

The Preparation of α -Alkyl- β -Amino Acids via β -Alanine Ni(II) Complex

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(A) General Methods

The reagents (chemicals) were purchased from commercial sources, and used without further purification. Analytical thin layer chromatography (TLC) was HSGF 254 (0.15-0.2 mm thickness). All products were characterized by their NMR and MS spectra. ^1H and ^{13}C NMR spectra were recorded in deuteriochloroform (CDCl_3) or deuterioxide (D_2O) on 300 MHz, 400Mz or 500Mz instrument. Chemical shifts were reported in parts per million (ppm, δ) downfield from tetramethylsilane. Proton coupling patterns are described as singlet (s), doublet (d), triplet (t), quartet (q), multiplet (m), and broad (br). Low- and high-resolution mass spectra (LRMS and HRMS) were measured on spectrometer.

(B) The Absolute Configuration of 4a

X-ray Single Crystal Structure Analysis of **4a**: X-ray crystallographic data of **4a** were solutions at $T = 293(2)$ K: $C_{29}H_{21}N_3NiO_3$, $M_r = 518.20$, monoclinic. Space group $P2(1)$, $a = 8.8486(13)$ Å, $b = 9.5964(14)$ Å, $c = 27.377(4)$ Å, $\alpha = 90.00^\circ$, $\beta = 96.322(2)^\circ$, $\gamma = 90.00^\circ$, $V = 2310.6(6)$ Å³, $Z = 4$.

CCDC 800889 contains the supplementary crystallographic data for this paper.

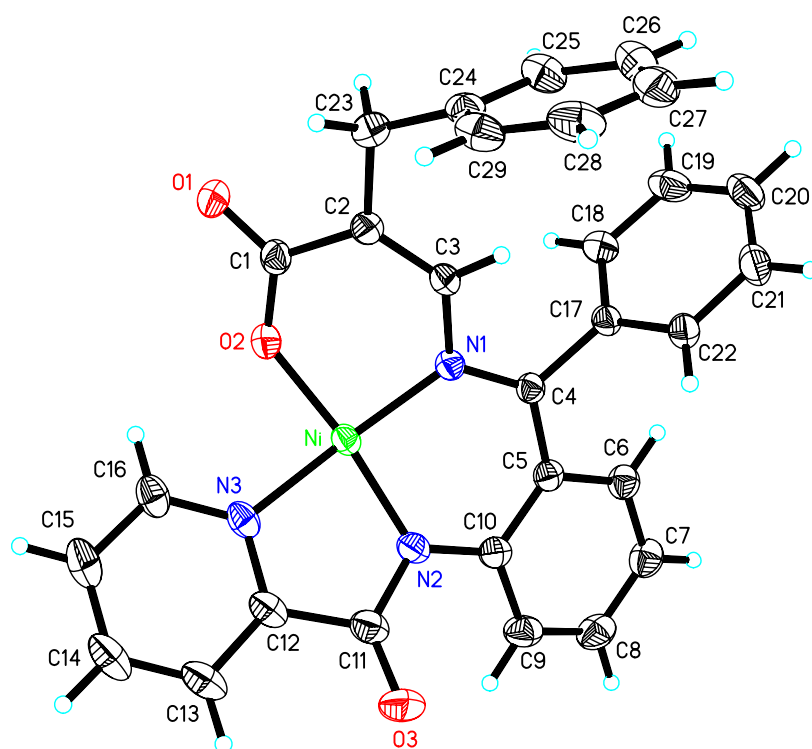
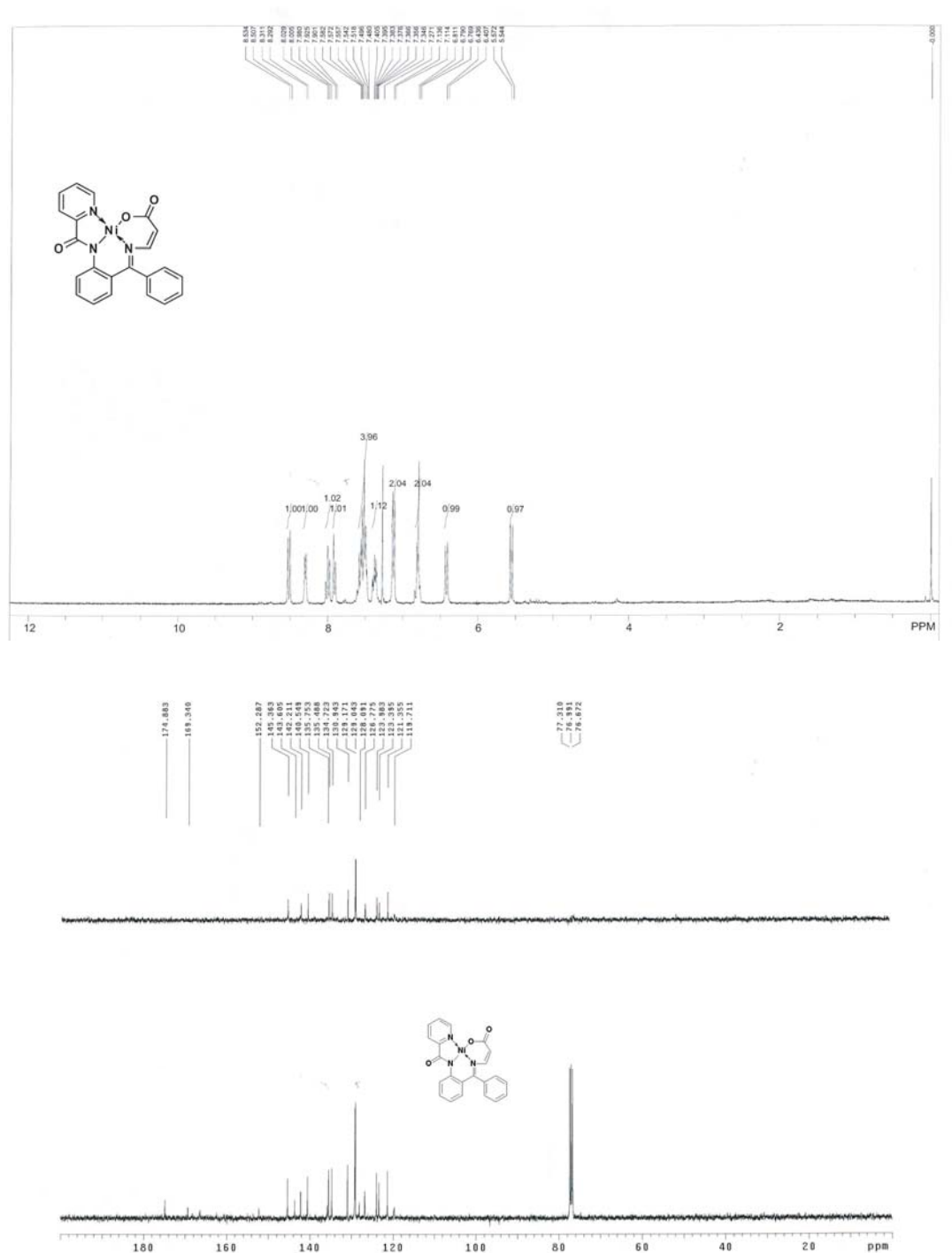


FIGURE S1. The crystal structure of **4a**.

These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

(C) Copies of ^1H NMR and ^{13}C NMR Spectra for the Products

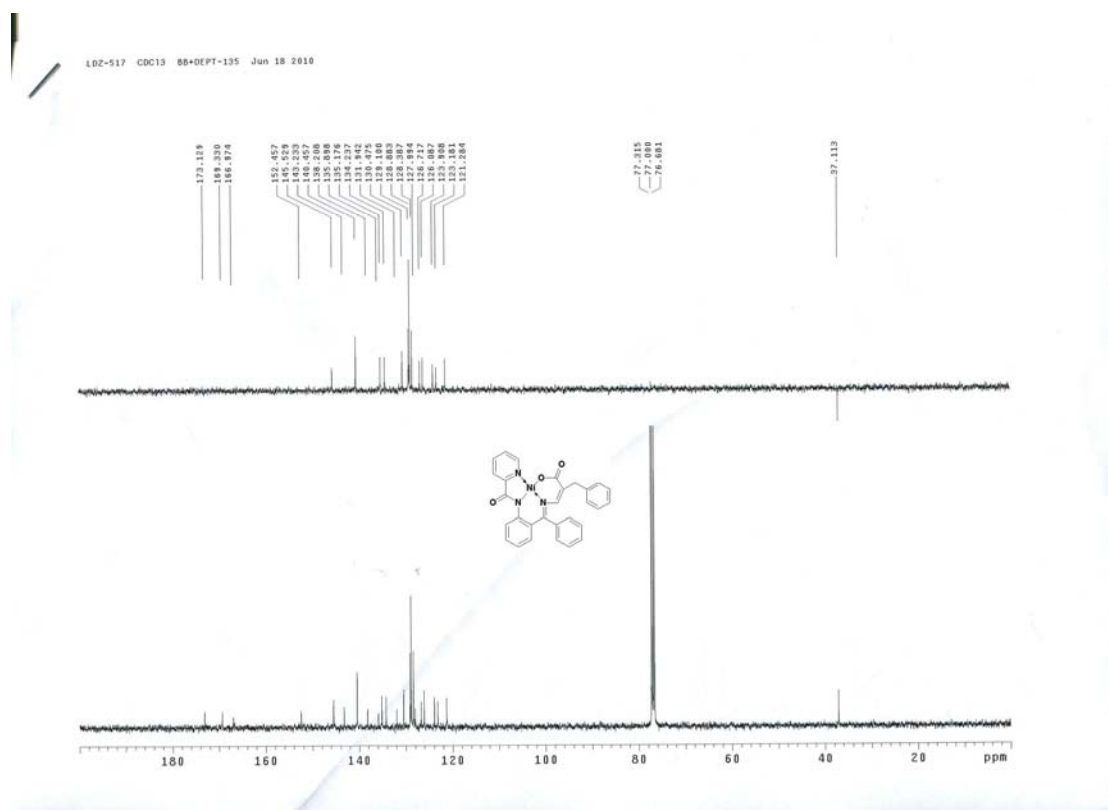
Ni(II)-PABP/3-amino-acrylic acid Schiff Base Complex 2.



