

ASIAN JOURNAL

OF ORGANIC CHEMISTRY

Supporting Information

Nickel-Catalyzed Cross-Coupling of (Hetero)aryl Chlorides with Aryllithium Compounds

Jian-Long Tao^[a] and Zhong-Xia Wang^{*[a, b]}

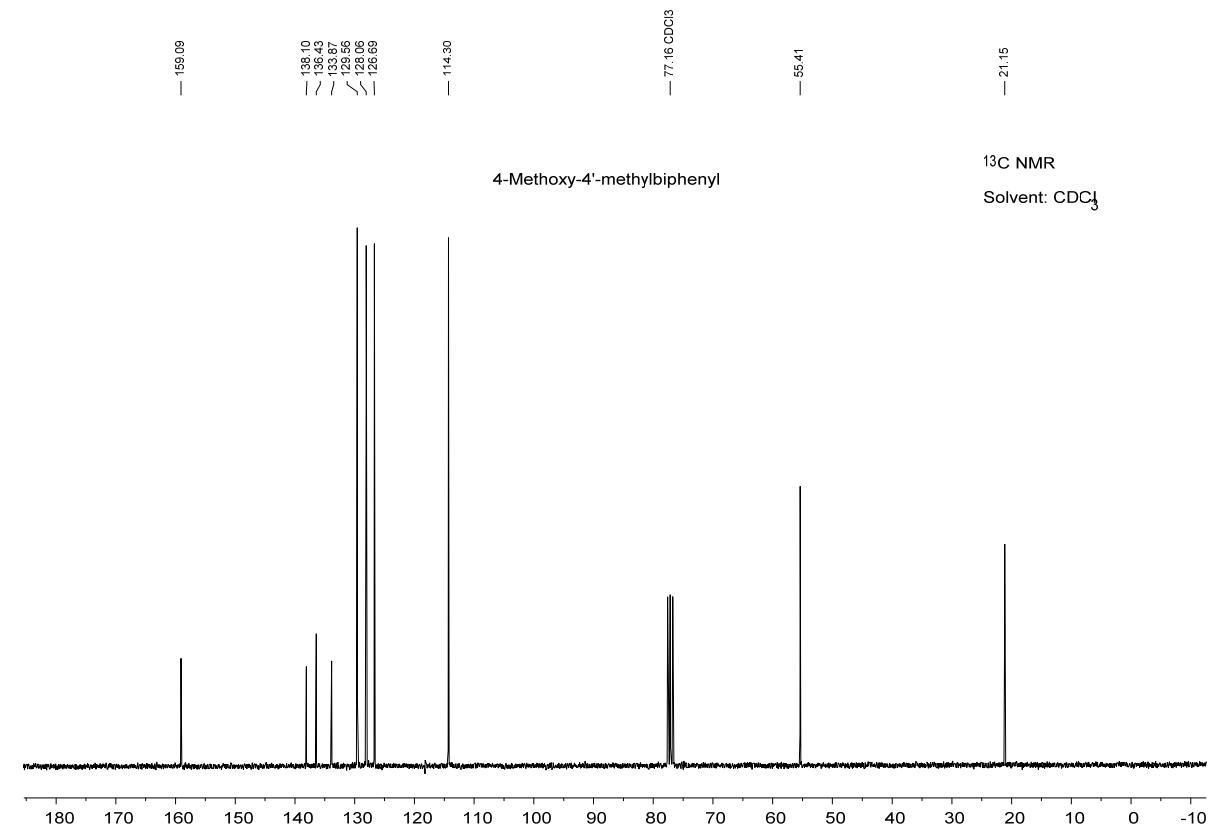
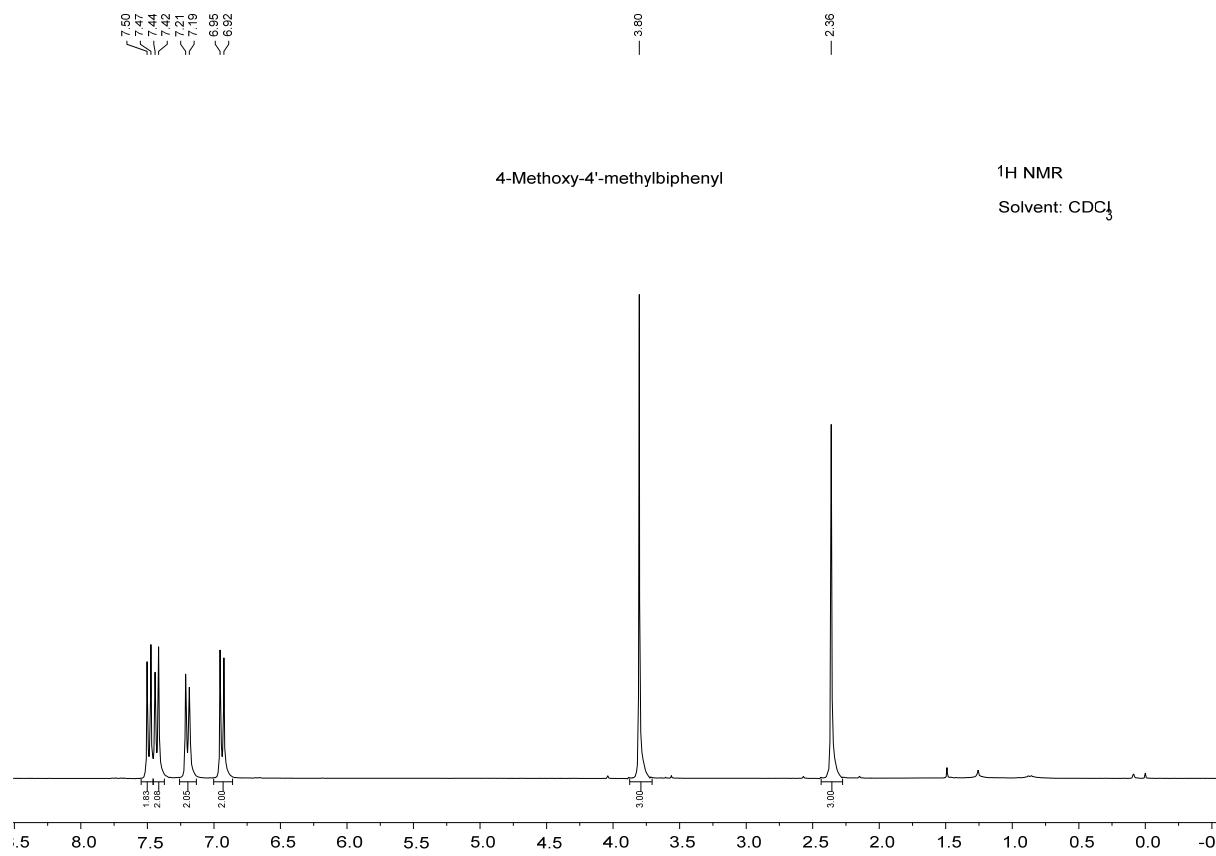
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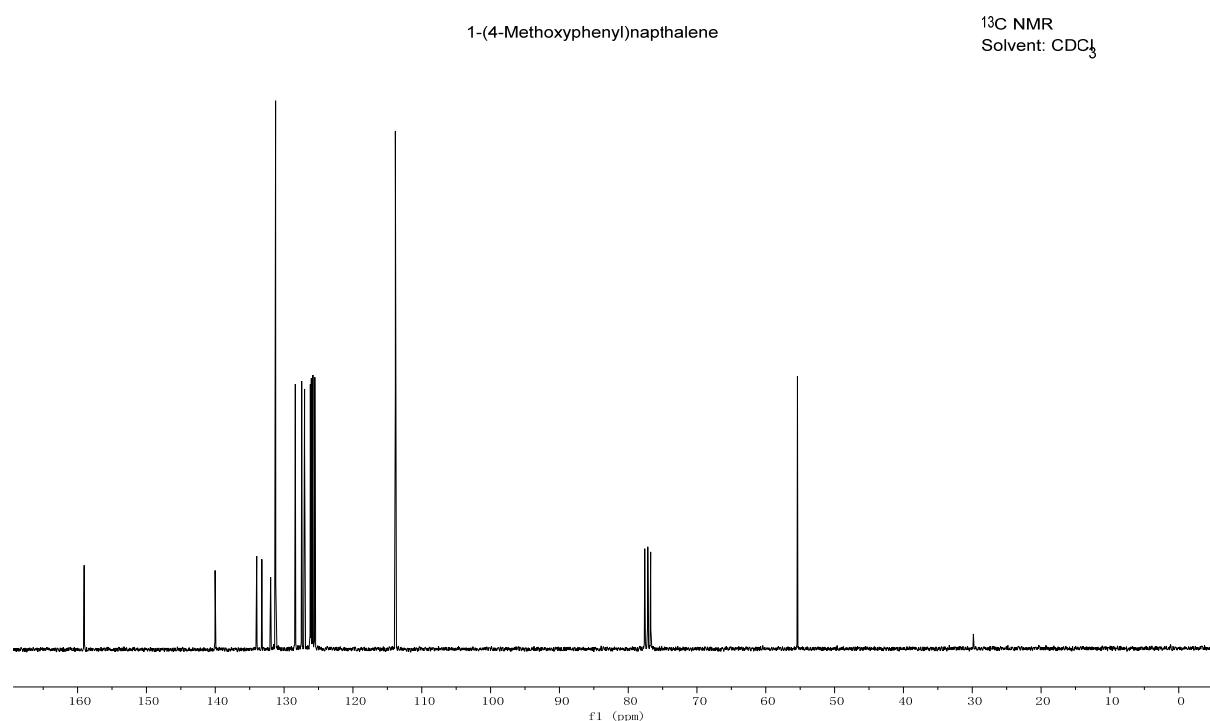
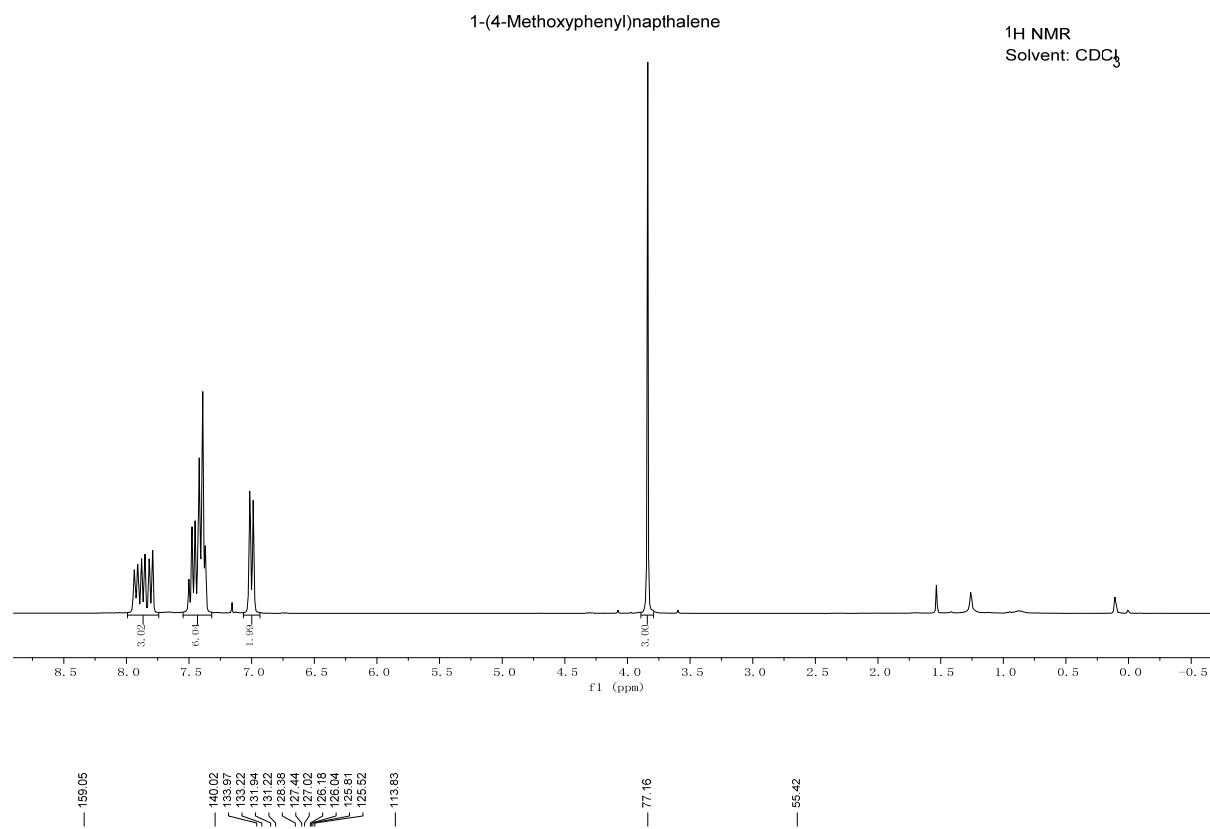
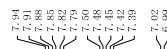
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Copies of NMR spectra for the cross-coupling products

