Supplementary Material (ESI) for Chemical Communications

Electronic Supplementary Information

Synthesis and Reactions of the First Fluoroalkylated Ni(II) N-Confused Porphyrins

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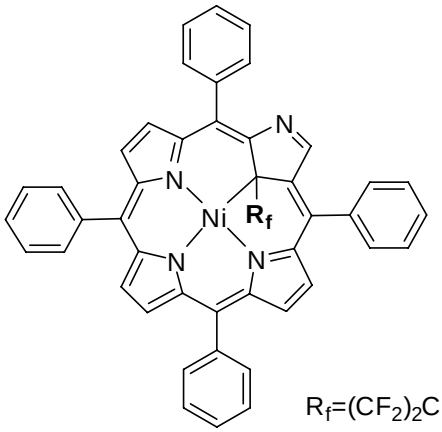
Contents

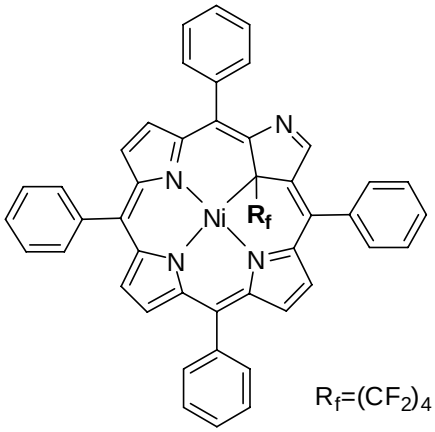
General: ^{1}H (300MHz) and ^{19}F (282MHz) NMR spectra were recorded with a Brucker AM-300 or Varian-VXR (300MHz) spectrometer. Chemical shifts are reported in parts per million (ppm) relative to TMS as an internal standard (δ_{TMS} = 0 ppm) for ^{1}H NMR spectra and $CFCl_3$ as an external standard (negative for upfield) for ^{19}F NMR spectra. Deuterated solvents for NMR were purchased from Cambridge Isotope Laboratories, Aldrich or Acros. MS and HRMS were recorded on a Hewlett-Packard HP-5989A spectrometer and a Finnigan MAT-8483 mass spectrometer. UV/Vis spectra were measured with a Varian Cary 100 spectrophotometer. Elementary analyses were obtained on a Perkin Elmer 2400 Series□ Elemental Analyzer. TLC analysis were performed on silica gel plate and column chromatography over silica gel (mesh 300-400).Unless otherwise noted, reagents were commercial available and used as received. The solvent DMSO was treated with CaH_2 and redistilled before using. The copper powder was prepared according the reported procedure (Liu, C.; Shen, D. –M.; Chen, Q. –Y. *Eur. J. Org. Chem.* 2006, 2703.). The starting N-confused porphyrins and Ni(II) N-Confused Porphyrins were synthesized according to the literatures (G. Richard Geier III, Denise M. Haynes, Jonathan S. Lindsey. 1999, **9**, 1455, and Chmielewski, P. J.; Latos-Grażyński, L.; Rachlewicz, K.; Głowiak, T. *Angew. Chem.* 1994, **104,** 805; *Angew. Chem. Int. Ed.* 1994, **33**, 779.).

Typical procedure for synthesis of 21-fluoroalkylated N-confused porphyrins. A mixture of **Ni1** (67 mg, 0.1 mmol), $Cl(CF_2)_4I$ (1.087 g, 3 mmol) and copper powder (1.000 g, 22 mmol) was stirred in 20 mL DMSO at 100 for 40-60 min. The reaction course was monitored by TLC. When **Ni1** was totally consumed, the reaction mixture was filtered. Then CH_2Cl_2 (100 ml) was added and washed several times with water. The organic layer was dried over anhydrous Na_2SO_4 and evaporated by rotary vaporator to dryness. After chromatography on silica gel column using CH_2Cl_2 as an eluent (the first band was collected) and crystallization from CH_2Cl_2/EtOH, a purple solid **Ni1b** was obtained.



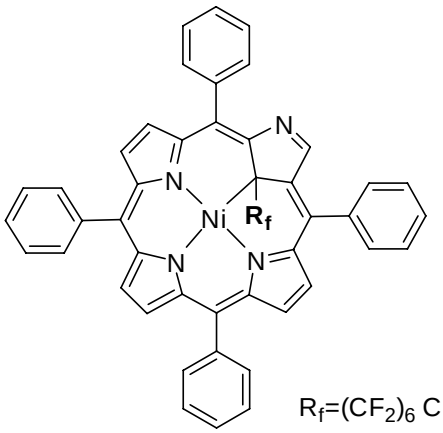
Ni1a

Ni1a: yield 37%. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 9.83 (s, 1H), 8.60 (d, *J* = 5.0 Hz, 1H), 8.58 (d, *J* = 5.0 Hz, 1H), 8.49 (d, *J* = 5.0 Hz, 2H), 8.45 (d, *J* = 4.9 Hz, 1H), 8.41 (d, *J* = 4.9 Hz, 1H), 7.62 ~ 8.18 (m, 20H). ^{19}F NMR (282 MHz, $CDCl_3$): δ = -63.47, -65.77 (AB, J_{AB} = 169.1 Hz, 2F), -92.58 (m, 2F). UV/Vis (CH_2Cl_2): λ_{max} (relative intensity) = 435 (35.4), 563 (sh), 607 (sh), 784 (1.0) nm. MS (MALDI): *m*/z 804.1 (M^+). Anal. Calcd for $C_{46}H_{27}ClF_4N_4Ni \cdot 0.25H_2O$: C, 68.18; H, 3.42; N, 6.91. Found: C, 68.13; H, 3.73; N, 6.55.



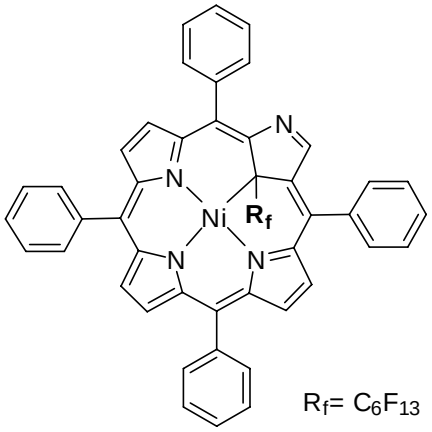
Ni1b

Ni1b: yield 88%. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 9.78 (s, 1H), 8.63 (d, *J* = 5.1 Hz, 1H), 8.60 (d, *J* = 5.1 Hz, 1H), 8.49 (d, *J* = 4.8 Hz, 2H), 8.45 (d, *J* = 4.9 Hz, 1H), 8.41 (d, *J* = 4.9 Hz, 1H), 7.62 ~ 8.18 (m, 20H). ^{19}F NMR (282 MHz, $CDCl_3$): δ = -68.49 (m, 2F), -93.69, -96.07 (AB, J_{AB} = 269.8 Hz, 2F), -117.25 ~ -123.26 (m, 4F). UV/Vis (CH_2Cl_2): λ_{max} (relative intensity) = 435 (40.2), 567 (sh), 610 (sh), 781 (1.0) nm. HRMS (MALDI): Calcd for $C_{48}H_{27}ClF_8N_4Ni^+$: 904.11500. Found: 904.11445. Anal. Calcd for $C_{46}H_{27}ClF_4N_4Ni{\cdot}CH_2Cl_2{\cdot}H_2O$: C, 58.34; H, 3.10; N, 5.55. Found: C, 58.35; H, 3.02; N, 5.48.



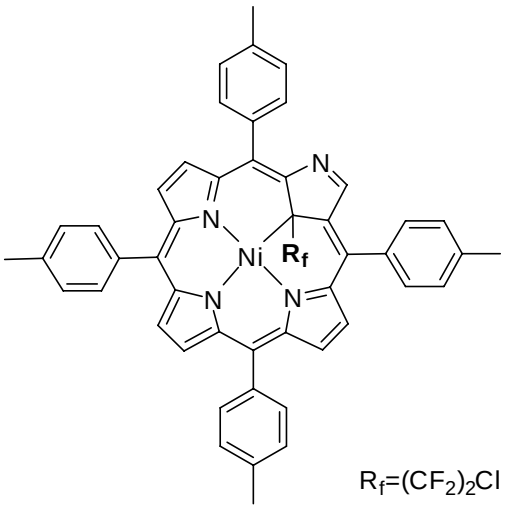
Ni1c

Ni1c: yield 78%. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 9.78 (s, 1H), 8.64 (d, *J* = 5.0 Hz, 1H), 8.61 (d, *J* = 5.0 Hz, 1H), 8.50 (d, *J* = 4.7 Hz, 2H), 8.46 (d, *J* = 4.9 Hz, 1H), 8.42 (d, *J* = 4.9 Hz, 1H), 7.62 ~ 8.18 (m, 20H). ^{19}F NMR (282 MHz, $CDCl_3$): δ = -68.17 (m, 2F), -93.11, -95.45 (AB, J_{AB} = 261.3 Hz, 2F), -117.37 ~ -122.50 (m, 8F). UV/Vis (CH_2Cl_2): λ_{max} (relative intensity) = 435 (40.2), 562 (sh), 612 (sh), 783 (1.0) nm. MS (MALDI): *m*/*z* 1004.1 (M^+). Anal. Calcd for $C_{50}H_{27}ClF_{12}N_4N{\cdot}H_2O$: C, 58.65; H, 2.85; N, 5.47. Found: C, 58.49; H, 2.86; N, 5.07.



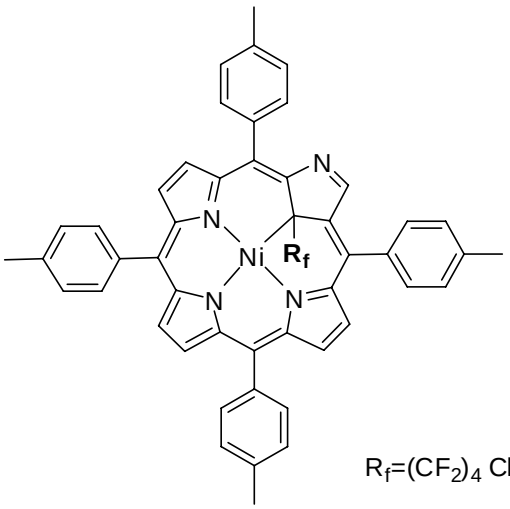
Ni1d

Ni1d: yield 78%. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 9.77 (s, 1H), 8.63 (d, *J* = 5.0 Hz, 1H), 8.61 (d, *J* = 5.0 Hz, 1H), 8.50 (d, *J* = 5.0 Hz, 2H), 8.46 (d, *J* = 5.0 Hz, 1H), 8.42 (d, *J* = 5.0Hz, 1H), 7.62 ~ 8.18 (m, 20H). ^{19}F NMR (282 MHz, $CDCl_3$): δ = -80.56 (m, 3F), -92.78, -95.21 (AB, J_{AB} = 279.3 Hz, 2F), -117.71 ~ -123.20 (m, 8F). UV/Vis (CH_2Cl_2): λ_{max} (relative intensity) = 436 (35.0), 563 (sh), 611 (sh), 779(1.0) nm. MS (MALDI): *m*/*z* 988.1 (M^+). Anal. Calcd for $C_{50}H_{27}F_{13}N_4Ni{\cdot}CH_3CH_2OH$: C, 60.31; H, 3.21; N, 5.41. Found: C, 60.39; H, 3.49; N, 4.93.



