Supporting Information 2

Synthesis of variously 3-substituted 1,2,4-oxadiazole-containing chiral β^3 - and α -aminoacids from Fmoc-protected aspartic acid.

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- Copies of ^1H NMR spectra of final compounds **4a** to **4g**, **7a** to **7f**, **10a** to **10d**. -----S2

815 2H₄ t_{max} (d1) 7.878 6.128 1H N⁺ H₂O 1.01
 8102 2H₄ t_{max} (d1) 7.13 5.17 1H CH₂ Arp₁ 1.01
 7192 2H₄ t_{max} (d1) 7.14 4.17 2H CH₂ F_{max} 1.01
 7165 2H₄ t_{max} (d1) 7.12 4.12 1H CH F_{max} 1.01
 7159 2H₄ t_{max} (d1) 7.13 3.52 1H CH₂ (d1) 4.17, 17.6
 715 2H₄ t_{max} (d1) 7.13 3.38 1H CH₂ (d1) 4.18, 17.6
 216 3H t_{max} (d1) 7.13 2.16 3H t_{max} (d1)

2H₄ 522/CDCl₃

4 b

Current Data Parameters
 NAME Mar04
 EXFO 190
 PROCNO 1
 F2 - Acquisition Parameters
 Date 500000
 Time 19.59
 INSTRUM spect
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 PULPROG zg30
 TD 32768
 SOLVENT CDCl₃
 NS 16
 DS 2
 SWE 8223.685 Hz
 FIDRES 0.250967 Hz
 AQ 1.9923444 sec
 RG 574.7
 DW 60.800 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 P1 10.00 usec
 DE 4.50 usec
 SF01 400.1324710 MHz
 NUC1 1H
 P11 -6.00 dB
 F2 - Processing parameters
 SI 16384
 SF 400.1324710 MHz
 KW 2K
 SS 0
 LB 0.30 Hz
 GB 0
 PC 1.00
 1D NMR plot parameters
 CX 30.00 cm
 FIP 11.000 ppm
 F1 4401.43 Hz
 F2 -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.40000 ppm/cm
 HZCM 160.05197 Hz/cm

4,25 14 CH₂NO₂ (t) 613
 3,2 14 CH₂(d) 5174
 3,1 14 CH₂(d) 4183 1714
 113 9H tBu (s)

775 2H_q Fmoc (d) 715
 716 2H_d Fmoc (d) 710
 714 2H_b Fmoc (t) 714
 715 2H_c Fmoc (t) 713
 610 14 NH₂ (d) 911
 514 14 CH₂ (m) 1
 415 24 CH₂ Fmoc (m) 1

Zan 524/CDC13

4 c

Current Data Parameters
 NAME Mar04
 EXPNO 180
 PROCNO 1
 F2 - Acquisition Parameters
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 Time 19.52
 INSTRUM spect
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 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.250967 Hz
 AQ 1.9923444 sec
 RG 456.1
 DW 60.800 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 P1 10.00 usec
 DE 4.50 usec
 SFO1 400.1324710 MHz
 NUC1 1H
 PL1 -6.00 dB
 F2 - Processing parameters
 SI 16384
 SF 400.1300104 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00
 1D NMR plot parameters
 CX 30.00 cm
 F1 11.000 ppm
 F2 4401.43 Hz
 F3 -1.000 ppm
 F4 -400.13 Hz
 F5 0.40000 ppm/cm
 F6 160.05200 Hz/cm

12,6 1H COOH (s)
 7,9 2H α β (d) 7,5
 7,65 2H α β (d) 6,8
 7,41 2H α β (t) 7,4
 7,3 2H α β (t) 7,4
 Zahn 526/dmso

5,2 1H CH₂ (q) 7,8; 14,6
 4,32 2H CH₂ (m)
 4,25 1H CH₂ (t) 6,6
 3,5 2H CH₂ (m) 6,1
 3,1 1H CH₂ (d) 6,3; 16,6
 2,91 1H CH₂ (d) 16,8

Current Data Parameters
 NAME 4d
 EXPNO 230
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 500000
 Time 8:57
 INSTRUM spect
 PULPROG 5 mm Dual 13
 F4PRG 2g30
 TD 32768
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 823.685 Hz
 FIDRES 0.250967 Hz
 AQ 1.9921444 sec
 RG 512
 DW 60.800 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 P1 10.00 usec
 DE 4.50 usec
 SFO1 400.1324710 MHz
 NUC1 1H
 PL1 -6.00 dB
 F2 - Processing parameters
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 SF 400.1300000 MHz
 WTM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00
 ID NMR plot parameters
 CX 30.00 cm
 FIP 13.200 ppm
 F1 5281.72 Hz
 F2P 0.600 ppm
 F2 240.08 Hz
 PPMCM 0.42000 ppm/cm
 HZCM 168.05461 Hz/cm

