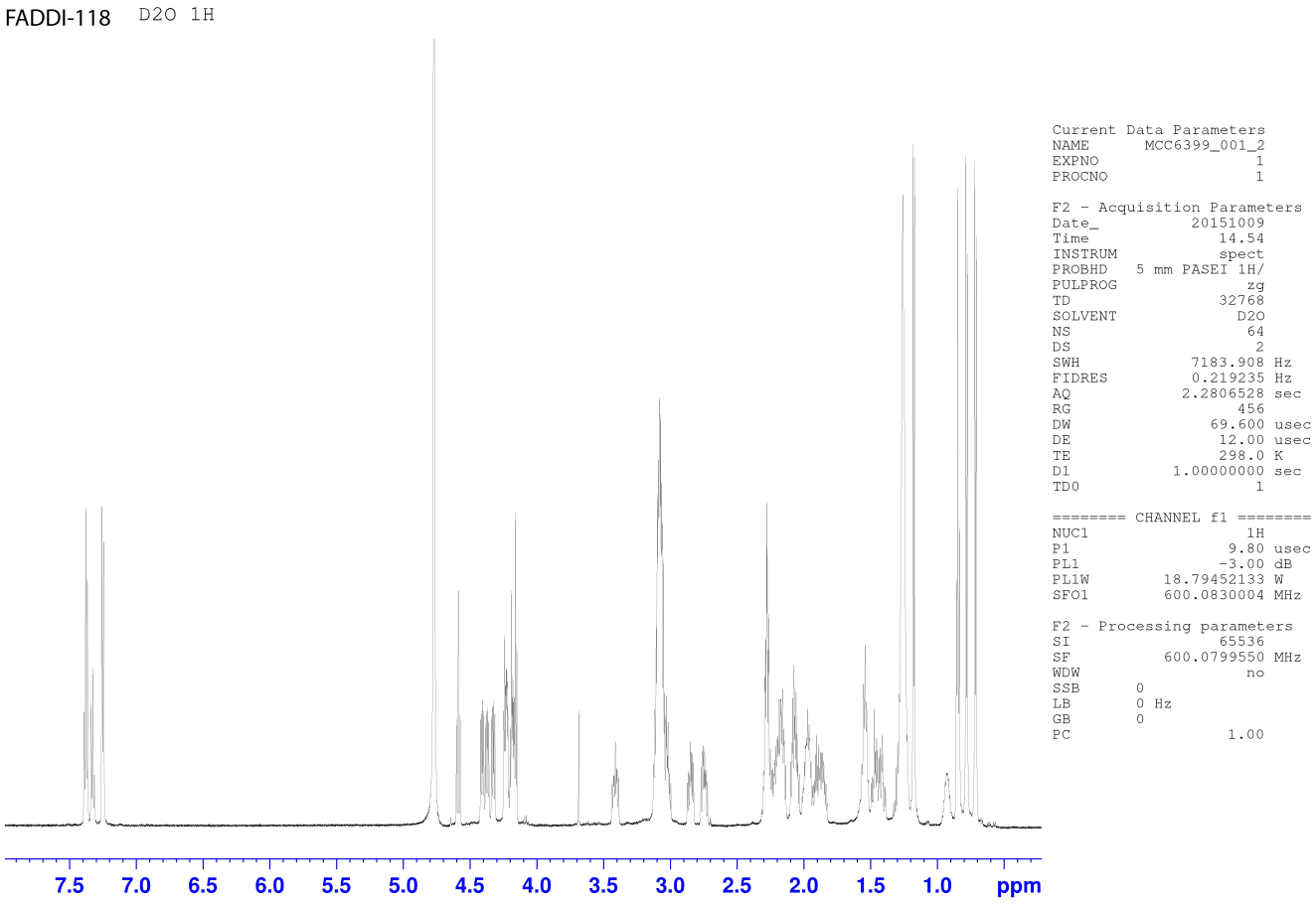
Data S1. NMR spectra, statistics and chemical shifts. Related to Figure 2