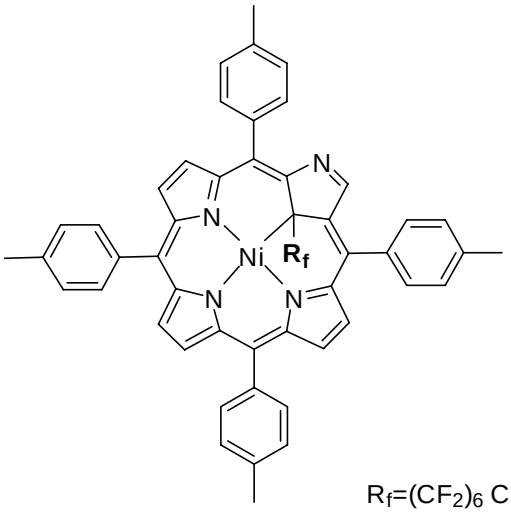
Ni2a

Ni2a: yield 32%. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 9.79 (s, 1H), 8.57 ~ 8.62(m, 2H), 8.49 (d, *J* = 5.0 Hz, 2H), 8.46 (d, *J* = 5.0 Hz, 1H), 8.41 (d, *J* = 5.0 Hz, 1H), 7.45 ~ 8.08 (m, 16H), 2.56 ~ 2.67 (m, 12H). ^{19}F NMR (282 MHz, $CDCl_3$): δ = -63.72, -65.78 (AB, J_{AB} = 168.3 Hz, 2F), -92.51 (m, 2F). UV/Vis (CH_2Cl_2): λ_{max} (relative intensity) = 438 (33.4), 567 (sh), 609 (sh), 790 (1.0) nm. MS (MALDI): *m*/*z* 860.2 (M^+). Anal. Calcd for $C_{50}H_{35}ClF_4N_4Ni{\cdot}H_2O$: C, 68.24; H, 4.24; N, 6.37. Found: C, 68.40; H, 3.95; N, 6.62.



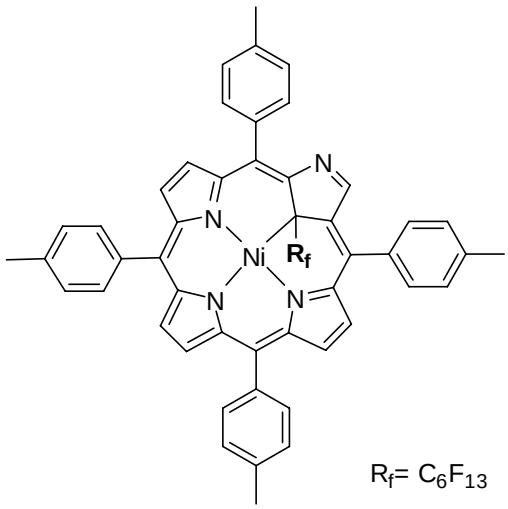
Ni2b

Ni2b: yield 92%. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 9.72 (s, 1H), 8.57 ~ 8.64 (m, 2H), 8.49 (d, *J* = 5.0 Hz, 2H), 8.45 (d, *J* = 4.8 Hz, 1H), 8.41 (d, *J* = 4.8Hz, 1H), 7.42 ~ 8.07 (m, 16H), 2.58 ~ 2.69 (m, 12H). ^{19}F NMR (282 MHz, $CDCl_3$): δ = -68.38 (m, 2F), -93.65, -96.02 (AB, J_{AB} = 269.5 Hz, 2F), -117.90 ~ -123.24 (m, 4F). UV/Vis (CH_2Cl_2): λ_{max} (relative intensity) = 439 (31.5), 567 (sh), 612 (sh), 779 (1.0) nm. MS (MALDI): *m*/*z* 960.2 (M^+). Anal. Calcd for $C_{52}H_{35}ClF_8N_4Ni{\cdot}1.5CH_2Cl_2$: C, 58.98; H, 3.52; N, 5.14. Found: C, 58.85; H, 3.21; N, 5.22.



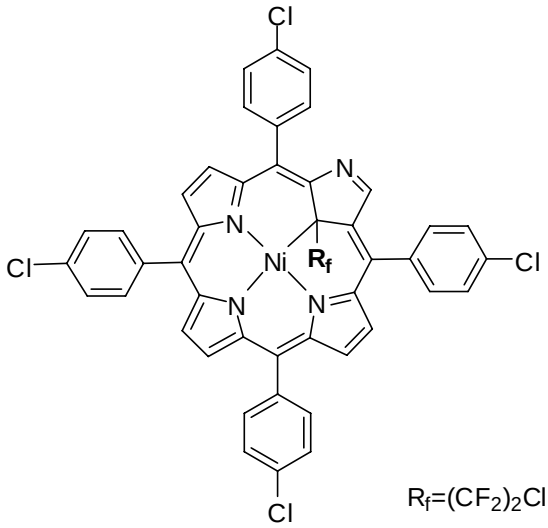
Ni2c

Ni2c: yield 91%. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 9.73 (s, 1H), 8.58 ~ 8.64 (m, 2H), 8.50 (d, *J* = 5.0 Hz, 2H), 8.46 (d, *J* = 4.8 Hz, 1H), 8.42 (d, *J* = 4.8Hz, 1H), 7.40 ~ 8.07 (m, 16H), 2.53 ~ 2.69 (m, 12H). ^{19}F NMR (282 MHz, $CDCl_3$): δ= -68.51 (m, 2F), -93.69, -96.13 (AB, J_{AB} = 268.9 Hz, 2F), -117.74 ~ -123.61 (m, 8F). UV/Vis (CH_2Cl_2): λ_{max} (relative intensity) = 439 (33.2), 568 (sh), 610 (sh), 779 (1.0) nm. MS (MALDI): *m*/*z* 1060.2 (M^+). Anal. Calcd for $C_{54}H_{35}ClF_{12}N_4Ni{\cdot}CH_2Cl_2{\cdot}CH_3CH_2OH{\cdot}0.5H_2O$: C, 56.96; H, 3.69; N, 4.66. Found: C, 57.25; H, 3.94; N, 4.26.



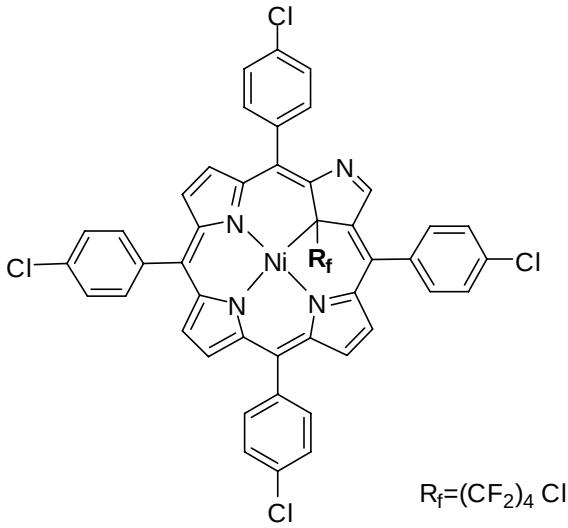
Ni2d

Ni2d: yield 90%. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 9.71 (s, 1H), 8.57 ~ 8.66 (m, 2H), 8.49 (d, *J* = 4.8 Hz, 2H), 8.45 (d, *J* = 4.9 Hz, 1H), 8.41 (d, *J* = 4.9 Hz, 1H), 7.37 ~ 8.00 (m, 16H), 2.57 ~ 2.72 (m, 12H). ^{19}F NMR (282 MHz, $CDCl_3$): δ = -80.51 (m, 3F), -92.79, -95.15 (AB, J_{AB} = 280.3 Hz, 2F), -117.74 ~ -123.17 (m, 8F). UV/Vis (CH_2Cl_2): λ_{max} (relative intensity) = 439 (33.5), 565 (sh), 612 (sh), 788 (1.0) nm. MS (MALDI): *m*/*z* 1044.2 (M^+). Anal. Calcd for $C_{54}H_{35}F_{13}N_4Ni$: C, 62.03; H, 3.37; N, 5.36. Found: C, 61.60; H, 3.65; N, 4.88.



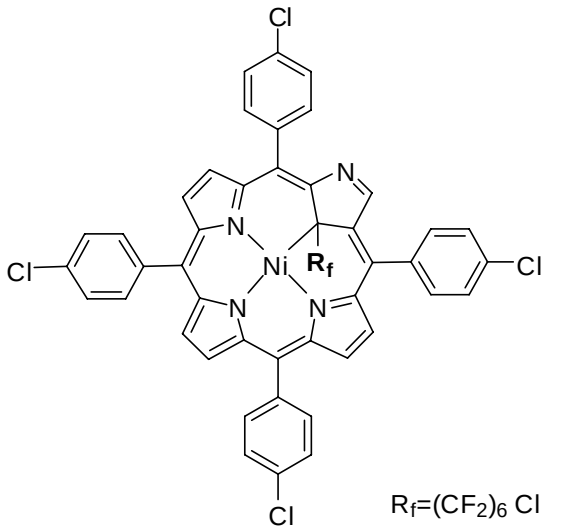
Ni3a

Ni3a: yield 33%. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 9.83 (s, 1H), 8.60 (d, *J* = 5.0 Hz, 1H), 8.58 (d, *J* = 5.0 Hz, 1H), 8.49 (d, *J* = 5.0 Hz, 2H), 8.45 (d, *J* = 4.9 Hz, 1H), 8.41 (d, *J* = 4.9 Hz, 1H), 7.63 ~ 8.18 (m, 16H).^{19}F NMR (282 MHz, $CDCl_3$): δ = -63.72, -65.77 (AB, J_{AB} = 167.8 Hz, 2F), -92.58 (m, 2F). UV/Vis (CH_2Cl_2): λ_{max} (relative intensity) = 439 (32.7), 567 (sh), 611 (sh), 767 (1.0) nm. MS (MALDI): *m*/*z* 940.0 (M^+). Anal. Calcd for $C_{46}H_{23}Cl_5F_4N_4Ni \cdot 2.25CH_2Cl_2 \cdot 0.5CH_3CH_2OH$: C, 51.09; H, 2.66; N, 4.84. Found: C, 51.33; H, 2.24; N, 4.36.