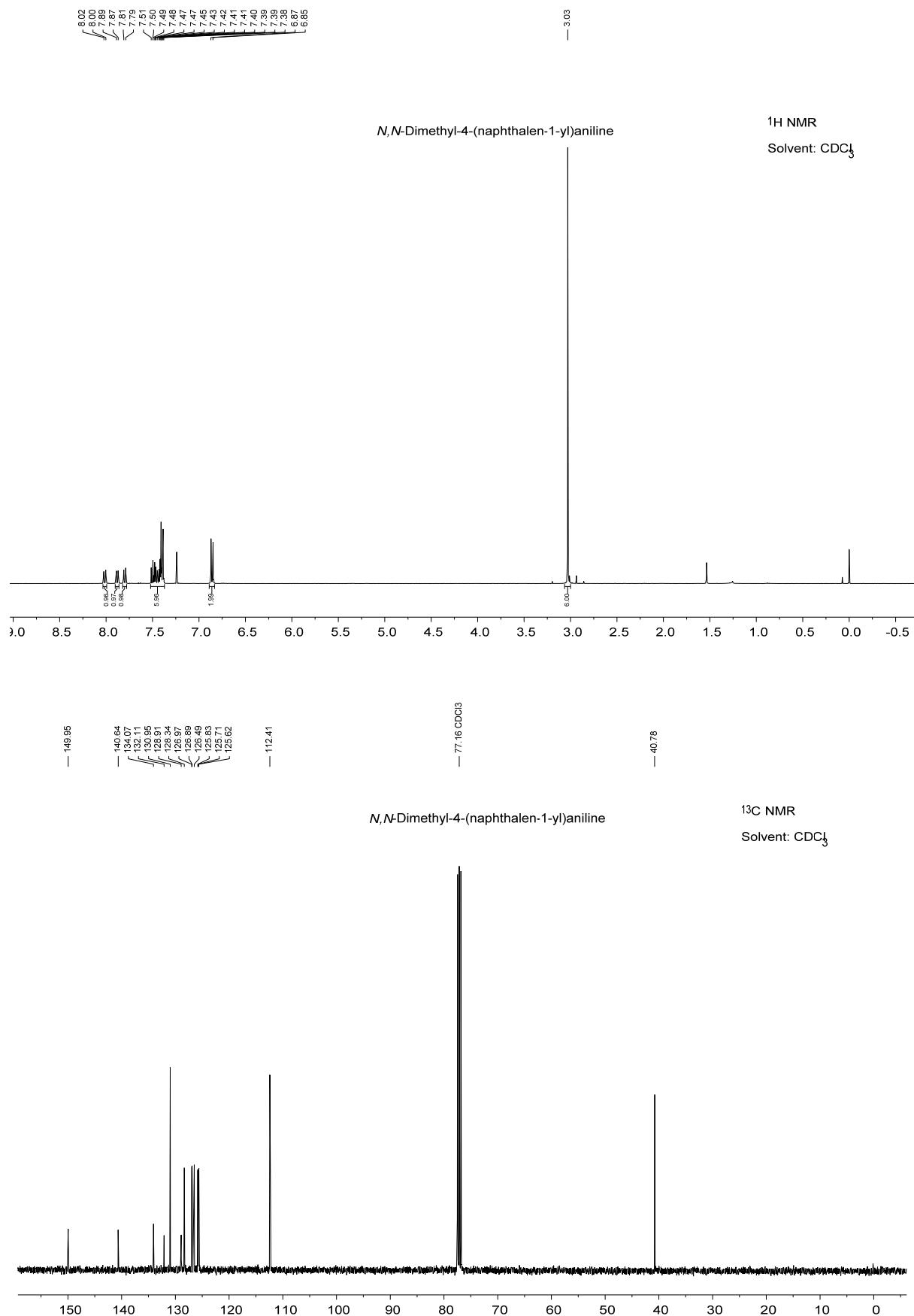
(1) 4-Methoxy-4'-methylbiphenyl



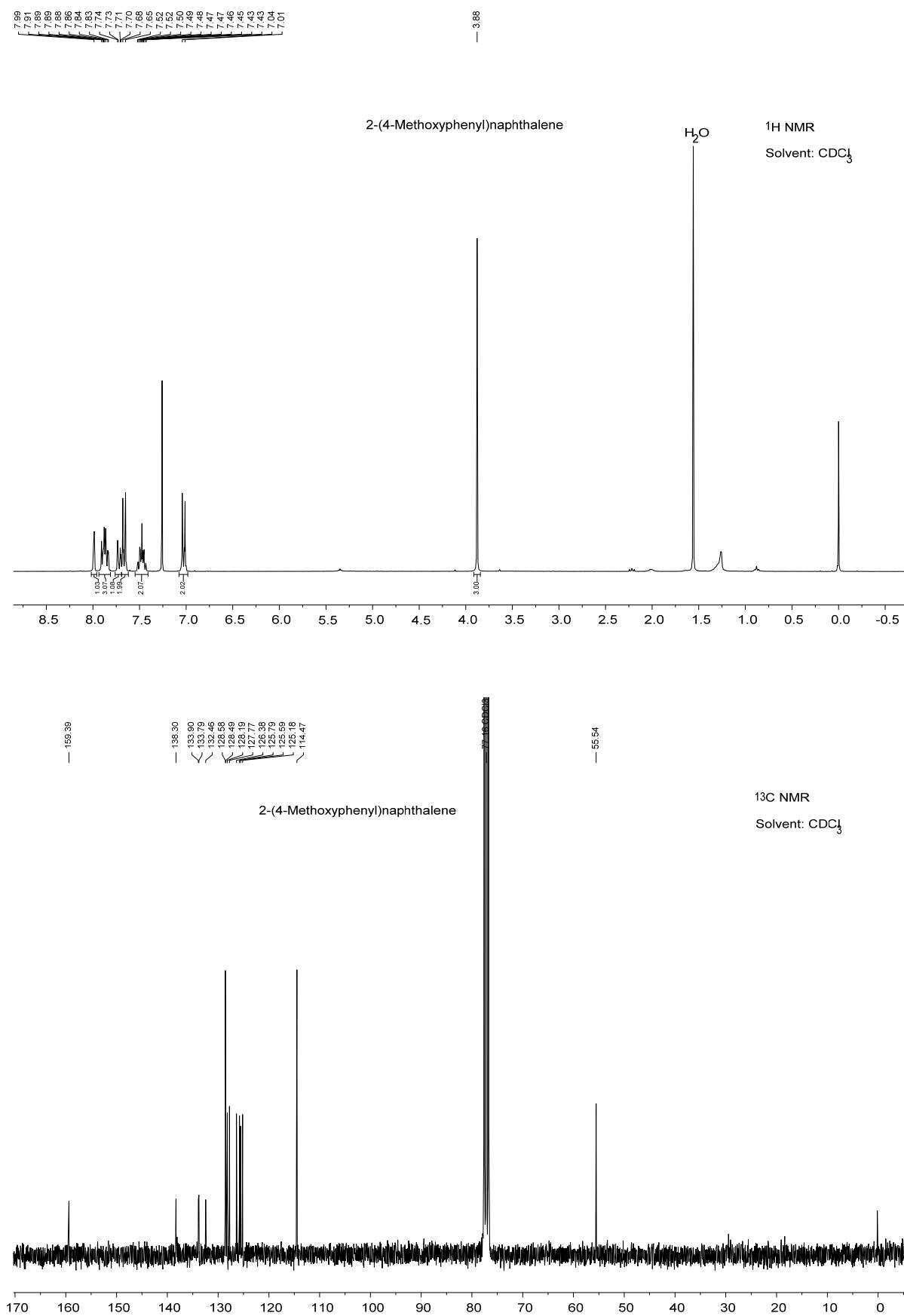
(2) 1-(4-Methoxyphenyl)naphthalene



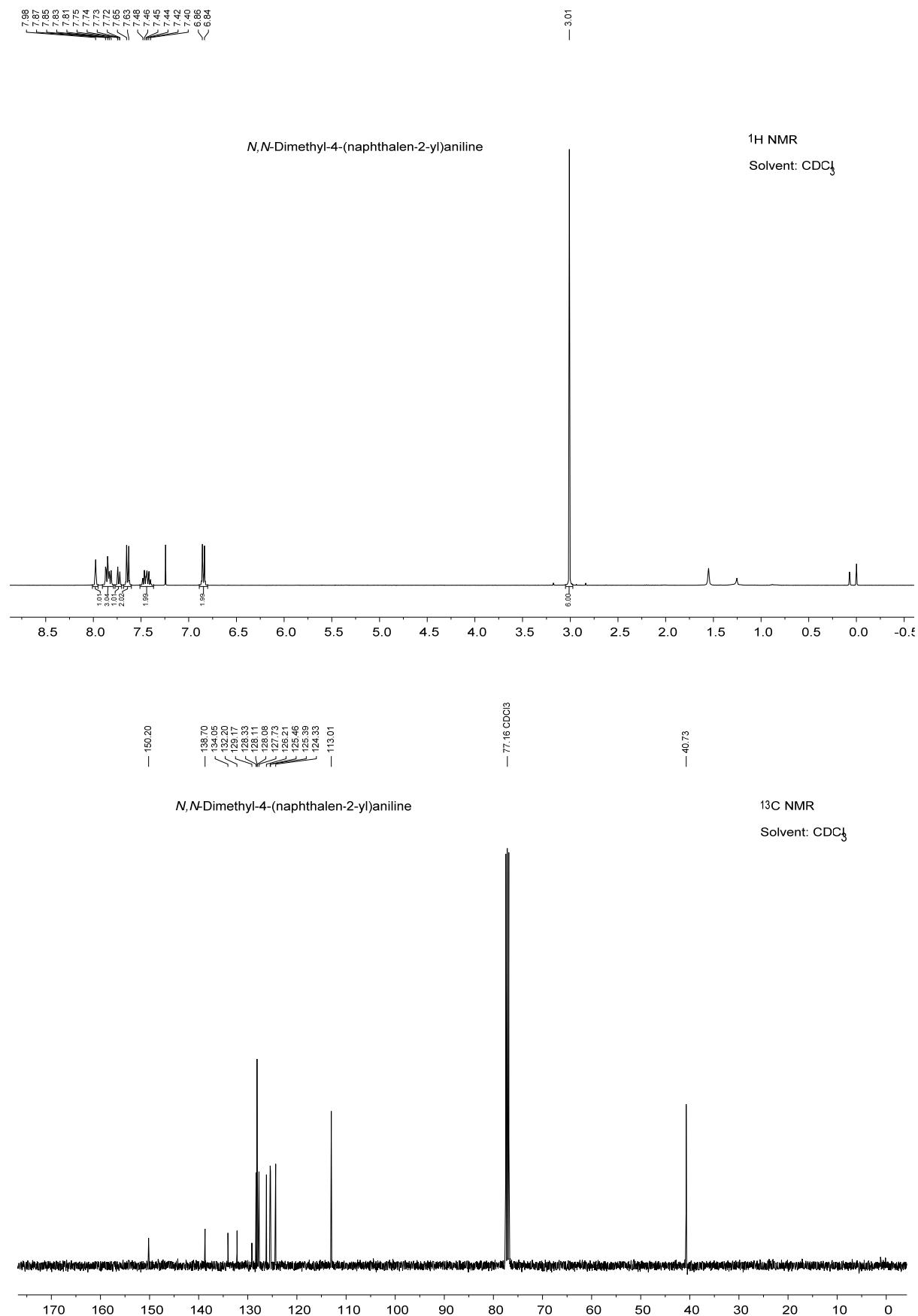
(3) *N,N*-Dimethyl-4-(naphthalen-1-yl)aniline