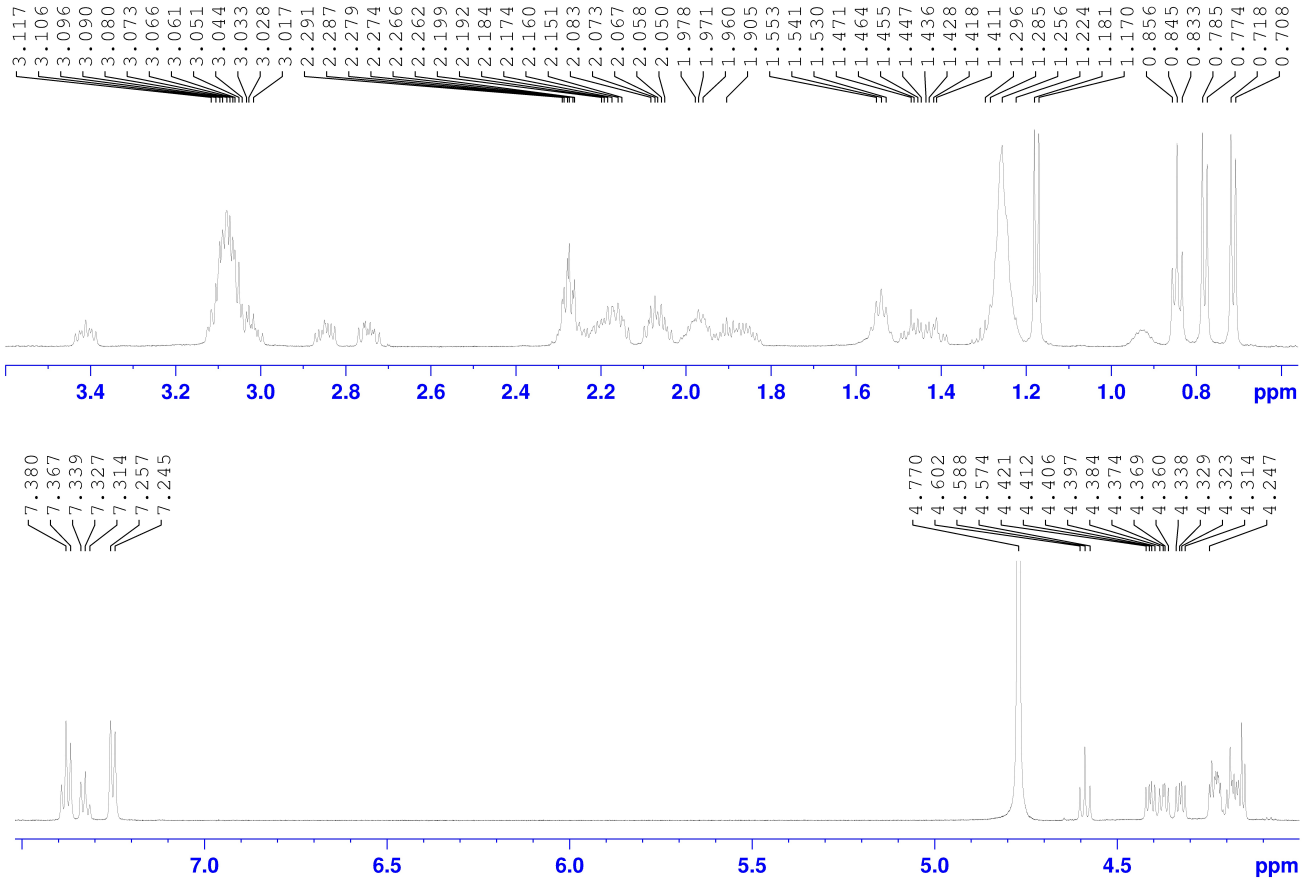
(A) 1 H NMR spectrum of FADDI-118 (D2 O, 600 MHz). **(B)** Expansions of 1 H NMR spectrum of FADDI-118 (D2 O, 600 MHz). **(C).** 13 C NMR spectrum of FADDI-118 (D2 O, 150 MHz). **(D)** Expansions of 13 C NMR spectrum of FADDI-118 (D2 O, 150 MHz). **(E)** COSY NMR spectrum of FADDI-118 (D2 O). **(F)** TOCSY NMR spectrum of FADDI-118 (D2 O). **(G)** edHSQC NMR spectrum of FADDI-118 (D2 O). **(H)** HMBC NMR spectrum of FADDI-118 (D2 O). **(I)** 1H and 13C Chemical shifts for octapeptin C4 peptide in water at 22°C. **(J)** NMR statistics for the solution structure of octapeptin C4 and FADDI-115 in DPC micelles. **(K)** NMR assignments of FADDI-118 TFA salt in D2O (1H 600 MHz, 13C 150 MHz) derived from analysis of 2D NMR spectra.

