Synthesis of Dendritic Catalysts and Application in Asymmetric Transfer Hydrogenation

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General procedure for condensation of Fréchet-type acid with (S, S)-1: (S, S)-*N*-Boc-*N'*-(4-aminophenylsulfonyl)-1,2-dipheylethylenediamine **1** (467 mg, 1.0 mmol),¹ Dendritic acid (1.05 eq.) and triphenyl phosphite (370 mg, 1.1 mmol) were stirred in Pyridine (2 mL) at 95 °C for 24 hours. The solution was poured into water (30 mL) and extracted with EtOAc (40 mL). The organic phase was washed successively with 0.5 M citric acid, sodium bicarbonate and brine, dried. Flash chromatography on silica gel gave the Boc-protected dendrimers **2a-5a**.

(*S,S*)-**2a**, 80% yield; mp 190-192°C; $[\alpha]_D^{28}$ -12.7° (*c* 0.30, acetone); ¹H NMR (CDCl₃, 300 MHz) δ 1.49 (s, 9H), 4.61 (t, *J* = 7.8 Hz, 1H), 4.80 (t, *J* = 8.1 Hz, 1H), 5.10 (s, 4H), 5.27 (d, *J* = 6.6 Hz, 1H), 6.30 (s, 1H), 6.76-7.52 (m, 27H), 7.86 (s, 1H) ppm; ¹³C NMR (DMSO+CD₃COCD₃, 75 MHz) δ 28.4, 59.4, 62.6, 70.1, 105.1, 107.2, 119.6, 127.0, 127.2, 127.7, 128.0, 128.1, 128.3, 128.6, 135.7, 136.7, 136.8, 139.6, 140.3, 142.3, 155.3, 159.7, 165.5 ppm; IR (KBr) 3376, 3305, 1686, 1518, 1160 cm⁻¹; ESI HRMS calcd for C₄₆H₄₅N₃O₇S+Na 806.2878, obsd 806.2828.

(*S, S*)-**3a**, 75% yield; mp 164-166°C; $[\alpha]_D^{28}$ -6.25° (*c* 0.30, acetone); ¹H NMR (CDCl₃, 300 MHz) δ 1.40 (s, 9H), 4.61 (br.s, 1H), 4.81 (t, *J* = 8.4 Hz, 1H), 5.00-5.04 (m, 12H), 5.30 (s, 1H), 6.31 (s, 1H), 6.59-7.49 (m, 43H), 7.96 (s, 1H) ppm; Partial ¹³C NMR (CD₃COCD₃, 75 MHz) δ 28.3, 59.8, 62.5, 69.9, 79.0, 101.4, 105.2, 106.4, 107.1, 119.6, 126.8, 126.9, 127.0, 127.1, 127.2, 127.5, 127.9, 128.0, 128.1, 128.5, 135.5, 136.7, 136.8, 138.9, 139.1, 142.3, 159.6, 160.0, 165.8 ppm; IR (KBr) 3365, 3301, 1685, 1596, 1516, 1159 cm⁻¹; FAB MS (*m/z*) 1230 [M+Na]⁺.

(*S, S*)-**4a**, 73% yield; mp 146-148 °C; $[\alpha]_D^{28}$ -4.90° (*c* 0.30, acetone); ¹H NMR (CDCl₃, 300 MHz) δ 1.49 (s, 9H), 4.60 (br.s, 1H), 4.77-4.79 (m, 1H), 4.96-5.01 (m, 28H), 5.27 (d,

$J = 6.6$ Hz, 1H), 6.26 (br.s, 1H), 6.56-7.48 (m, 75H), 7.85 (s, 1H) ppm; Partial ^{13}C NMR (CD_3COCD_3 , 75 MHz) δ 28.3, 61.2, 64.8, 69.9, 70.0, 80.7, 101.5, 101.6, 106.3, 106.4, 119.2, 127.2, 127.4, 127.5, 127.7, 128.0, 128.3, 128.5, 136.4, 136.6, 138.6, 139.1, 159.9, 160.0, 160.1, 165.3 ppm; IR (KBr) 3371, 3306, 1683, 1596, 1450, 1157 cm^{-1} ; Anal. Calcd for $\text{C}_{130}\text{H}_{117}\text{N}_3\text{O}_{19}\text{S}$: C, 75.89; H, 5.73; N, 2.04; S, 1.56. Found: C, 75.76; H, 5.67; N, 2.00; S, 1.30.

