Supplementary Materials



Figure S1. ¹H-NMR Spectrum of Compound 7a.

Figure S2. ¹³C-NMR Spectrum of Compound 7a.





Figure S3. HPLC Spectra of Compound 7a.











Figure S7. ¹H-NMR Spectrum of Compound **7c**.

Figure S8. ¹³C-NMR Spectrum of Compound 7c.



Figure S9. HPLC Spectra of Compound 7c.

Figure S11. ¹³C-NMR Spectrum of Compound 7d.

Figure S13. ¹H-NMR Spectrum of Compound 7e.

Figure S15. HPLC Spectra of Compound 7e.

Figure S17. ¹³C-NMR Spectrum of Compound 7f.

Figure S18. HPLC Spectra of Compound 7f.

Figure S19. ¹H-NMR Spectrum of Compound 7g.

Figure S20. ¹³C-NMR Spectrum of Compound 7g.

9.5

9.0

8.0

8.5

7.5 7.0 6.5

5.0 4.5 fl (ppm)

6.0

5.5

4.0

3.5

3.0 2.5

2.0

1.5

1.0

0.5

0.0

-0.5

Figure S21. HPLC Spectra of Compound 7g.

Figure S23. ¹³C-NMR Spectrum of Compound 7h.

Figure S24. HPLC Spectra of Compound 7h.

Figure S25. ¹H-NMR Spectrum of Compound 7i.

Figure S26. ¹³C-NMR Spectrum of Compound 7i.

Figure S29. ¹³C-NMR Spectrum of Compound 7j.

Figure S31. ¹H-NMR Spectrum of Compound 7k.

Figure S33. HPLC Spectra of Compound 7k.

Figure S35. ¹³C-NMR Spectrum of Compound 7l.

Figure S37. ¹H-NMR Spectrum of Compound 7m.

Figure S41. ¹³C-NMR Spectrum of Compound 7n.

Figure S43. ¹H-NMR Spectrum of Compound 70.

Figure S45. HPLC Spectra of Compound 70.

Figure S46. ¹H-NMR Spectrum of Compound 7p.

Figure S47. ¹³C-NMR Spectrum of Compound 7p.

Figure S49. ¹H-NMR Spectrum of Compound 7q.

Figure S51. HPLC Spectra of Compound 7q.

Figure S53. ¹³C-NMR Spectrum of Compound 7r.

Figure S55. ¹H-NMR Spectrum of Compound 7s.

7.5

7.0

6.5

6.0

5.5

5.0

8. 0

). o

8.5

Figure S57. HPLC Spectra of Compound 7s.

4.5 4.0 f1 (ppm) 3.0

3.5

2.5

2.0

1.5

1.0

0.0

0.5

Figure S59. ¹³C-NMR Spectrum of Compound 7t.

Figure S60. HPLC Spectra of Compound 7t.

f1 (ppm) ò

-10

 Figure S61. ¹H-NMR Spectrum of Compound 7u.

Figure S63. HPLC Spectra of Compound 7u.

Figure S64. ¹H-NMR Spectrum of Compound 7v.

Figure S67. ¹H-NMR Spectrum of Compound 7w.

Figure S69. HPLC Spectra of Compound 7w.

Figure S71. ¹³C-NMR Spectrum of Compound 8a.

Figure S72. X-ray Single Crystal Structure Analysis of (*S*, *2S*, *3R*)-7a.

Empirical formula	C ₃₇ H ₃₁ N ₅ NiO ₃
Formula weight	652.38
Temperature/K	293.15
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
a/Å	11.6716(5)
b/Å	14.4772(6)
c/Å	18.6850(7)
α/°	90.00
β/°	90.00
γ/°	90.00
Volume/Å ³	3157.2(2)
Ζ	4
$\rho_{calc} mg/mm^3$	1.372
m/mm^{-1}	0.660
F(000)	1360.0
Crystal size/mm ³	$0.38 \times 0.20 \times 0.08$
2Θ range for data collection	6.04 to 49.98°
Index ranges	$-13 \le h \le 11, -17 \le k \le 13, -13 \le l \le 22$
Reflections collected	8050
Independent reflections	5166[R(int) = 0.0237]
Data/restraints/parameters	5166/0/415
Goodness-of-fit on F ²	1.032
Final R indexes [I>= 2σ (I)]	$R_1 = 0.0388, wR_2 = 0.0649$
Final R indexes [all data]	$R_1 = 0.0512, wR_2 = 0.0698$
Largest diff. peak/hole / e $Å^{-3}$	0.36/-0.20
Flack parameter	-0.029(12)

 Table S1. Crystal data and structure refinement for 7a.

Figure S73. X-ray Single Crystal Structure Analysis of (*S*, *2S*, *3R*, *4S*)-7q.

Empirical formula	$C_{41}H_{40}Cl_2N_4NiO_6$
Formula weight	814.36
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	$P2_{1}2_{1}2_{1}$
a/Å	9.8656(5)
b/Å	17.5526(8)
c/Å	22.7136(9)
α/°	90
β/°	90
$\gamma/^{\circ}$	90
Volume/Å ³	3933.2(3)
Z	4
$\rho_{calc} mg/mm^3$	1.372
m/mm^{-1}	2.387
F(000)	1688.0
Crystal size/mm ³	0.4 imes 0.2 imes 0.02
2Θ range for data collection	6.364 to 134.456°
Index ranges	$-8 \le h \le 11, -20 \le k \le 20, -27 \le l \le 27$
Reflections collected	25555
Independent reflections	7055[R(int) = 0.0855]
Data/restraints/parameters	7055/1686/510
Goodness-of-fit on F ²	1.183
Final R indexes [I>= 2σ (I)]	$R_1 = 0.1069, wR_2 = 0.2999$
Final R indexes [all data]	$R_1 = 0.1291, wR_2 = 0.3355$
Largest diff. peak/hole / e $Å^{-3}$	1.23/-0.72
Flack parameter	0.090(18)

Table S2. Crystal data and structure refinement for 7q.

Crystallographic data (excluding structure factors) for the structures **7a** (CCDC 951535) and **7q** (CCDC 949234) in this paper have been deposited with the Cambridge Crystallographic Data Centre. Copies of the data can be obtained, free of charge, on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: +44 (0)1223 336033 or e-mail: deposit@ccdc.cam.ac.Uk).