A



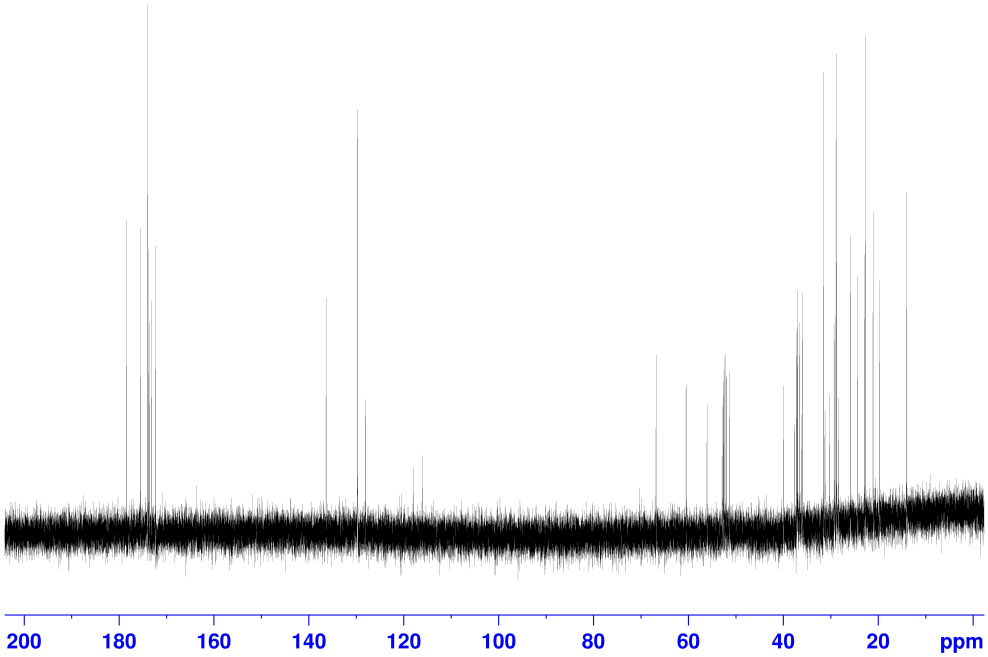
B

FADDI-118 D2O 1H



C

FADDI-118 D2O 13C

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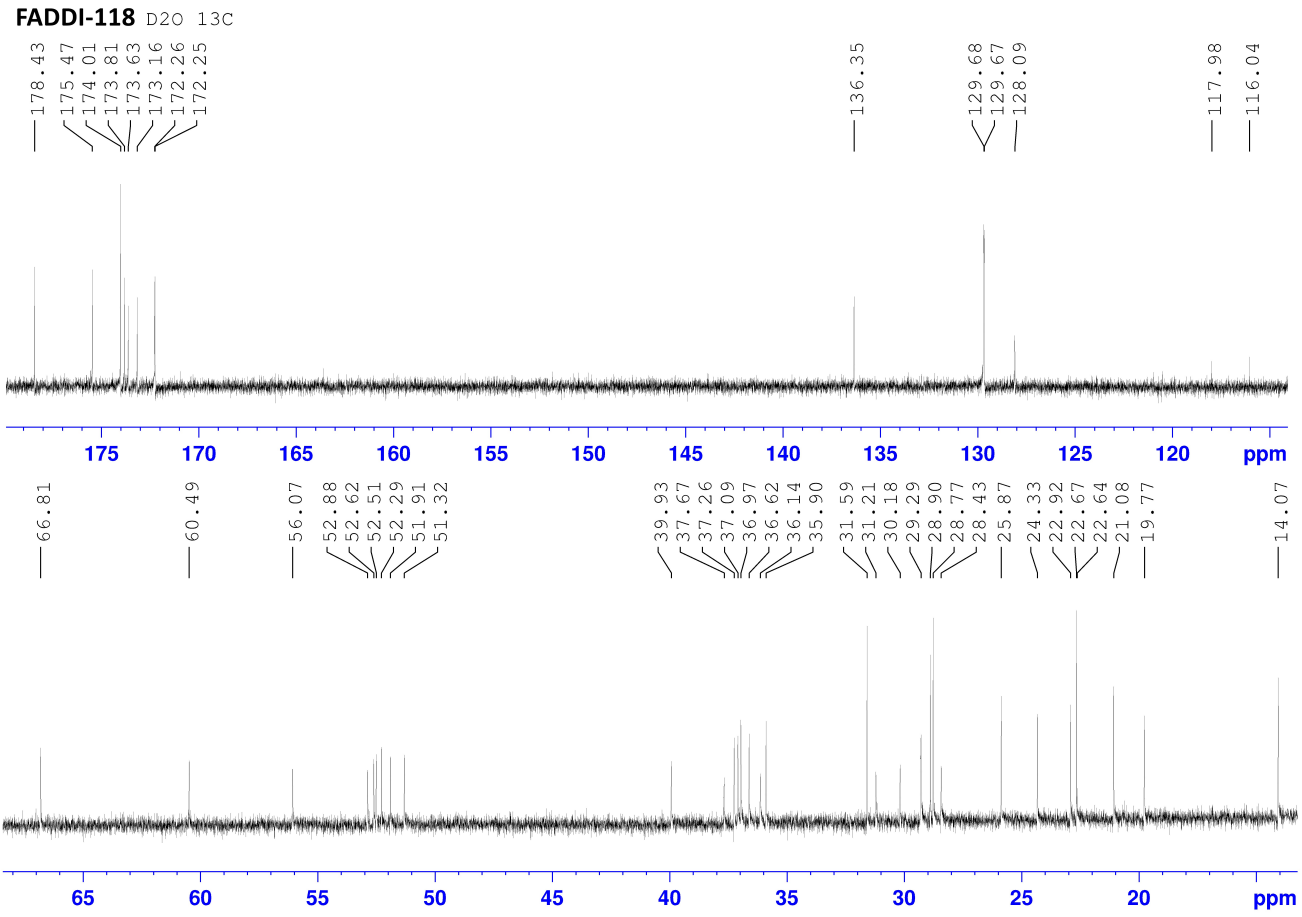
D


FADDI-118 D2O 13C
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173.81
173.63
173.16
172.26
172.25
136.35
129.68
129.67
128.09
117.98
116.04
175
170
165
160
155
150
145
140
135
130
125
120
ppm
66.81
60.49
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52.88
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51.32
39.93
37.67
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36.14
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31.59
31.21
30.18
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28.77
28.43
25.87
24.33
22.92
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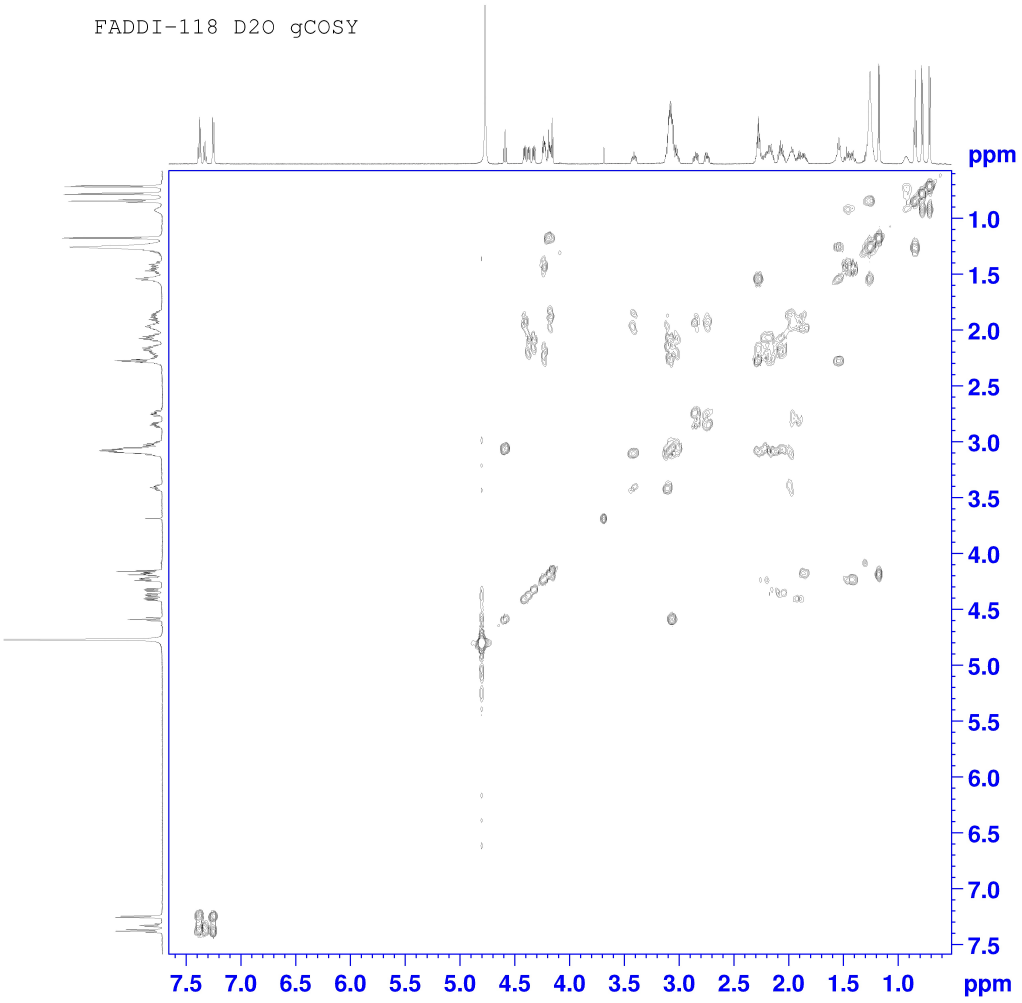
ppm

E

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TE                298.1 K
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GB        0
PC                  1.00

