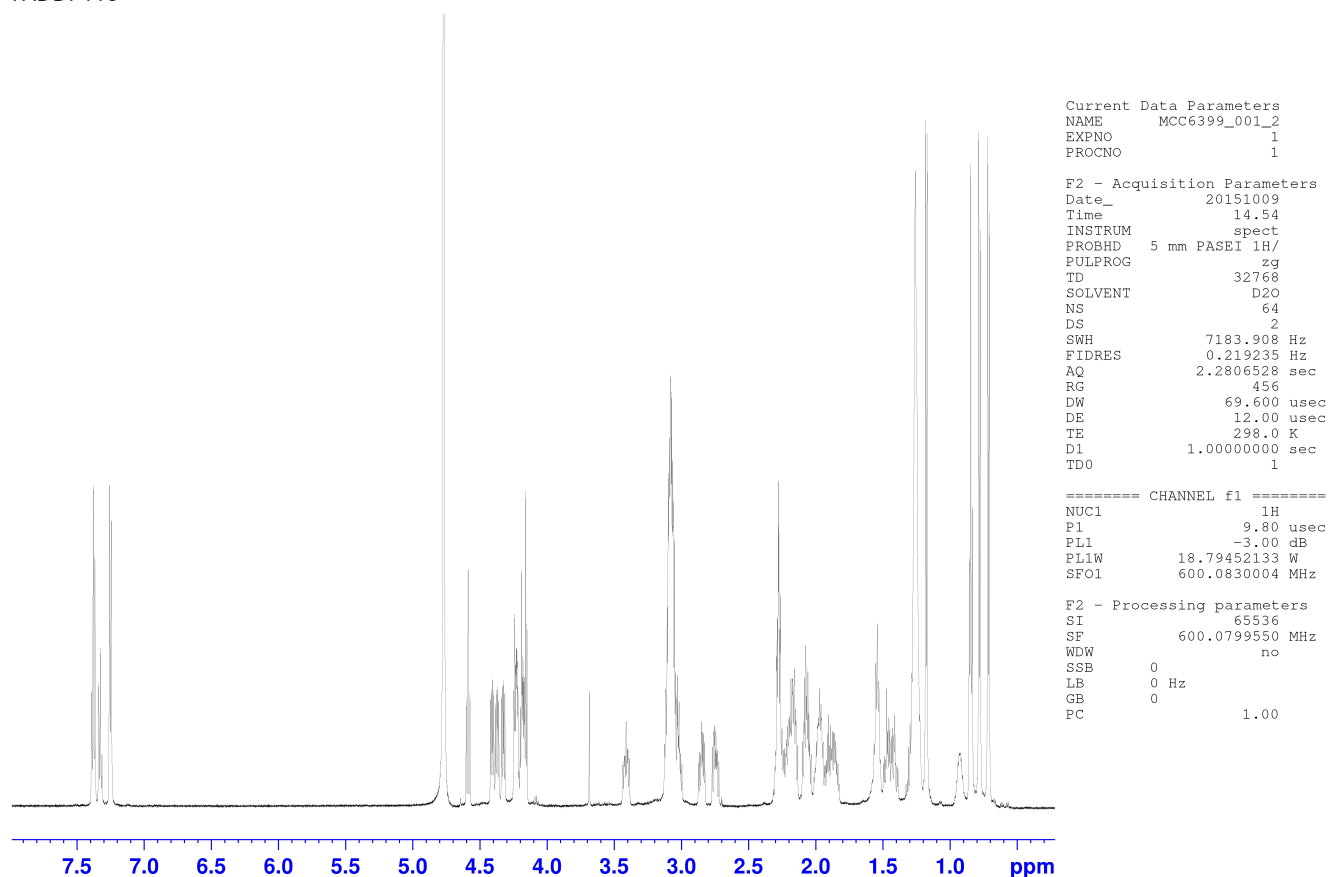


## Data S1. NMR spectra, statistics and chemical shifts. Related to Figure 2

**(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.

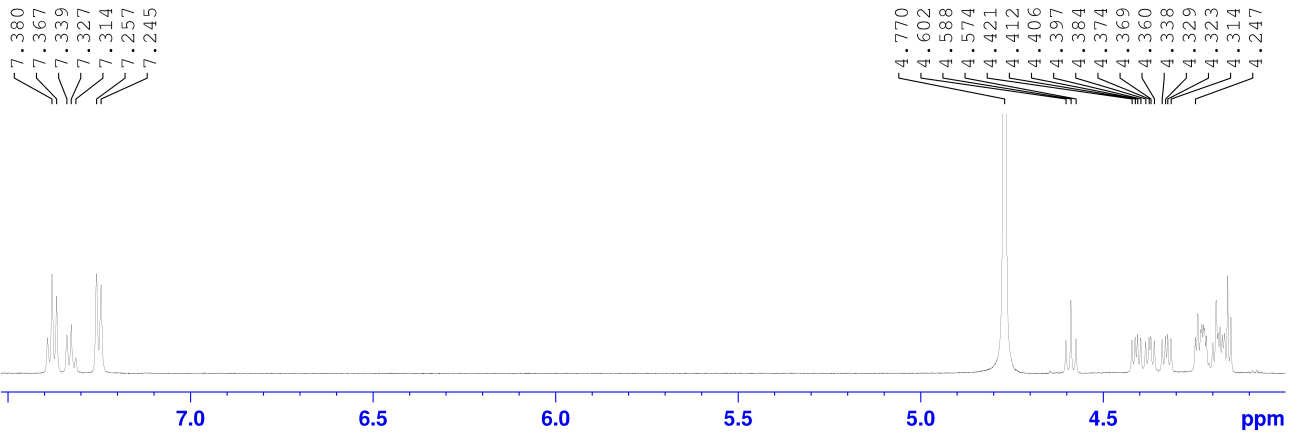
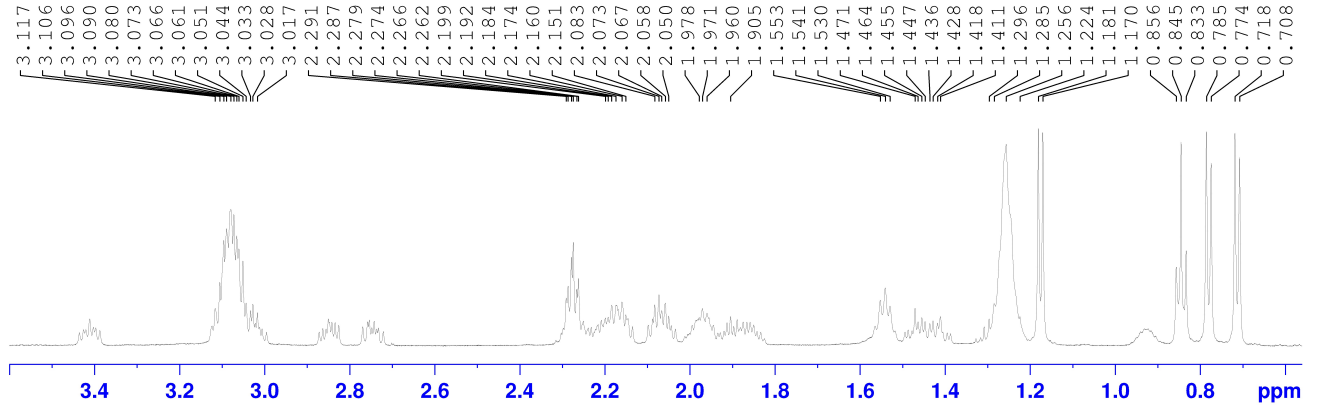
**A**

FADDI-118 D2O 1H



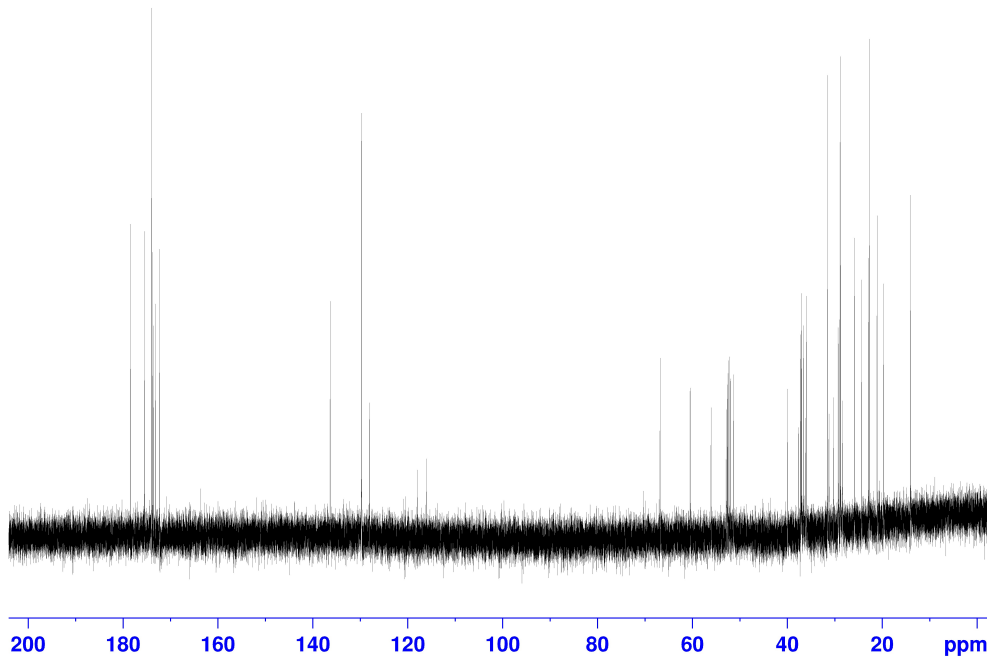
**B**

FADDI-118 D2O 1H



C

FADDI-118 D2O 13C



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Current Data Parameters
NAME      MCC6399_001
EXPNO     7
PROCNO    1

F2 - Acquisition Parameters
Date_     20151010
Time      10.45
INSTRUM   spect
PROBHD    5 mm CPTCI 1H/
PULPROG   zgpg
TD         65536
SOLVENT   D2O
NS         7000
DS         4
SWH        39062.500 Hz
FIDRES     0.596046 Hz
AQ         0.8388608 sec
RG         6502
DW         12.800 usec
DE         21.96 usec
TE         298.0 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1