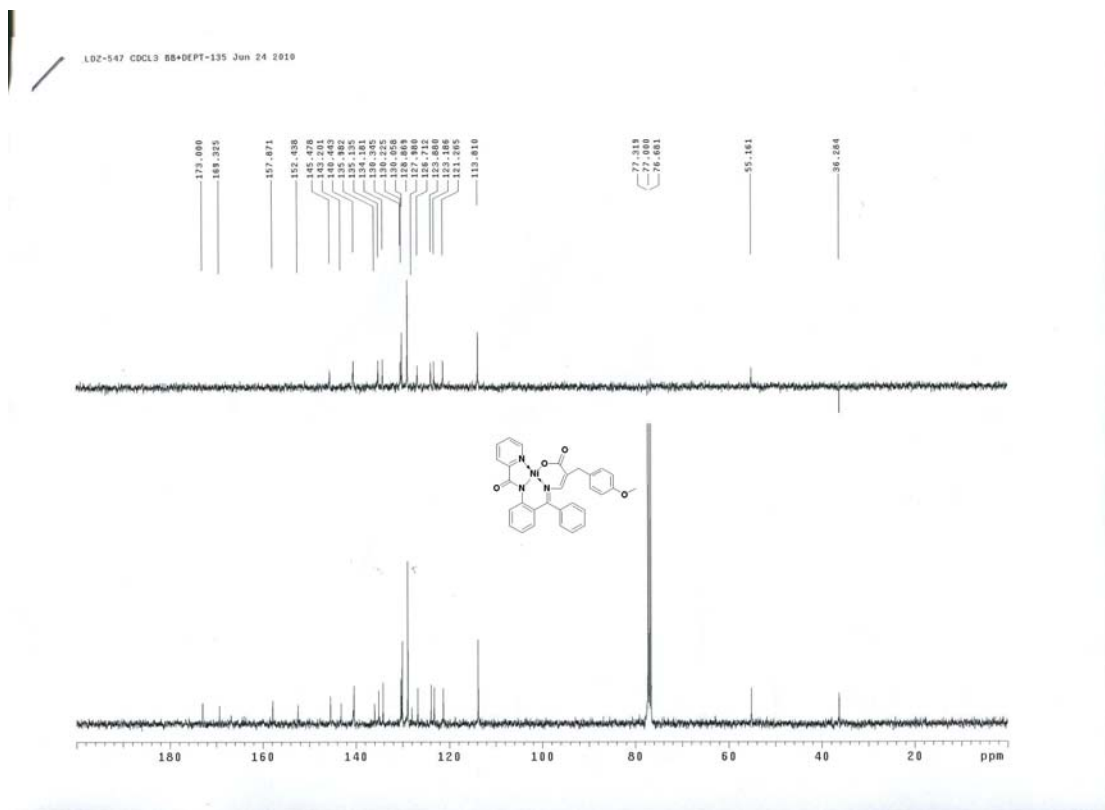
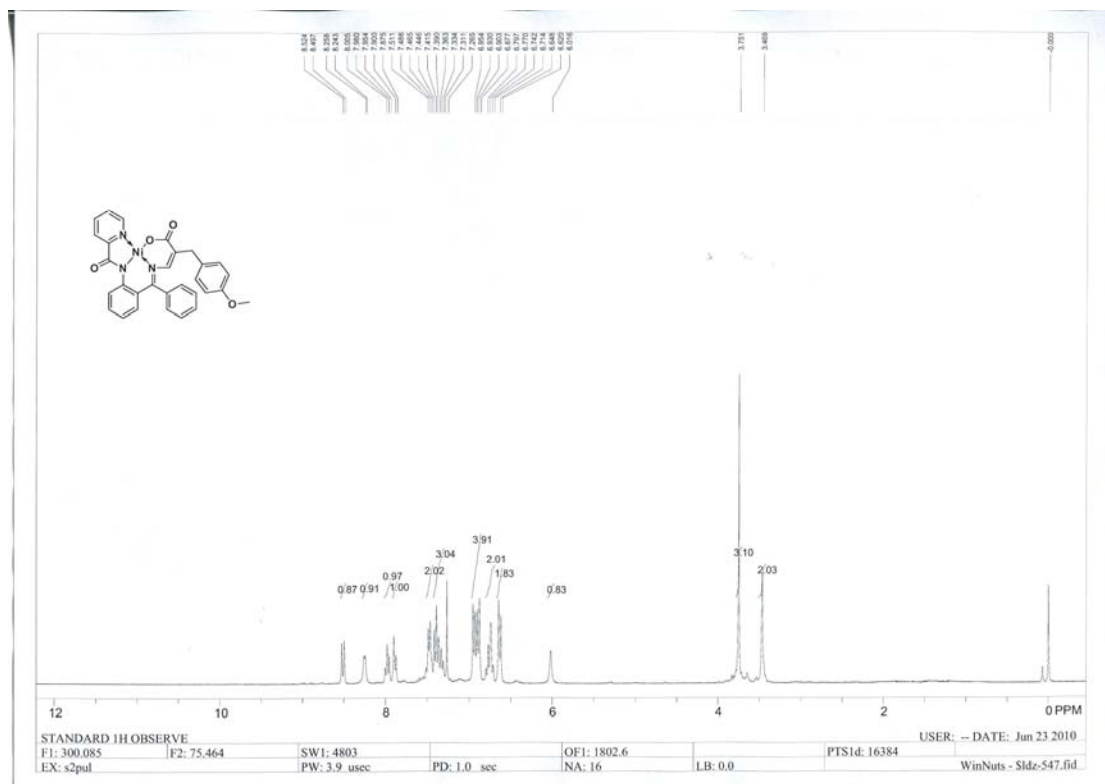
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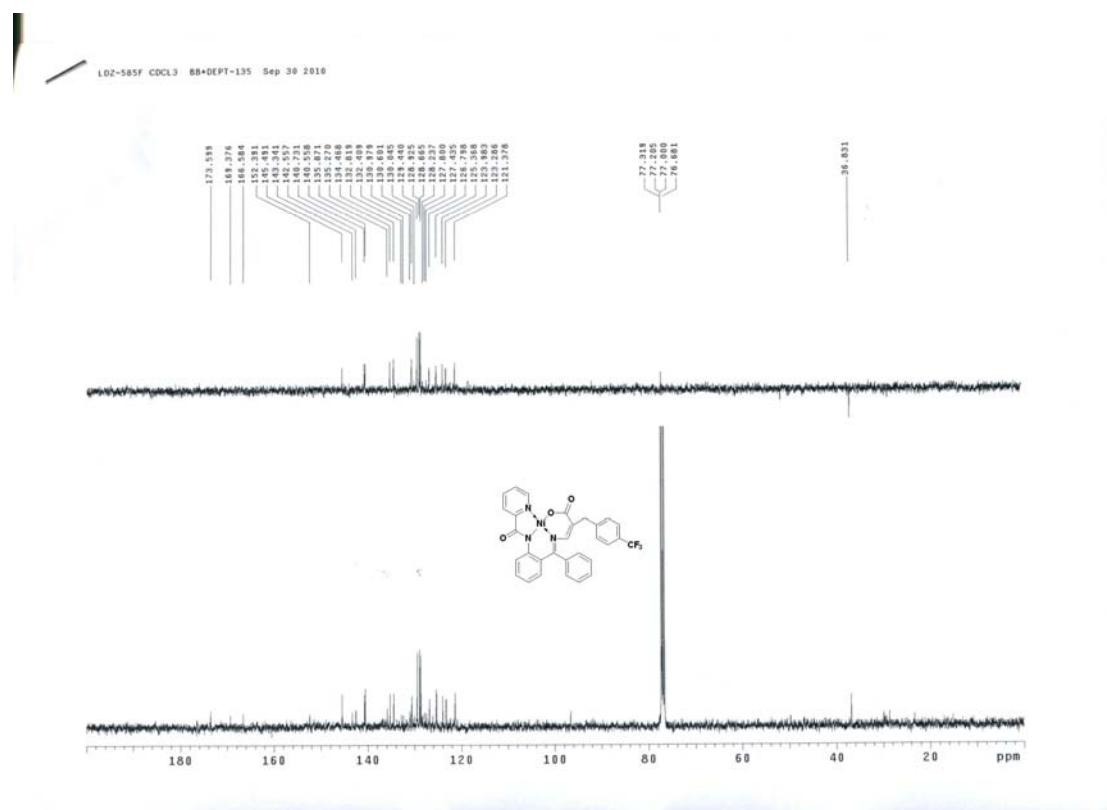
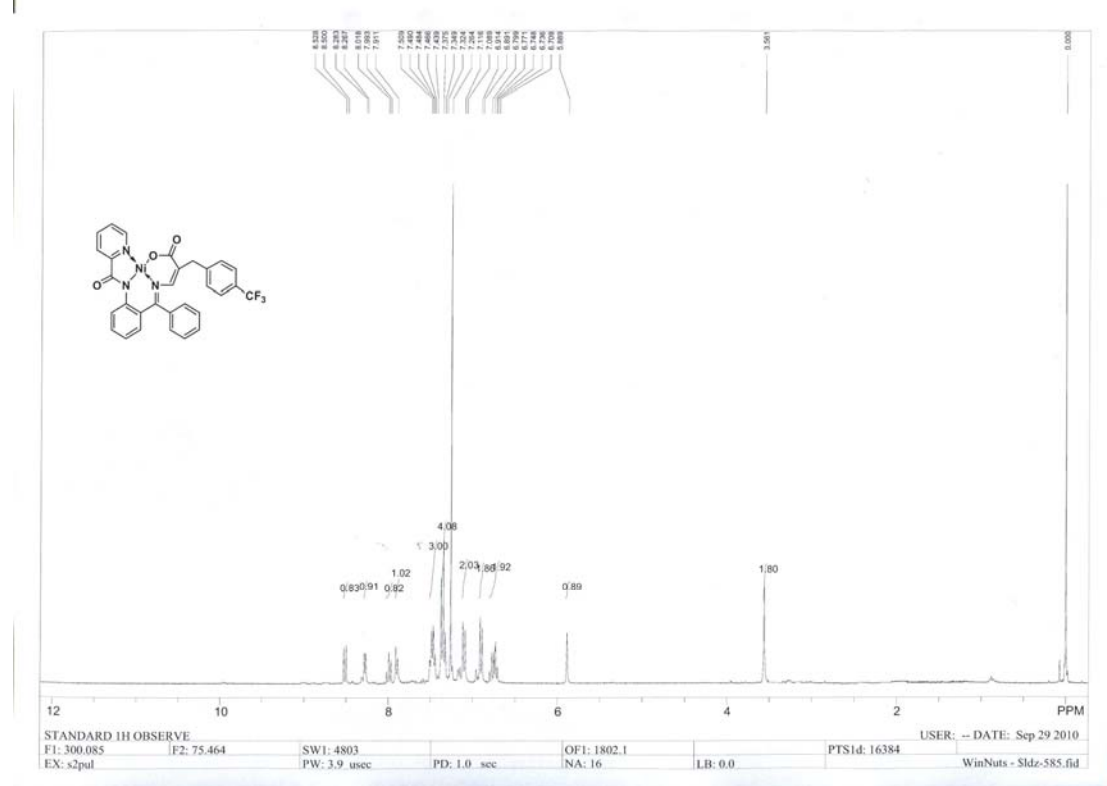
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Ni(II)-PABP/ 3-amino-2-(4-methoxybenzyl)acrylic acid Schiff Base Complex 4b



**Ni(II)-PABP/ 3-amino-2-(4-(trifluoromethyl)benzyl)acrylic acid Schiff Base
Complex 4c**

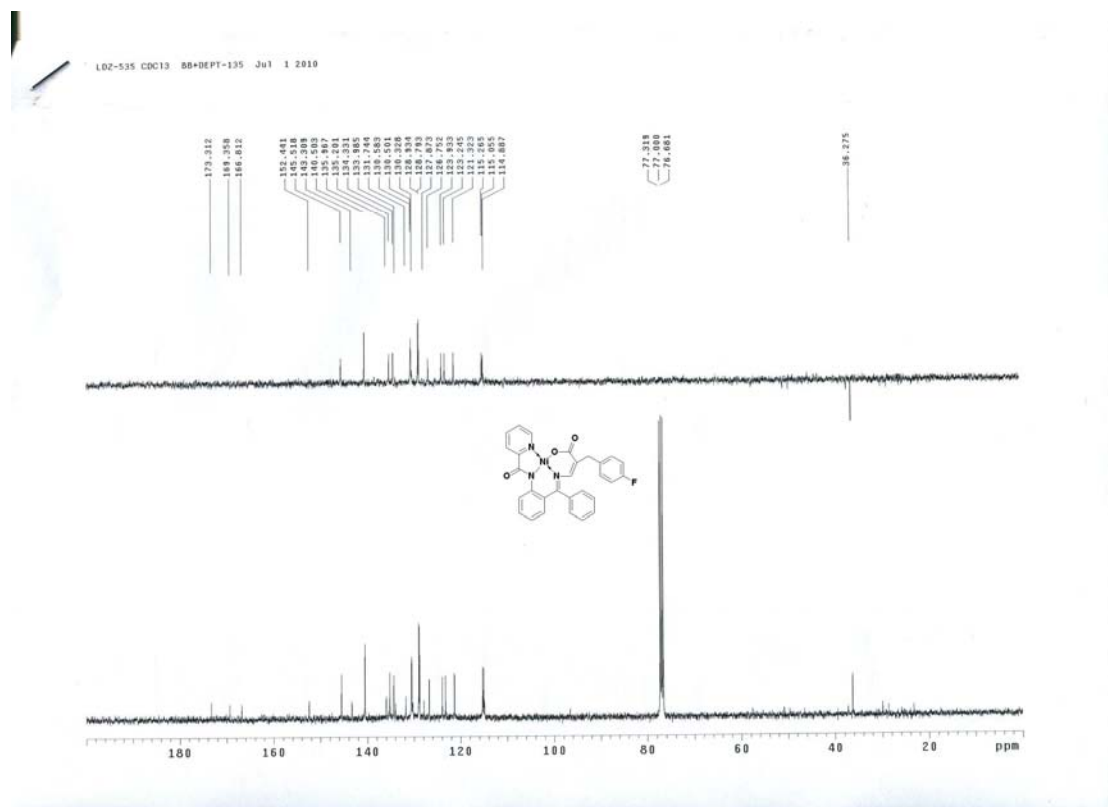


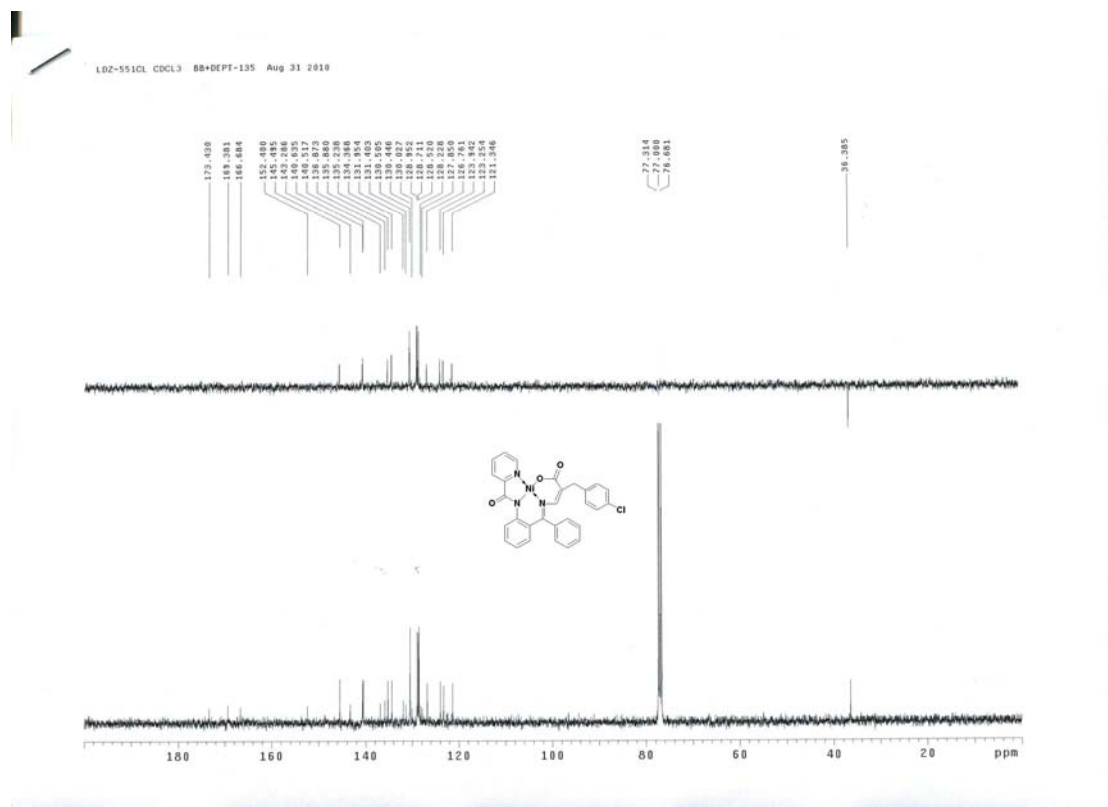
O=C1NC(=O)c2ccccc2N1C(=O)C(c3ccccc3)=C(c4ccccc4)c5ccccc5

Chemical structure of the compound is shown above the spectrum. The structure is a complex molecule featuring a central benzene ring substituted with a carboxylic acid group, a methyl group, and a 4-fluorophenyl group. The spectrum displays several peaks corresponding to the protons in the molecule, with integration values provided for each major peak.