General procedure for the synthesis of Boc-protected hybrid dendrimers: Branched ligand (**R, R**)-**6** (192 mg, 0.1 mmol),² Fréchet-type acid (1.05 eq.), EDCI (25 mg, 0.13 mmol) and HOBT (14 mg, 0.1 mmol) were stirred in DCM (5 mL) and cooled in ice water. NEt_3 (18 μL , 0.13 mmol) was added and the solution was stirred overnight. The solution was washed successively with 0.5M citric acid, saturated sodium bicarbonate and brine, and dried. Flash chromatography on silica gel gave the Boc-protected hybrid dendrimers.

(**R, R**)-**8a**, 70% yield; $[\alpha]_{\text{D}}^{20} +13.5^\circ$ (c 0.43, THF); ^1H NMR (CD_3COCD_3 , 400 MHz) δ 1.32 (s, 27H), 2.44 (br.s, 6H), 3.61 (br.s, 6H), 3.72 (br.s, 6H), 4.07 (br.s, 8H), 4.70-4.95 (m, 66H), 6.51-6.67 (m, 45H), 6.96-7.49 (m, 122H), 7.86 (br.s, 3H), 9.57 (br.s, 3H) ppm (the six NCH protons of DPEN was overlapped by ArCH_2); Partial ^{13}C NMR (CD_3COCD_3 , 50 MHz) δ 28.6, 37.1, 44.6, 60.7, 61.4, 63.9, 68.2, 70.5, 79.6, 102.1, 107.3, 119.6, 127.9, 128.4, 128.6, 128.8, 129.2, 136.6, 136.9, 138.1, 139.8, 140.3, 140.6, 140.7, 142.6, 156.6, 160.7, 160.9, 161.0, 167.9, 169.3, 171.2, 173.1 ppm; IR (KBr) 3407, 3032, 1690, 1596, 1498, 1372 cm^{-1} ; Anal. Calcd. for $\text{C}_{313}\text{H}_{300}\text{N}_{14}\text{O}_{53}\text{S}_3$: C, 72.27; H, 5.81; N, 3.77; S, 1.85. Found: C, 72.07; H, 5.85; N, 3.72; S, 1.62.

General procedure for deprotection of Boc-group: Boc-protected dendrimer (0.2 mmol) was dissolved in DCM (1 mL) and cooled with ice water. TFA (1 mL) was added and the solution was stirred for 1 hour. The solvent was removed under vacuum and water (10 mL) was added. The mixture was neutralized with ammonia and stirred at room temperature for 2 hours. The solid was collected, washed with water, and dried under vacuum.

(S, S)-3b, 90% yield; $[\alpha]_D^{20}$ -25.2° (c 0.55, CH₂Cl₂); ¹H NMR (CDCl₃, 300 MHz) δ 4.23 (br.s, 1H), 4.46 (br.s, 1H), 5.01, 5.03 (s×2, 12H), 6.43-6.75 (m, 9H), 7.08-7.59 (m, 34H), 8.04 (s, 1H) ppm; IR (KBr) 3430, 3261, 3031, 1676, 1594, 1321, 1157 cm⁻¹; ESI HRMS calcd for C₆₉H₆₁N₃O₉S+H 1108.4207, obsd 1108.4179.

(S, S)-4b, 90% yield; $[\alpha]_D^{20}$ -13.1° (c 0.50, CH₂Cl₂); ¹H NMR (CDCl₃, 300 MHz) δ 4.04-4.08 (m, 2H), 4.88-5.00 (m, 28H), 6.54-7.62 (m, 75H) ppm; IR (KBr) 3440, 3032, 1677, 1595, 1452, 1321, 1157, 1053 cm⁻¹; ESI HRMS calcd for C₁₂₅H₁₀₉N₃O₁₇S+H 1956.7556, obsd 1956.7929.