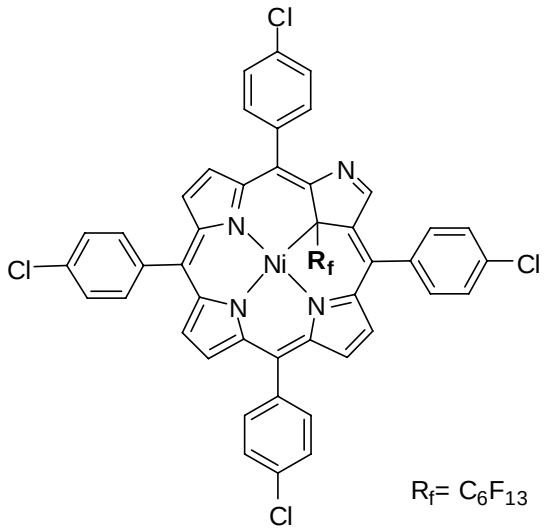
Ni3b

Ni3b: yield 62%. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 9.74 (s, 1H), 8.50 ~ 8.56 (m, 2H), 8.49 (d, *J* = 5.0 Hz, 2H), 8.46 (d, *J* = 5.0 Hz, 1H), 8.42 (d, *J* = 5.0 Hz, 1H), 7.55 ~ 8.07 (m, 16H). ^{19}F NMR (282 MHz, $CDCl_3$): δ = -68.05 (m, 2F), -93.49, -95.50 (AB, J_{AB} = 292.3 Hz, 2F), -117.81 ~ -122.21 (m, 4F). UV/Vis (CH_2Cl_2): λ_{max} (relative intensity) = 442 (35.1), 567 (sh), 612 (sh), 782 (1.0) nm. MS (MALDI): *m*/*z* 1040.0 (M^+). Anal. Calcd for $C_{48}H_{23}Cl_5F_8N_4Ni \cdot CH_2Cl_2 \cdot H_2O$: C, 51.33; H, 2.37; N, 4.89. Found: C, 51.41; H, 2.62; N, 4.69.



Ni3c

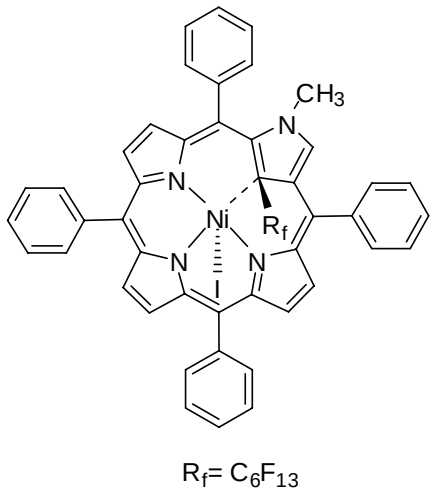
Ni3c: yield 56%. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 9.76 (s, 1H), 8.57 ~ 8.64 (m, 2H), 8.50 (d, *J* = 5.0 Hz, 2H), 8.47 (d, *J* = 4.8 Hz, 1H), 8.43 (d, *J* = 4.8 Hz, 1H), 7.58 ~ 8.17 (m, 16H). ^{19}F NMR (282 MHz, $CDCl_3$): δ = -68.20 (m, 2F), -93.10, -95.47 (AB, J_{AB} = 263.5 Hz, 2F), -117.24 ~ -122.45 (m, 8F). UV/Vis (CH_2Cl_2): λ_{max} (relative intensity) = 441 (33.2), 575 (sh), 613 (sh), 780 (1.0) nm. MS (MALDI): *m*/*z* 1140.0 (M^+). Anal. Calcd for $C_{50}H_{23}Cl_5F_{12}N_4Ni \cdot 0.5CH_2Cl_2 \cdot CH_3CH_2OH$: C, 51.17; H, 2.45; N, 4.55. Found: C, 51.29; H, 2.19; N, 4.20.



Ni3d

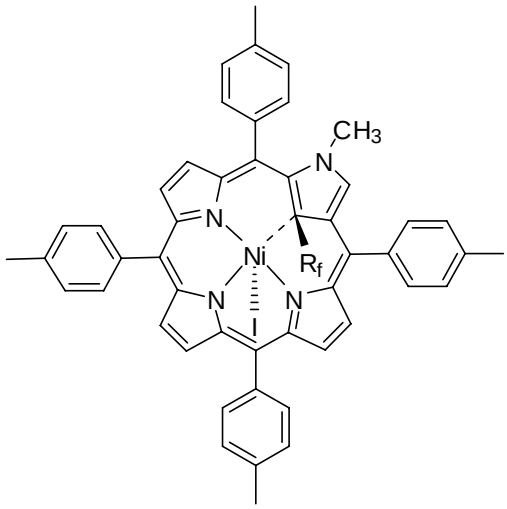
Ni3d: yield 58%. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 9.72 (s, 1H), 8.56 ~ 8.64 (m, 2H), 8.49 (d, *J* = 5.0 Hz, 2H), 8.46 (d, *J* = 5.0 Hz, 1H), 8.42 (d, *J* = 5.0 Hz, 1H), 7.61 ~ 8.15 (m, 16H). ^{19}F NMR (282 MHz, $CDCl_3$): δ = -81.36 (m, 3F), -93.77, -95.90 (AB, J_{AB} = 265.6 Hz, 2F), -117.65 ~ -127.18 (m, 8F). UV/Vis (CH_2Cl_2): λ_{max} (relative intensity) = 441 (35.1), 574 (sh), 617 (sh), 781 (1.0) nm. MS (MALDI): *m*/*z* 1124.0 (M^+). Anal. Calcd for $C_{50}H_{23}Cl_4F_{13}N_4Ni{\cdot}CH_2Cl_2{\cdot}2CH_3CH_2OH{\cdot}H_2O$: C, 49.96; H, 2.97; N, 4.24. Found: C, 50.22; H, 2.68; N, 3.77.

Typical Procedure for the Synthesis of 2-Aza-2-CH_3-21-fluoroalkyl -5,10,15,20-tetra-aryl-21-carbaporphyrinatonickel(II) Iodide. Ni1d (20 mg, 0.029 mmol) and methyl iodide (5mL, 98.6 mmol) were dissolved in 20 mL of dichloromethane and stirred under reflux for 24 h. The reaction mixture was evaporated by rotary vaporator to dryness and dissolved in dichloromethane again. Precipitation with *n*-hexane gave the methylated product **Ni1da**.



Ni1da

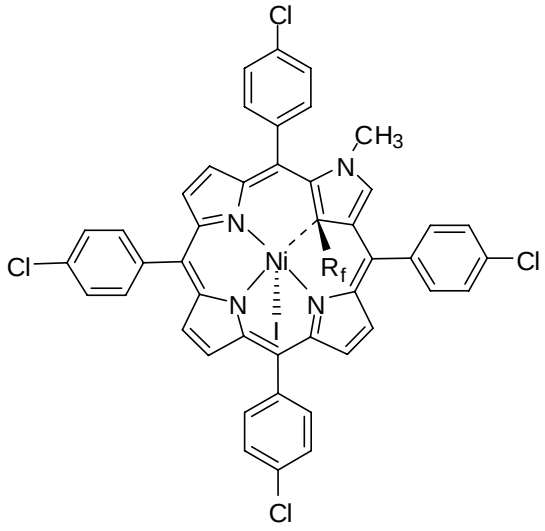
Ni1da: yield 75%. UV/Vis (CH_2Cl_2): λ_{max} (relative intensity) = 455 (32.2), 501 (sh), 684 (sh), 750 (1.0) nm. MS (MALDI): *m*/z, 1003.2 ($[M\text{-}I]^+$). Anal. Calcd for $C_{51}H_{30}F_{13}IN_4Ni{\cdot}3H_2O$: C, 51.67; H, 3.06; N, 4.73. Found: C, 51.29; H, 3.28; N, 4.50.



Ni2da

R_f= C_6F_{13}

Ni2da: yield 73%. UV/Vis (CH_2Cl_2): λ_{max} (relative intensity) = 453 (35.0), 502 (sh), 687 (sh), 756 (1.0) nm. MS (MALDI): *m*/*z* 1059.2 ([M-I]$^+$). Anal. Calcd for $C_{55}H_{38}F_{13}IN_4Ni \cdot C_6H_{14} \cdot 2.5H_2O$: C, 55.56; H, 4.36; N, 4.25. Found: C, 55.23; H, 4.56; N, 3.95.