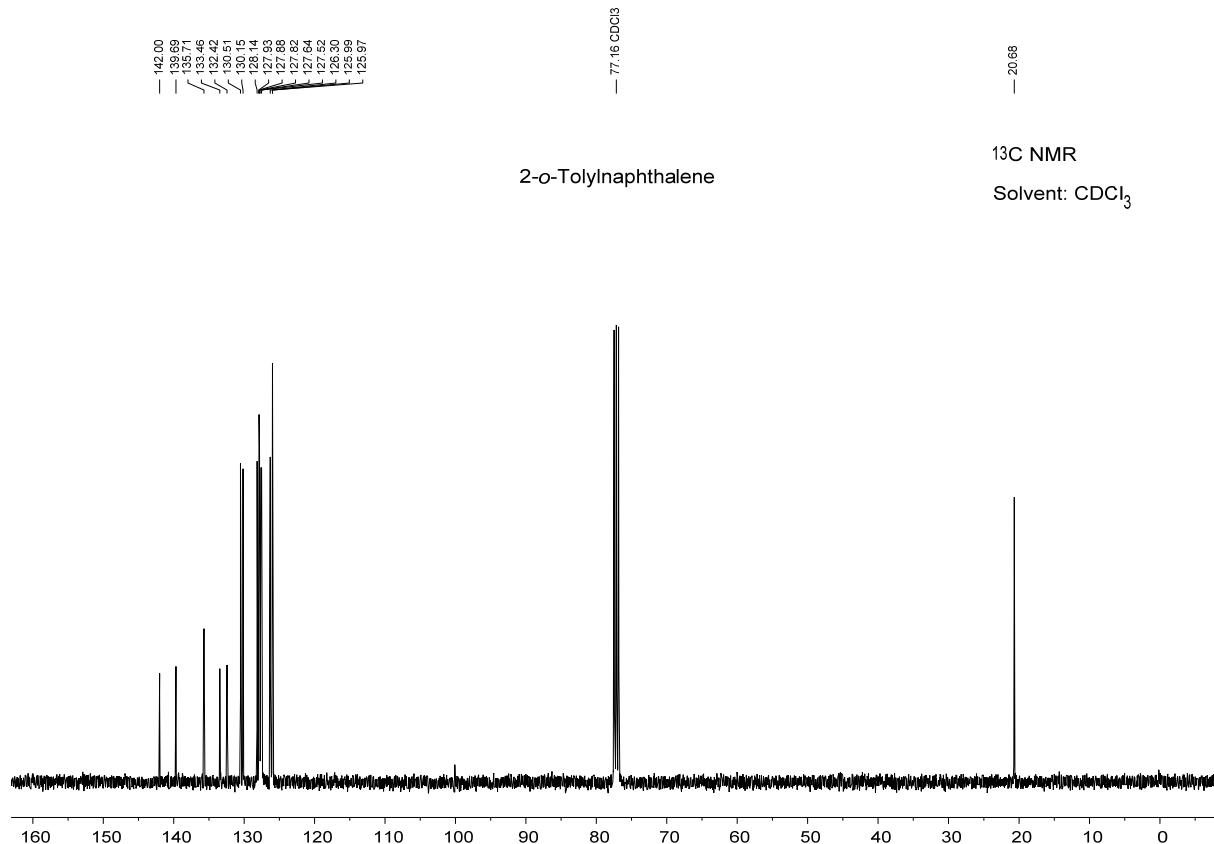
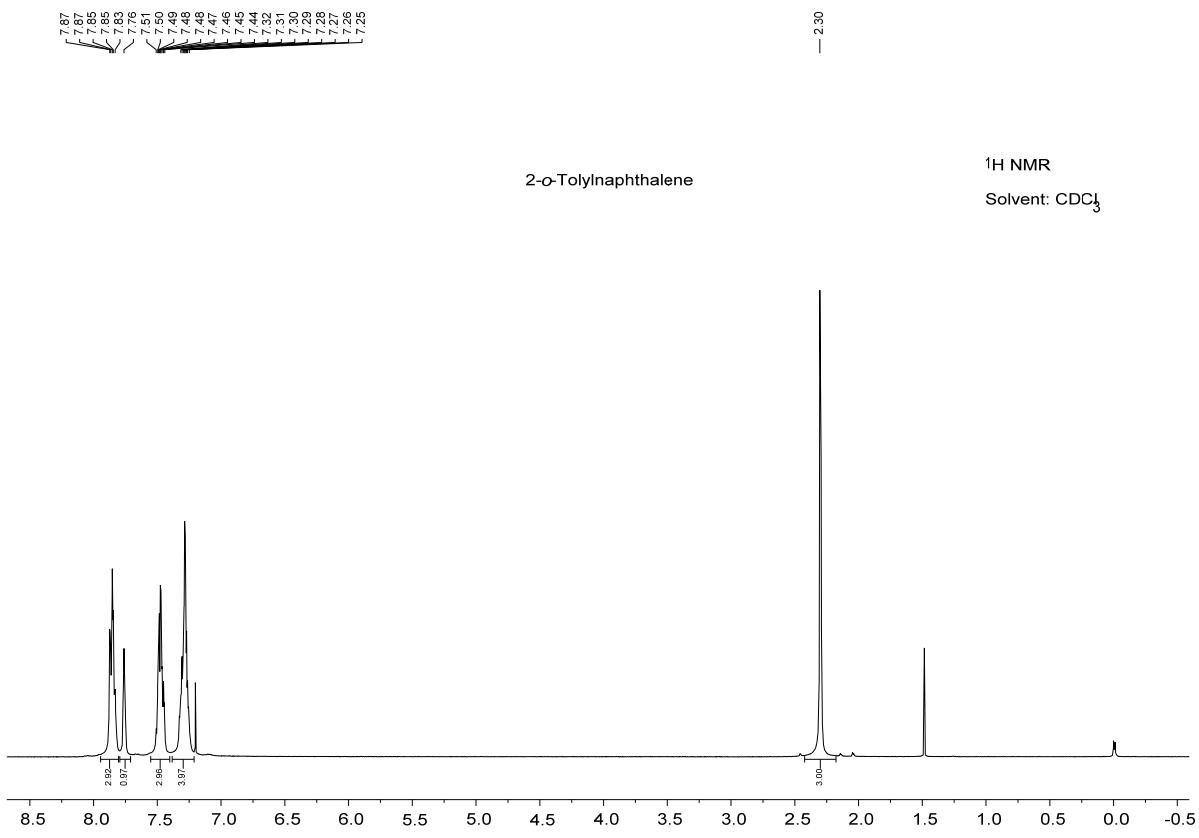
(4) 2-(4-Methoxyphenyl)naphthalene



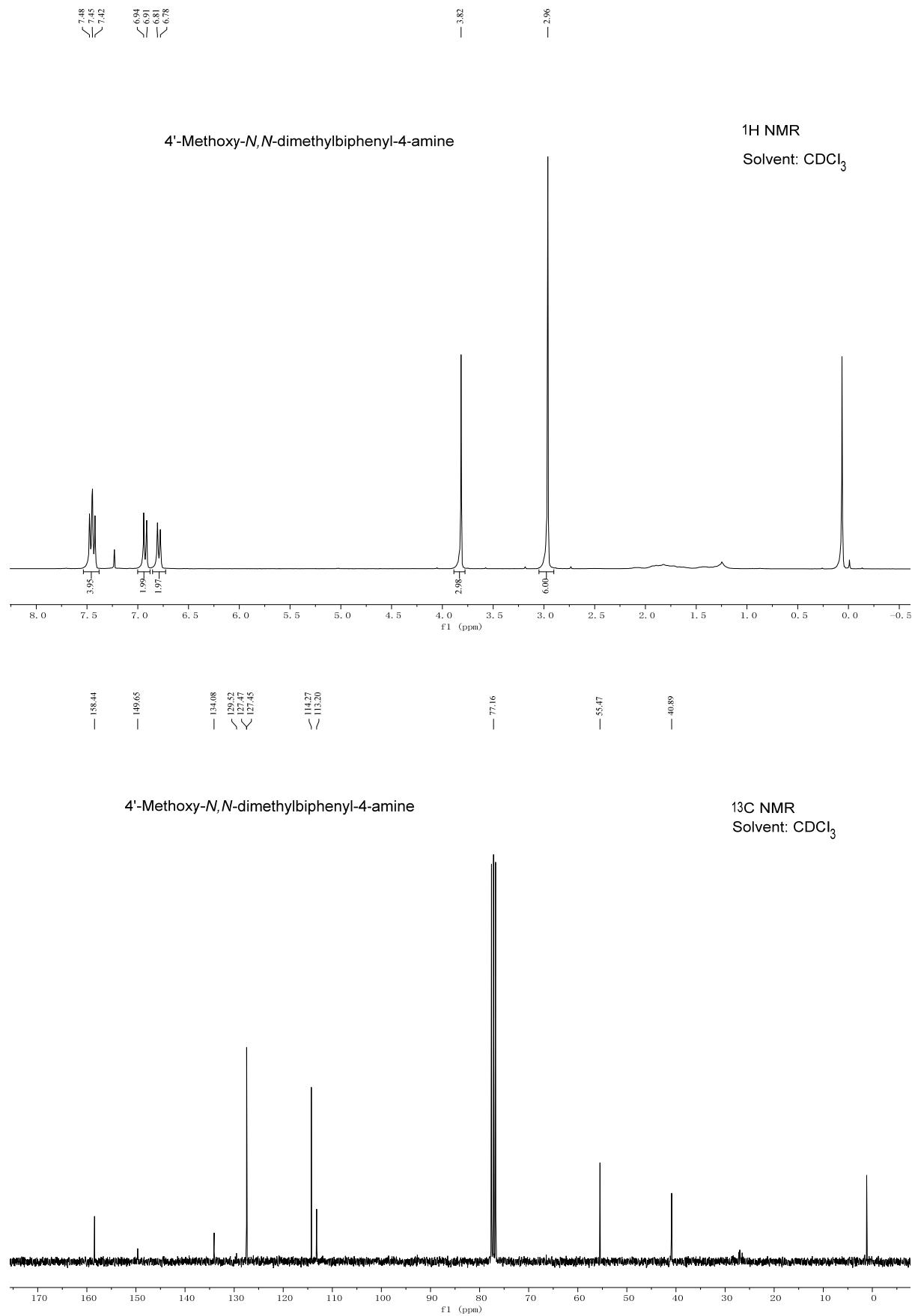
(5) *N,N*-Dimethyl-4-(naphthalen-2-yl)aniline