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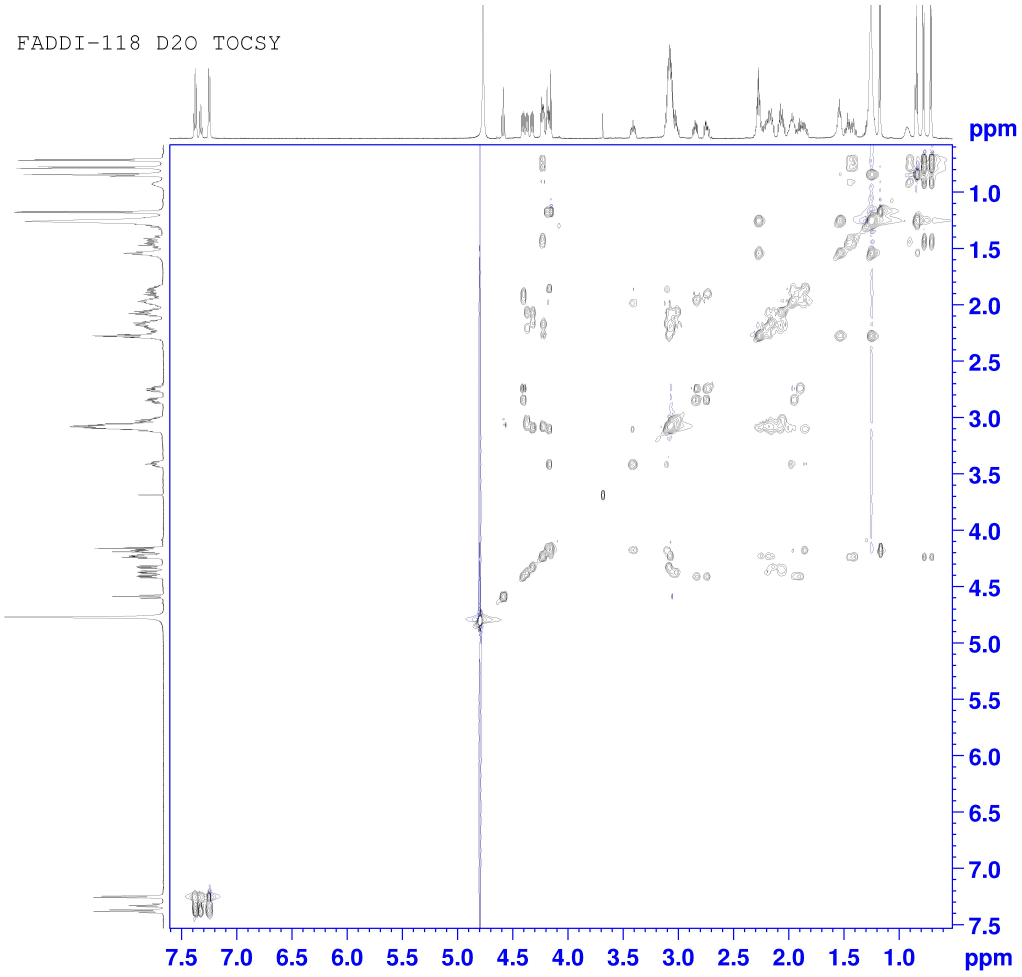
F

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DS                    16
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D12             0.00002000 sec
D16             0.00020000 sec
IN0             0.00013920 sec
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P2                 14.50 usec
P5                 18.68 usec
P6                 28.00 usec
P7                 56.00 usec
P12              2400.00 usec
P17              2500.00 usec
PL0               120.00 dB
PL1                 2.00 dB
PL10               13.74 dB
PL0W      0 W
PL1W          9.65199947 W
PL10W         0.64657265 W
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GPNAM[2]        sine.100
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GPZ2               11.00 %
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F1 - Acquisition parameters
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SFO1          600.133 MHz
FIDRES         56.124283 Hz
SW              11.971 ppm
FnMODE       States-TPPI

F2 - Processing parameters
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SF            600.1299364 MHz
WDW                 QSINE
SSB                     2
LB        0 Hz
GB        0
PC                   1.00

F1 - Processing parameters
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SSB                     2
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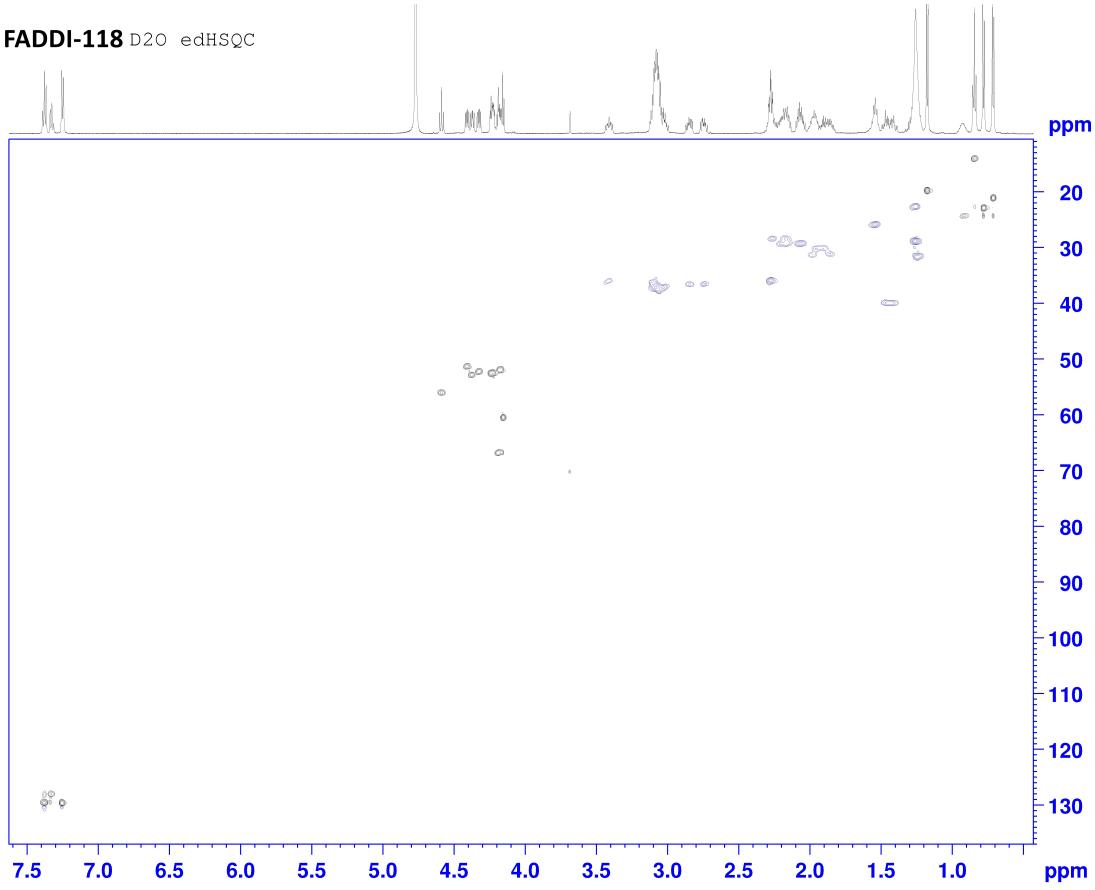
G