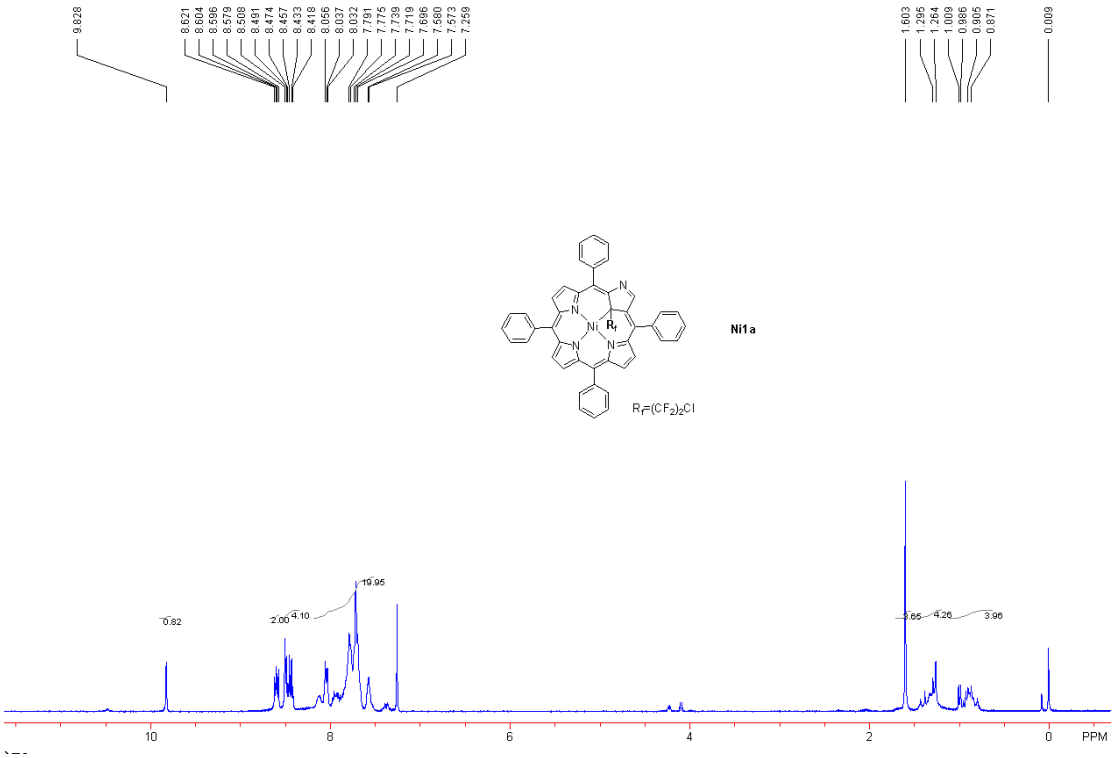


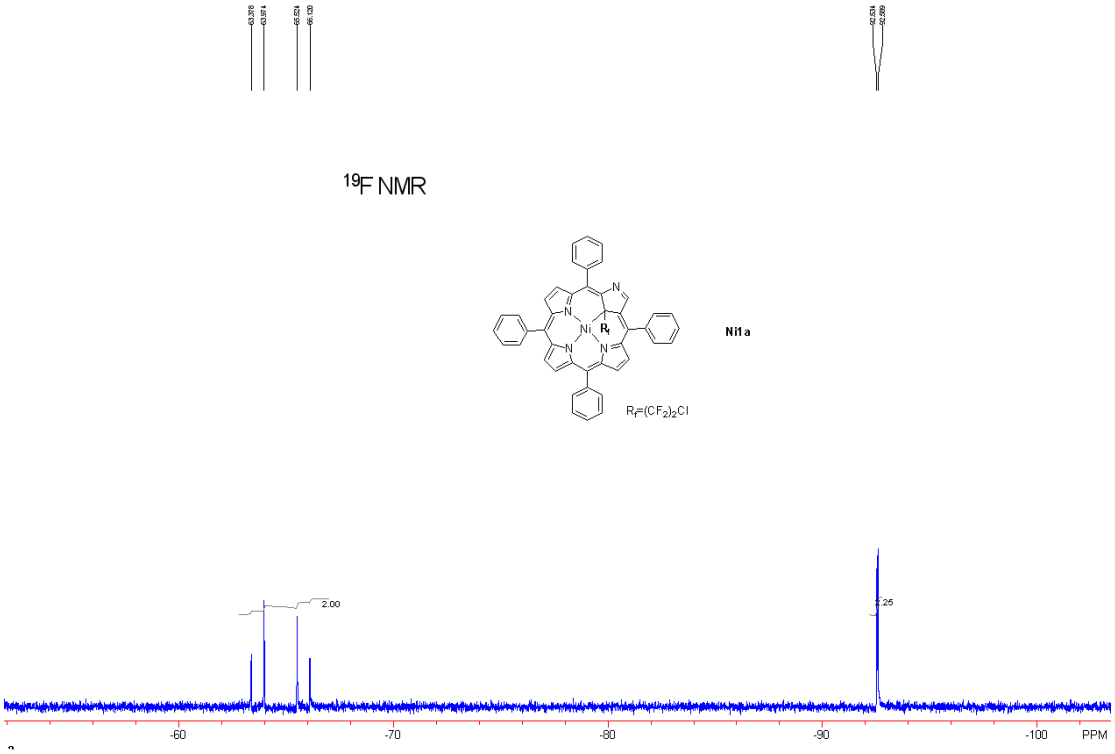
Ni3da

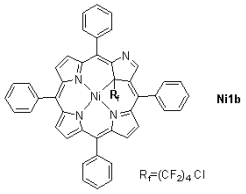
R_f= C_6F_{13}

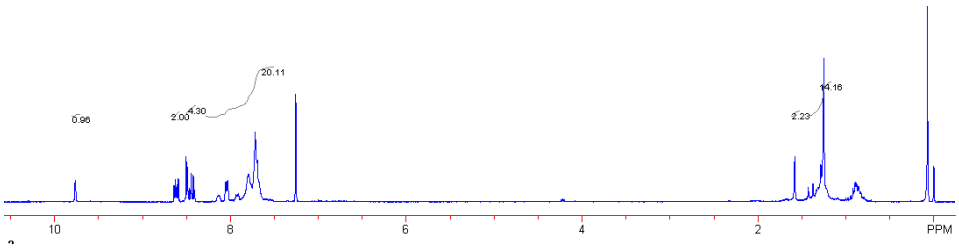
Ni3da: yield 78%. UV/Vis (CH_2Cl_2): λ_{max} (relative intensity) = 451 (32.3), 501 (sh), 683 (sh), 752 (1.0) nm. MS (MALDI): *m*/*z* 1139.0 ([M-I]$^+$). Anal. Calcd for $C_{51}H_{26}Cl_4F_{13}IN_4Ni \cdot C_6H_{14} \cdot H_2O$: C, 49.85; H, 3.08; N, 4.08. Found: C, 49.70; H, 3.19; N, 3.90.

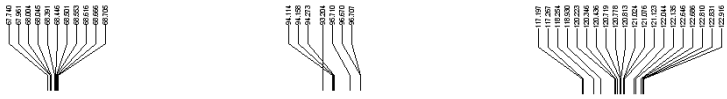
Copies of ^{1}H and ^{19}F NMR spectra of new fluoroalkylated porphyrins:



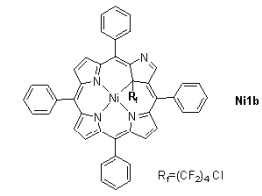


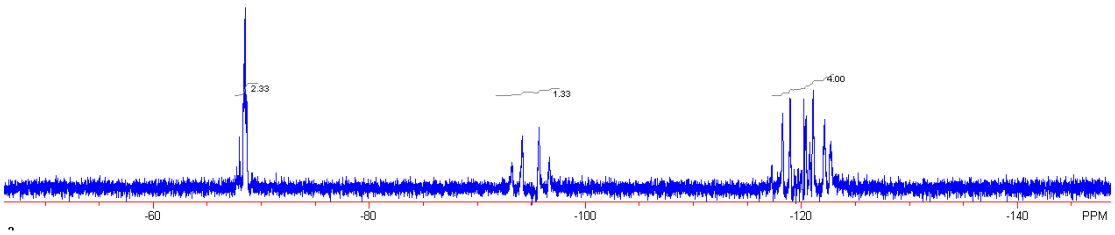

Ni1b
R_f=$(CF_2)_4$ Cl

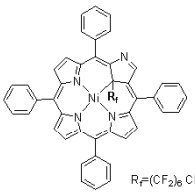

0.96
2.00
4.30
20.11
2.23
14.16
10
8
6
4
2
PPM



^{19}F NMR

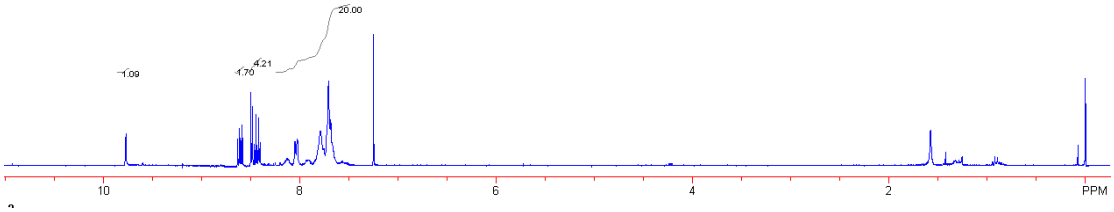

Ni1b
R_f=$(CF_2)_4$ Cl

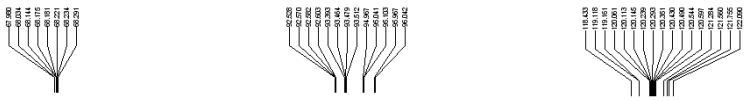

2.33
1.33
4.00
-60
-80
-100
-120
-140
PPM



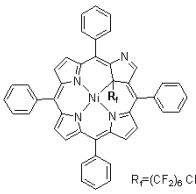
Ni1c

R_f=$(CF_2)_6$ Cl



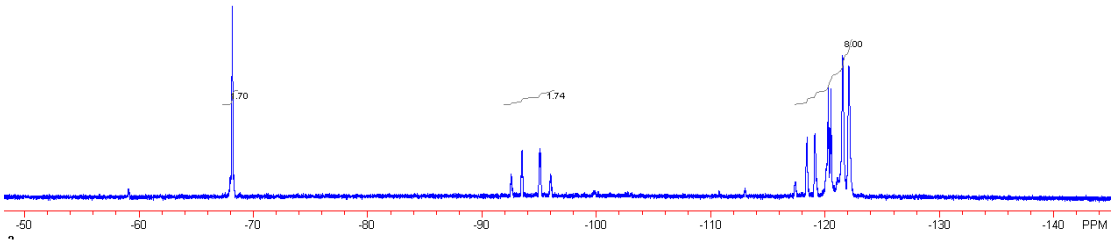


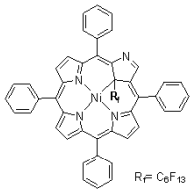
^{19}F NMR



Ni1c

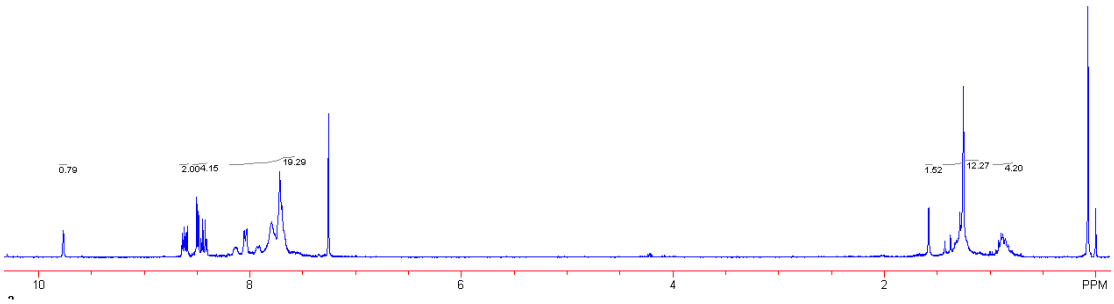
R_f=$(CF_2)_6$ Cl



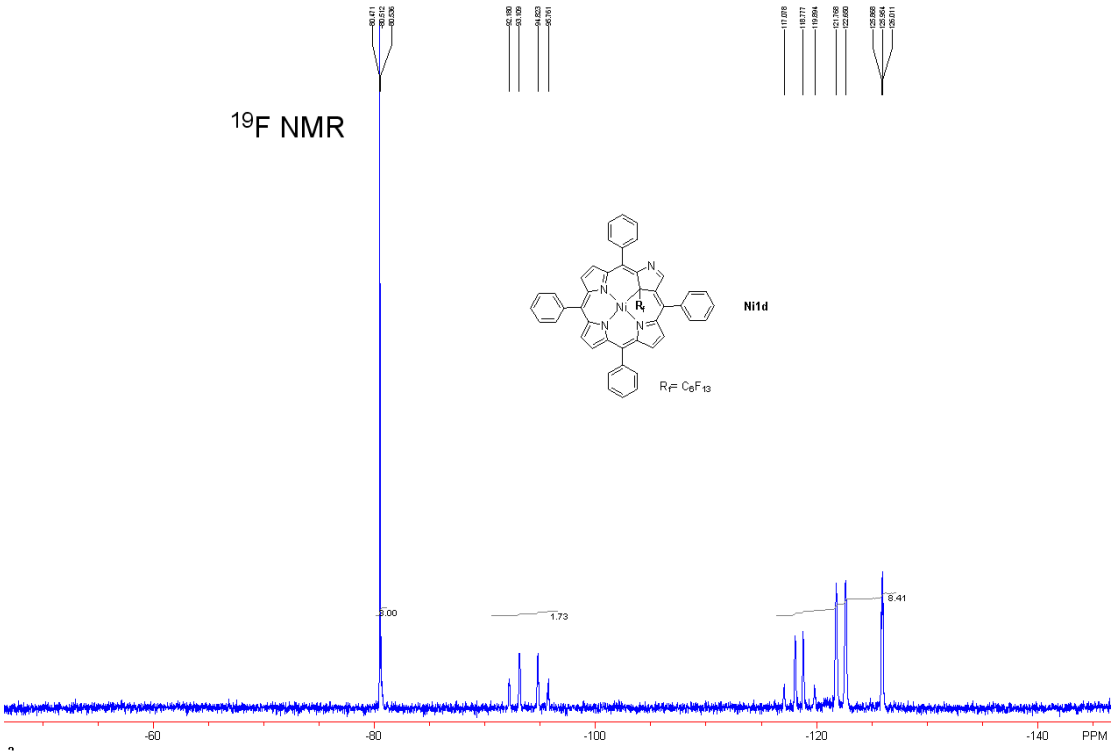


Ni1d

R_f= C_6F_{13}

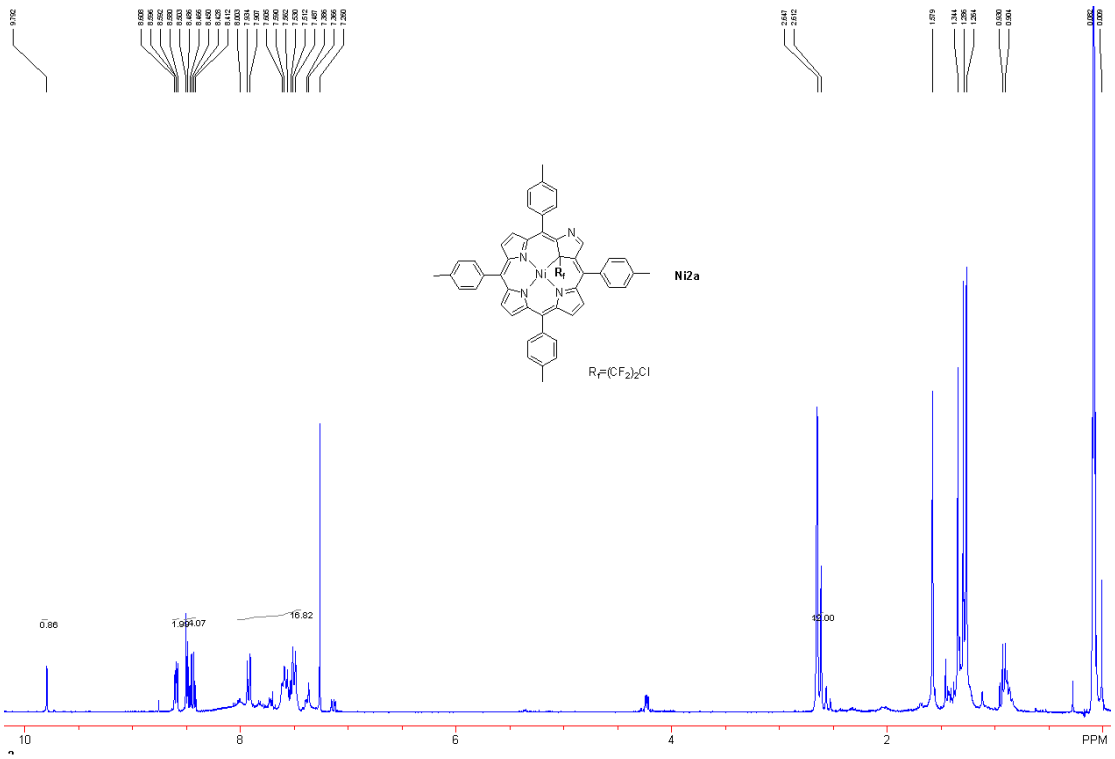