(6) 2-*o*-Tolylnaphthalene



(7) 4'-Methoxy-*N,N*-dimethylbiphenyl-4-amine



(8) 4-Methoxybiphenyl

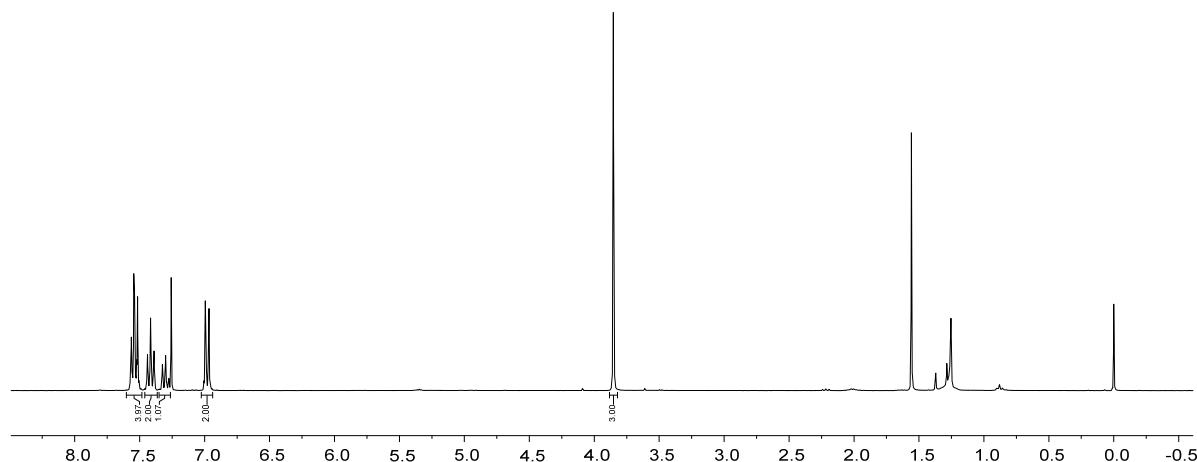
7.67
7.59
7.56
7.55
7.53
7.52
7.44
7.42
7.39
7.32
7.32
7.30
6.97