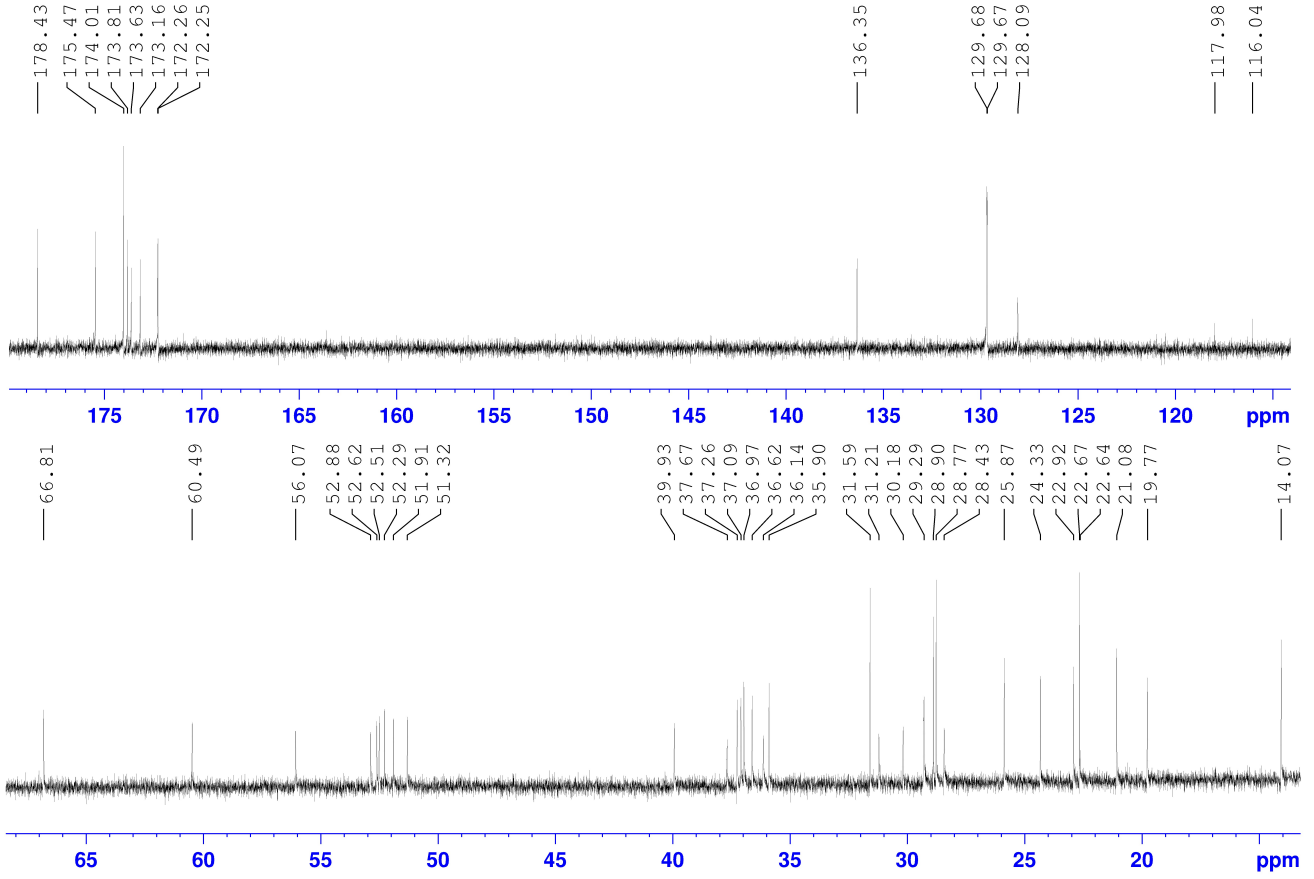
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NUC1       13C
P1         12.00 usec
PL1        -2.40 dB
PL1W       120.04185486 W
SFO1       150.9194078 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2       1H
PCPD2      80.00 usec
PL2         2.00 dB
PL12        16.83 dB
PL13         120.00 dB
PL2W        9.65199947 W
PL12W       0.31740758 W
PL13W       0 W
SFO2       600.1330006 MHz