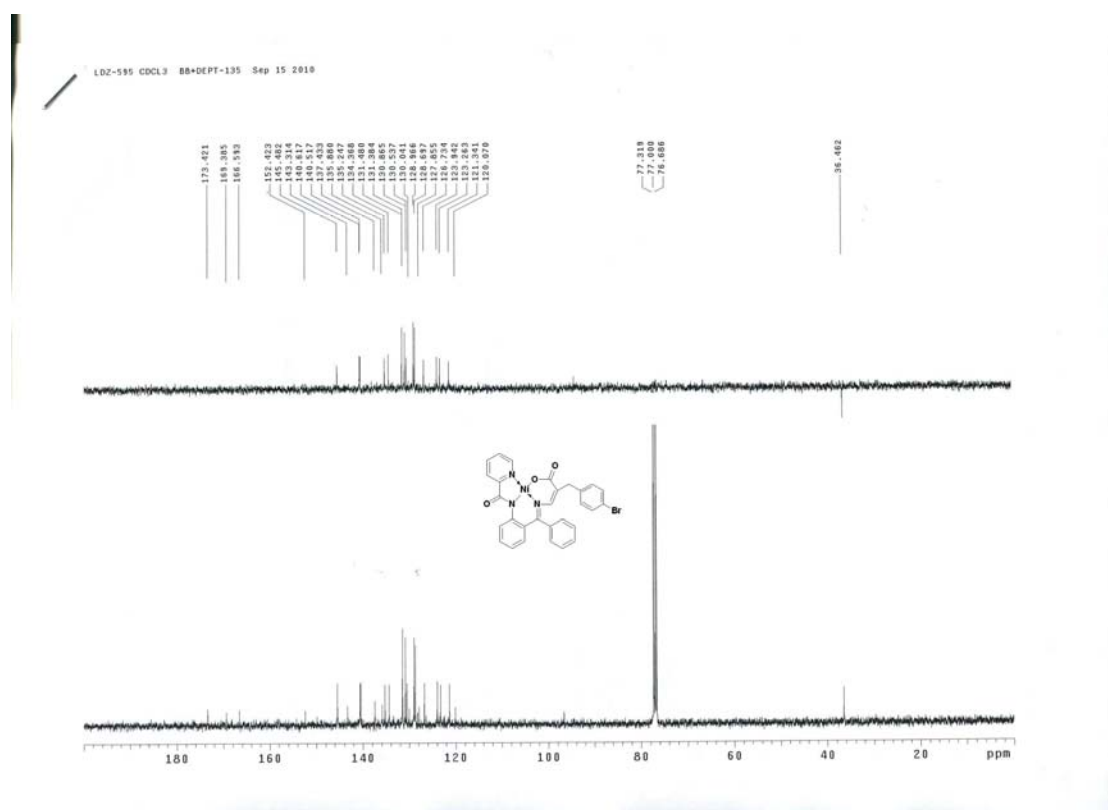
Chemical Shift (ppm)	Integration
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~7.6	1.00
~7.4	1.00
~7.2	2.18
~7.0	3.17
~6.8	4.04
~6.6	3.83
~6.4	0.93
~3.8	1.88

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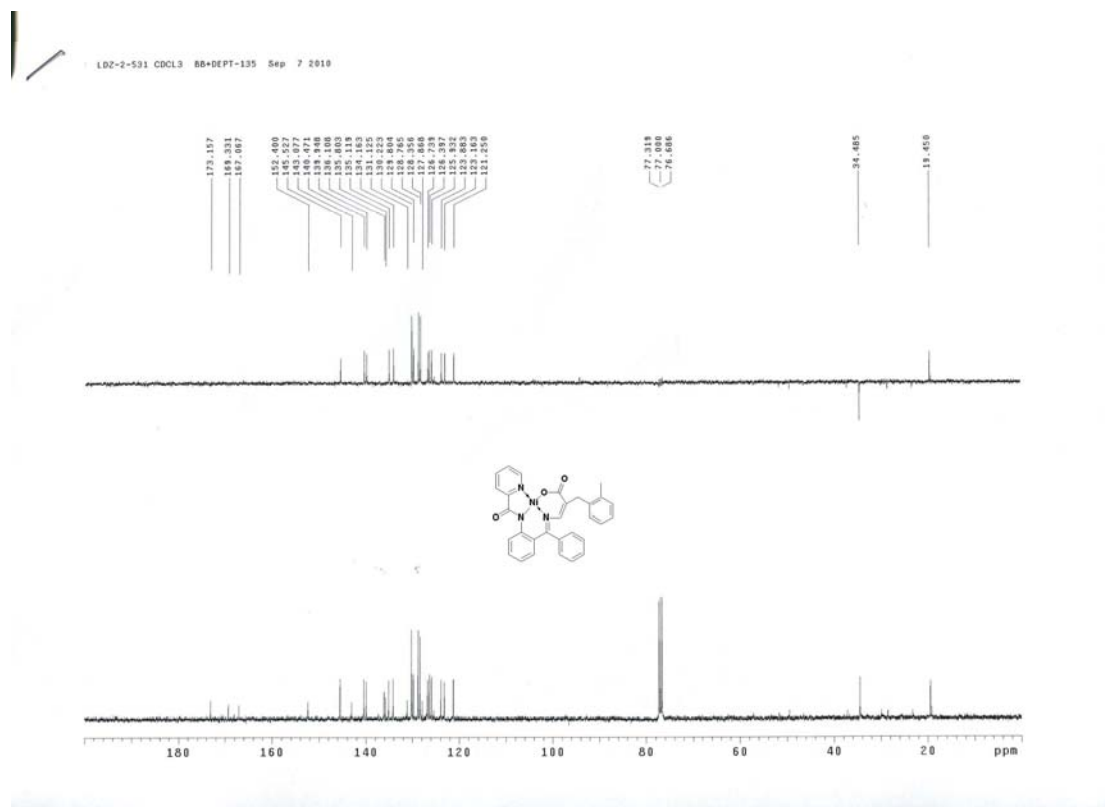
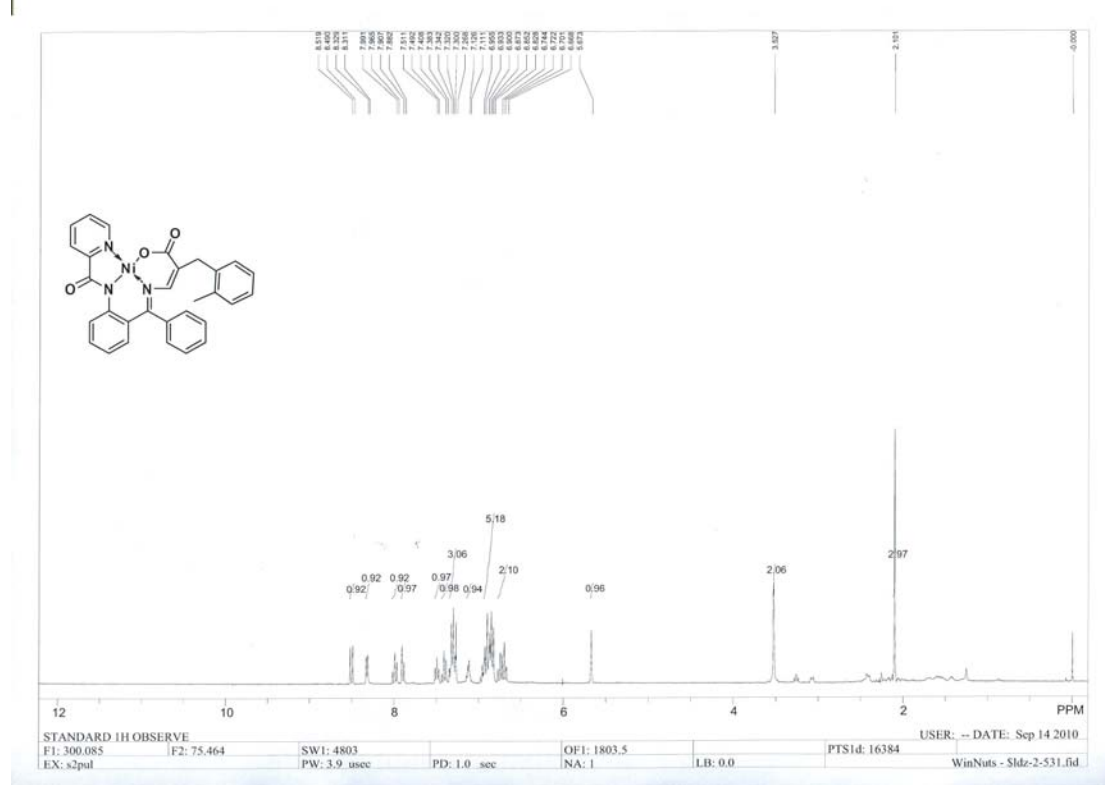


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10 8 6 4 2 0 PPM

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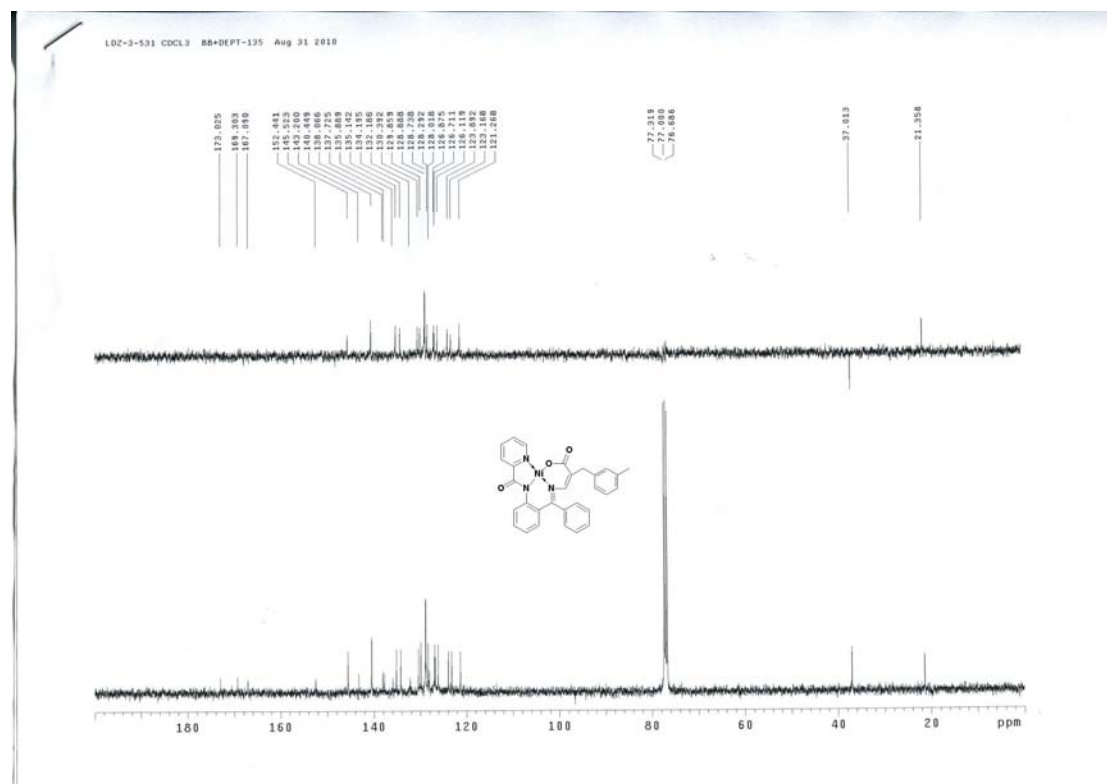
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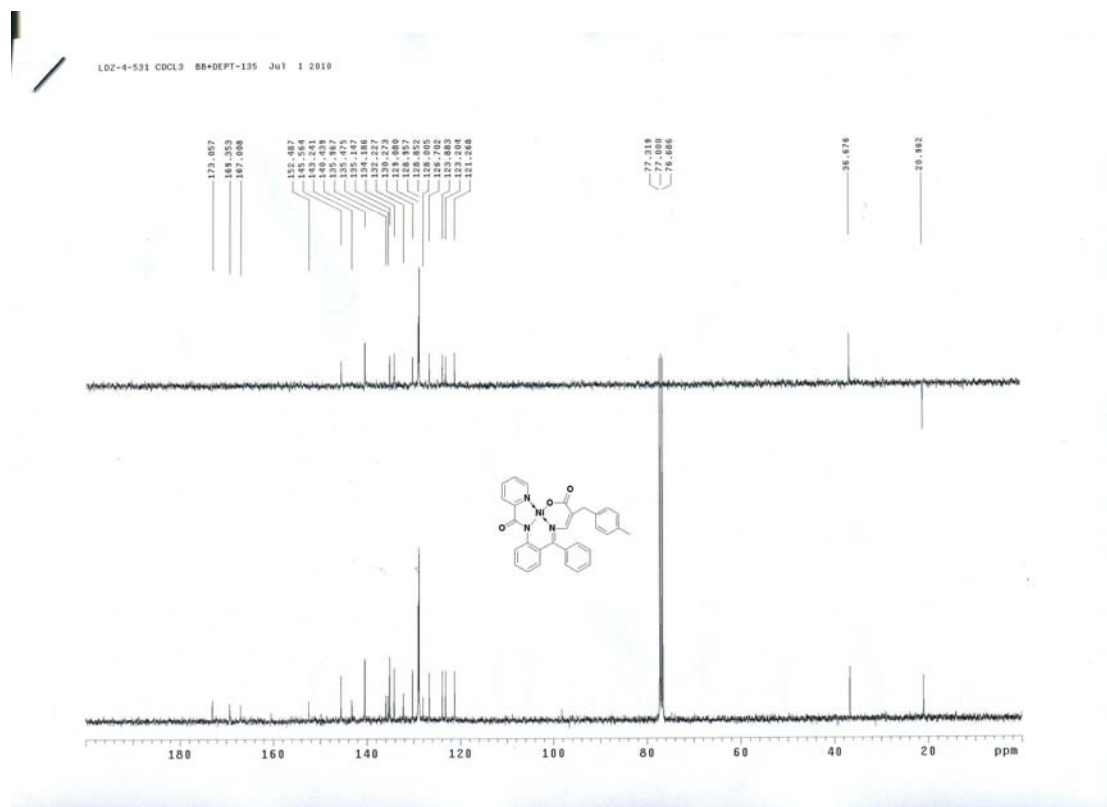
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STANDARD 1H OBSERVE