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TD 2048
SOLVENT D2O
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DS 32
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D11 0.03000000 sec
D16 0.00020000 sec
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D24 0.00092593 sec
IN0 0.00001950 sec
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P2 14.50 usec
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PLW 9.65199947 W
SFO1 600.1327006 MHz

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P24 2000.00 usec
P63 1500.00 usec
PLO 120.00 dB
PL2 -2.40 dB
PL12 13.21 dB
PLW0 0 W
PLW 120.04185486 W
PL12W 1.29862309 W
SFO2 150.9148808 MHz
SP3 4.47 dB
SP7 4.47 dB
SP14 4.95 dB
SP31 11.97 dB
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SPNAM[7] Crp60comp.4
SPNAM[14 Crp32,1.5,20.2
SPNAM[31 Crp32,1.5,20.2
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SPOAL7 0.500
SPOAL14 0.500
SPOAL31 0.500
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SPOFFS7 0 Hz
SPOFFS14 0 Hz
SPOFFS31 0 Hz

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GPNAM[4] sine.100
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GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
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P19 600.00 usec

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FIDRES 200.433823 Hz
SW 170.000 ppm
FnMODE Echo-Antiecho

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WDW QSINE
SSB 2
LB 0 Hz
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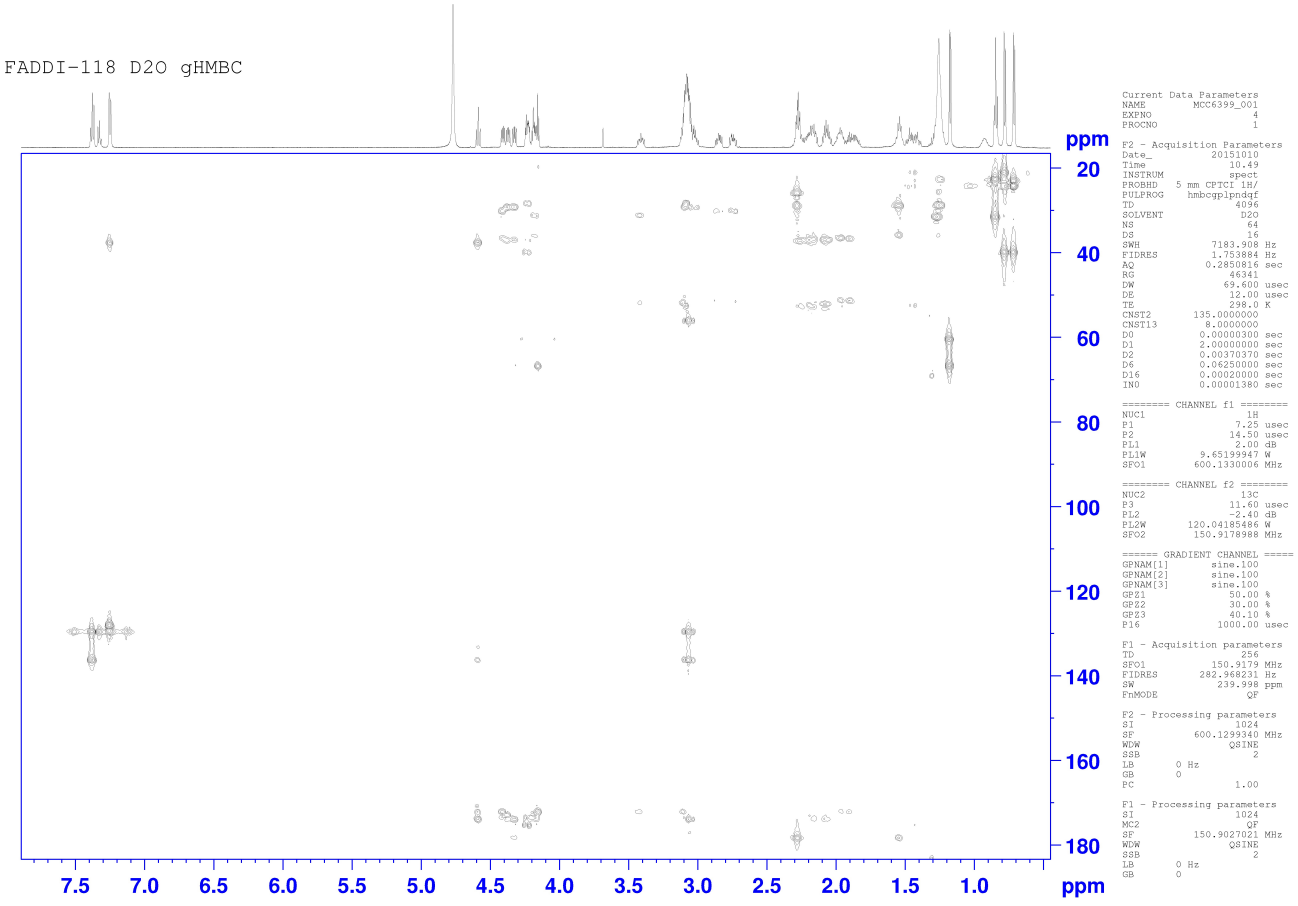
H

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======== CHANNEL f1 ========
NUC1                  1H
P1                  7.25 usec
P2                 14.50 usec
PL1                 2.00 dB
PL1W          9.65199947 W
SFO1        600.1330006 MHz

======== CHANNEL f2 ========
NUC2                 13C
P3                 11.60 usec
PL2                -2.40 dB
PL2W        120.04185486 W
SFO2        150.9178988 MHz

====== GRADIENT CHANNEL =====
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GPNAM[2]         sine.100
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GPZ2                30.00 %
GPZ3                40.10 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            150.9179 MHz
FIDRES          282.968231 Hz
SW                239.998 ppm
FnMODE                QF

F2 - Processing parameters
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SF            600.1299340 MHz
WDW                  QSINE
SSB                      2
LB        0 Hz
GB        0
PC                    1.00

F1 - Processing parameters
SI                   1024
MC2                    QF
SF            150.9027021 MHz
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SSB                      2
LB        0 Hz
GB        0
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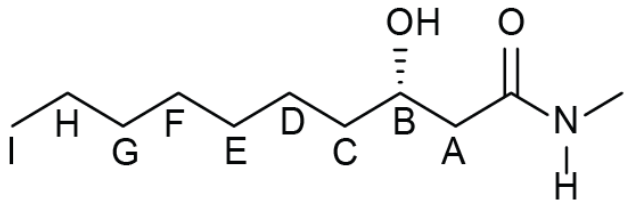
I

^{1}H and ^{13}C Chemical shifts for octapeptin C4 peptide in water at 22°C.