F2 - Processing parameters
SI         65536
SF         150.9026950 MHz
WDW        no
SSB        0
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GB         0
PC         1.00
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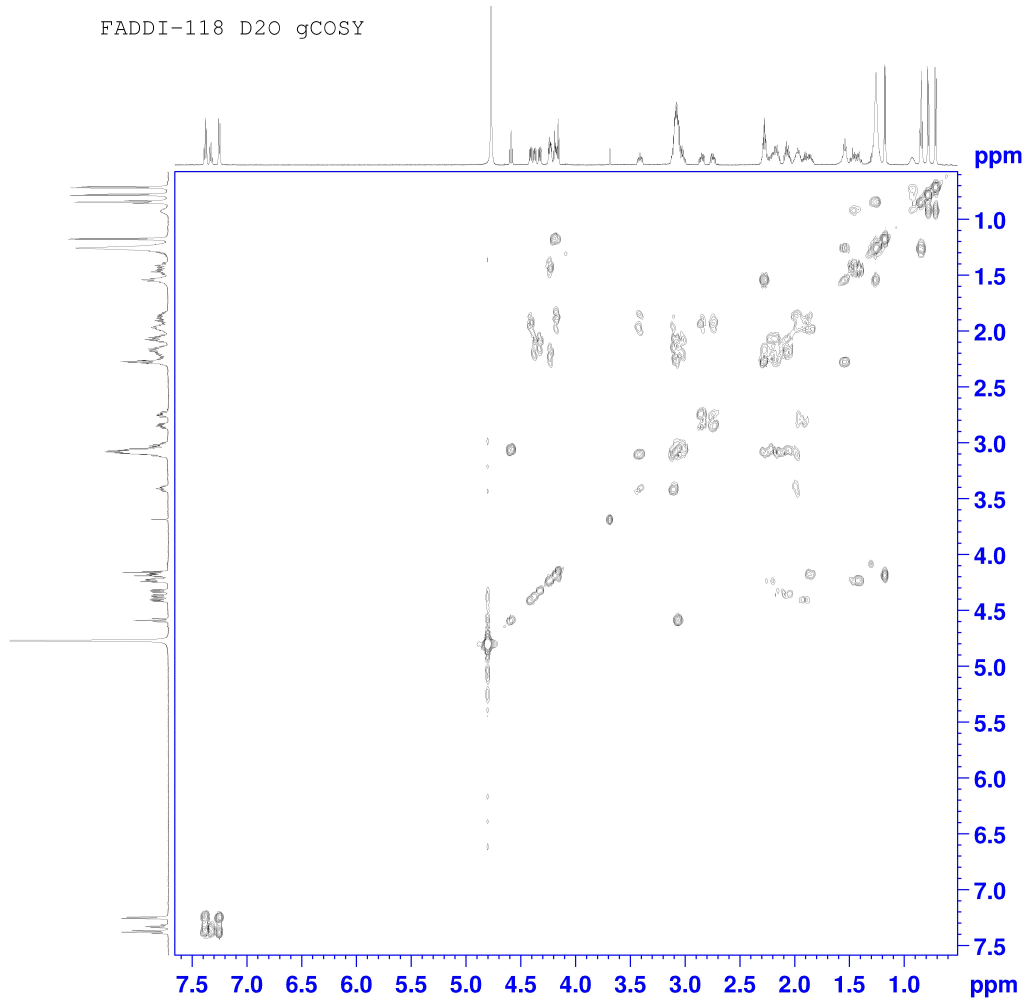
D

FADDI-118 D2O 13C



E

FADDI-118 D2O gCOSY



```
Current Data Parameters
NAME      MCC6399_001
EXPNO    2
PROCNO   1

F2 - Acquisition Parameters
Date_    20151008
Time     17.53
INSTRUM  spect
PROBHD   5 mm CPTCI 1H/
PULPROG  cosygpgf
TD       2048
SOLVENT  D2O
NS       8
DS       8
SWH      7183.908 Hz
FIDRES   3.507768 Hz
AQ       0.1425408 sec
RG       812.7
DW       69.600 usec
DE       12.00 usec
TE       298.1 K
D0       0.0000300 sec
D1       1.00000000 sec
D13      0.00000400 sec
D16      0.00020000 sec
IN0      0.00013920 sec

===== CHANNEL f1 =====
NUC1     1H
PQ       7.25 usec
F1       7.25 usec
PL1      2.00 dB
PL1W     9.65199947 W
SFO1     600.1330006 MHz

===== GRADIENT CHANNEL =====
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GPZ1     10.00 %
P16      1000.00 usec

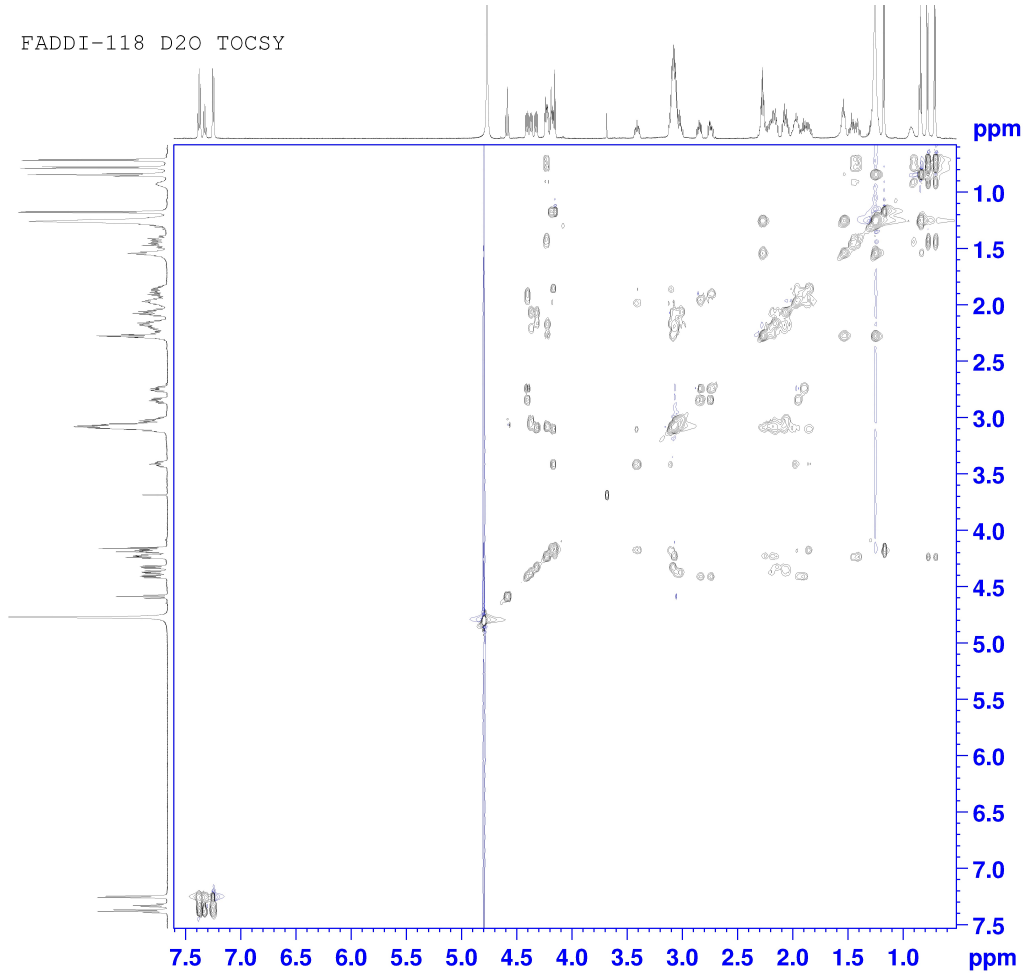
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TD       256
SFO1     600.133 MHz
FIDRES   56.124283 Hz
SW       11.971 ppm
FnMODE   QF

F2 - Processing parameters
SI       1024
SF       600.1299348 MHz
WDW      QSINE
SSB      0
LB       0 Hz
GB       0
PC       1.00

F1 - Processing parameters
SI       1024
MC2      QF
SF       600.1299369 MHz
WDW      QSINE
SSB      0
LB       0 Hz
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F

FADDI-118 D2O TOCSY