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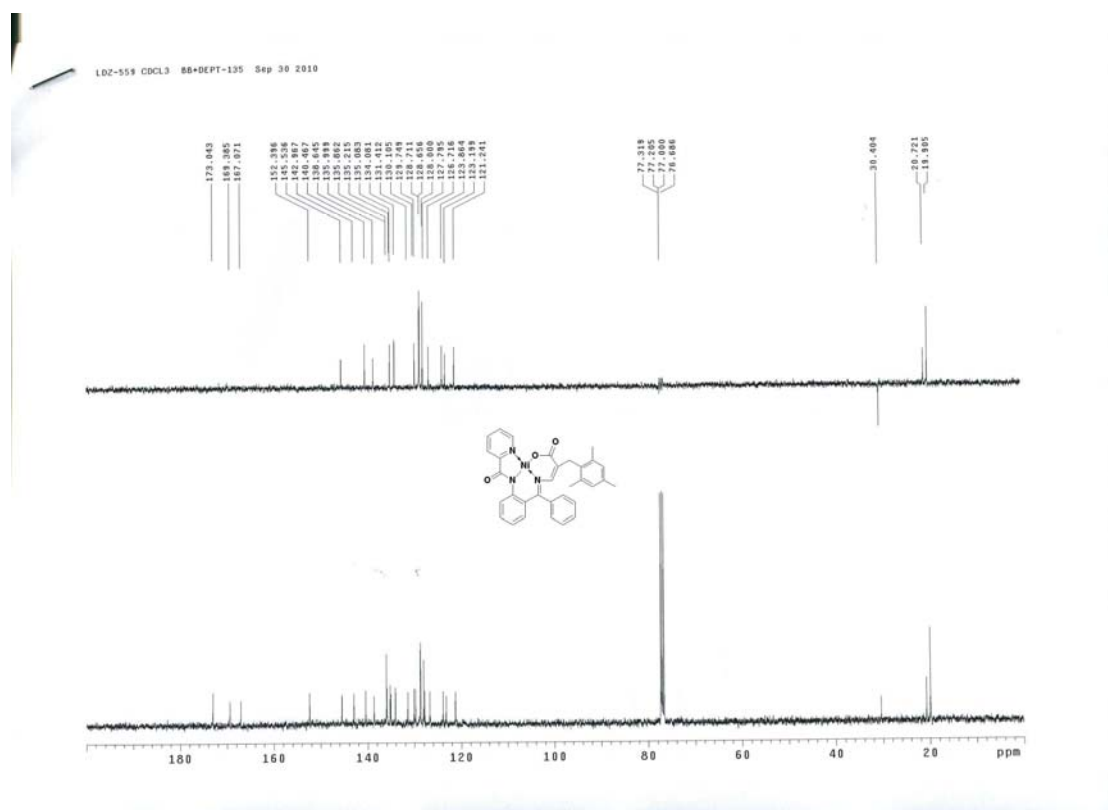
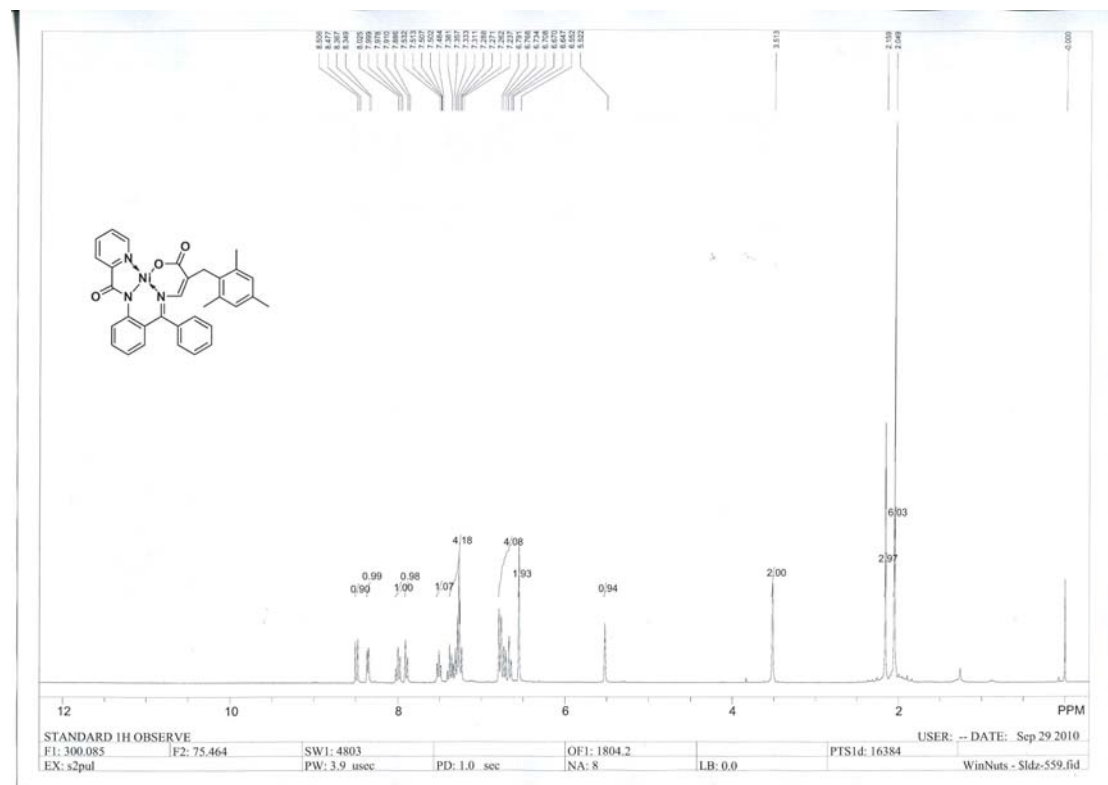
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Ni(II)-PABP/ 3-amino-2-(2,4,6-trimethylbenzyl)acrylic acid Schiff Base Complex

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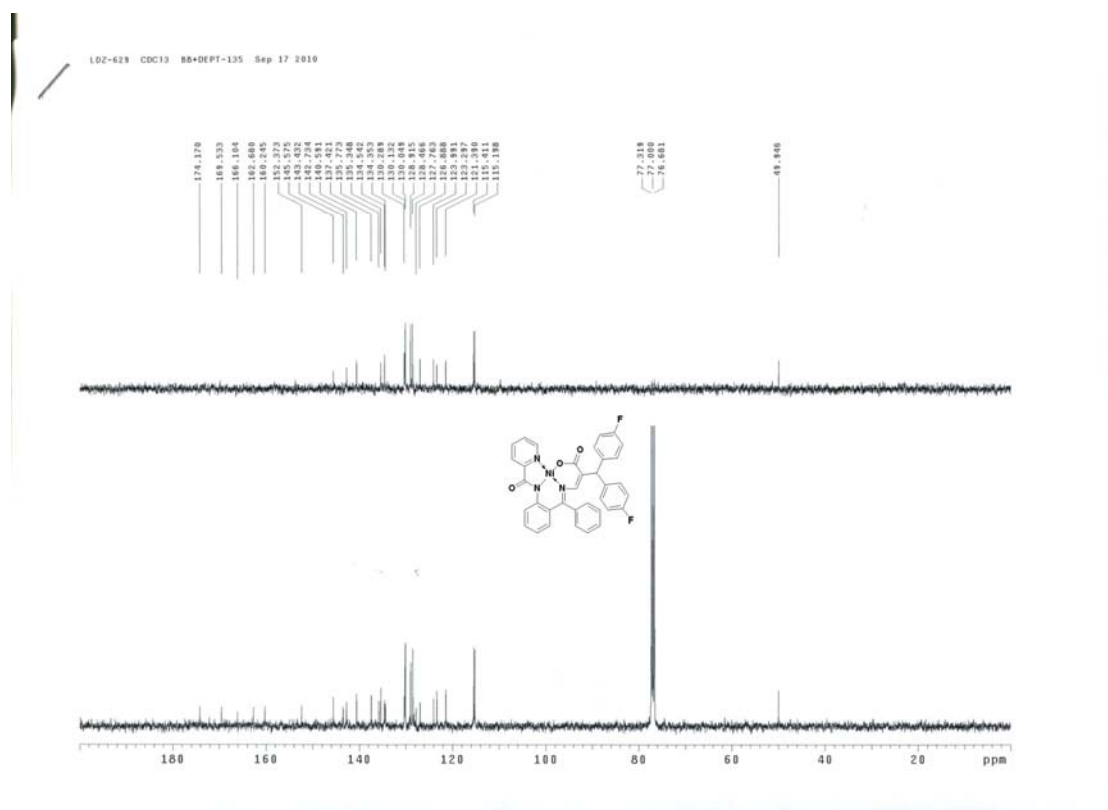
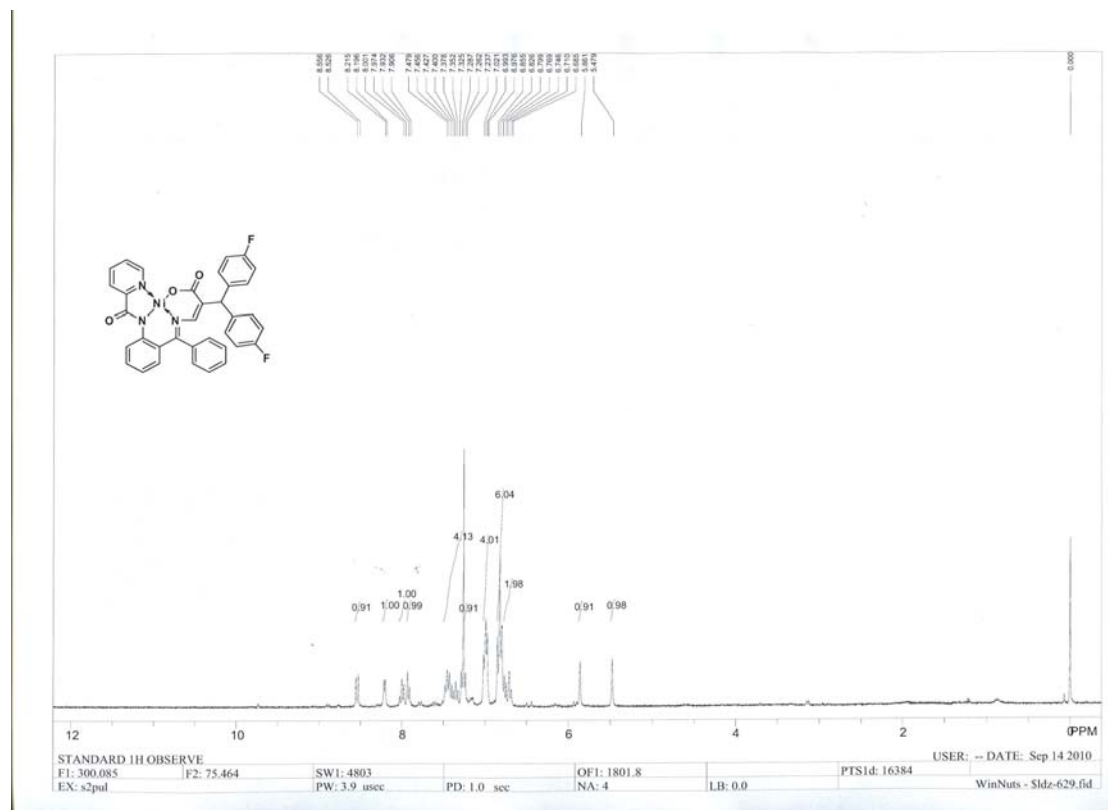
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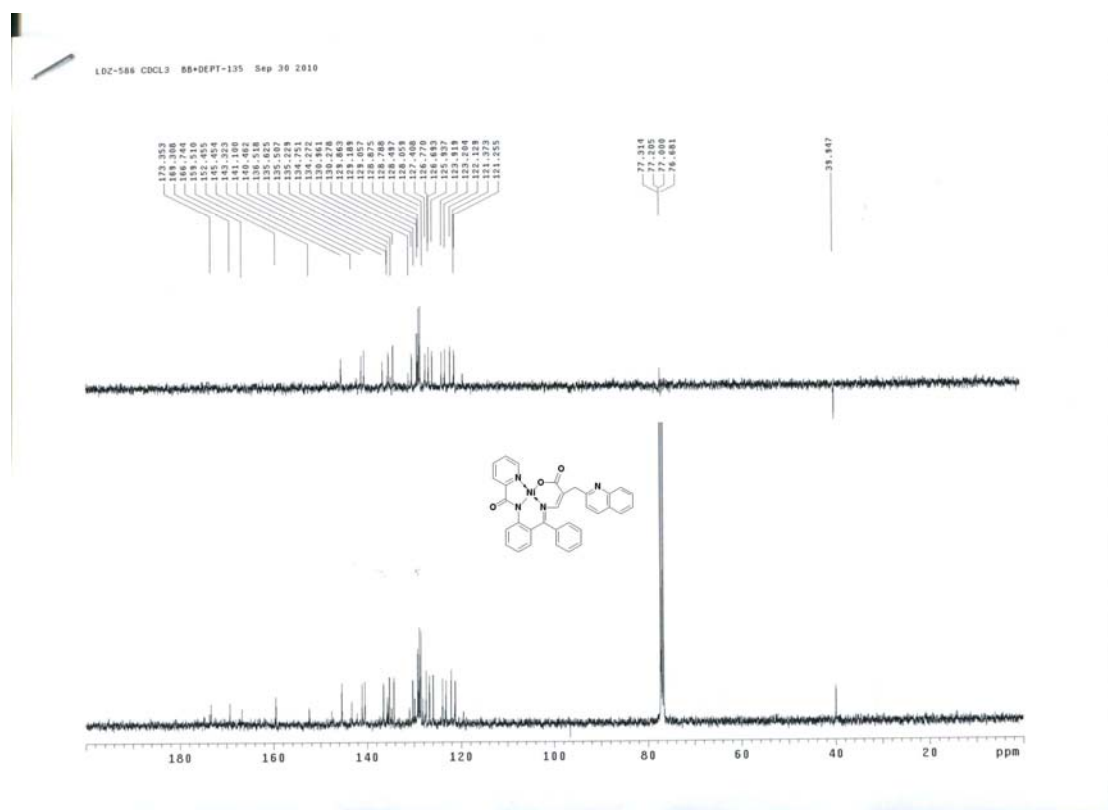
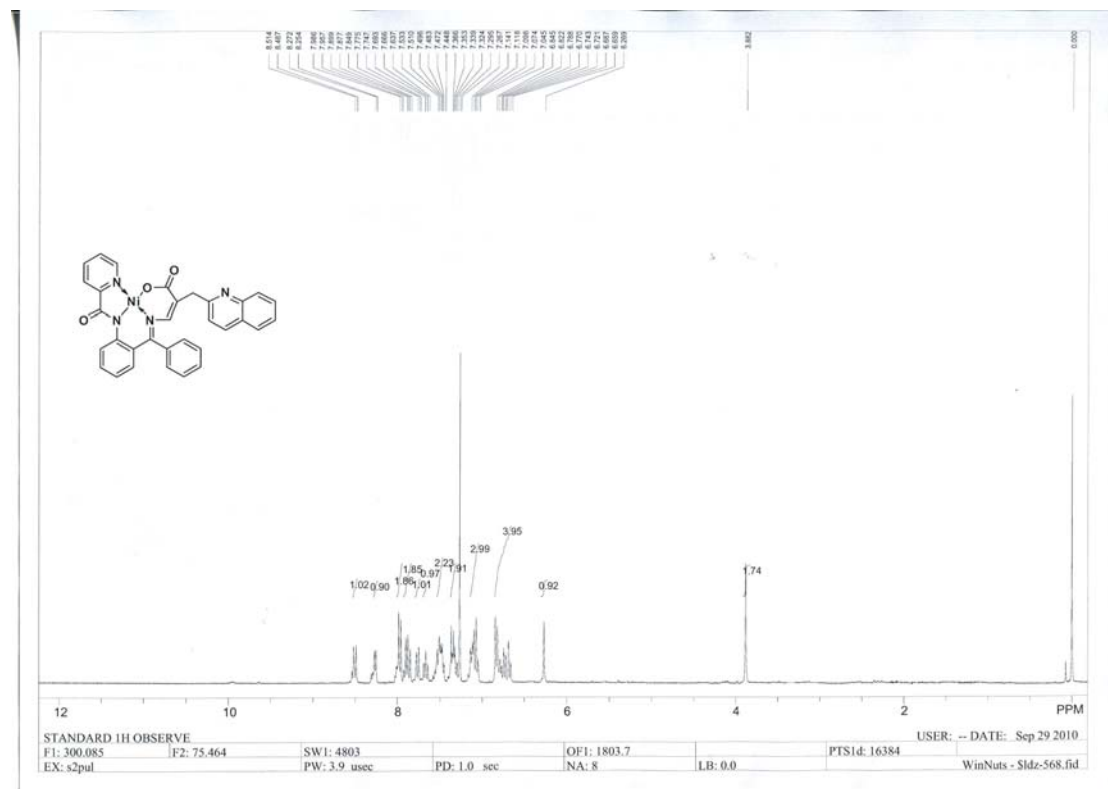