— 3.65

4-Methoxybiphenyl

¹H NMR

Solvent: CDCl₃

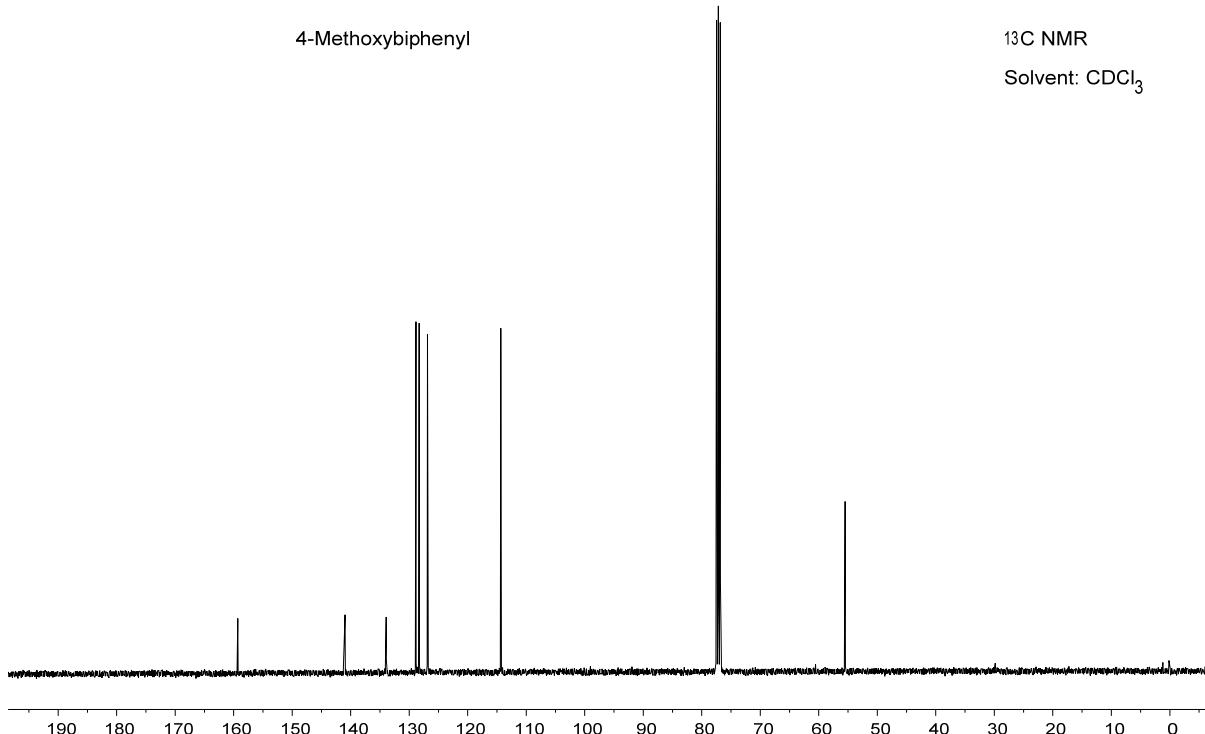


— 3.65

4-Methoxybiphenyl

¹³C NMR

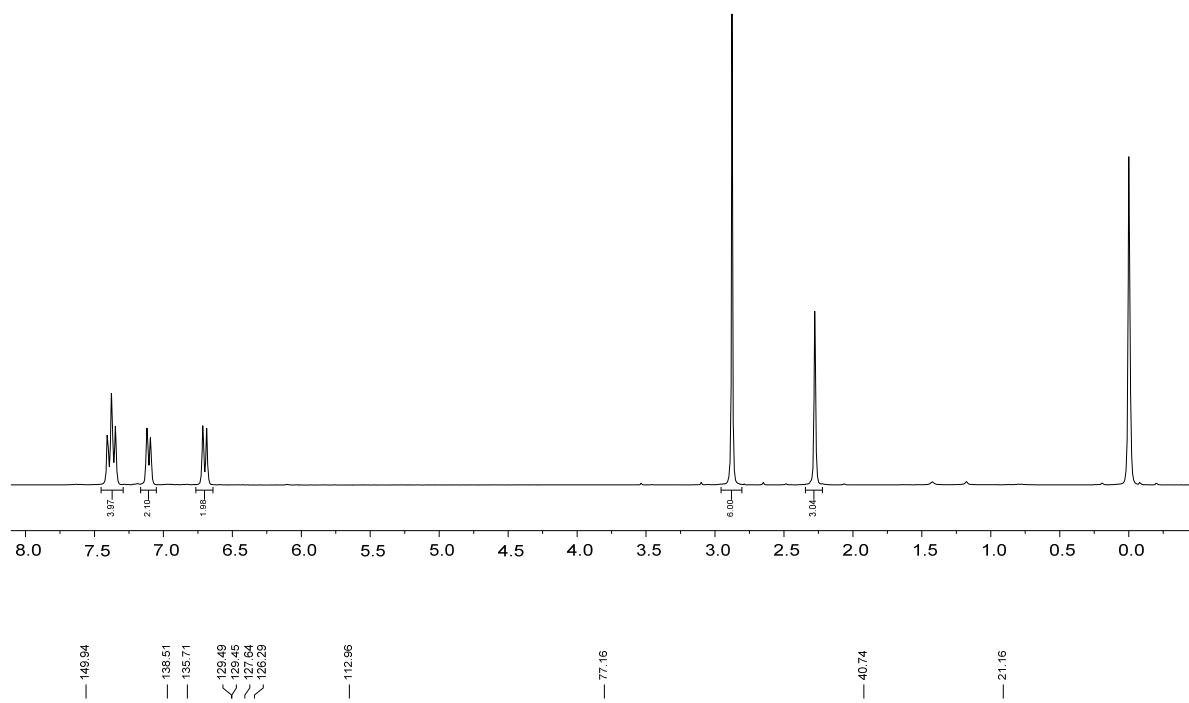
Solvent: CDCl₃



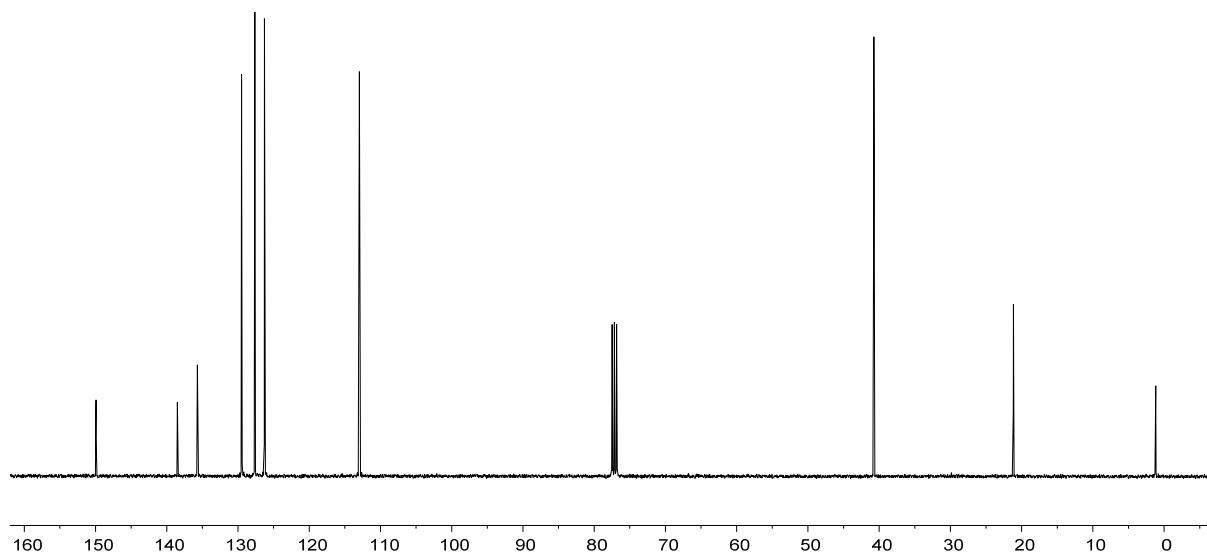
(9) *N,N*,4'-Trimethylbiphenyl-4-amine

✓ 7.41
✓ 7.38
✓ 7.35
✓ 7.12
✓ 7.09
✓ 6.98
✓ 6.69

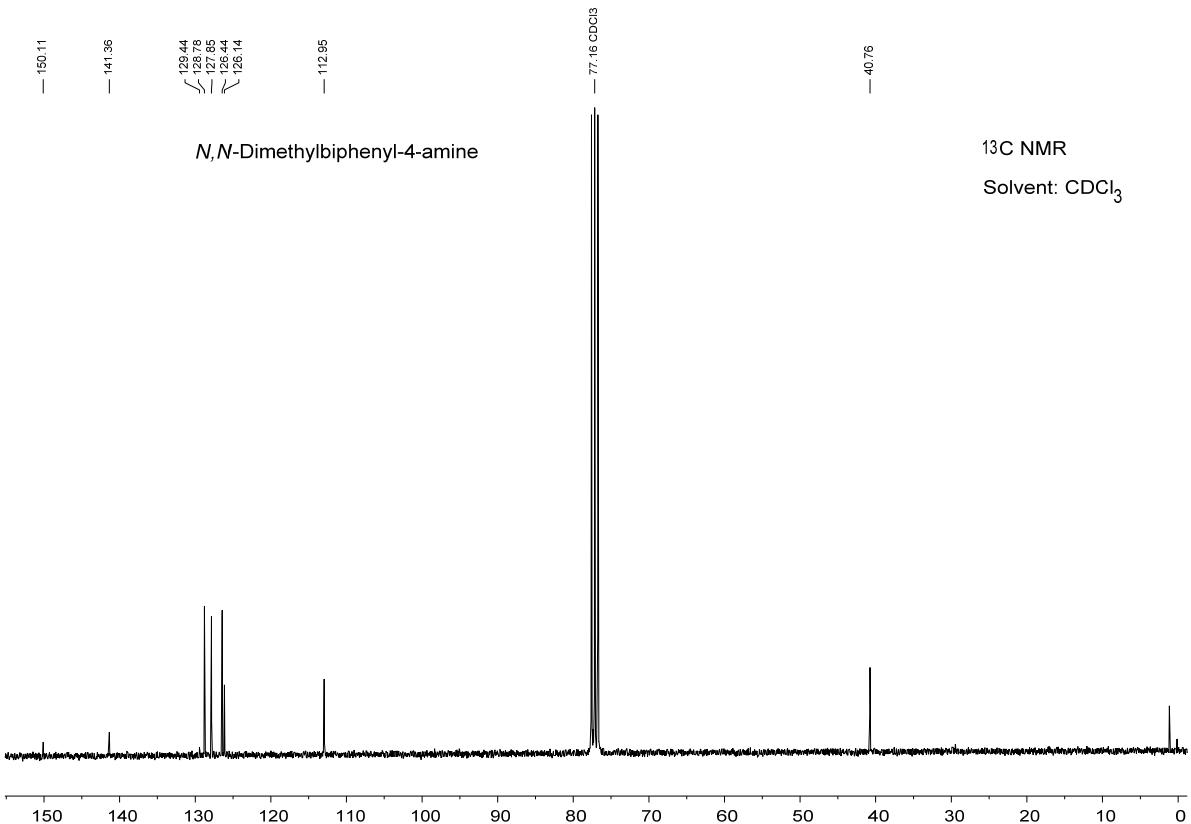
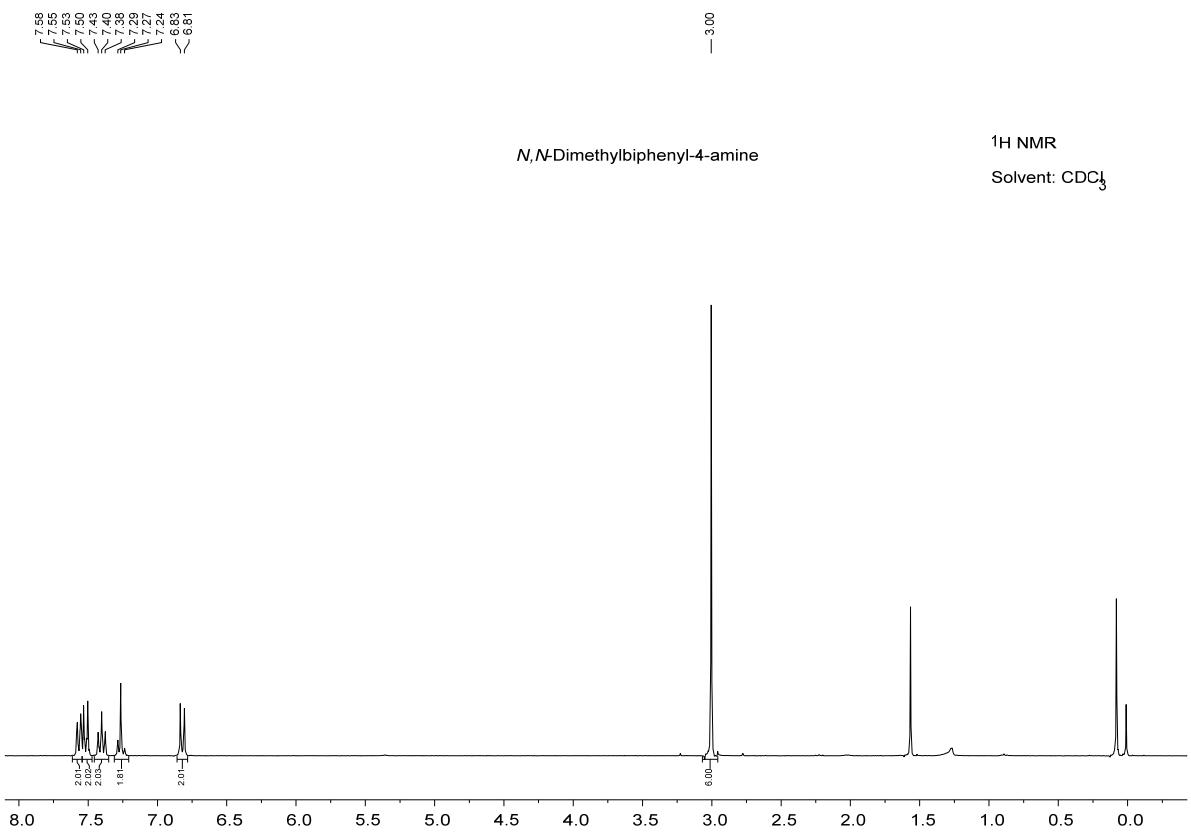
1H NMR
N,N,4'-Trimethylbiphenyl-4-amine
Solvent: CDCl₃