^{19}F NMR

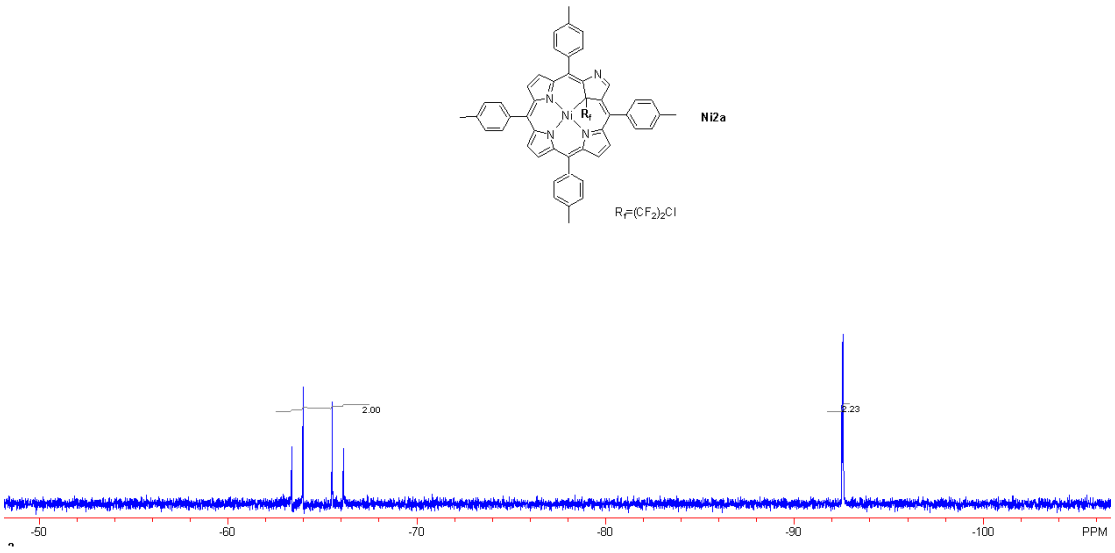


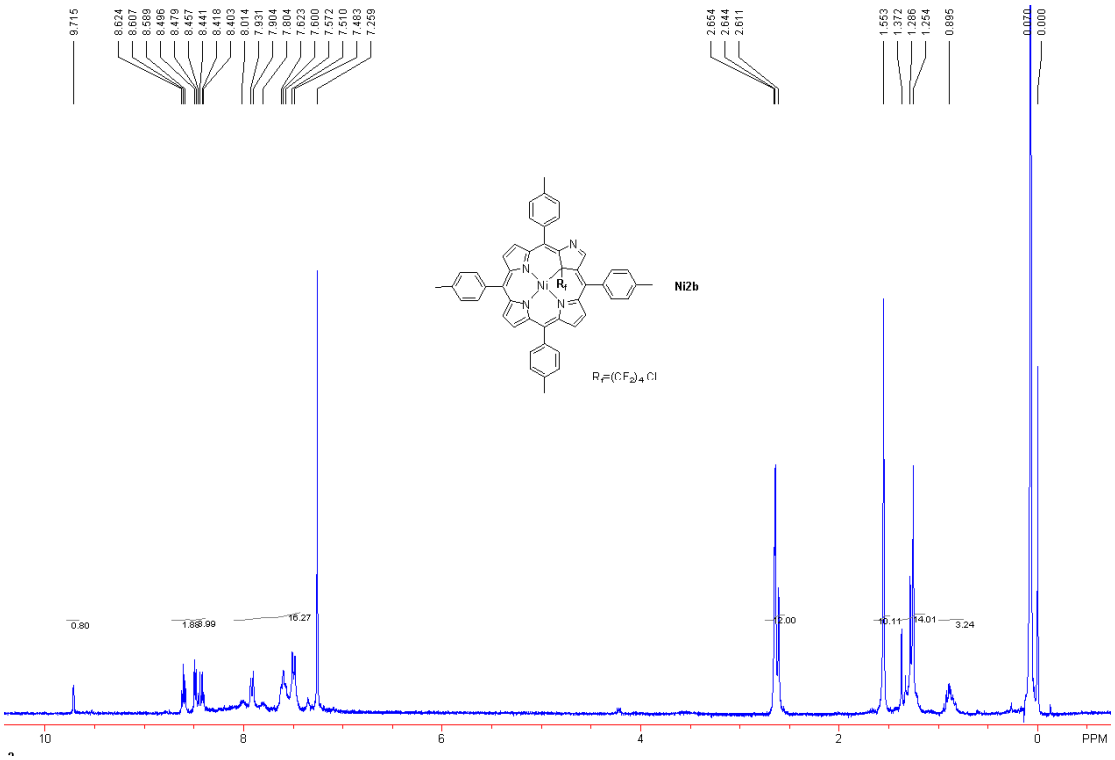
Ni1d

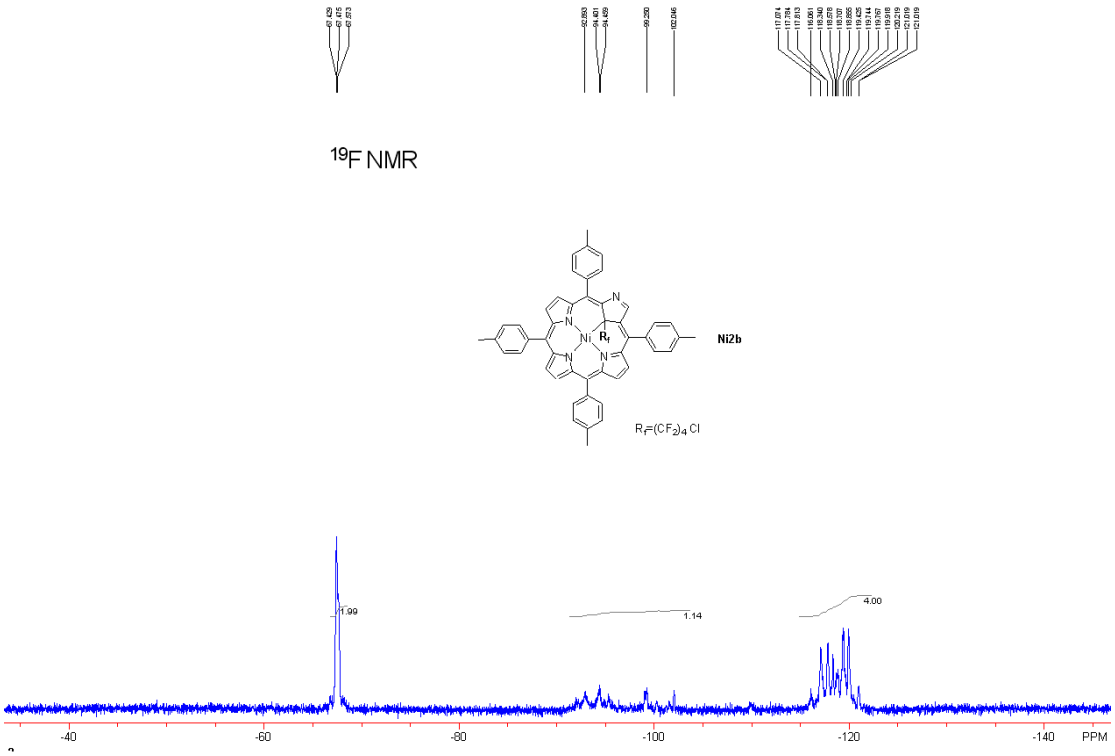
R_f= C_6F_{13}

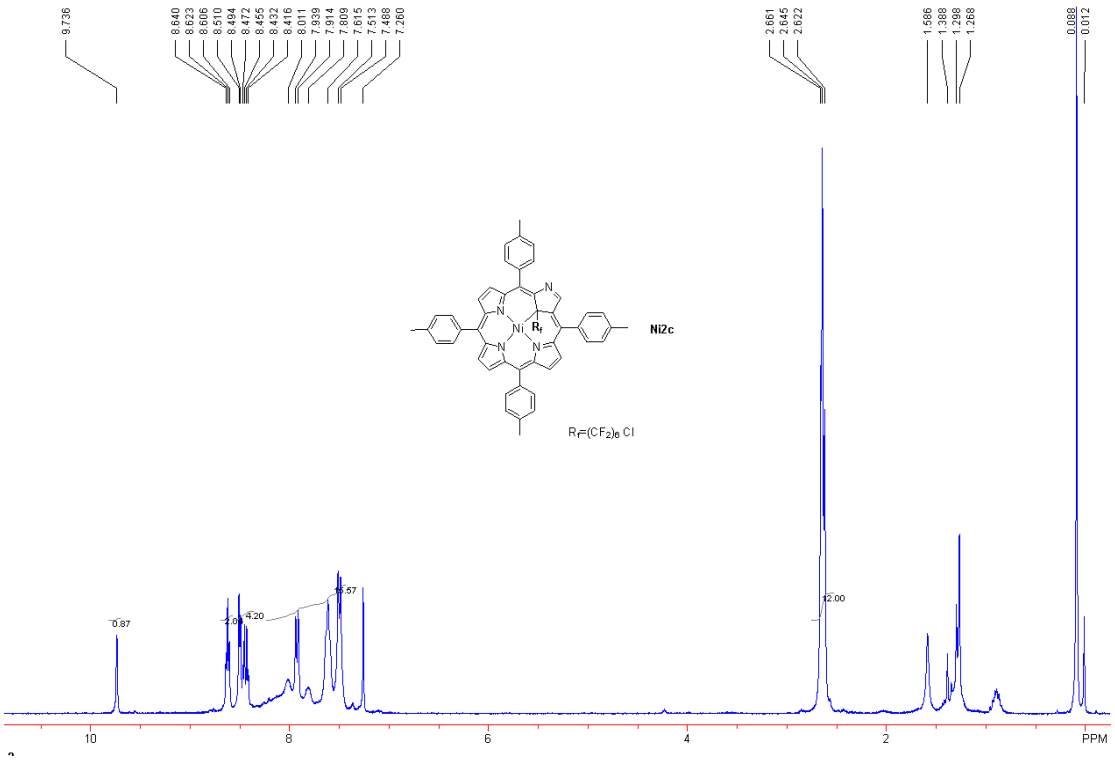

Ni2a
R_f=$(CF_2)_2Cl$
0.86
1.99
4.07
16.82
12.00
10
8
6
4
2
PPM

^{19}F NMR

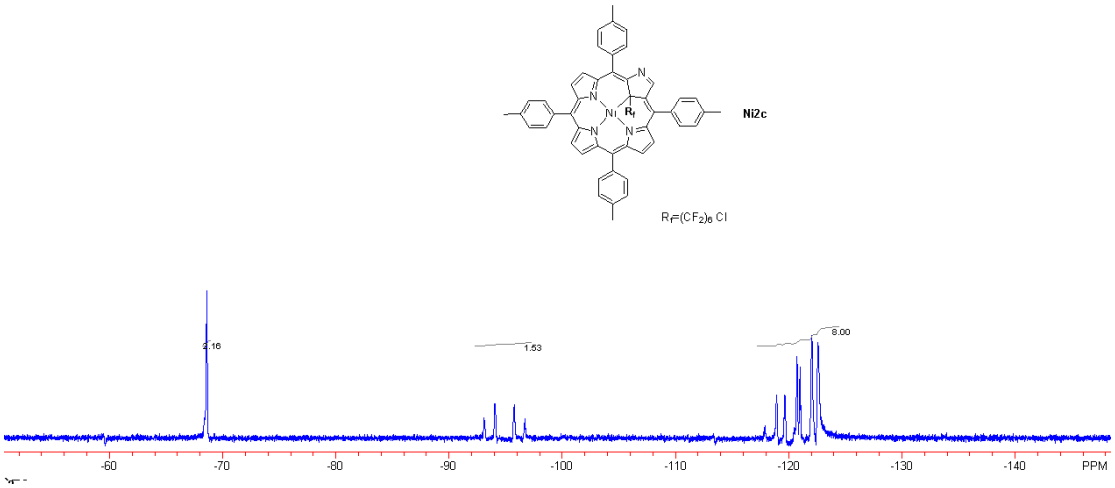

Ni2a
R_f=$(CF_2)_2Cl$
2.00
2.23
-50
-60
-70
-80
-90
-100
PPM

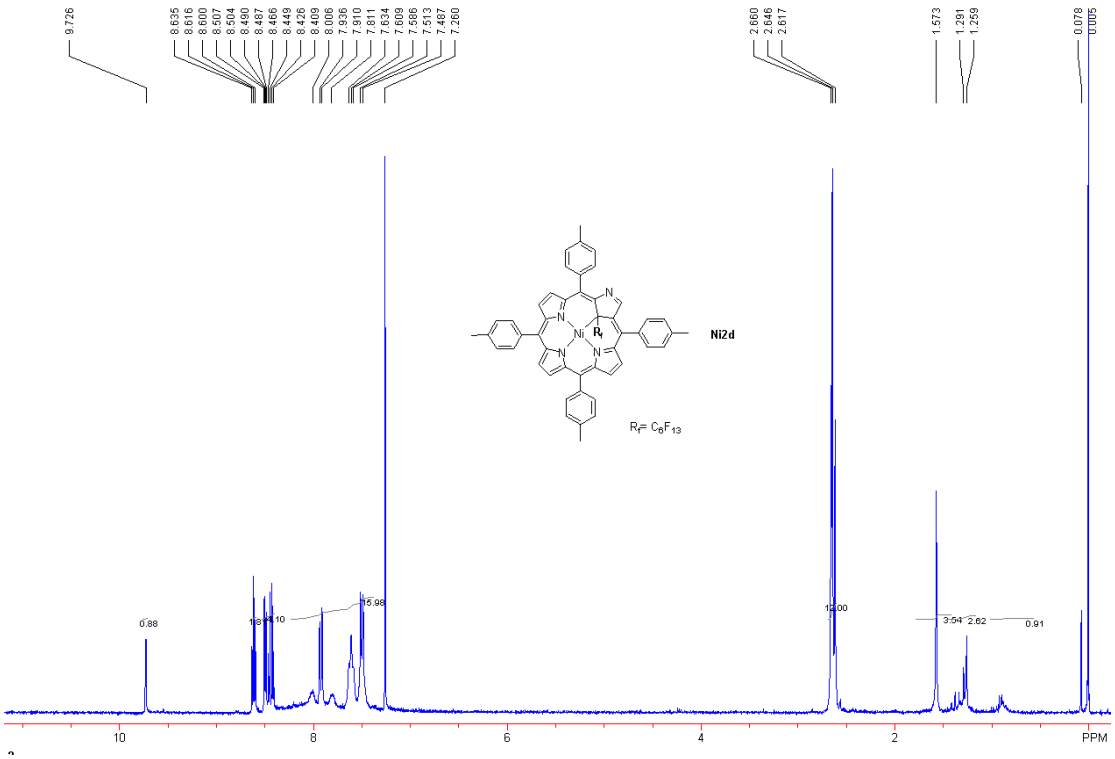

9.715
8.624
8.607
8.589
8.496
8.479
8.457
8.441
8.418
8.403
8.014
7.931
7.904
7.804
7.623
7.600
7.572
7.510
7.483
7.259
2.654
2.644
2.611
1.553
1.372
1.266
1.234
0.895
0.070
0.000
Ni2b
R_f=$(CF_2)_4$Cl
0.80
1.88
8.99
16.27
12.00
10.11
14.01
3.24
10
8
6
4
2
0
PPM