**Ni(II)-PABP/ 3-amino-2-(bis(4-fluorophenyl)methyl)acrylic acid Schiff Base
Complex 4m**

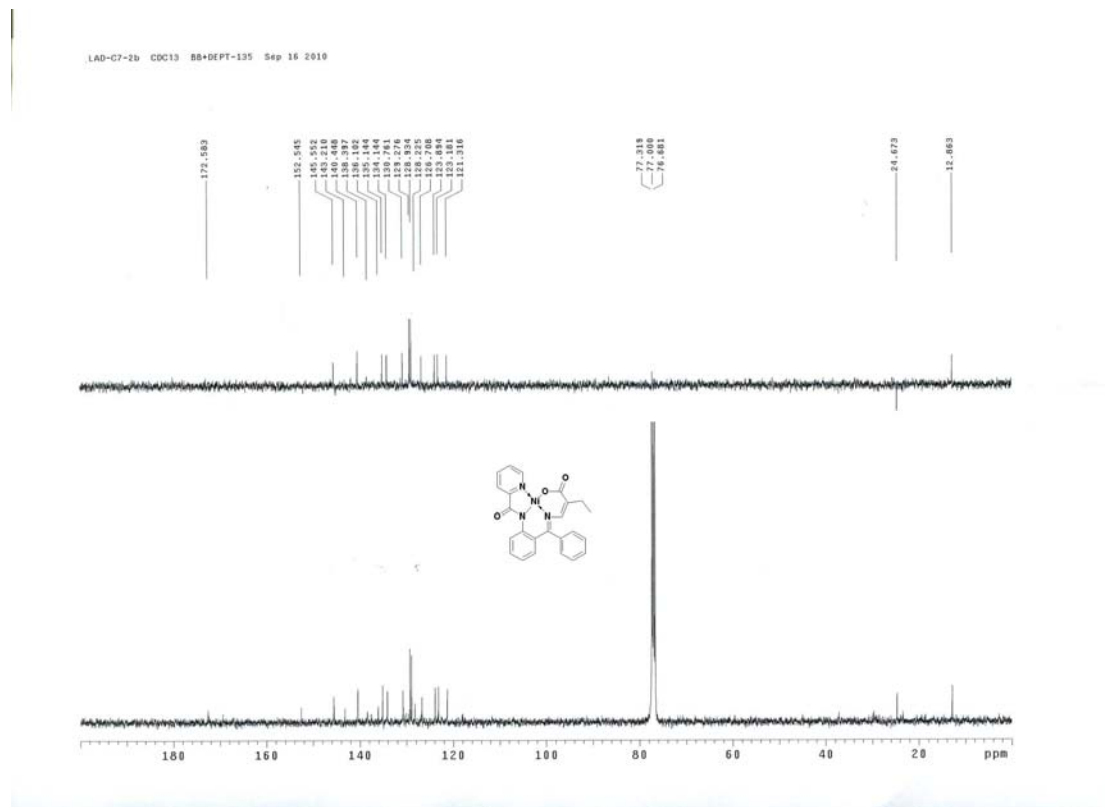
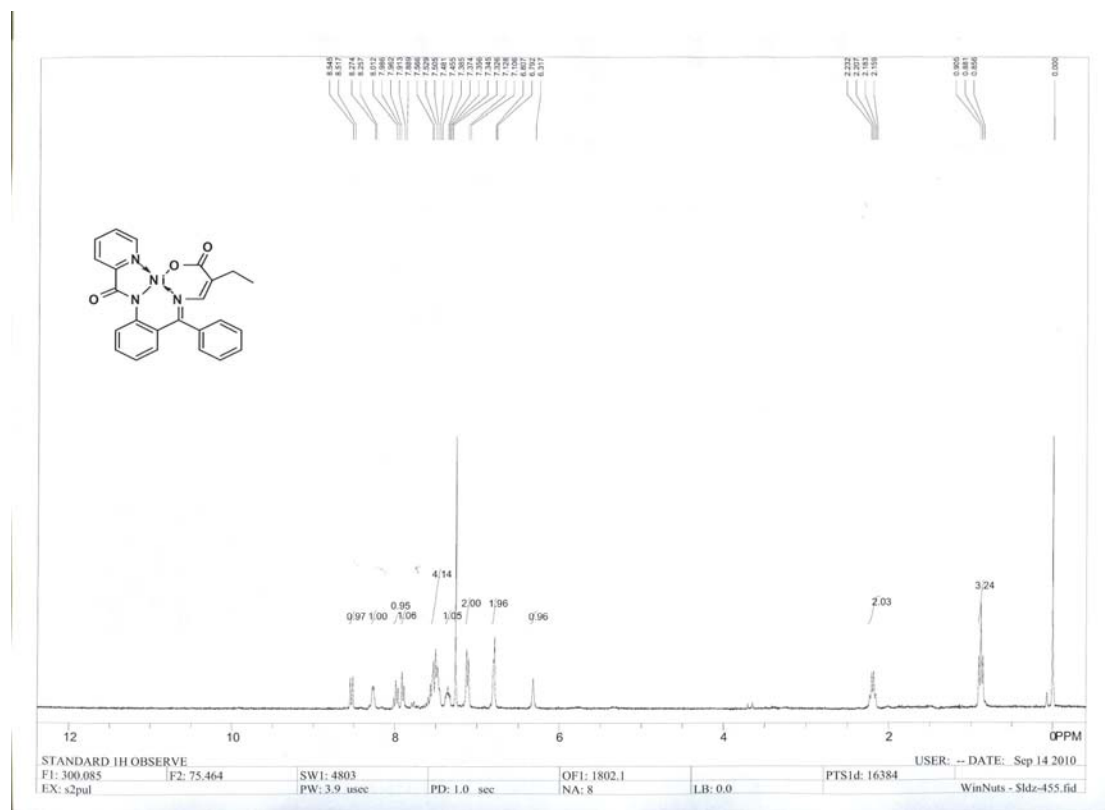


Ni(II)-PABP/ 3-amino-2-(quinolin-2-ylmethyl)acrylic acid Schiff Base Complex

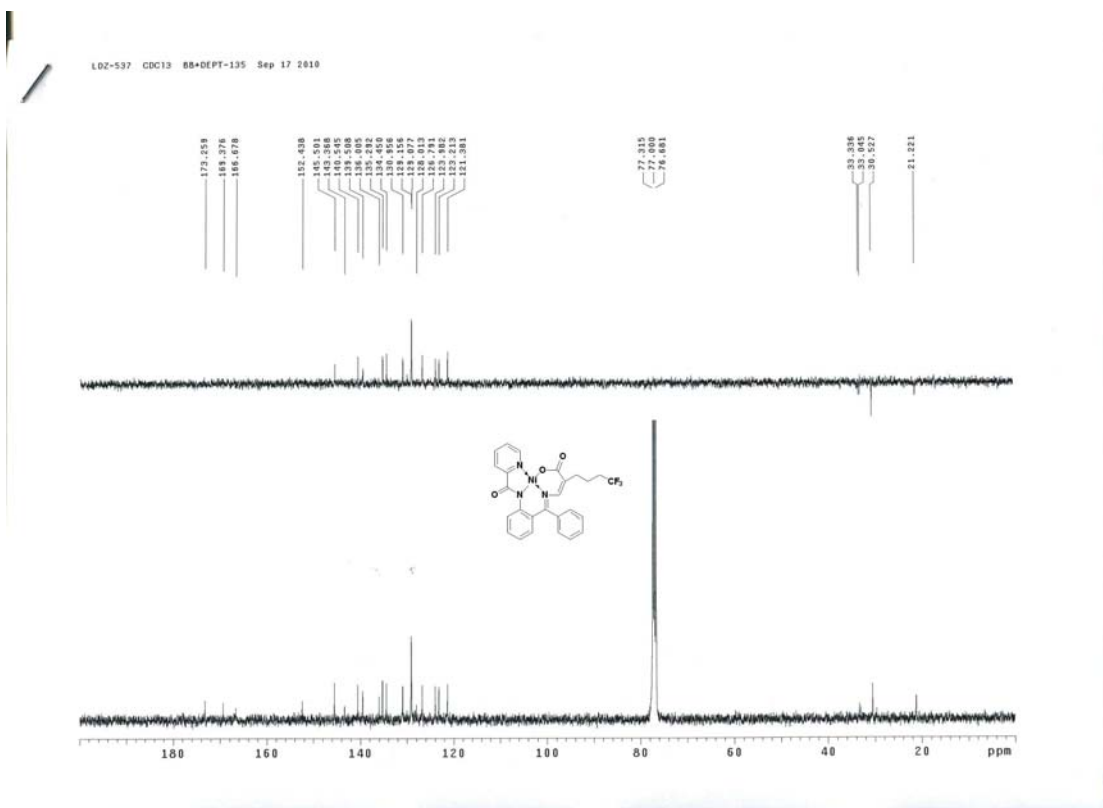
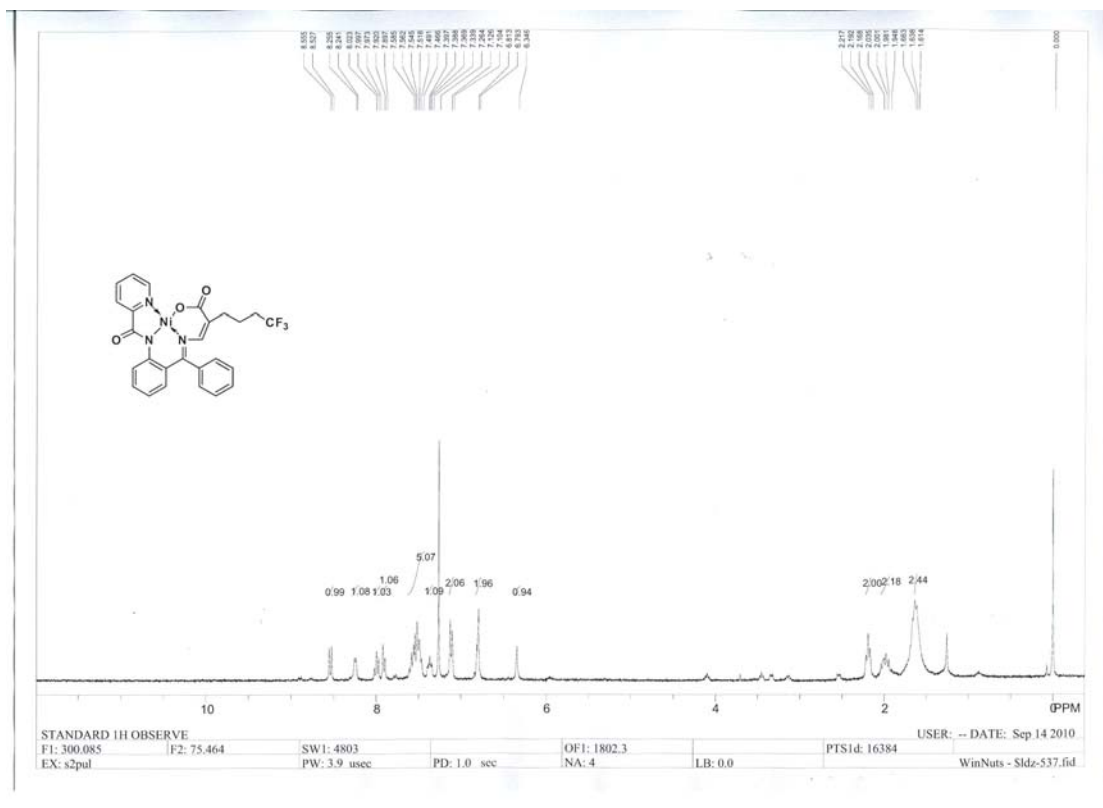
4n