4 d

4 e

7.16 2H₂Phen (d) 7.0
 7.18 2H₂Phen
 7.25 9H {5H phen} m
 {+4H₂Phen}
 6.18 1H NH₂Arp (d) g
 5.8 1H NH₂ SI
 Zahn 513/CDCl₃ 5.28 1H (H₂Arp(m))

Current Data Parameters
 NAME Mar03
 EXPNO 250
 PROCNO 1

F2 - Acquisition Parameters
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 Time 18.36
 INSTRUM spect
 PROBED 5 mm Dual 13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl₃
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.250967 Hz
 AQ 1.9923444 sec
 RG 456.1
 DW 60.800 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 P1 10.00 usec
 DE 4.50 usec
 SF01 400.1324710 MHz
 NUC1 1H
 PL1 -6.00 dB

F2 - Processing parameters
 SI 16384
 SF 400.1300551 MHz
 WNW 0
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 30.00 cm
 P1P 11.000 ppm
 F1 440.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 FREQM 0.40000 ppm/cm
 FZCM 160.05203 Hz/cm

$4, 3, 8, 24 \text{ CH}_{12}\text{Foc (a)}$
 $4, 18, 14 \text{ CH}_{12}\text{Foc (t)}$ 7, 0
 $3, 12, 14 \text{ CH}^{\text{F}}\text{Foc}$ 5, 0 ; 17
 $3, 0, 24, 14 \text{ CH}^{\text{F}}\text{Foc}$
 $1, 18, 6, 14 \text{ 2 CH}_{12}\text{Foc}$ (d) 6, 8

4 g

7.78 2H Fmoc (t) 7.5
7.6 2H Fmoc (t) 7.3
7.4 2H Fmoc (t) 7.4
7.35 2H Fmoc (t) 7.4
6.18 1H NH₂ Arg (t) 8.8
5.14 1H CH₂ Arg (m)
4.46 2H CH₂ Arg (m)
4.18 1H CH₂ Arg (t) 7.0
3.28 1H CH₂ Arg (t) 7.5
3.12 1H CH₂ Arg (t) 7.5
2.75 2H CH₂-C=N (t) 7.6
1.18 2H CH₂-CH₂-CH₂ (m)
1.14 2H CH₂-CH₂-CH₂ (m)
0.91 3H CH₃ (t) 7.3

Zah503/CDCl₃

11.5 1H COOH (s)
 7.85 2H a Fmoc d 7RM 6.2 1HNH α ANP d 9.13
 7.68 2H d Fmoc (d) 7.44S 5.4 1H CH α ANP (m)
 7.55 2H e Ph (m) 7.1 2H (H₁Fmoc (m)
 7.31 2H b Fmoc (t) 7.44S 4.2 1H CH α Fmoc (t) 7.61
 7.25 2H c Fmoc (t) 7.44S 3.22 1H CH β ANP dd 4.11; 1.74
 7.12 2H d Ph (m) 2.1 1H CH β ANP (m)

7.12 2H_a -woc & 7.10
 7.55 2H_d -woc (d) 6.7
 7.38 2H_b -woc (t) 7.4
 7.32 2H_c -woc (t) 7.4
 5.96 1H N_H (d) 9.1
 1.28 gH tBu (S)

41.28 1H CH₂CO₂ (s, 6.7)
 3.16 2H (CH₂-C) (s)
 3.02 1H (CH₂CO₂) (s, 6.7)
 2.95 1H (CH₂CO₂) (s, 6.7)

58.38 2H Fmoc (s, 7.2)
 7.19 2H Fmoc (s, 7.4)
 7.15 2H Fmoc (s, 7.4)
 7.13 2H Fmoc (s, 7.4)
 5.12 1H CH₂CO₂ (s)
 4.14 2H CH₂CO₂ (s)