```
Current Data Parameters
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EXPNO    5
PROCNO   1

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Date_    20151008
Time     20.52
INSTRUM  spect
PROBHD   5 mm CPTCI 1H/
PULPROG  mlevaegpph
TD       2048
SOLVENT  D2O
NS       16
DS       16
SWH      7183.908 Hz
FIDRES   3.507768 Hz
AQ       0.1425408 sec
RG       574.7
DW       69.600 usec
DE       12.00 usec
TE       298.0 K
D0       0.0000498 sec
D1       2.0000000 sec
D9       0.0800000 sec
D12      0.0002000 sec
D16      0.0002000 sec
IN0      0.00013920 sec
LI       42

----- CHANNEL f1 -----
NUC1     1H
P1       7.25 usec
P2       14.50 usec
P5       15.65 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
PL1W     0 W
PL1W     9.65199947 W
PL1W     0.64657265 W
SFO1     600.1330006 MHz
SF1      41.76 dB
SFNAM[1] Sincl1.1000
SFOAL1   0 Hz
SFOFFS1  0.500

===== GRADIENT CHANNEL =====
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GFNAM[2]  sine.100
GPZ1     31.00 %
GPZ2     11.00 %
P16     1000.00 usec

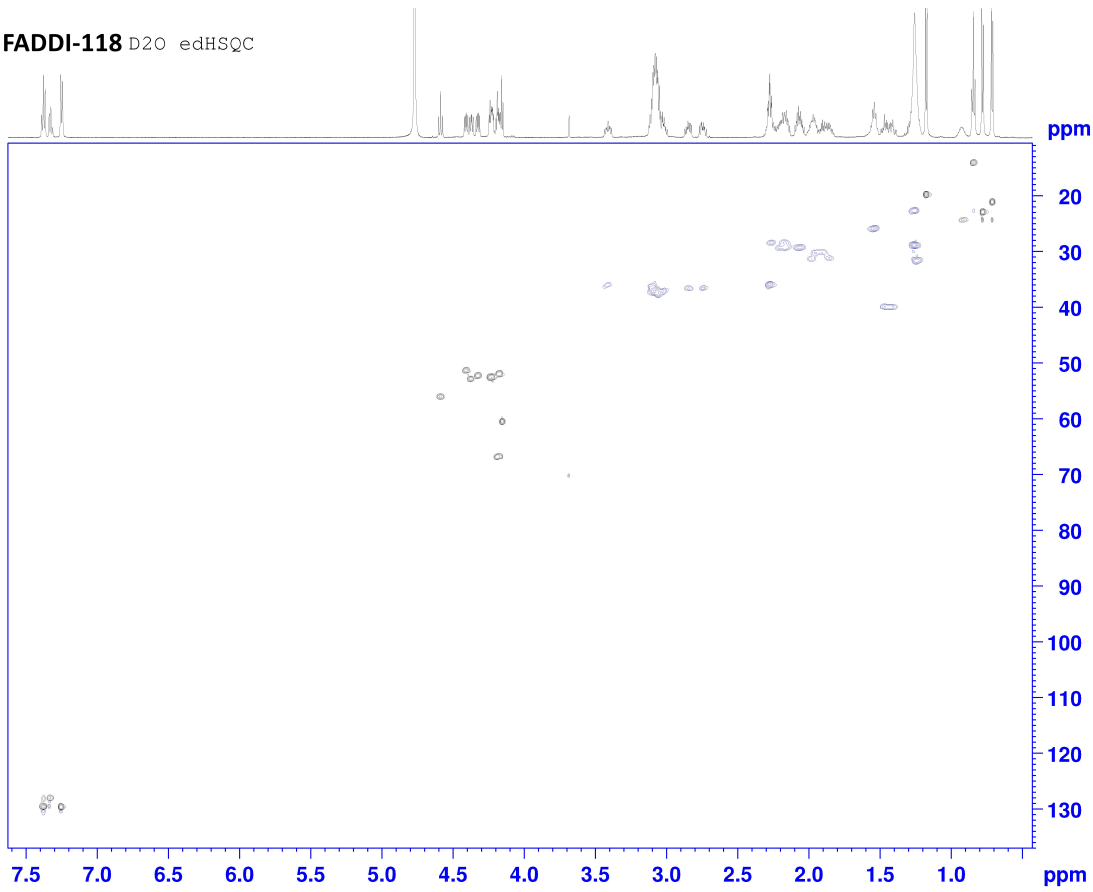
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FIDRES   56.124283 Hz
SN       11.971 ppm
F2MODE   States-TPPI