Ni(II)-PABP/ 2-(aminomethylene)butanoic acid Schiff Base Complex 4o

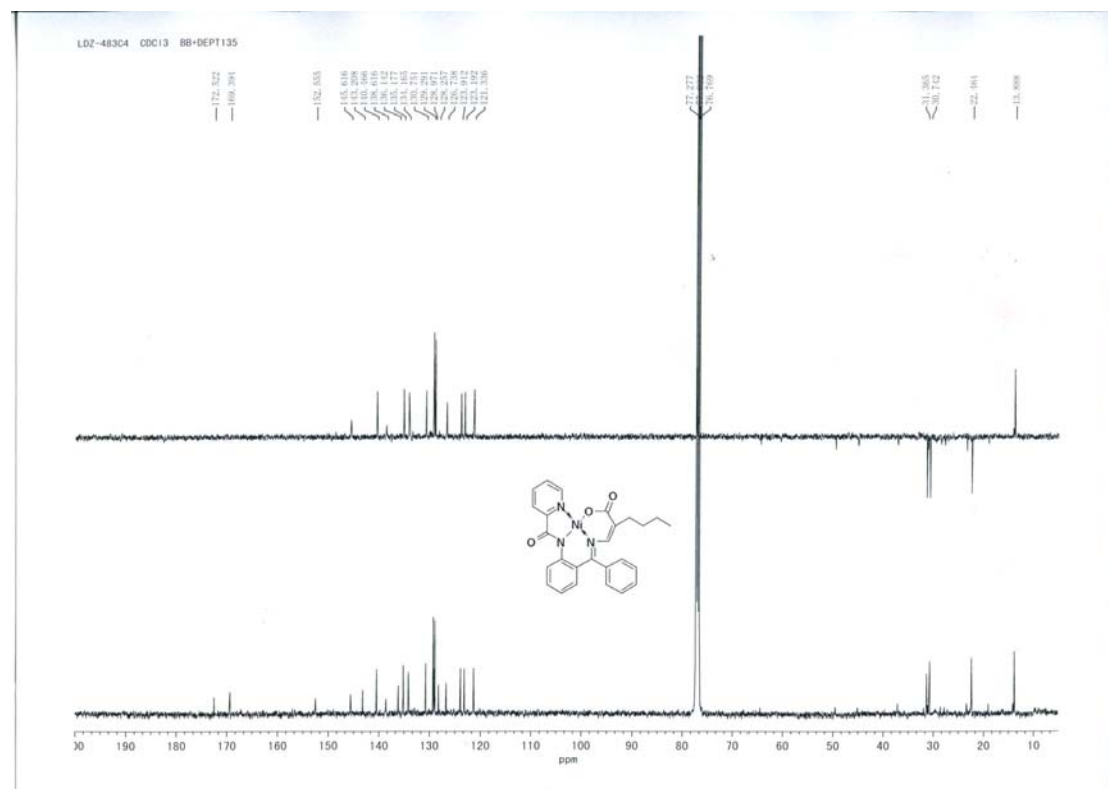


**Ni(II)-PABP/ 2-(aminomethylene)-6,6,6-trifluorohexanoic acid Schiff Base
Complex 4p**



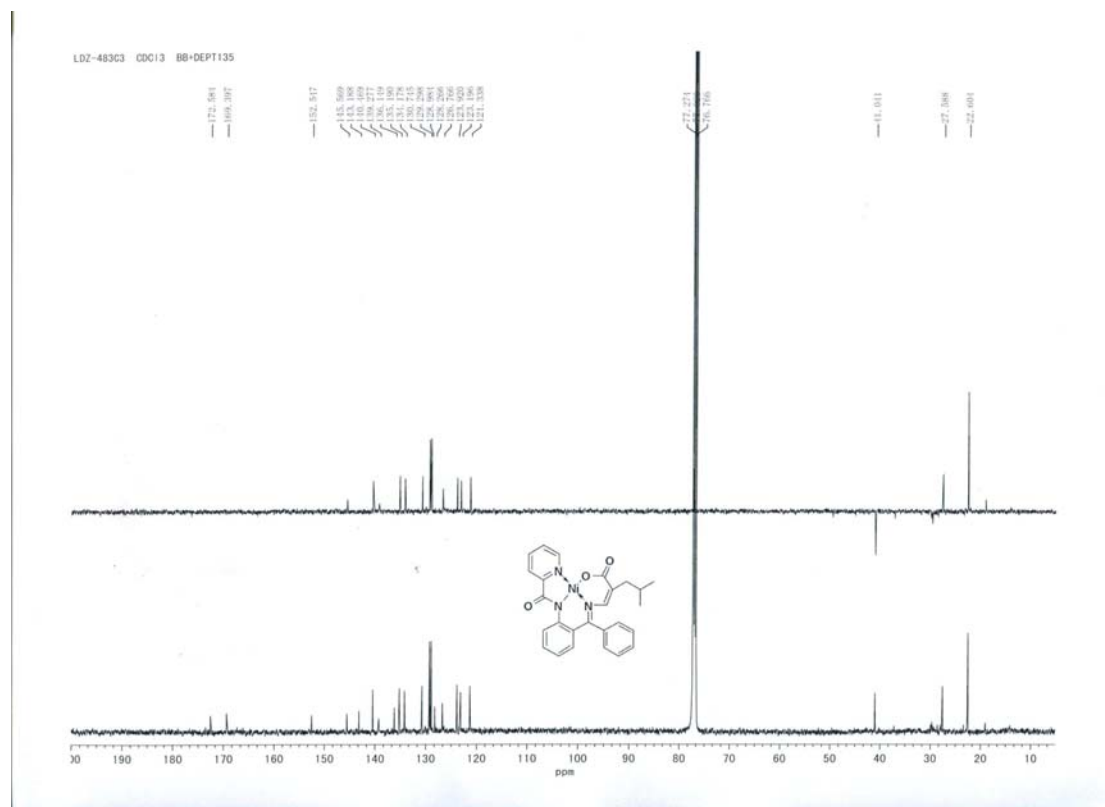
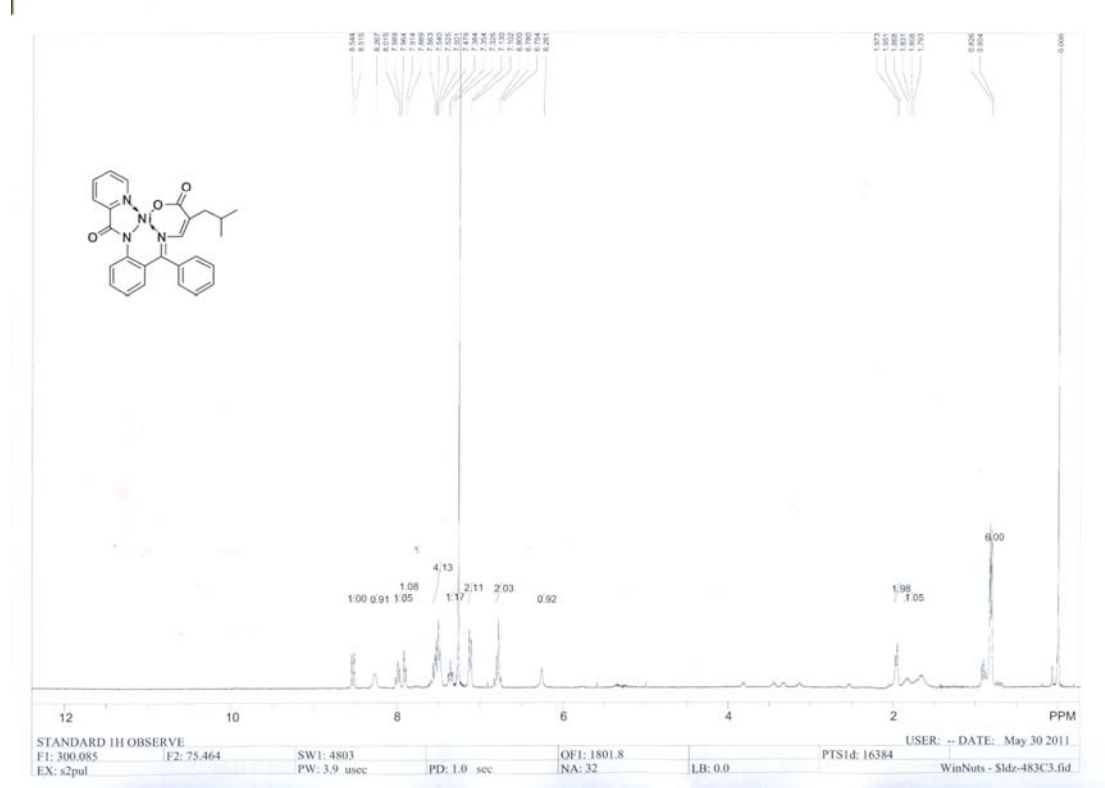
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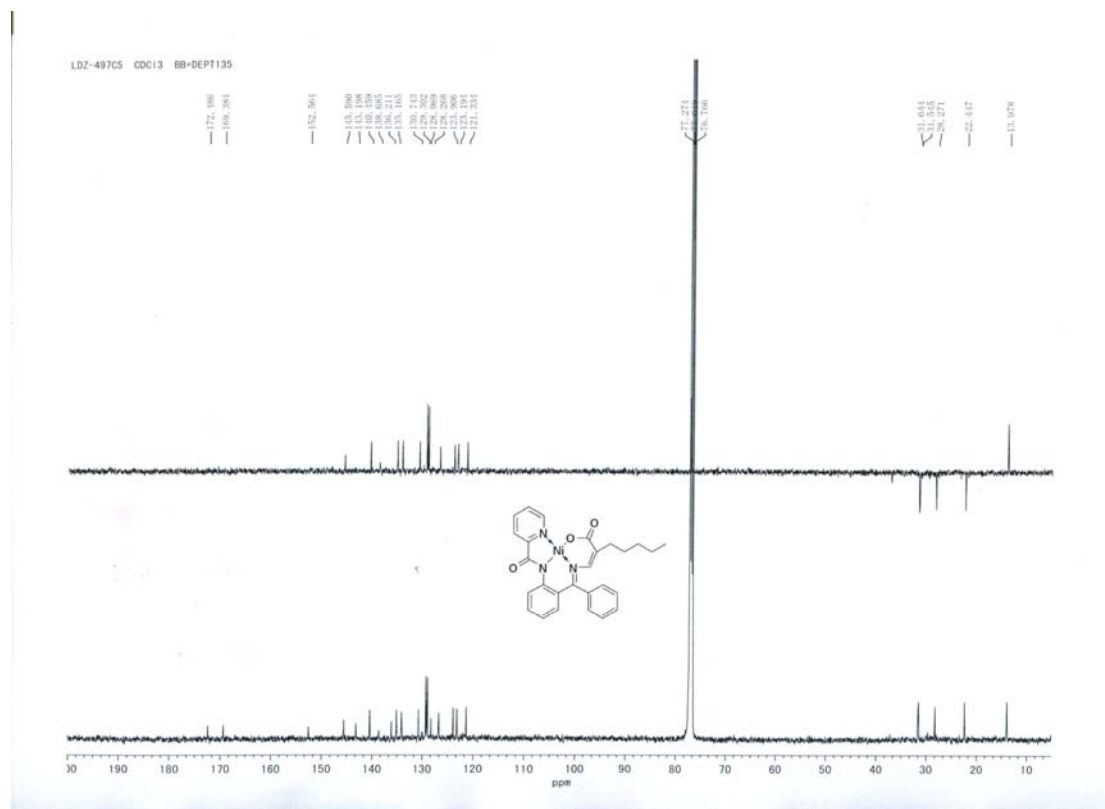
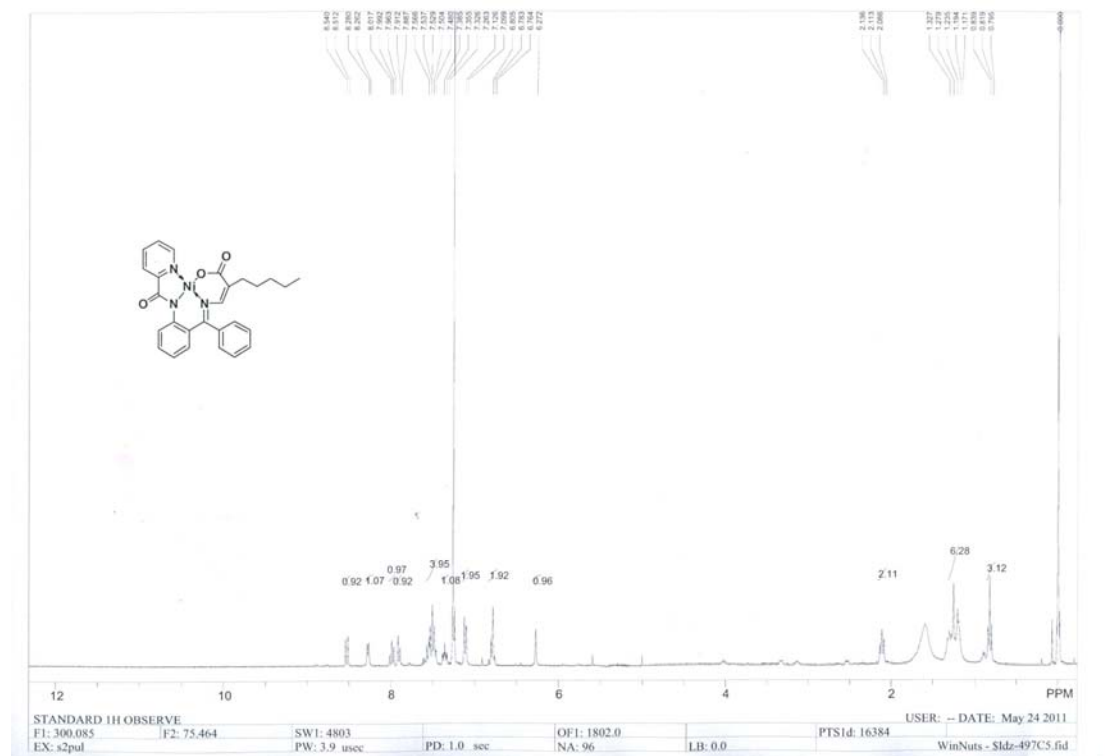
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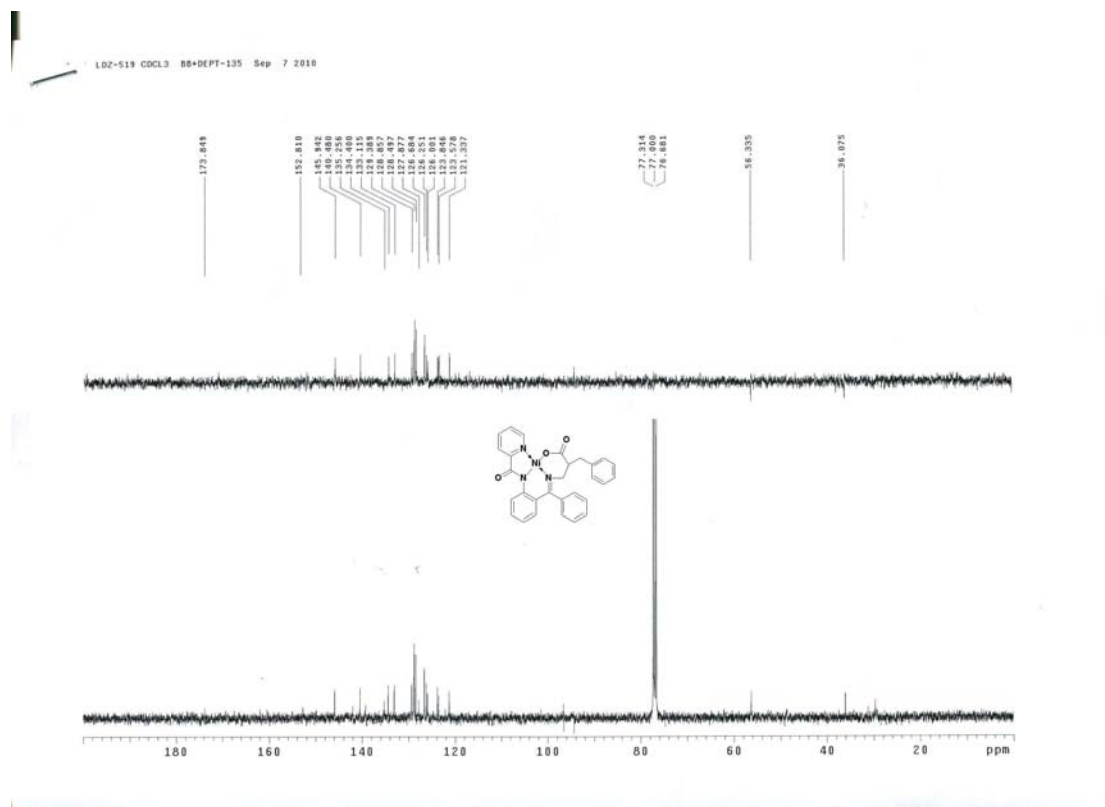
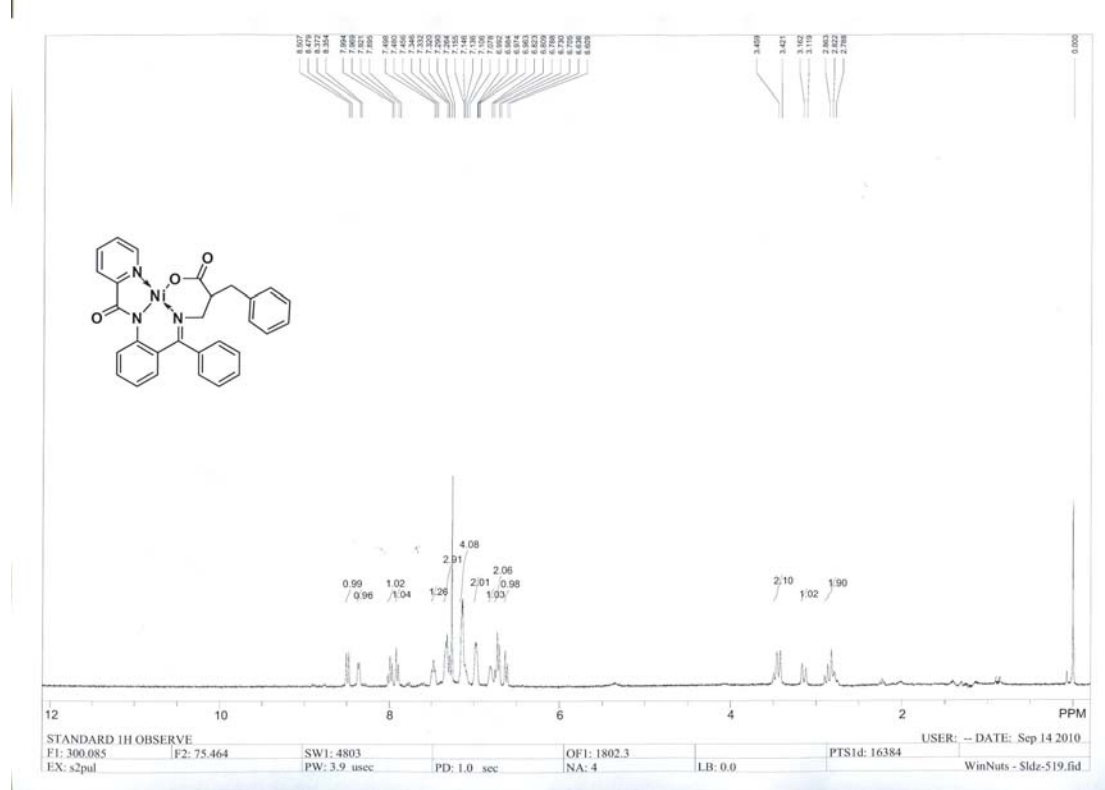
Ni(II)-PABP/ 2-(aminomethylene)-4-methylpentanoic acid Schiff Base Complex