50min

Zah 51H/dmso-d6

7d

Current Data Parameters
 Name: Mar18
 ExpNo: 80
 ProcNo: 1
 F2 - Acquisition Parameters
 Date_: 500000
 Time: 17.32
 INSTRUM: spect
 PROBD: 5 mm Dual 13
 PULPROG: zg30
 TD: 32768
 SOLVENT: DMSO
 NS: 16
 DS: 2
 SWH: 8223.685 Hz
 FIDRES: 0.250967 Hz
 AQ: 1.9923444 sec
 RG: 362
 DW: 60.800 usec
 DE: 4.50 usec
 TE: 300.0 K
 D1: 1.00000000 sec
 PL: 10.00 usec
 DE: 4.50 usec
 SFO1: 400.1324710 MHz
 NUC1: 1H
 P1: -6.00 dB
 F2 - Processing parameters
 SI: 16384
 SF: 400.1300000 MHz
 WDW: EM
 SSB: 0
 LB: 0.10 Hz
 GB: 0
 PC: 1.00
 LD NMR plot parameters
 CX: 30.00 cm
 F1P: 11.500 ppm
 F1: 5401.75 Hz
 F2P: 0.000 ppm
 F2: 0.00 Hz
 F2FREQ: 0.45000 ppm/cm
 F2CN: 180.05849 Hz/cm

7e

Current Data Parameters
 NAME Feb26
 EXPNO 70
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 500000
 Time_ 12.34
 INSTRUM Spect
 PROBED 5 mm Dual 13
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8231.685 Hz
 FIDRES 0.250867 Hz
 AQ 1.9923444 sec
 RG 363
 DW 60.800 usec
 DE 4.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 10.00 usec
 DE 4.50 usec
 SFO1 400.1324710 MHz
 NUC1 1H
 P11 -6.00 dB

F2 - Processing parameters
 SI 16384
 SF 400.129353 MHz
 EX 0
 WDW 0
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 30.00 cm
 FIP 9.000 ppm
 F1 3601.17 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCK 0.30000 ppm/cm
 HZCM 120.03899 Hz/cm

7.9 2H t m (d) / 7.1
 7.8 2H t m (d) /
 7.45 9H (2H s, 2H t m + 5H m) / m
 6.42 1H m (d) / 9.1
 6.3 1H m (d) /
 5.52 1H m (m)
 2.054 3H s
 1.110 3H s

4735 CH₂Fur (d) 6,9
4718 CH₂Fur (t) 6,9.
4735 CH₂PP 47
4735 CH₂PP 5,7,16,7
4728 CH₂PP 5,7,16,7

Zah498/CDCL3

10 c

Current Data Parameters	
NAME	Feb17
EXPNO	60
PROCNO	1
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F2 - Acquisition Parameters	
Date_	500000
Time	19 02
INSTRUM	spect
PROBHD	5 mm Dual 13
PULPRG	Zg30
TD	32768
SOLVENT	CDCl3
DS	16
NS	2
DS NS	2
FIDRES	8231.685 Hz
AQ FWHM	0.250957 Hz
RG	1.3923444 sec
AG	1024
DW	60.800 usec
DE	4.50 usec
TE	300.0 K
DT	1.00000000 sec
DELTA	10.00 usec
DELTA DELTA	4.50 usec
NUC1	400.1324710 MHz
NUC1	1H
PL1	-6.00 dB
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F2 - Processing parameters	
SF	16394
WDW	EM
SSB	0
GB	0.30 Hz
LB	0
PC	1.00
<hr/>	
L2 LMR plot parameters	
CX	30.00 cm
F1P	11.000 ppm
F2P	4401.43 Hz
F2P2	-1.000 ppm
F2P3	-400.13 Hz
PPPMCK	0.40000 ppm/cm
HZCMCK	160.05002 Hz/cm

4.95 1H C=O (s)
 7.9 2H aromatic
 7.15 2H aromatic
 7.41 2H aromatic
 7.35 2H aromatic
 4.5 1H CH₂ (m)
 4.3 2H CH₂ (m)

Zah 496/DMSO-d₆

10 d

Current Data Parameters
 NAME Mar03
 EXPNO 230
 PROCNO 1
 F2 - Acquisition Parameters
 Date 500000
 Time 19.08
 INSTRUM spect
 PROBD 5 mm Dual 13
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.350957 Hz
 AQ 1.9921444 sec
 RG 574.7
 DW 60.800 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 P1 10.00 usec
 DE 4.50 usec
 SPOL 400.1324710 MHz
 NUC1 1H
 PUL1 -6.00 dB
 F2 - Processing parameters
 SI 16384
 SF 400.1300000 MHz
 EM
 MDW 0
 SSB 0.30 Hz
 LB 0
 GB 0
 PC 1.00
 ID NMR plot parameters
 CX 30.00 cm
 FIP 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.40000 ppm/cm
 HZCM 160.05200 Hz/cm