13C NMR
N,N,4'-Trimethylbiphenyl-4-amine
Solvent: CDCl₃



(10) *N,N*-Dimethylbiphenyl-4-amine



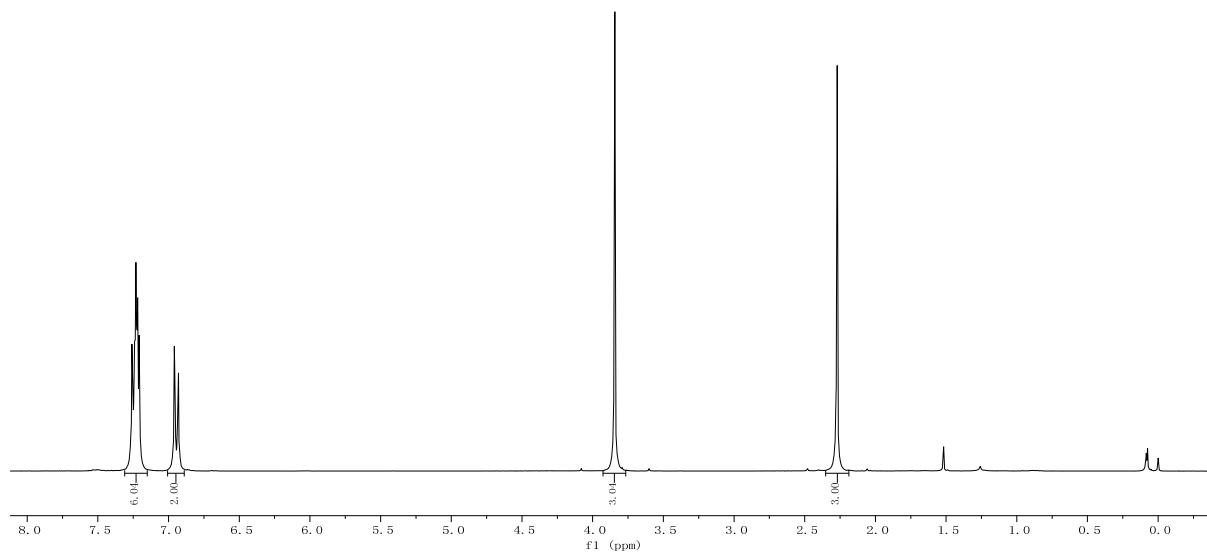
(11) 4'-Methoxy-2-methylbiphenyl



4'-Methoxy-2-methylbiphenyl

¹H NMR

Solvent: CDCl₃



— 158.69
— 141.72
— 135.62
— 134.55
— 130.43
— 130.39
— 130.04
— 127.11
— 125.89

— 113.65

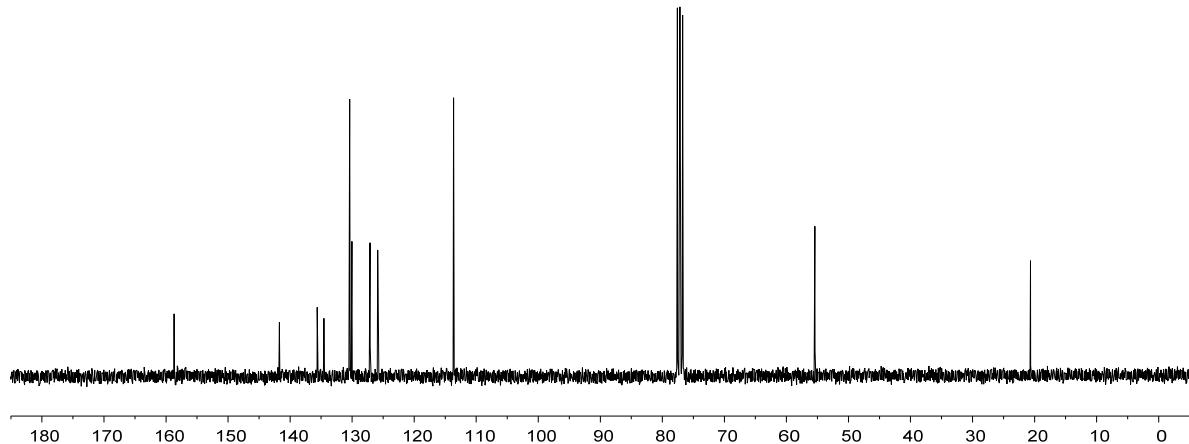
— 55.42

— 20.66

4'-Methoxy-2-methylbiphenyl

¹³C NMR

Solvent: CDCl₃



(12) *N,N*,2'-Trimethylbiphenyl-4-amine

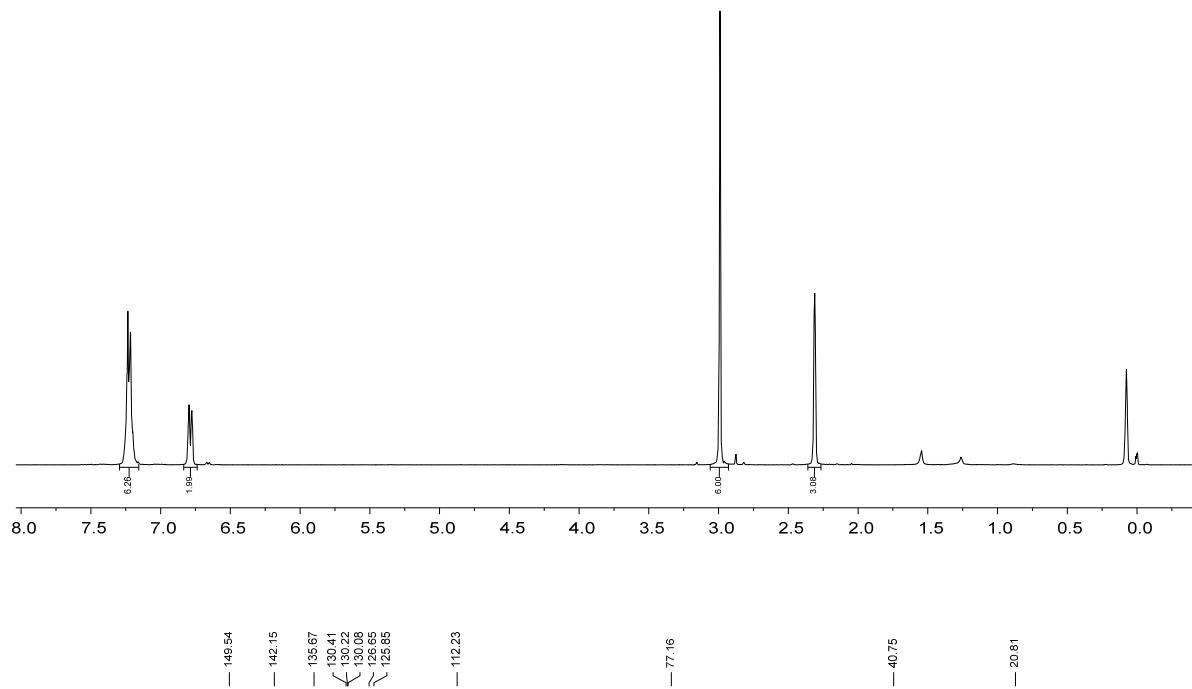
7.24
7.22
7.22
7.20
6.80
< 6.78

— 2.99
— 2.31

N,N,2'-Trimethylbiphenyl-4-amine

¹H NMR

Solvent: CDCl₃



— 149.54

— 142.15

— 135.67

— 130.41

— 130.22

— 130.08

— 126.89

— 125.85

— 112.23

— 77.16

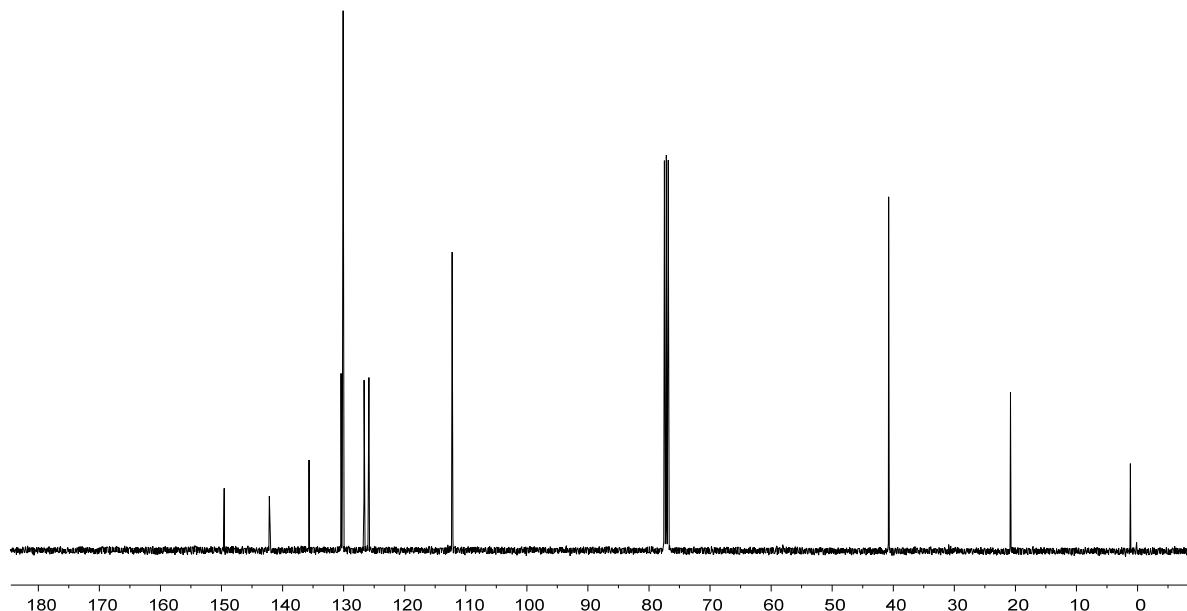
— 40.75

— 20.81

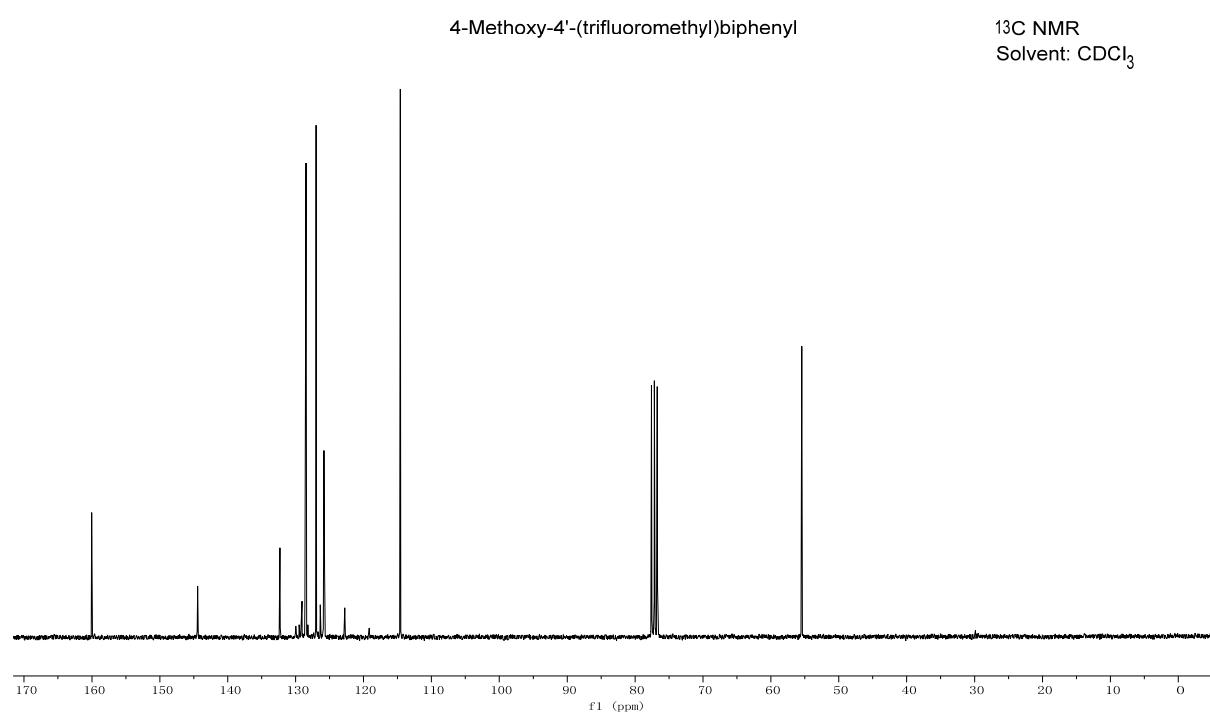
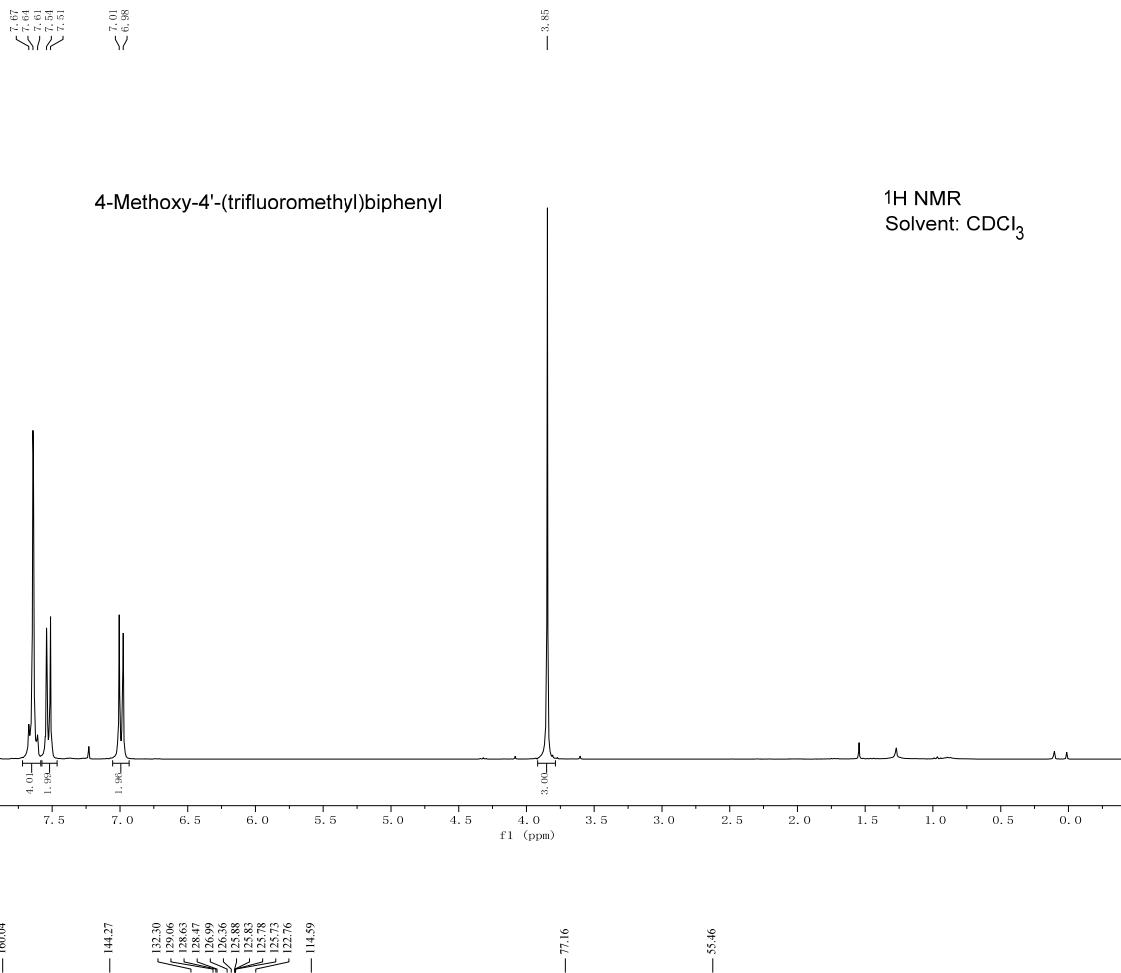
N,N,2'-Trimethylbiphenyl-4-amine