(S, S)-5b. The Boc-group was removed with HCl-EtOAc solution in 90% yield; $[\alpha]_D^{20}$ -6.6° (c 0.62, CH₂Cl₂); ¹H NMR (CDCl₃, 400 MHz) δ 4.82-5.07 (m, 60H), 6.48-6.81 (m, 45H), 7.04-7.42 (m, 94H) ppm, the two NCHs of DPEN are too small to be detected; IR (KBr) 3473, 3432, 3031, 1596, 1450, 1374, 1157, 1053 cm⁻¹; MALDI-TOF MS calcd for C₂₃₇H₂₀₅N₃O₃₃S+Na 3675.41, obsd 3676.03; calcd for C₂₃₇H₂₀₅N₃O₃₃S+K 3691.52, obsd 3692.01.

(R, R)-7b, 93% yield; $[\alpha]_D^{20}$ +5.47° (c 0.38, THF); ¹H NMR (CD₃OD+CDCl₃, 400 MHz) δ 2.44 (t, *J* = 5.6 Hz, 6H), 3.63-3.72 (m, 12H), 3.98 (br.s, 8H), 4.03 (d, *J* = 8.4 Hz, 3H), 4.39 (d, *J* = 8.4 Hz, 3H), 4.72-4.86 (m, 28H), 6.41-7.36 (m, 103H), 7.67 (s, 1H) ppm; Partial ¹³C NMR (CD₃OD+CDCl₃, 50 MHz) δ 35.6, 42.6, 59.9, 63.7, 66.6, 69.0, 69.2, 100.9, 105.7, 118.3, 126.6, 126.8, 127.1, 127.3, 127.7, 134.5, 136.2, 137.1, 138.4, 138.5, 138.8, 141.1, 159.2, 159.3, 159.4, 167.8, 172.5 ppm; IR (KBr) 3407, 3104, 1674, 1595, 1453, 1322 cm⁻¹; MALDI-TOF MS calcd for C₁₈₆H₁₈₀N₁₄O₃₁S₃+Na 3224.2, obsd 3224.7.

(R, R)-8b, 95% yield; $[\alpha]_D^{20}$ +4.50° (c 0.38, THF); ¹H NMR (CD₃OD+CDCl₃, 400 MHz)

δ 2.43 (br.s, 6H), 3.60-3.66 (m, 12H), 4.04 (br.s, 8H), 4.49 (d, $J = 9.2$ Hz, 3H), 4.83-4.91 (m, 60H), 6.46-6.60 (m, 45H), 6.79-7.46 (m, 122H), 7.57 (s, 1H) ppm (the other three NCH protons of DPEN were overlapped by H₂O in CD₃OD); Partial ¹³C NMR (CD₃OD+CDCl₃, 50 MHz) δ 35.8, 43.0, 59.8, 63.4, 66.8, 69.5, 100.0, 101.2, 104.8, 106.0, 118.6, 125.0, 126.8, 127.0, 127.4, 127.6, 128.0, 134.6, 135.1, 136.3, 137.0, 138.0, 138.7, 138.9, 141.2, 157.8, 159.6, 167.9, 169.5, 172.6 ppm; IR (KBr) 3410, 3249, 3119, 1677, 1596, 1452, 1376 cm⁻¹; MALDI-TOF MS calcd for C₂₉₈H₂₇₆N₁₄O₄₇S₃+Na, 4921, obsd 4926.

References

- (1) Chen, Y.-C.; Wu, T.-F.; Deng, J.-G.; Liu, H.; Jiang, Y.-Z.; Choi, M. C. K.; Chan, A. S. *C. Chem. Commun.* **2001**, 1488.
- (2) Chen, Y.-C.; Wu, T.-F.; Deng, J.-G.; Liu, H.; Cui, X.; Zhu, J.; Jiang, Y.-Z.; Choi, M. C. K.; Chan, A. S. *C. J. Org. Chem.* **2002**, 67, 5301.