F2 - Processing parameters
SI       1024
SF       600.129364 MHz
WDW      QSINE
SSB      2
LB       0 Hz
GB       0
PC       1.00

F1 - Processing parameters
SI       1024
MC2     States-TPPI
SF       600.129347 MHz
WDW      QSINE
SSB      2
LB       0 Hz
GB       0
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G

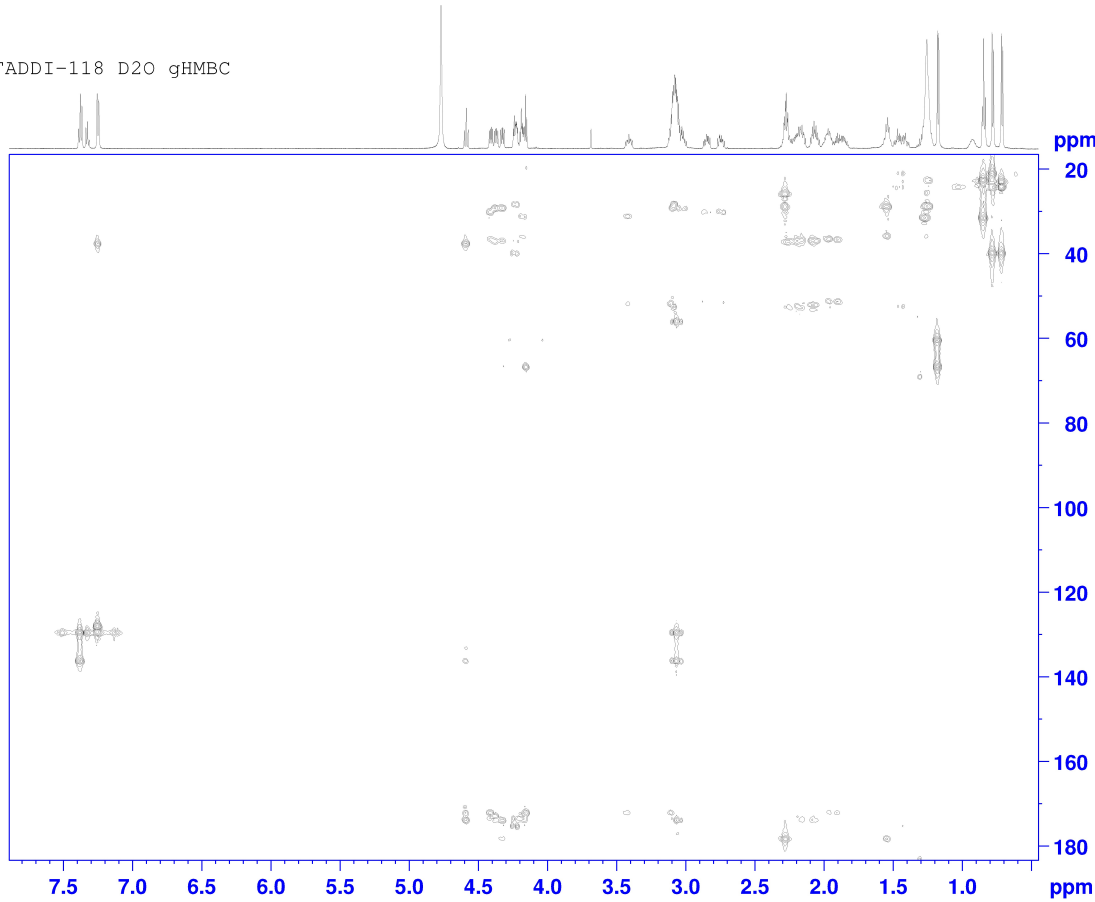
FADDI-118 D2O edHSQC



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PROCNO   1
F2 - Acquisition Parameters
Date_    20110908
Time     18.16
INSTRUM  spect
PROBHD   5 mm CPT1 1H/
PULPROG  zgpg30
TD        65536
SOLVENT  D2O
NS        16
DS        4
SFO1     718.908 MHz
FIDRES   0.007168 Hz
AQ        0.1415408 sec
RG         500
SWH       49.600 usec
TE        12.00 usec
TE        298.0 K
CHU1     135.9000000
CHU2     -0.5000000
D1        0.0000000 sec
D2        0.0018185 sec
D3        0.0000000 sec
D4        0.0018185 sec
D5        0.0000000 sec
D6        0.0000000 sec
D7        0.0000000 sec
D8        0.0000000 sec
D9        0.0000000 sec
D10       0.0000000 sec
D11       0.0000000 sec
D12       0.0000000 sec
D13       0.0000000 sec
D14       0.0000000 sec
D15       0.0000000 sec
D16       0.0000000 sec
D17       0.0000000 sec
D18       0.0000000 sec
D19       0.0000000 sec
D20       0.0000000 sec
L31       1
===== CHANNEL f1 =====
NUC1      1H
P1        7.12 usec
PC        14.50 usec
PL1       0 usec
PL2       2.00 dB
PL3       0.6199947 dB
PL4       600.1317006 MHz
===== CHANNEL f2 =====
CPDPRG2  zgpg30
NUC2      13C
P2        11.80 usec
PC        11.80 usec
PL2       2000.00 usec
PL3       1500.00 usec
PL4       120.00 dB
PL5       -2.40 dB
PL6       13.21 dB
PL7       0 W
PL8       100.0418586 W
PL9       3.2986208 MHz
SFO1     150.9188008 MHz
SFO2     4.47 MHz
SFO3     4.47 MHz
SFO4     3.85 MHz
SFO5     11.97 MHz
SFO6     0.2001 MHz
SFO7     0.2001 MHz
SFO8     0.2001 MHz
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SFO12    0.2001 MHz
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F2       718.908 MHz
F3       150.90400 ppm
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F96      Echo-antecho
F97      Echo-antecho
F98      Echo-antecho
F99      Echo-antecho
F100     Echo-antecho
F1 - Processing parameters
SI        32768
SF        600.1317006 MHz