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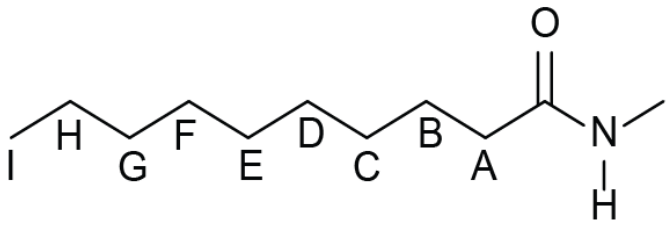
HDec	CB	71.58	2	CB	33.22	4	HN	8.78	7	CB	31.48
HDec	CC	38.88	2	CG	38.03	4	HZ	7.34	7	CG	39.08
HDec	CD	27.24	2	HA	4.15	4	QB	3.08	7	HA	4.32
HDec	CE	31.01	2	HB2	2	4	QD	7.26	7	HB2	2.15
HDec	CF	30.99	2	HB3	1.86	4	QE	7.4	7	HB3	2.03
HDec	CG	33.62	2	HD	7.92				7	HG2	3.06
HDec	CH	24.61	2	HG2	3.44	5	CA	54.39	7	HG3	3
HDec	CI	15.97	2	HG3	3.08	5	CB	41.89	7	HN	8.34
HDec	HA1	2.52	2	HN	8.56	5	CD1	24.78			
HDec	HA2	2.39				5	CD2	22.98	8	CA	55.62
HDec	HB	3.99	3	CA	53.13	5	CG2	26.13	8	CB	41.13
HDec	QC	1.51	3	CB	32.13	5	HA	4.24	8	CD1	24.46
HDec	HD1	1.3	3	CG	38.66	5	HG	0.87	8	CD2	23.55
HDec	HD2	1.39	3	HA	4.47	5	HN	8.56	8	CG2	26.84
HDec	QE	1.3	3	HB2	2	5	QB	1.44	8	HA	4.24
HDec	QF	1.27	3	HB3	1.93	5	QD1	0.78	8	HG	1.54
HDec	QG	1.26	3	HG2	2.89	5	QD2	0.71	8	HN	8.29
HDec	QH	1.28	3	HG3	2.77				8	QB	1.62
HDec	QI	0.86	3	HN	8.31	6	CA	54.72	8	QD1	0.92
1	CA	54.19				6	CB	30.28	8	QD2	0.87
1	CB	31.23	4	CA	58.16	6	CG	39.28			
1	CG	39.07	4	CB	39.34	6	HA	4.21			
1	HA	4.38	4	CD	131.53	6	HB2	2.26			
1	HB2	2.21	4	CE	131.48	6	HB3	2.2			
1	HB3	2.1	4	CZ	129.93	6	HN	8.42			
1	HN	8.52				6	QG	3.1			
1	QG	3.13									

The nomenclature of the *R*-3-hydroxydecanoyl (HDec) group is shown below. Protons with the same apparent chemical shift in the ^{1}H NMR spectrum are denoted by the pseudoatom Q.

^{1}H and ^{13}C Chemical shifts for FADDI-115 peptide in water at 22°C



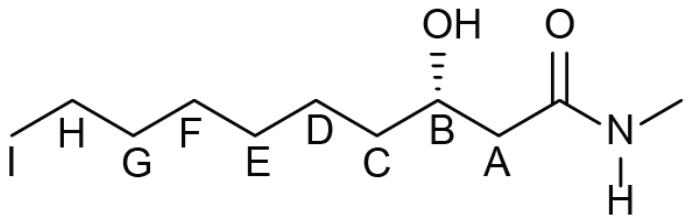
Res	Atom	Shift	Res	Atom	Shift	Res	Atom	Shift	Res	Atom	Shift
Dec	CA	38.42	2	CA	54.58	4	HA	4.57	7	CA	55.05
Dec	CB	28.36	2	CB	33.85	4	HN	8.72	7	CB	32.14
Dec	CC	31.62	2	CG	38.65	4	HZ	7.32	7	CG	39.79
Dec	C-DEF	31.82	2	HA	4.14	4	QB	3.07	7	HA	4.32
Dec	CG	34.34	2	HB2	1.96	4	QD	7.25	7	HB2	2.14
Dec	CH	25.24	2	HB3	1.84	4	QE	7.38	7	HB3	2.01
Dec	CI	16.6	2	HD	7.93				7	HG2	3.03
Dec	QA	2.28	2	HG2	3.44	5	CA	55.03	7	HG3	2.97
Dec	QB	1.54	2	HG3	3.06	5	CB	42.52	7	HN	8.33
Dec	QC	1.26	2	HN	8.58	5	CD1	25.4			
Dec	Q-DEF	1.27				5	CD2	23.61	8	CA	56.23
Dec	QG	1.27	3	CA	53.83	5	CG2	26.82	8	CB	41.82
Dec	QH	1.26	3	CB	32.72	5	HA	4.24	8	CD1	25.09
Dec	QI	0.84	3	CG	39.34	5	HG	0.9	8	CD2	24.17
			3	HA	4.42	5	HN	8.54	8	CG2	27.47
1	CA	54.91	3	HB2	1.96	5	QB	1.42	8	HA	4.23
1	CB	31.9	3	HB3	1.91	5	QD1	0.78	8	HG	1.52
1	CG	40.01	3	HG2	2.87	5	QD2	0.71	8	HN	8.26
1	HA	4.32	3	HG3	2.75				8	QB	1.59
1	HB2	2.16	3	HN	8.24	6	CA	55.38	8	QD1	0.91
1	HB3	2.08				6	CB	30.81	8	QD2	0.82
1	HN	8.43	4	CA	58.66	6	CG	39.68			
1	QG	3.1	4	CB	40.08	6	HA	4.18			
			4	CD	132.18	6	HB2	2.26			
			4	CE	132.11	6	HB3	2.17			
			4	CZ	130.56	6	HN	8.46			
						6	QG	3.1			

The nomenclature of the decanoyl (Dec) group is shown below. Protons with the same apparent chemical shift in the ^{1}H NMR spectrum are denoted by the pseudoatom Q.