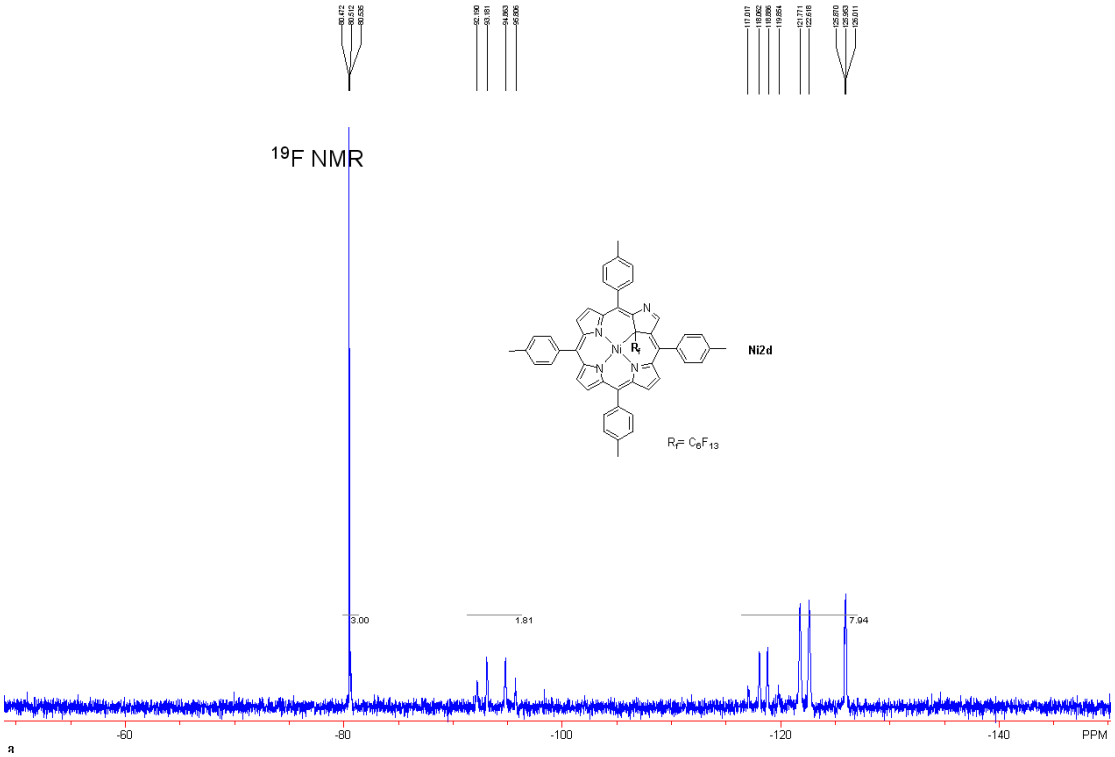

^{19}F NMR
Ni2b
R_f=$(CF_2)_4$Cl
1.99
1.14
4.00
-40
-60
-80
-100
-120
-140
PPM


9.736
8.640
8.623
8.606
8.510
8.494
8.472
8.455
8.432
8.416
8.011
7.939
7.914
7.809
7.615
7.513
7.488
7.260
2.661
2.645
2.622
1.586
1.388
1.298
1.268
0.088
0.012
Ni2c
Rf=(CF2)6 CF3
0.87
2.08
4.20
6.57
12.00
10
8
6
4
2
PPM

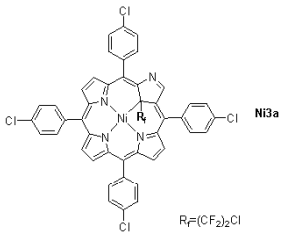
^{19}F NMR

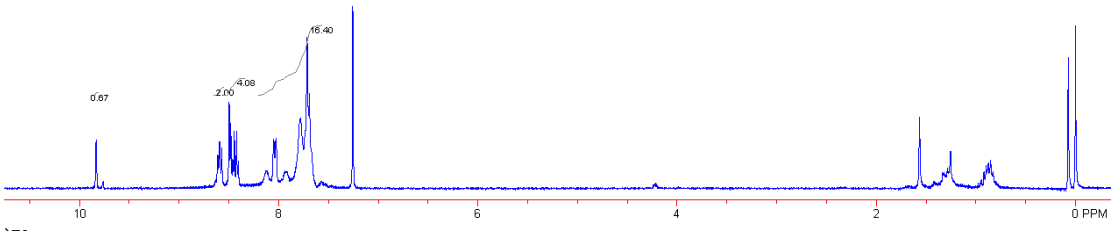

Ni2c
Rf=(CF2)6 CF3
2.16
1.53
8.00
-60
-70
-80
-90
-100
-110
-120
-130
-140
PPM


9.726
8.635
8.616
8.600
8.507
8.504
8.490
8.487
8.466
8.449
8.426
8.409
8.006
7.936
7.910
7.811
7.634
7.609
7.586
7.513
7.487
7.260
2.660
2.646
2.617
1.573
1.291
1.259
0.078
0.005
Ni2d
R_F= C_6F_{13}
0.88
15.98
12.00
3.54
2.62
0.91
10
8
6
4
2
PPM


^{19}F NMR
Ni2d
R_F= C_6F_{13}
3.00
1.81
7.94
-60
-80
-100
-120
-140
PPM

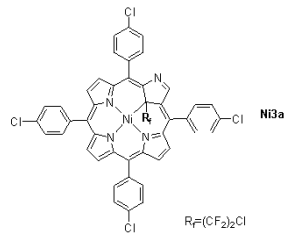

9.832
8.612
8.595
8.571
8.497
8.480
8.462
8.446
8.423
8.406
8.050
8.027
7.780
7.735
7.714
7.692
7.266
1.566
1.266
1.254
0.895
0.875
0.852
0.072
-0.000