¹³C NMR

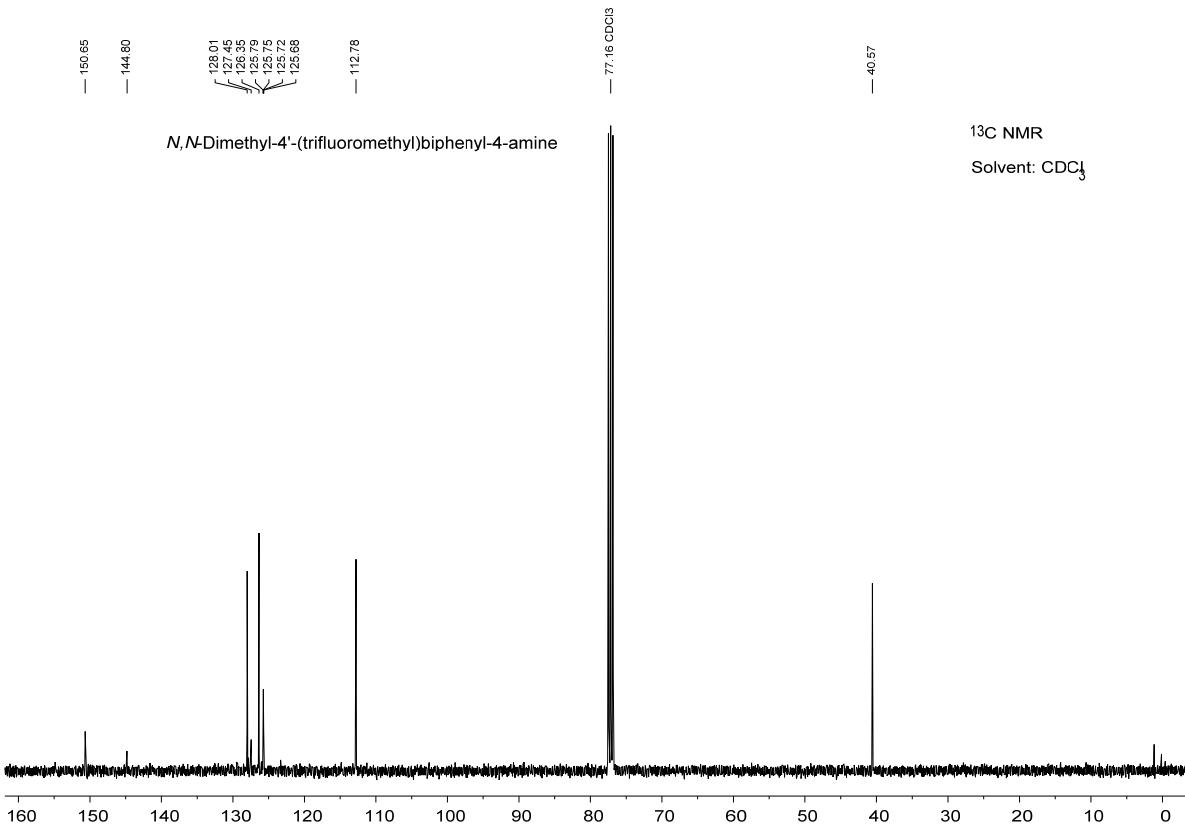
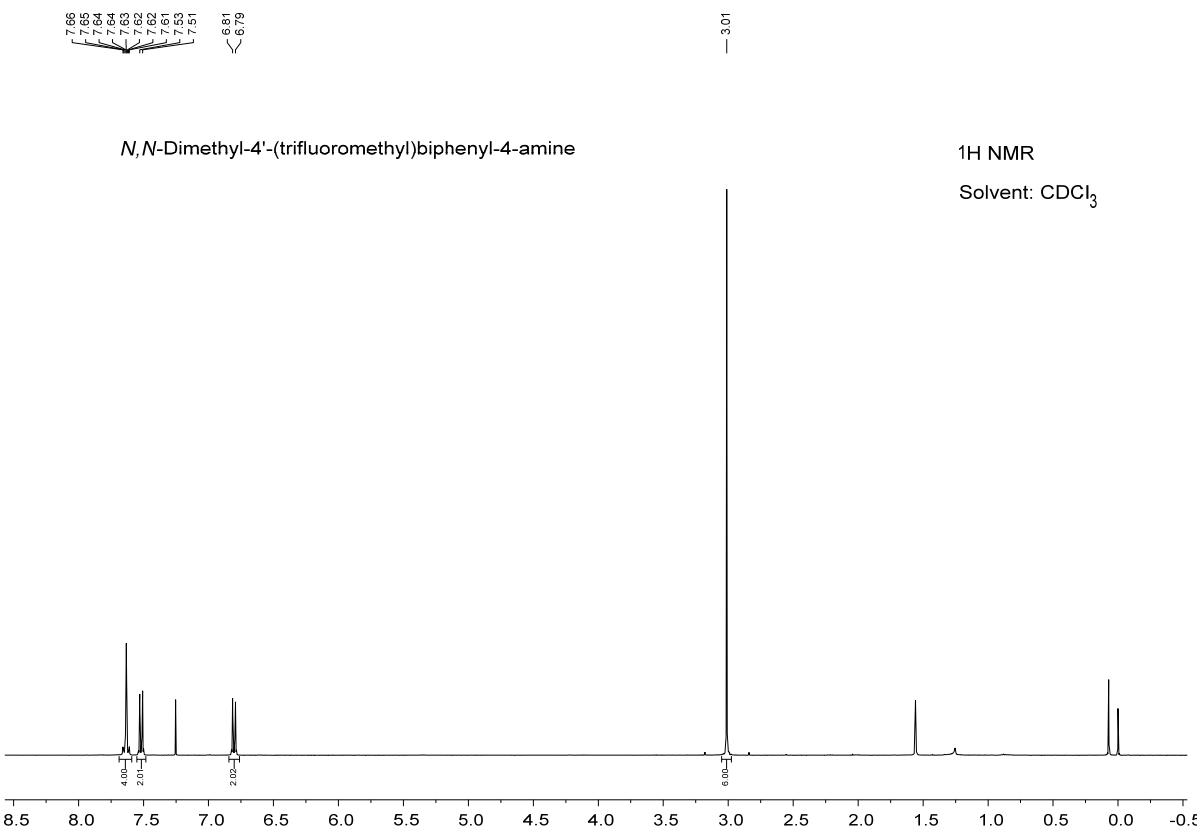
Solvent: CDCl₃



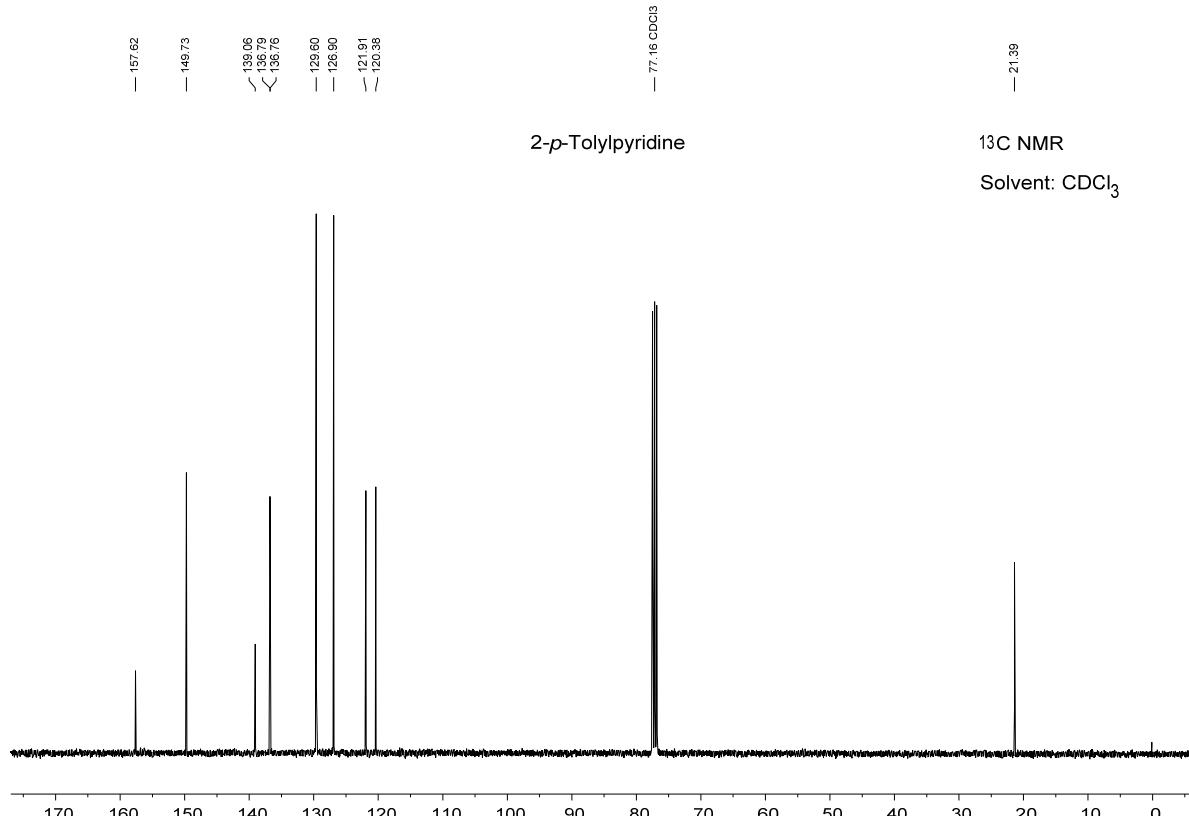
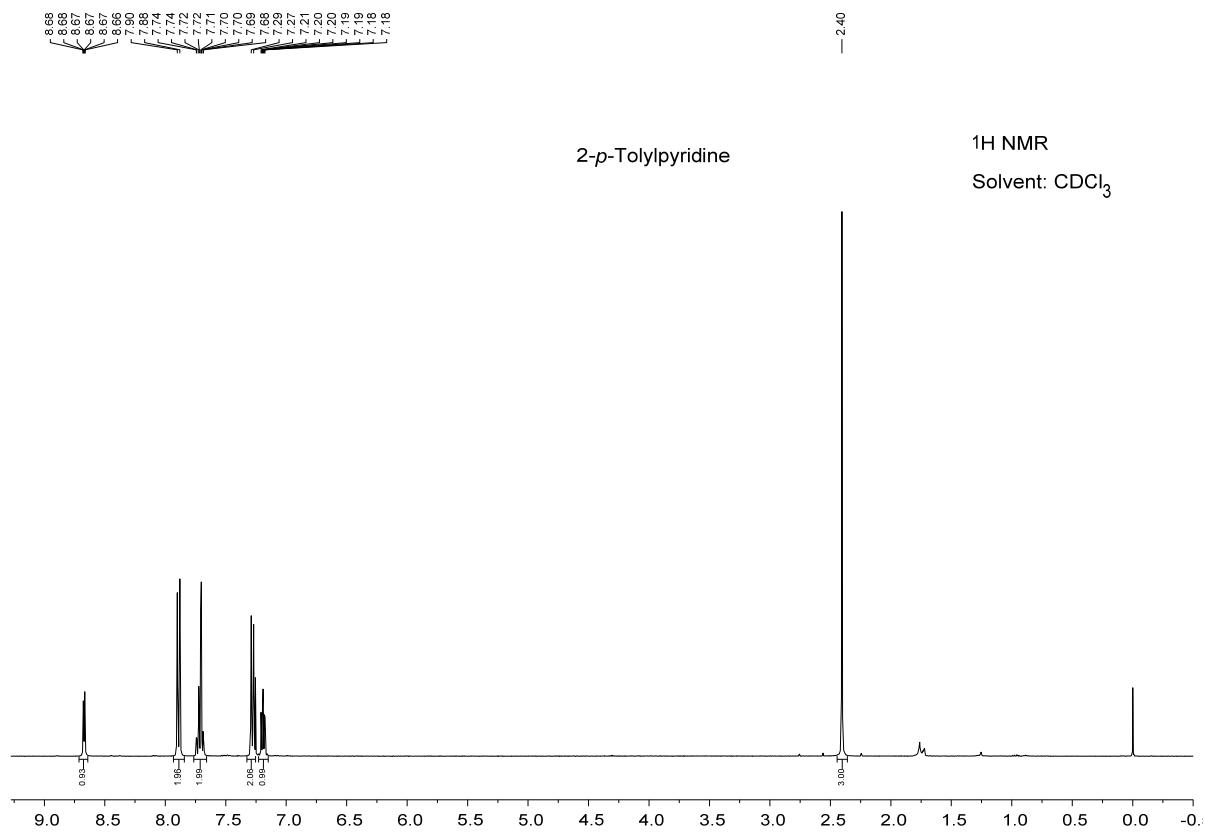
(13) 4-Methoxy-4'-(trifluoromethyl)biphenyl