$^{3}J_{HNH\alpha}$ (Hz) and ^{1}H amide temperature coefficients (ΔT_{HN}) x 10^{3} for octapeptin C4 and FADDI-115 peptide in water at 22°C

Octapeptin C4				FADDI-115		
Residue	$^{3}J_{HNH\alpha}$ (Hz)	ΔT_{HN} x 10^{3}		Residue	$^{3}J_{HNH\alpha}$ (Hz)	ΔT_{HN} x 10^{3}
1	6.75	-6.73 ± 0.25		1	6.3	-7.8 ± 0.14
2	6.86	-6.80 ± 0.25		2	6.98	-7.6 ± 0.17
3	8.28	-4.90 ± 0.25		3	7.4	-4.5 ± 0.13
4	5.8	-9.10 ± 0.08		4	5.90	-8.9 ± 0.14
5	8.12	-8.76 ± 0.03		5	7.89	-9.8 ± 0.22
6	5.3	-4.23 ± 0.06		6	6.5	-4.6 ± 0.09
7	4.4	-0.87 ± 0.13		7	5.12	-2.0 ± 0.13
8	6.38	-9.70 ± 0.13		8	6.7	-10.1 ± 0.23
2HD	8.2, 4.5	-8.40 ± 0.22		2HD	8.6,4.3	-8.6 ± 0.27

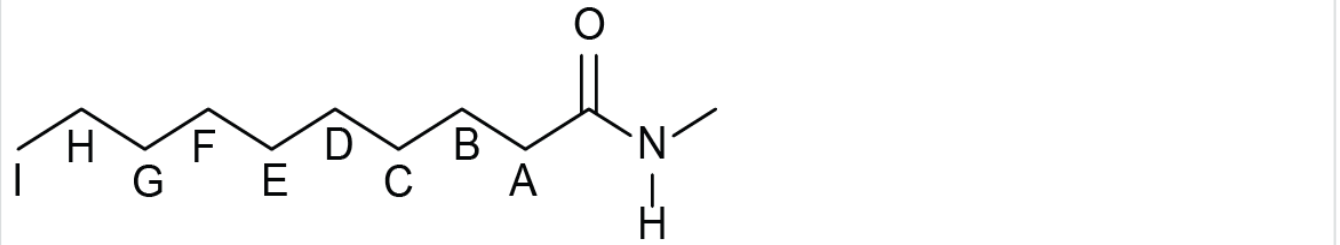
^{1}H and ^{13}C Chemical shifts for octapeptin C4 peptide in 120 mM DPC at 25ºC



Res	Atom	Shift	Res	Atom	Shift	Res	Atom	Shift	Res	Atom	Shift
Dec	CA	44.5	2	CA	52.09	4	HA	4.48	7	CA	53.31
Dec	CB	70.27	2	CB	30.73	4	HB2	2.96	7	CB	29.67
Dec	CC	38.37	2	CG	36.14	4	HB3	3.02	7	CG	37.44
Dec	CD	26.83	2	HA	3.92	4	HN	8.9	7	HA	4.25
Dec	CE	30.62	2	HB2	2.07	4	HZ	7.11	7	HB2	2.08
Dec	CF	31.13	2	HB3	1.92	4	QD	7.19	7	HB3	1.99
Dec	CG	32.93	2	HD	7.43	4	QE	7.21	7	HG2	3.01
Dec	CH	23.6	2	HG2	3.5				7	HN	8.42
Dec	CI	14.85	2	HG3	2.95	5	CA	52.19			
Dec	HA1	2.4	2	HN	8.51	5	CB	39.86	8	CA	53.85
Dec	HA2	2.3				5	CD1	24.02	8	CB	39.7
Dec	QB	3.88	3	CA	51.57	5	CD2	22.07	8	CD1	23.62
Dec	HC1	1.48	3	CB	29.78	5	CG2	25.56	8	CD2	22.1
Dec	HC2	1.43	3	CG	37.18	5	HA	4.29	8	CG2	25.98
Dec	HD1	1.43	3	HA	4.42	5	HG	1.49	8	HA	4.12
Dec	HD2	1.28	3	HB2	1.97	5	HN	8.14	8	HG	1.52
Dec	QE	1.26	3	HB3	1.95	5	QB	1.43	8	HN	8.09
Dec	QF	1.18	3	HG3	2.87	5	QD1	0.77	8	QB	1.64
Dec	QG	1.24	3	HN	7.98	5	QD2	0.7	8	QD1	0.89
Dec	QH	1.24							8	QD2	0.82
Dec	QI	0.83	4	CA	56.07	6	CA	53.94			
1	CA	53.86	4	CB	37.64	6	CB	29.02			
1	CB	29.04	4	CD	130.26	6	CG	37.67			
1	CG	37.61	4	CE	129.27	6	HA	4.22			
1	HA	4.19	4	CZ	127.49	6	HB2	2.17			
1	HB2	2.11				6	HB3	2.14			
1	HB3	2.08				6	HN	8.53			
1	HN	8.86				6	QG	3.1			
1	QG	3.04									

The nomenclature of the R-3-hydroxydecanoyl (HDec) group is shown below. Protons with the same apparent chemical shift in the ^{1}H NMR spectrum are denoted by the pseudoatom Q.