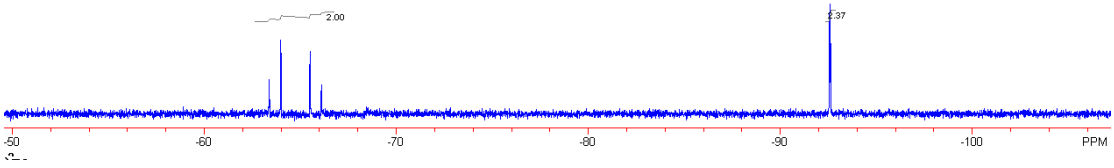

Cl
N
Ni
Rf
Cl
Cl
Cl
Ni3a
Rf=(CF2)2Cl

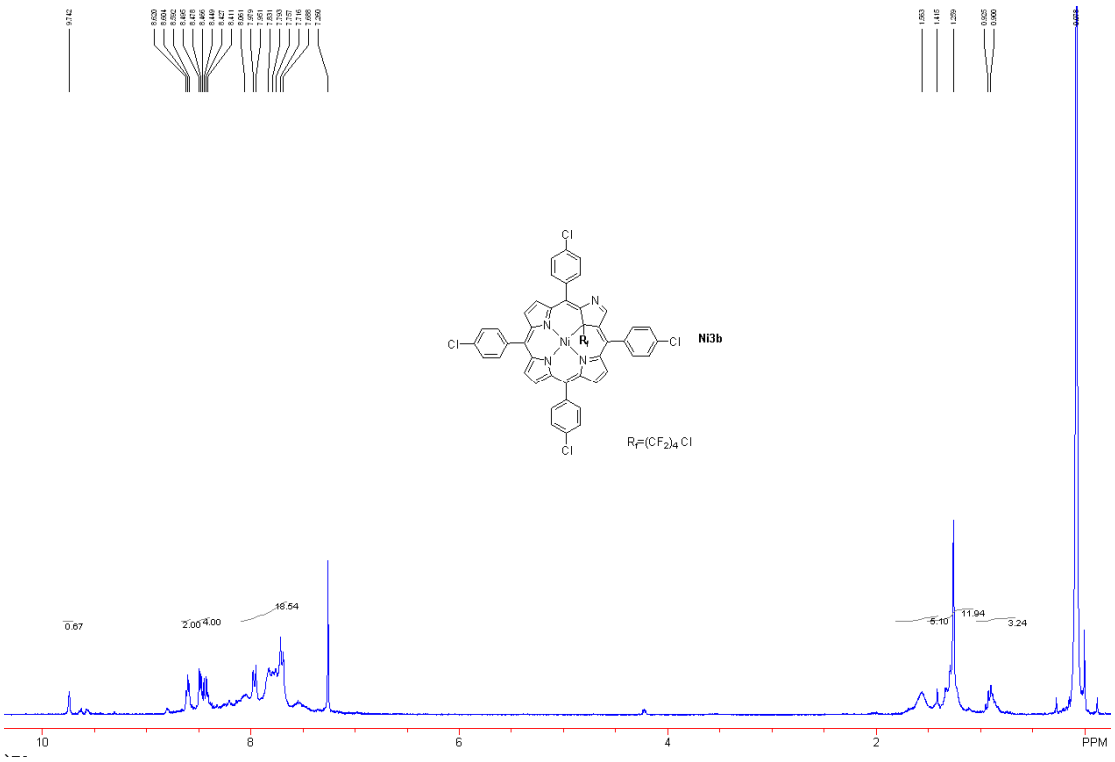

16.40
4.08
2.00
0.67
10
8
6
4
2
0 PPM


-63.396
-63.990
-65.515
-66.111
-82.591
-82.691

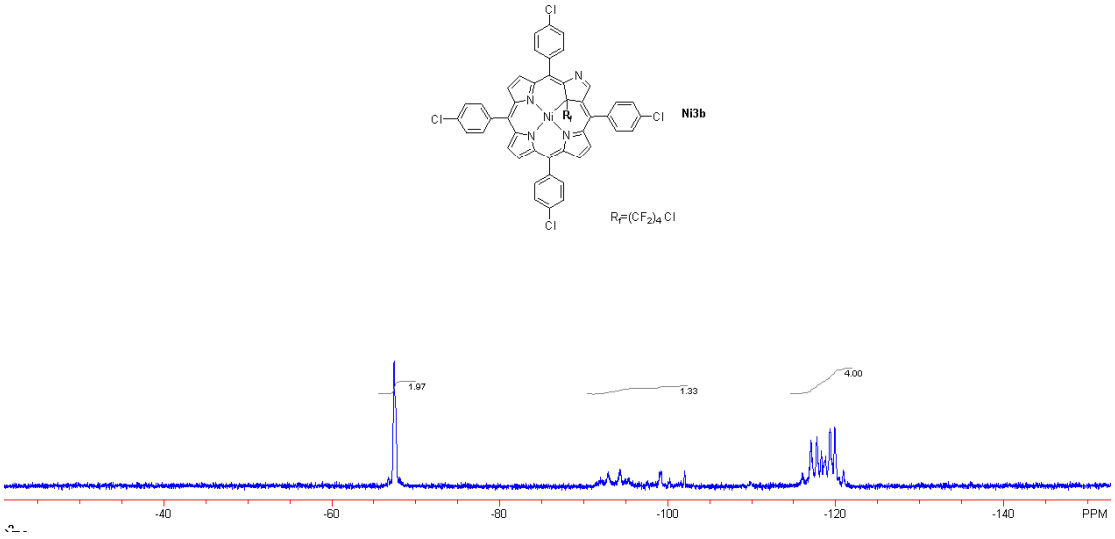
^{19}F NMR

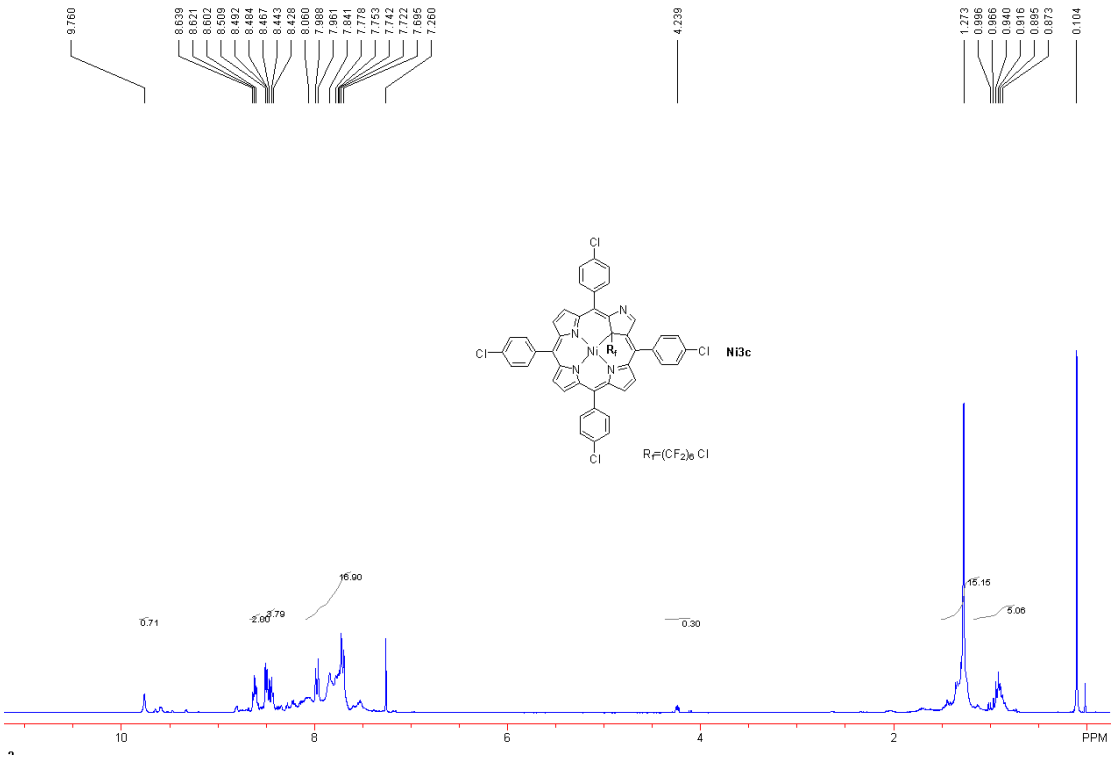

Cl
N
Ni
Rf
Cl
Cl
Cl
Ni3a
Rf=(CF2)2Cl


2.00
2.37
-50
-60
-70
-80
-90
-100
PPM

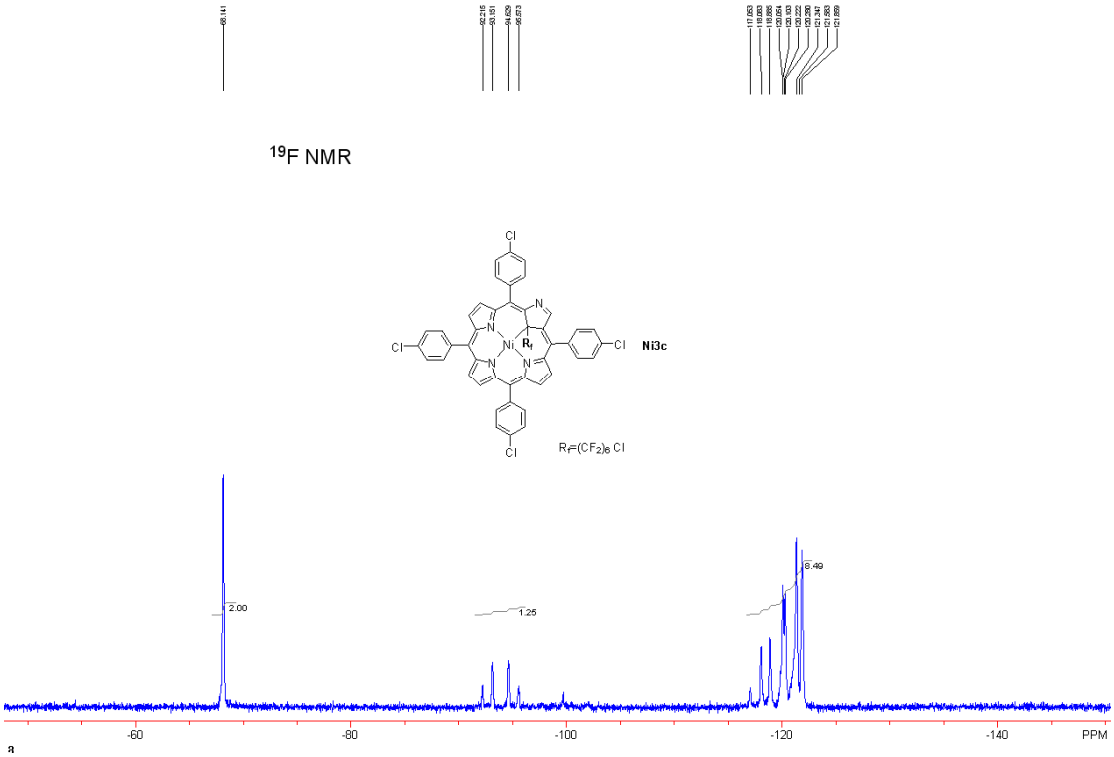

Ni3b
R_F=$(CF_2)_4$CF$_3$
0.67
2.00
4.00
16.54
5.10
11.94
3.24
10
8
6
4
2
PPM

^{19}F NMR

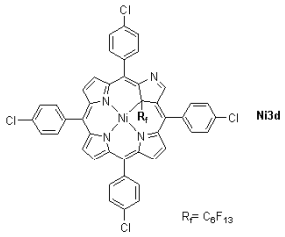

Ni3b
R_F=$(CF_2)_4$CF$_3$
1.97
1.33
4.00
-40
-60
-80
-100
-120
-140
PPM


9.760
8.639
8.621
8.602
8.509
8.492
8.484
8.467
8.443
8.428
8.060
7.988
7.961
7.841
7.778
7.753
7.742
7.722
7.695
7.260
4.239
1.273
0.996
0.966
0.940
0.916
0.895
0.873
0.104
Cl
Cl
Cl
Cl
Ni
N
N
N
N
Rf
Ni3c
Rf=(CF2)6 Cl
16.90
15.15
5.06
3.79
2.00
0.71
0.30
10
8
6
4
2
PPM

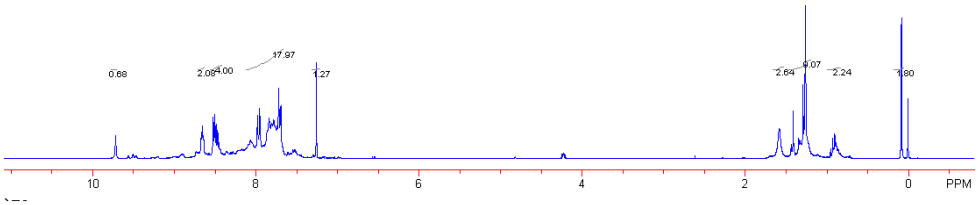
^{19}F NMR

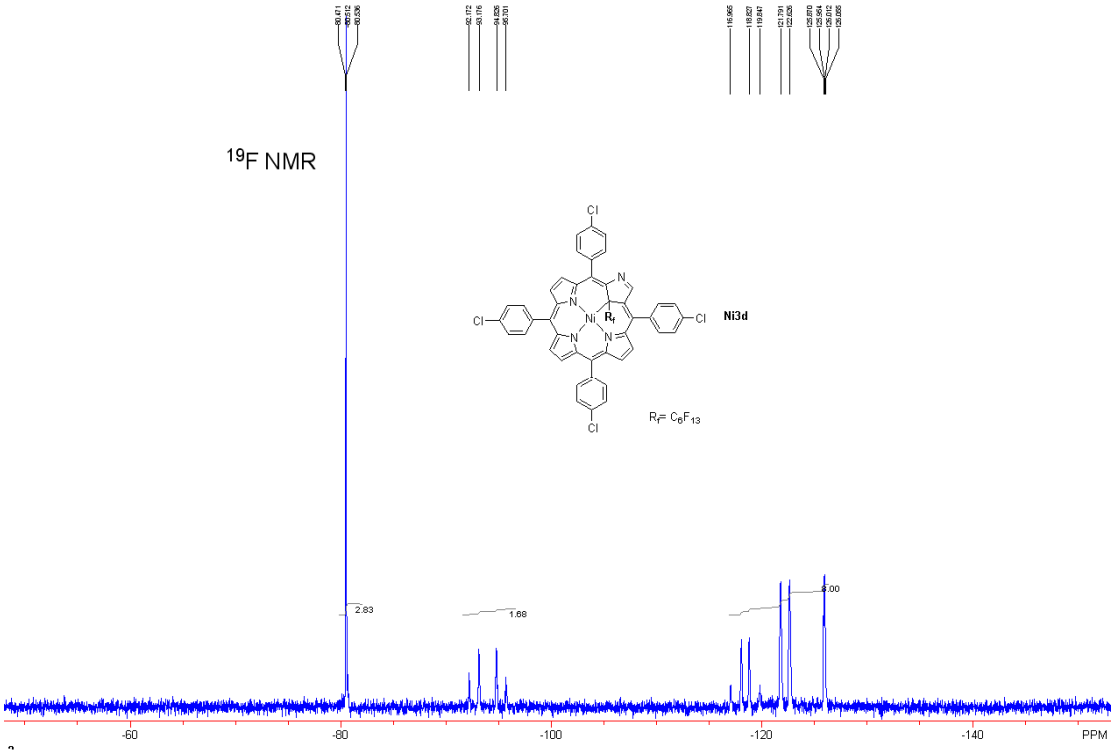

Cl
Cl
Cl
Cl
Ni
N
N
N
N
Rf
Ni3c
Rf=(CF2)6 Cl
6.49
2.00
1.25
-60
-80
-100
-120
-140
PPM


9.720
8.671
8.658
8.643
8.524
8.507
8.488
8.470
8.454
8.064
7.982
7.954
7.838
7.808
7.783
7.743
7.721
7.694
7.260
1.415
1.587
1.347
1.331
1.295
1.265
1.236
0.931
0.906
0.888
0.087
0.008


Cl
N
Ni
R_f
Cl
Cl
Cl
R_f= C_6F_{13}

Ni3d


0.68
2.08
4.00
17.97
7.27
2.64
9.07
2.24
1.80
10
8
6
4
2
0
PPM


^{19}F NMR
Cl
N
Ni
R_f
Cl
Cl
Cl
R_f= C_6F_{13}
2.83
1.68
8.00
-60
-80
-100
-120
-140
PPM

Ni3d