4r.

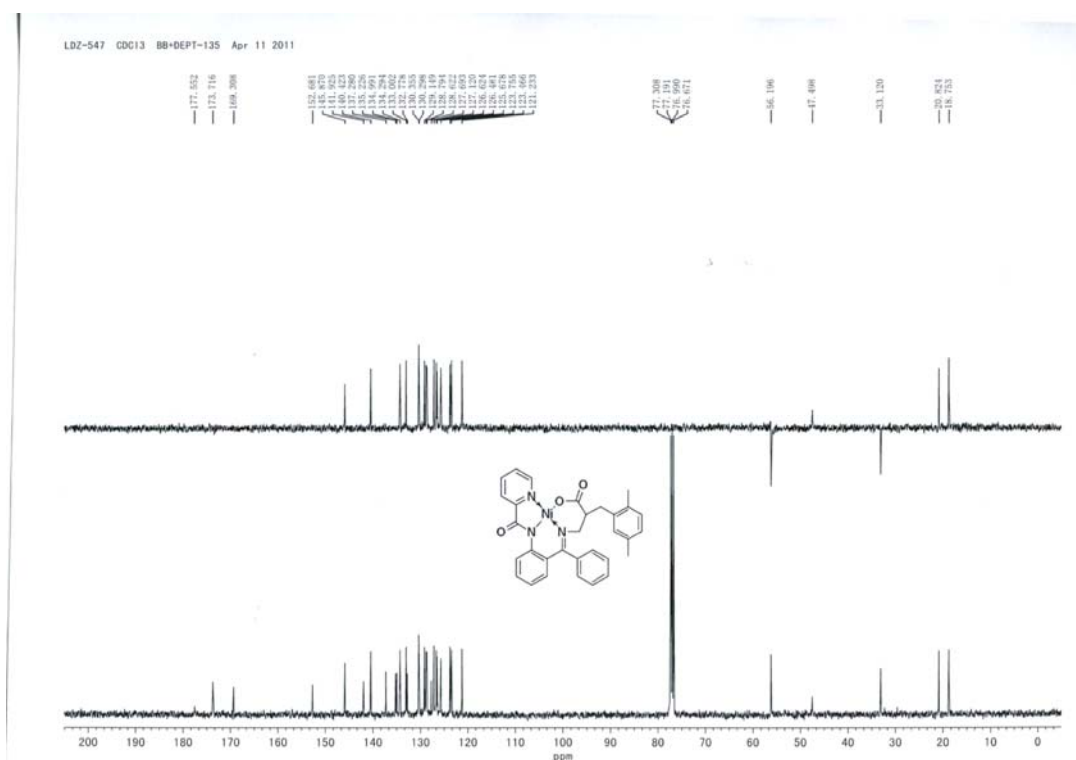
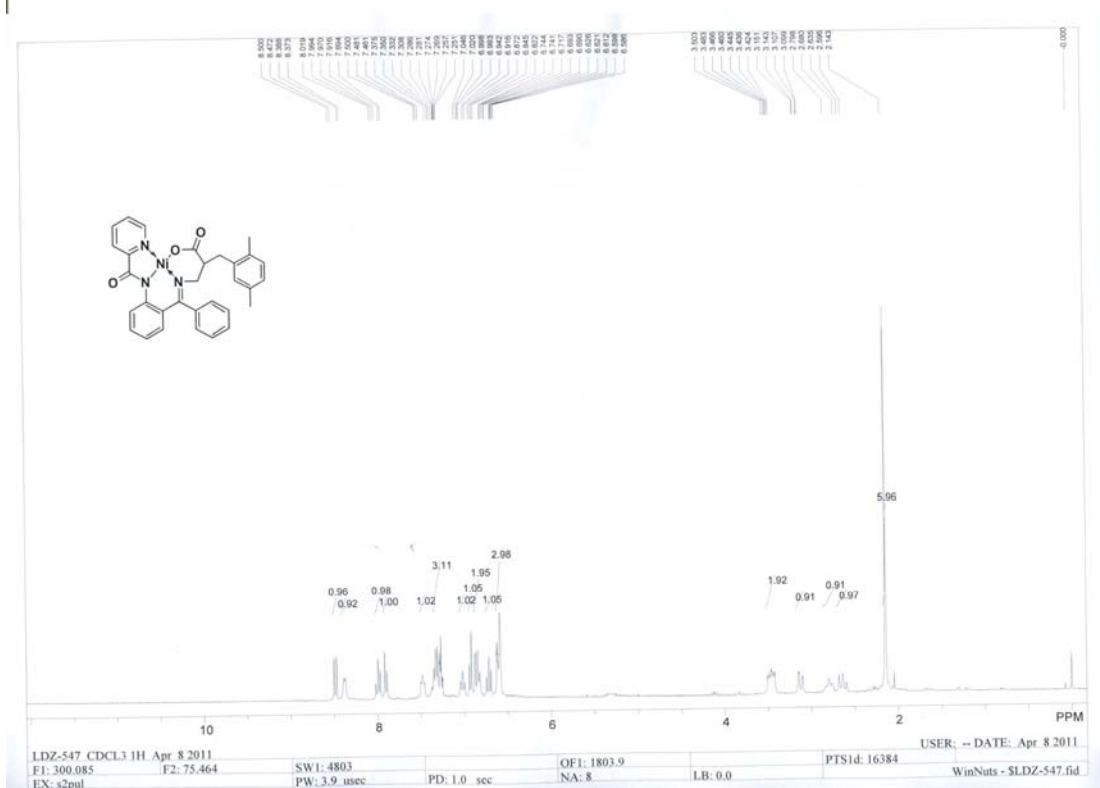