NMR data and GC or HPLC conditions for the reduced products

¹H NMR (CDCl₃, 300 MHz) δ 1.52 (d, $J = 6.3$ Hz, 3H), 4.94 (q, $J = 6.4$ Hz, 1H), 7.30-7.42 (m, 5H) ppm; GC: CP-Cyclodex-236, 110 °C, $t_R = 5.098$ min, $t_S = 5.423$ min.

¹H NMR (CDCl₃, 300 MHz) δ 1.47 (d, $J = 6.4$ Hz, 3H), 4.87 (q, $J = 6.4$ Hz, 1H), 7.26 (d, $J = 8.4$ Hz, 2H), 7.47 (d, $J = 8.4$ Hz, 2H) ppm; GC: CP-Cyclodex-236, 110

°C, t_R = 9.198 min, t_S = 9.832 min.

^1H NMR (CDCl_3 , 300 MHz) δ 1.59 (d, J = 6.5 Hz, 3H), 2.26 (s, 1H), 5.04 (q, J = 6.5 Hz, 1H), 7.47-7.54 (m, 3H), 7.80-7.86 (m, 4H) ppm; GC: CP-Cyclodex-236, 110 °C, t_R = 9.957 min, t_S = 10.182 min.

^1H NMR (CDCl_3 , 300 MHz) δ 2.96-3.09 (m, 2H), 4.91 (t, J = 6.9 Hz, 1H), 7.19-7.37 (m, 10H) ppm; HPLC: chiral OD column, 15% 2-propanol/hexane, 1.0 mL/min, UV 254 nm, t_R = 12.79 min, t_S = 15.79 min.

^1H NMR (CDCl_3 , 300MHz), δ 1.40 (d, J = 6.3 Hz, 3H), 2.42 (s, 1H), 4.46-4.55 (m, 1H), 6.28 (dd, J = 6.6, 15.9 Hz, 1H), 6.58 (d, J = 15.9 Hz, 1H), 7.29-7.42 (m, 5H) ppm; ^{13}C NMR (CDCl_3 , 75MHz) δ 23.3, 68.8, 126.4, 127.6, 128.5, 129.3, 133.5, 136.6 ppm; HPLC: chiral OD column, 15% 2-propanol/hexane, 1.0 mL/min, UV 254 nm, t_{major} = 6.78 min, t_{minor} = 9.67 min.

^1H NMR (CDCl_3 , 300MHz), δ 1.39 (d, J = 6.6 Hz, 3H), 1.91 (3H, s), 4.41 (q, J = 6.6 Hz, 1H), 6.54 (s, 1H), 7.23-7.38 (m, 5H), ppm; ^{13}C NMR (CDCl_3 , 75MHz) δ 13.4, 21.7, 73.5, 124.3, 126.3, 128.1, 128.9, 137.6, 141.6 ppm; HPLC: chiral OD column, 2.5% 2-propanol/hexane, 1.0 mL/min, UV 254 nm, t_{major} = 13.62 min, t_{minor} = 15.96 min.

^1H NMR (CDCl_3 , 300MHz) δ 1.28 (d, J = 6.3 Hz, 3H), 1.96 (s, 3H), 3.83 (s, 3H), 4.39 (q, J = 6.0 Hz, 1H), 6.47 (s, 1H), 6.89 (d, J = 8.7 Hz, 2H), 7.24 (d, J = 8.7 Hz, 2H) ppm; HPLC: chiral AD column, 2.5% 2-propanol/hexane, 1.0 mL/min, UV 254 nm, t_{major} = 20.97 min, t_{minor} = 29.35 min.

^1H NMR (CDCl_3 , 300MHz) δ 1.53 (s, 9H), 4.85 (s, 1H), 7.90-7.66 (m, 4H) ppm; HPLC: chiral OD column, 20% 2-propanol/hexane, 1.0 mL/min, UV 254 nm, t_S = 6.78 min, t_R = 13.29 min.