WDW       EM
SSB       0 Hz
GB        0 Hz
PC        1.00
F1 - Processing parameters
SI        1024
NUC1     echo-antecho
SF        150.9028942 MHz
WDW       EM
SSB       0 Hz
GB        0 Hz
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H

FADDI-118 D2O gHMBC



Current Data Parameters  
NAME MCC6399\_001  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20151010  
Time 10.49  
INSTRUM spect  
PROBHD 5 mm CPTCI 1H/  
PULPROG hmbcgp1pdqf  
TD 4096  
SOLVENT D2O  
NS 64  
DS 4  
SWH 7183.908 Hz  
FIDRES 1.753884 Hz  
AQ 0.2850816 sec  
RG 46341  
RW 69.400 usec  
DE 12.00 usec  
TE 298.0 K  
CNST2 135.0000000  
CNST13 8.0000000  
D0 0.00000300 sec  
D1 2.00000000 sec  
D2 0.00370370 sec  
D6 0.00250000 sec  
D16 0.00020000 sec  
IN0 0.00001380 sec

==== 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 120.04184846 W  
SFO2 150.9178988 MHz

==== GRADIENT CHANNEL =====  
GPNAM[1] sine.100  
GPNAM[2] sine.100  
GPNAM[3] sine.100  
GP21 50.00 %  
GP22 30.00 %  
GP23 40.10 %  
P16 1000.00 usec

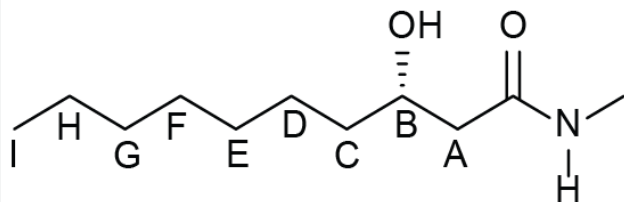
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TD 256  
SFO1 150.9179 MHz  
FIDRES 282.968231 Hz  
SW 239.298 ppm  
FnMODE QF

F2 - Processing parameters  
SI 1024  
SF 600.1299340 MHz  
SE  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0  
PC 1.00

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



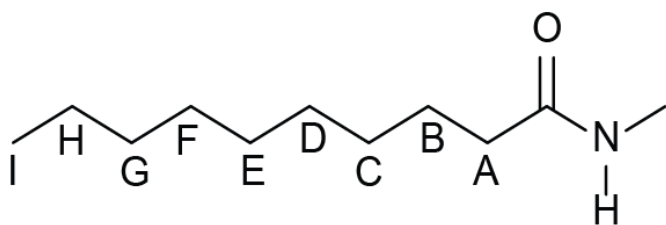
<sup>1</sup>H and <sup>13</sup>C Chemical shifts for octapeptin C4 peptide in water at 22°C.



Res	Atom	Shift	Res	Atom	Shift	Res	Atom	Shift	Res	Atom	Shift
HDec	CA	45.61	2	CA	54	4	HA	4.58	7	CA	54.49
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 <sup>1</sup>H NMR spectrum are denoted by the pseudoatom Q.

<sup>1</sup>H and <sup>13</sup>C Chemical shifts for FADDI-115 peptide in water at 22°C



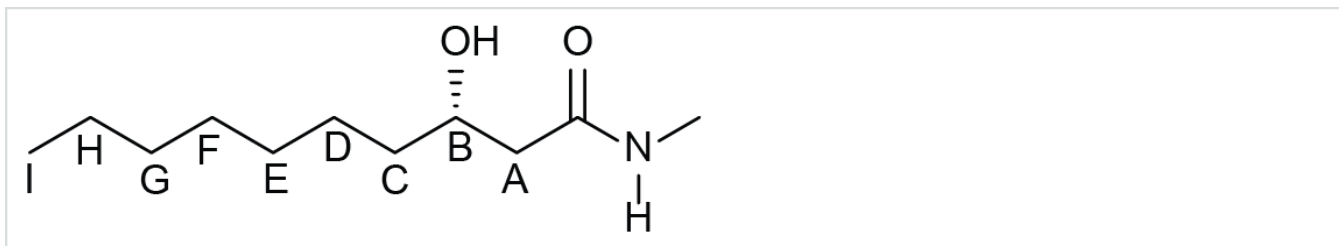
Res	Atom	Shift	Res	Atom	Shift	Res	Atom	Shift	Res	Atom	Shift
Dec	CA	38.42	2	CA	54.58	4	HA	4.57	7	CA	55.05
Dec	CB	28.36	2	CB	33.85	4	HN	8.72	7	CB	32.14
Dec	CC	31.62	2	CG	38.65	4	HZ	7.32	7	CG	39.79
Dec	C-DEF	31.82	2	HA	4.14	4	QB	3.07	7	HA	4.32
Dec	CG	34.34	2	HB2	1.96	4	QD	7.25	7	HB2	2.14
Dec	CH	25.24	2	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 <sup>1</sup>H NMR spectrum are denoted by the pseudoatom Q.