Ni(II)-PABP/ α -benzyl- β -alanine Schiff Base Complex 5a

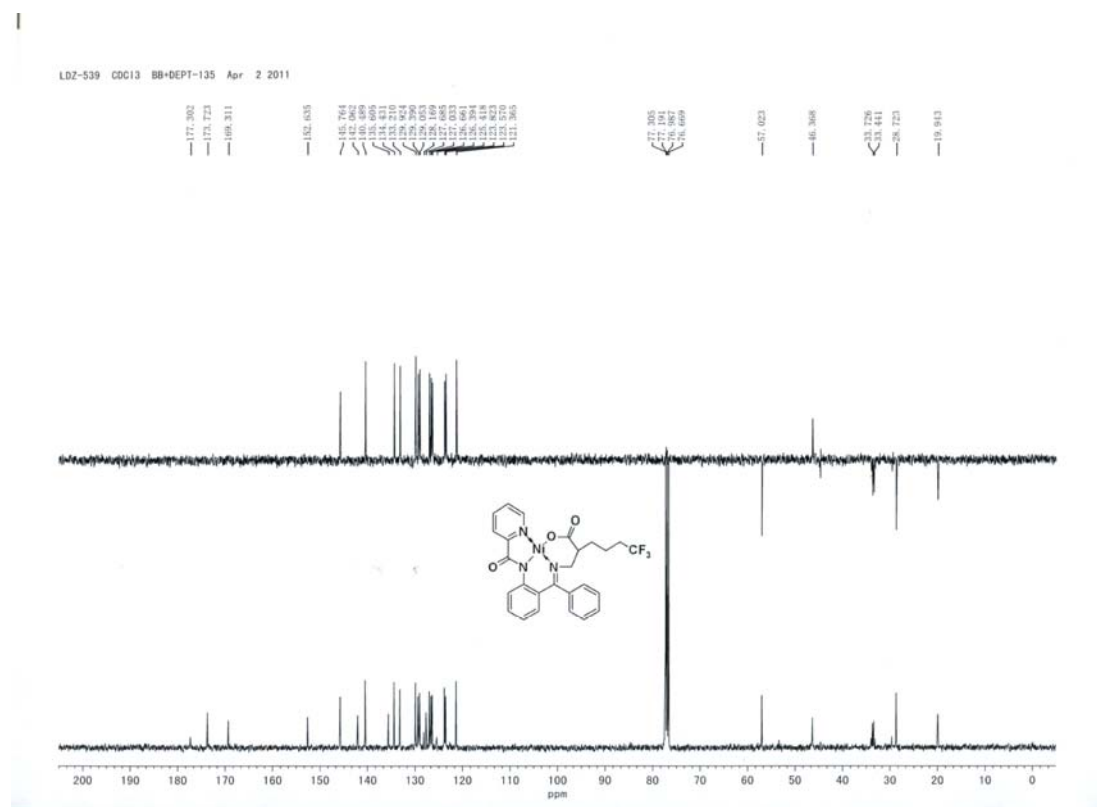
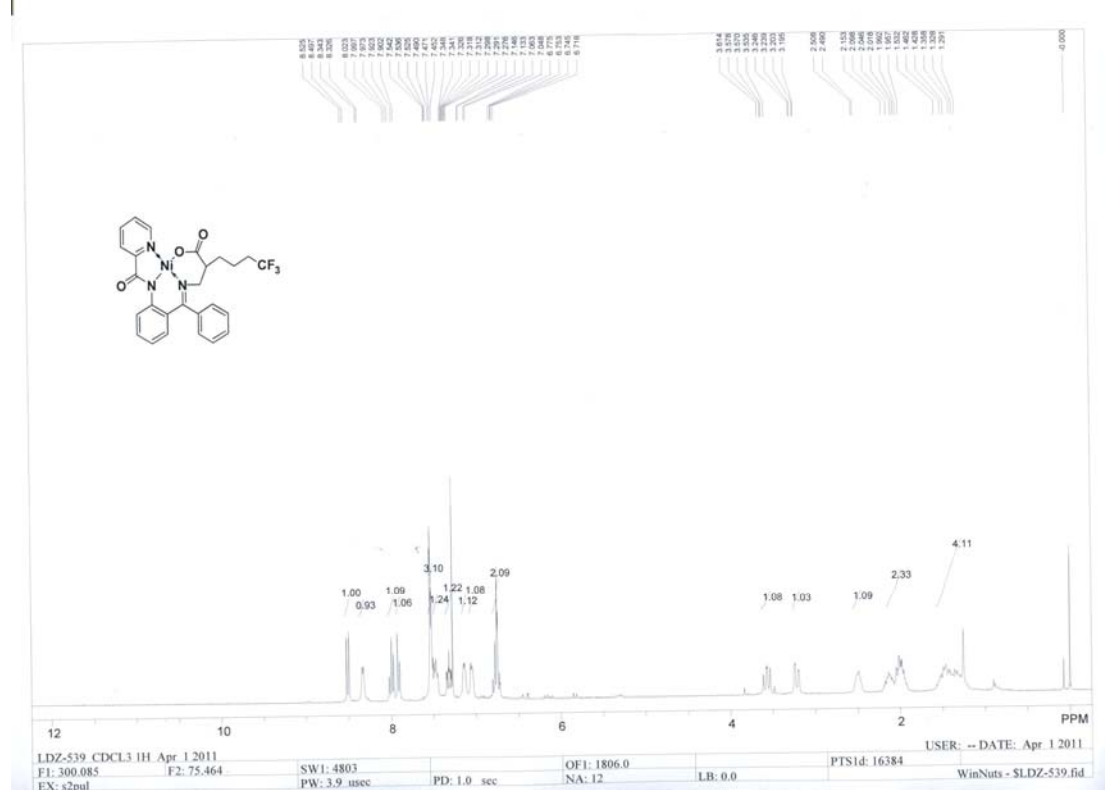


Ni(II)-PABP/ 3-amino-2-(2,5-dimethylbenzyl)propanoic acid Schiff Base Complex 5j.



Ni(II)-PABP/ 2-(aminomethyl)-6,6,6-trifluorohexanoic acid Schiff Base Complex

5p.



Chemical structure: NCC(C(=O)O)Cc1ccccc1

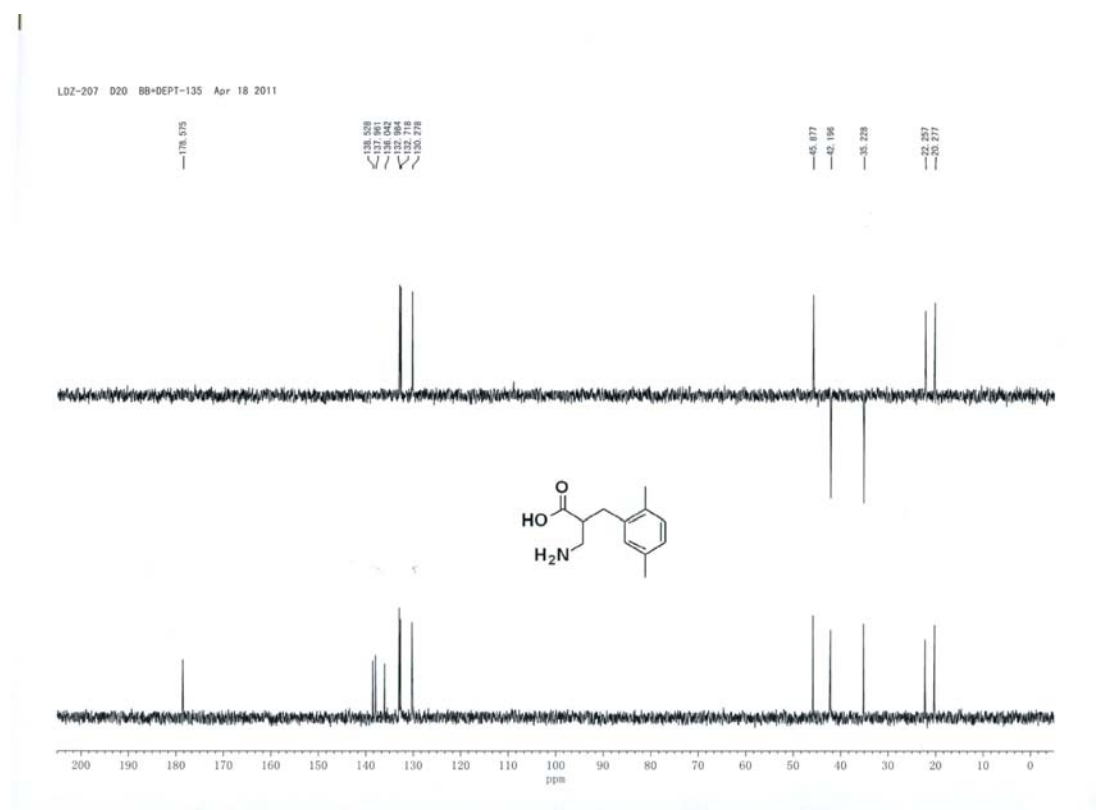
¹H NMR spectrum (D₂O, 1H) showing peaks at approximately 7.30-7.40 ppm (aromatic, 5H), 4.80 ppm (NH₂, 2H), and 2.80-3.40 ppm (CH₂, 2H). Integration values of 5.00 and 5.11 are shown for the aromatic and CH₂ regions respectively.

LDZ-179, D2O, 1H, Aug 25 2010	SW1: 4803	OF1: 1864.9	PTS1d: 16384	USER: -- DATE: Aug 25 2010
F1: 300.086	F2: 75.464	NA: 20	LB: 0.0	
EX: s2pul	PW: 3.9 usec	PD: 1.0 sec		WinNuts - ldx-179

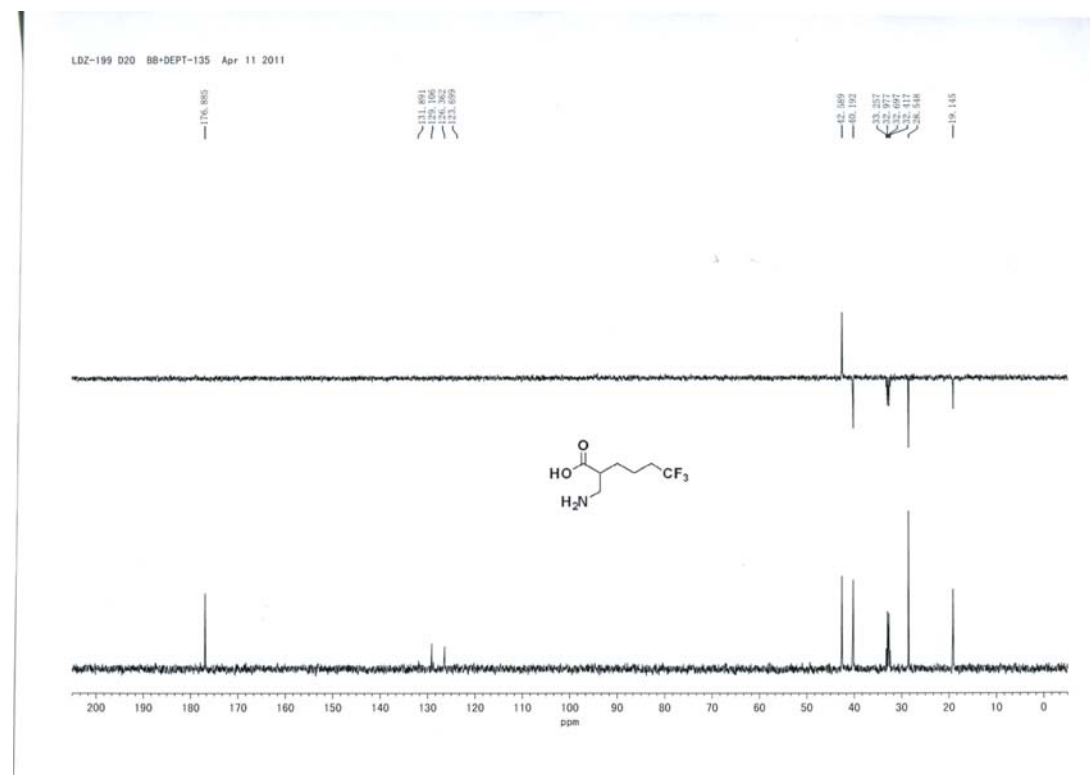
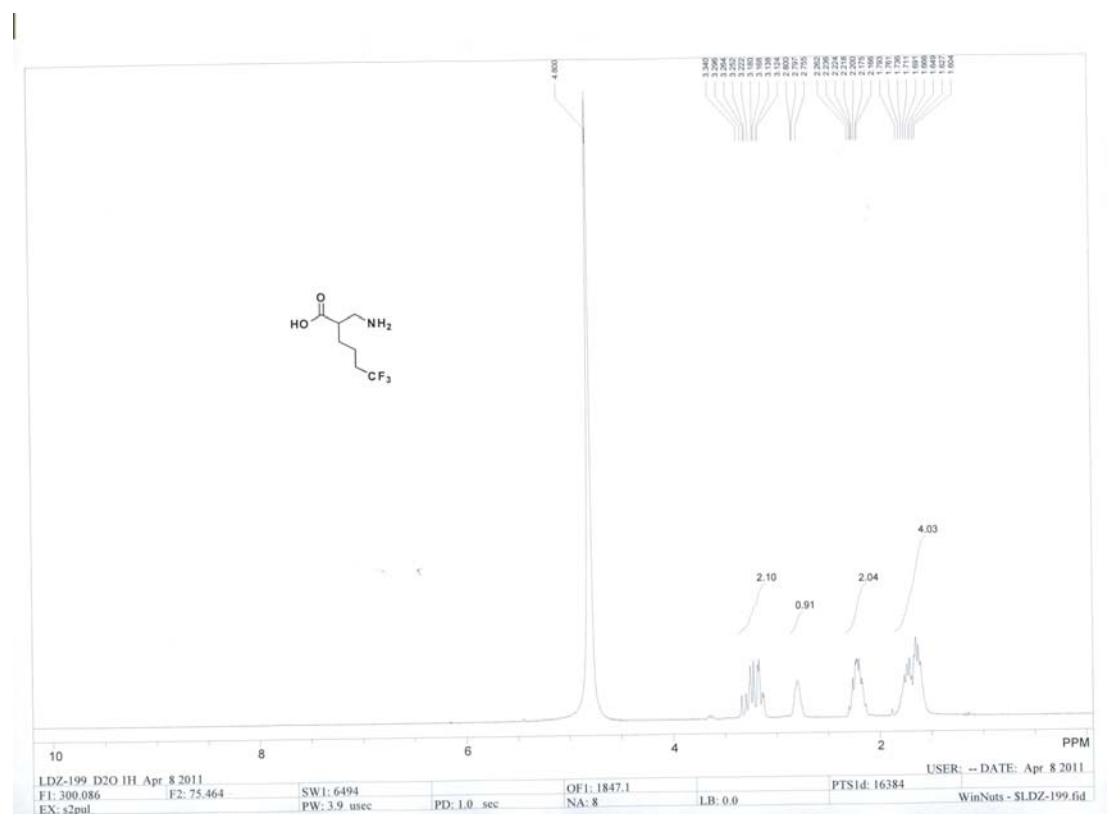


NC(Cc1ccc(C)cc1)C(=O)O

LDZ-207 1H Apr 18 2011
F1: 400.168 F2: 100.631 SW1: 6410 OF1: 2482.3 PTS1d: 32768
EX: s2pul PW: 3.8 usec PD: 0.2 sec NA: 28 LB: 0.0 WinNuts - \$LDZ-207.fid



2-(aminomethyl)-6,6,6-trifluorohexanoic acid 6p.



3-phenylpropanal 7a