^1H NMR (CDCl_3 , 300 MHz), δ 1.85-1.87 (m, 1H), 1.99-2.14 (m, 2H), 2.25-

2.30 (m, 1H), 2.83-2.92 (m, 2H), 3.53 (q, $J = 6.3$ Hz, 1H), 4.13 (d, $J = 6.3$ Hz, 1H), 7.17-7.25 (m, 4H) ppm; ^{13}C NMR (CDCl_3 , 75 MHz), δ 19.6, 26.7, 28.8, 29.4, 39.2, 112.1, 112.91, 126.4, 127.9, 128.1, 130.0, 131.9, 138.0 ppm; HPLC on chiral OD column, 20% 2-propanol/hexane, 1.0 mL/min, UV 254 nm, $t_{\text{major}} = 12.97$ min, $t_{\text{minor}} = 20.04$ min.

Spectra of dendritic lignads

2G-DPEN-BOC 1H NMR bbi probe

3a

Current Data Parameters
NAME scien
EXPNO 26
PROCNO 1

F2 - Acquisition Parameters
Date_ 20001127
Time 20.44
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 24
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SFO1 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 11.487 ppm
F1 3447.72 Hz

2G-DPEN-BOC 13C NMR bbi robe

3a

Current Data Parameters
NAME first-13c
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20001201
Time 8.24
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 10000
DS 2
SWH 14970.060 Hz
FIDRES 0.228425 Hz
AQ 2.1889524 sec
RG 8192
DW 33.400 usec
DE 6.00 usec
TE 300.0 K
D1 3.0000000 sec
d11 0.0300000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.30 usec
PL1 2.00 dB
SFO1 75.4752658 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 27.00 dB
SFO2 300.1315007 MHz

F2 - Processing parameters
SI 65536
SF 75.4677570 MHz
WDW EN
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 198.679 ppm
F1 14993.84 Hz
F2P 0.315 ppm
F2 23.78 Hz
PPMCH 9.91818 ppm/cm
HZCM 746.50293 Hz/cm

2G-NH2 1H NMR bbi probe

3b

Current Data Parameters
NAME scien
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20001113
Time 10.42
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 40
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SFO1 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 9.222 ppm
F1 2767.67 Hz

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PROCNO 1

F2 - Acquisition Parameters
Date_ 20001127
Time 20.59
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 24
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SF01 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 8.178 ppm
F1 2454.49 Hz
F2P 0.680 ppm
F2 204.05 Hz
PPMCM 0.37491 ppm/
HZCM 112.52192 Hz/c

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Current Data Parameters
NAME first-13c
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20001129
Time 6.35
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 6000
DS 2
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400300 sec
RG 8192
DW 26.550 usec
DE 6.00 usec
TE 300.0 K
D1 4.00000000 sec
d11 0.03000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.30 usec
PL1 2.00 dB
SF01 75.4752658 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD02 80.00 usec
PL2 120.00 dB
PL12 27.00 dB
SF02 300.1315007 MHz

F2 - Processing parameters
SI 65536
SF 75.4677570 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 178.332 ppm
F1 13458.25 Hz
F2P -5.162 ppm
F2 -389.55 Hz
PPMCM 9.17471 ppm/cm
HZCM 692.39450 Hz/cm

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3G-DPEN 1H NMR bbi probe

4b

Current Data Parameters
NAME scien
EXPNO 29
PROCNO 1

F2 - Acquisition Parameters
Date_ 20010321
Time 9.41
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 24
DM 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SF01 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 9.491 ppm
F1 2848.50 Hz
F2P -0.447 ppm
F2 -134.08 Hz
PPMCM 0.49688 ppm/cm
HZCM 149.12920 Hz/cm

4G-DPEN (BOC) 1H NMR bbi probe

5a

Current Data Parameters
NAME scien
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20010326
Time 16.28
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 14
DM 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SFO1 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 8.470 ppm
F1 2542.13 Hz
F2P -0.342 ppm
F2 -102.54 Hz
PPMCM 0.44059 ppm/
HZCM 132.23389 Hz/c

5b 4G-DPEN