^{1}H and ^{13}C Chemical shifts for FADDI-115 peptide in 120 mM DPC at 25ºC



Res	Atom	Shift	Res	Atom	Shift	Res	Atom	Shift	Res	Atom	Shift
Dec	CA	36.15	2	CA	51.47	4	HA	4.51	7	CA	54.05
Dec	CB	26.42	2	CB	30.82	4	HN	8.72	7	CB	29.54
Dec	CC	30.69	2	CG	35.97	4	HZ	7.11	7	HA	4.26
Dec	C-DEF	31.28	2	HA	4.09	4	QB	2.97	7	HB2	2.08
Dec	CG	32.92	2	HB2	2.12	4	QD	7.2	7	HB3	1.97
Dec	CH	23.69	2	HB3	1.81	4	QE	7.2	7	HG2	3.03
Dec	CI	14.88	2	HG2	3.51				7	HG3	3
Dec	HA2	2.29	2	HG3	2.95	5	CB	39.7	7	HN	8.79
Dec	HA3	2.18	2	HN	8.65	5	CD1	23.99			
Dec	HB2	1.52	2	HND	7.43	5	CD2	22.14	8	CA	53.58
Dec	HB3	1.47				5	CG2	30.36	8	CB	39.83
Dec	QC	1.23	3	CA	51.9	5	HA	4.35	8	CD1	23.56
Dec	Q-DEF	1.21	3	CB	29.61	5	HB2	1.47	8	CD2	22.01
Dec	QG	1.23	3	CG	37.21	5	HB3	1.44	8	CG2	25.33
Dec	QH	1.23	3	HA	4.36	5	HG	1.16	8	HA	4.17
Dec	QI	0.82	3	QB	1.94	5	HN	8.33	8	HB2	1.66
			3	QG	2.84	5	QD1	0.8	8	HB3	1.62
1	CA	53.55	3	HN	7.96	5	QD2	0.72	8	HG	1.49
1	CB	29.23							8	HN	8.06
1	CG	37.64	4	CA	55.58	6	CA	53.29	8	QD1	0.89
1	HA	4.13	4	CB	37.66	6	CB	28.8	8	QD2	0.81
1	HN	8.71	4	CD	130.1	6	CG	37.53			
1	QB	2.11	4	CE	129.2	6	HA	4.26			
1	QG	3.08	4	CZ	127.36	6	HN	8.59			
						6	QB	2.17			
						6	QG	3.09			

The nomenclature of the decanoyl (Dec) group is shown below. Protons with the same apparent chemical shift in the ^{1}H NMR spectrum are denoted by the pseudoatom Q.

J

NMR statistics for the solution structure of octapeptin C4 and FADDI-115 in DPC micelles.

NOE distance restraints	**Octapeptin C4**	**FADDI-115**
Total Number	217	192
Intra residual, |i – j|=0	60	53
Sequential, |i – j|=1	83	88
Mediumrange,1<|i – j|<5	41	33
Long range[a], |i – j| ≥ 5	36	21
Maximal violation	0.06	0.12
Final CYANA target function value	0.0084+/-0.0009Å^2	0.12+/-0.0003Å^2
RMSD to mean coordinates:		
Back bone atoms N,C$^\alpha$,C'	0.05+/-0.01Å	0.06+/-0.01Å
All heavy atoms	0.38+/-0.05Å	0.38+/-0.08Å

[a]4 upper and 3 lower distance restraints were implemented to maintain an amide bond with trans geometry between Dab3 and Leu9 during the calculation and are included in the table.

K

NMR assignments of FADDI-118 TFA salt in D_2O (^1H 600 MHz, ^{13}C 150 MHz) derived from analysis of 2D NMR spectra.[a]

Amino Acid[b]	^{13}C δ (ppm)[c]	^1H δ (mult., *J* (Hz))[d]	Amino Acid[b]	^{13}C δ (ppm)[c]	^1H δ (mult., *J* (Hz))[d]
Dab1			**Dab1**		
1	174.0*		**1**	173.6	
2	52.3	4.33 (dd, 5.4, 9.2)	**2**	52.6	4.24 (dd, o)
3	29.3*	2.07 (m) 2.15 (m)	**3**	28.4	2.19 (m) 2.25 (m)
4	37.0 [e]	3.09 (m)	**4**	36.9 [e]	3.08 (o)
Dab2			**Dab7**		
1	173.8		**1**	173.2	
2	51.9	4.17 (o)	**2**	52.9	4.37 (dd, 5.8, 8.8)
3	31.2	1.86 (m) 1.99 (m)	**3**	29.3*	2.07 (m) 2.19 (m)
4	36.1	3.10 (o) 3.41 (ddd, 6.7, 9.3, 14.4)	**4**	37.3	3.02 (o) 3.05 (o)
Dab3			**Thr8**		
1	172.26		**1**	172.25	
2	51.3	4.41 (dd, 5.4, 9.2)	**2**	60.1	4.16 (d, 5.4))
3	30.2	1.88 (m) 1.92 (m)	**3**	39.2	4.19 (o)
4	36.6	2.75 (ddd, 6.7, 9.3, 13.0) 2.85 (ddd, 5.1, 9.7, 13.0)	**4**	19.8	1.18 (d, 6.3)
Phe4			***n*-C8 fatty acid**		
1	174.0*		**1**	178.4	
2	56.1	4.59 (t, 8.2)	**2**	35.9	2.28 (o)
3	37.7	3.06 (o)	**3**	25.9	1.54 (tt, 6.5, 6.5)
4	136.4		**4**	29.9	1.26 (o)
7	128.1	7.33 (dd, 7.5, 7.5)	**5**	28.8	1.26 (o)
5,9	129.67	7.25 (d, 7.5)	**6**	31.6	1.24 (o)
6,8	129.68	7.38 (dd, 7.5, 7.5)	**7**	22.7	1.25 (o)
Leu5			**8**	14.1	0.85 (t, 7.1)
1	175.5				
2	52.5	4.24 (o)			
3	39.9	1.41 (ddd, 4.5, 10.8, 14.0) 1.47 (ddd, 4.5, 10.4, 14.0)			
4	24.3	0.90 (br m)			
5	21.1	0.71 (d, 6.5)			
6	22.9	0.78 (d, 6.5)			

[a] The ^1H and ^{13}C NMR spectra were externally calibrated to NaOAc (δ_H 1.90 and 8.44 and δ_C 24.0 and 171.7; 10 mg in 500 μL D_2O) (H. E. Gottlieb, V. Kotlyar and A. Nudelman, *J. Org. Chem.*, 1997, **62**, 7512). [b] Numbering from the carbonyl group of the amino acids. [c] ^{13}C NMR chemical shifts quoted to one decimal except where resonances resolved, [d] s = singlet, d = doublet, t = triplet, o = overlap. [e] assignment may be interchanged, * = co-incident resonances.