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

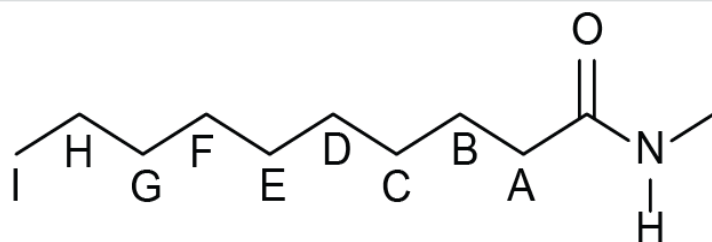
Octapeptin C4			FADDI-115		
Residue	$^3J_{\text{HNH}\alpha}$ (Hz)	$\Delta T_{\text{HN}} \times 10^3$	Residue	$^3J_{\text{HNH}\alpha}$ (Hz)	$\Delta T_{\text{HN}} \times 10^3$
1	6.75	$-6.73 \pm 0.25$	1	6.3	$-7.8 \pm 0.14$
2	6.86	$-6.80 \pm 0.25$	2	6.98	$-7.6 \pm 0.17$
3	8.28	$-4.90 \pm 0.25$	3	7.4	$-4.5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

<sup>1</sup>H and <sup>13</sup>C Chemical shifts for octapeptin C4 peptide in 120 mM DPC at 25°C



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 <sup>1</sup>H NMR spectrum are denoted by the pseudoatom Q.

<sup>1</sup>H and <sup>13</sup>C Chemical shifts for FADDI-115 peptide in 120 mM DPC at 25°C

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 <sup>1</sup>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.

<b>NOE distance restraints</b>	<b>Octapeptin C4</b>	<b>FADDI-115</b>
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 <sup>a</sup> , $ i - j  \geq 5$	36	21
Maximal violation	0.06	0.12
Final CYANA target function value	0.0084 $\pm$ 0.0009 $\text{\AA}^2$	0.12 $\pm$ 0.0003 $\text{\AA}^2$
RMSD to mean coordinates:		
Back bone atoms N,C $^\alpha$ ,C'	0.05 $\pm$ 0.01 $\text{\AA}$	0.06 $\pm$ 0.01 $\text{\AA}$
All heavy atoms	0.38 $\pm$ 0.05 $\text{\AA}$	0.38 $\pm$ 0.08 $\text{\AA}$

<sup>a</sup>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<sub>2</sub>O (<sup>1</sup>H 600 MHz, <sup>13</sup>C 150 MHz) derived from analysis of 2D NMR spectra.<sup>a</sup>

Amino Acid <sup>b</sup>	<sup>13</sup> C δ (ppm) <sup>c</sup>	<sup>1</sup> H δ (mult., J (Hz)) <sup>d</sup>	Amino Acid <sup>b</sup>	<sup>13</sup> C δ (ppm) <sup>c</sup>	<sup>1</sup> H δ (mult., J (Hz)) <sup>d</sup>
<b>Dab1</b>			<b>Dab1</b>		
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)	3	28.4	2.19 (m)
4	37.0 <sup>e</sup>	2.15 (m)	4	36.9 <sup>e</sup>	2.25 (m)
		3.09 (m)			3.08 (o)
<b>Dab2</b>			<b>Dab7</b>		
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)	3	29.3*	2.07 (m)
		1.99 (m)			2.19 (m)
4	36.1	3.10 (o)	4	37.3	3.02 (o)
		3.41 (ddd, 6.7, 9.3, 14.4)			3.05 (o)
<b>Dab3</b>			<b>Thr8</b>		
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)	3	39.2	4.19 (o)
		1.92 (m)			
4	36.6	2.75 (ddd, 6.7, 9.3, 13.0)	4	19.8	1.18 (d, 6.3)
		2.85 (ddd, 5.1, 9.7, 13.0)			
<b>Phe4</b>			<b>n-C8 fatty acid</b>		
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)
<b>Leu5</b>			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)			

<sup>a</sup> The <sup>1</sup>H and <sup>13</sup>C NMR spectra were externally calibrated to NaOAc ( $\delta_{\text{H}}$  1.90 and 8.44 and  $\delta_{\text{C}}$  24.0 and 171.7; 10 mg in 500  $\mu\text{L}$  D<sub>2</sub>O) (H. E. Gottlieb, V. Kotlyar and A. Nudelman, *J. Org. Chem.*, 1997, **62**, 7512). <sup>b</sup> Numbering from the carbonyl group of the amino acids. <sup>c</sup> <sup>13</sup>C NMR chemical shifts quoted to one decimal except where resonances resolved, <sup>d</sup> s = singlet, d = doublet, t = triplet, o = overlap. <sup>e</sup> assignment may be interchanged, \* = co-incident resonances.