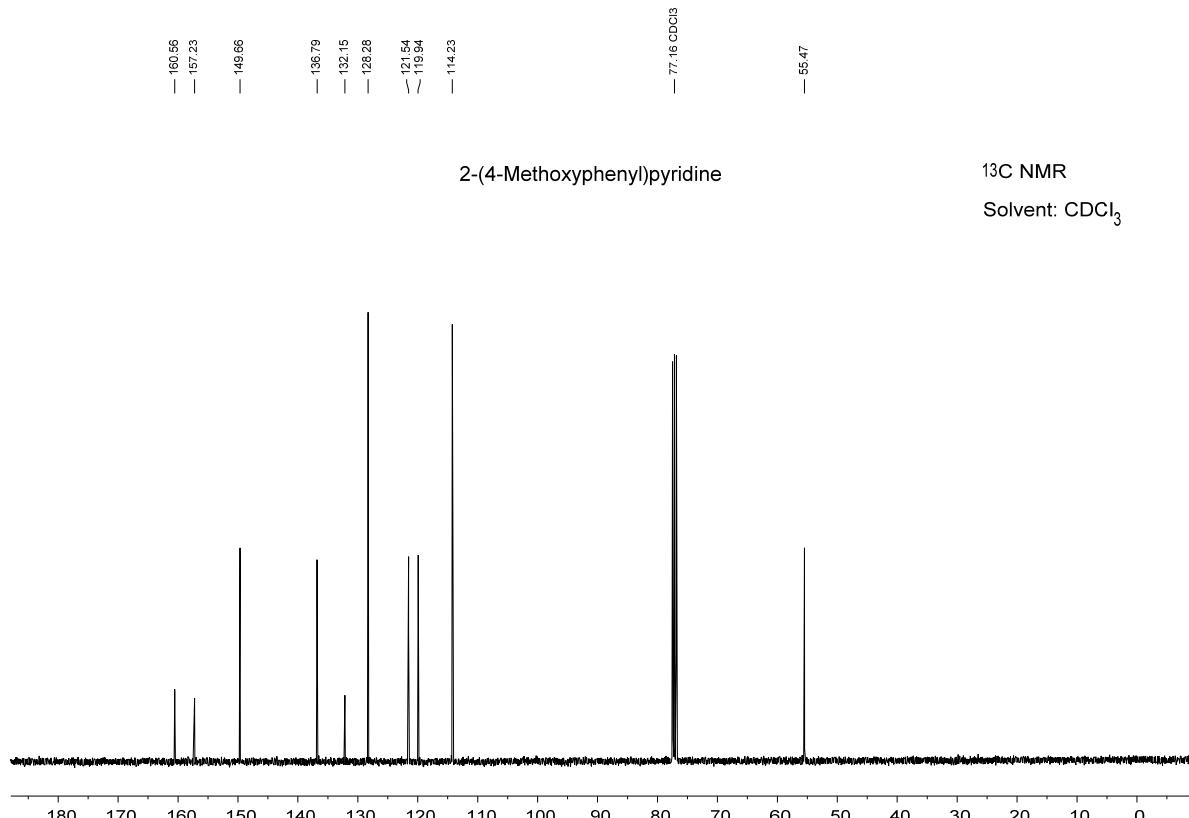
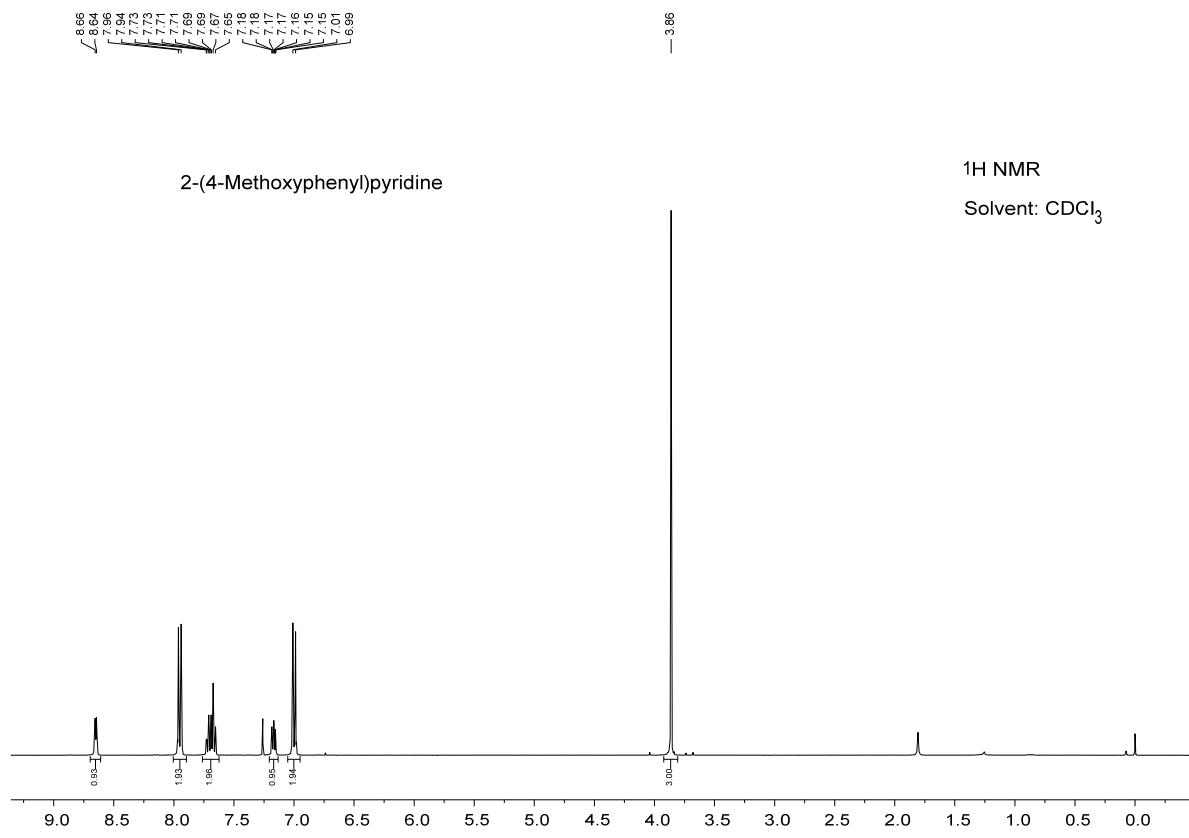
(14) *N,N*-Dimethyl-4'-(trifluoromethyl)biphenyl-4-amine



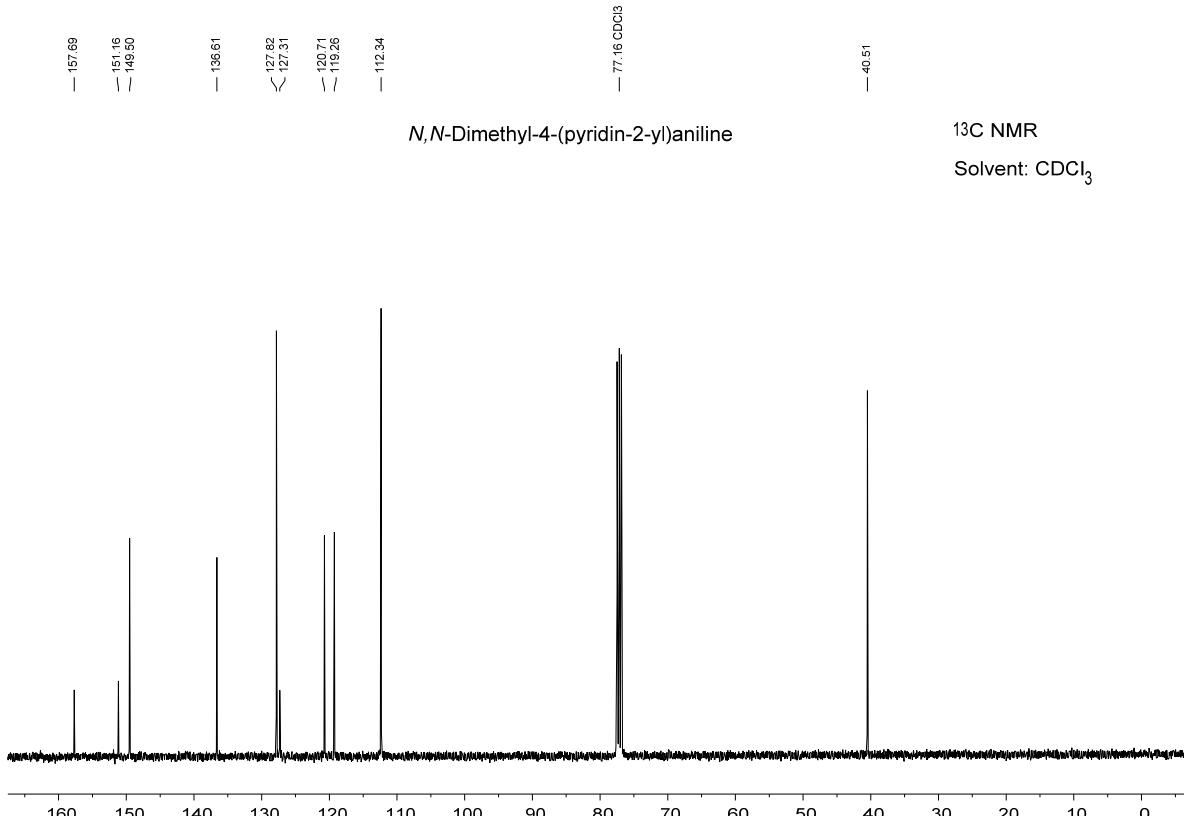
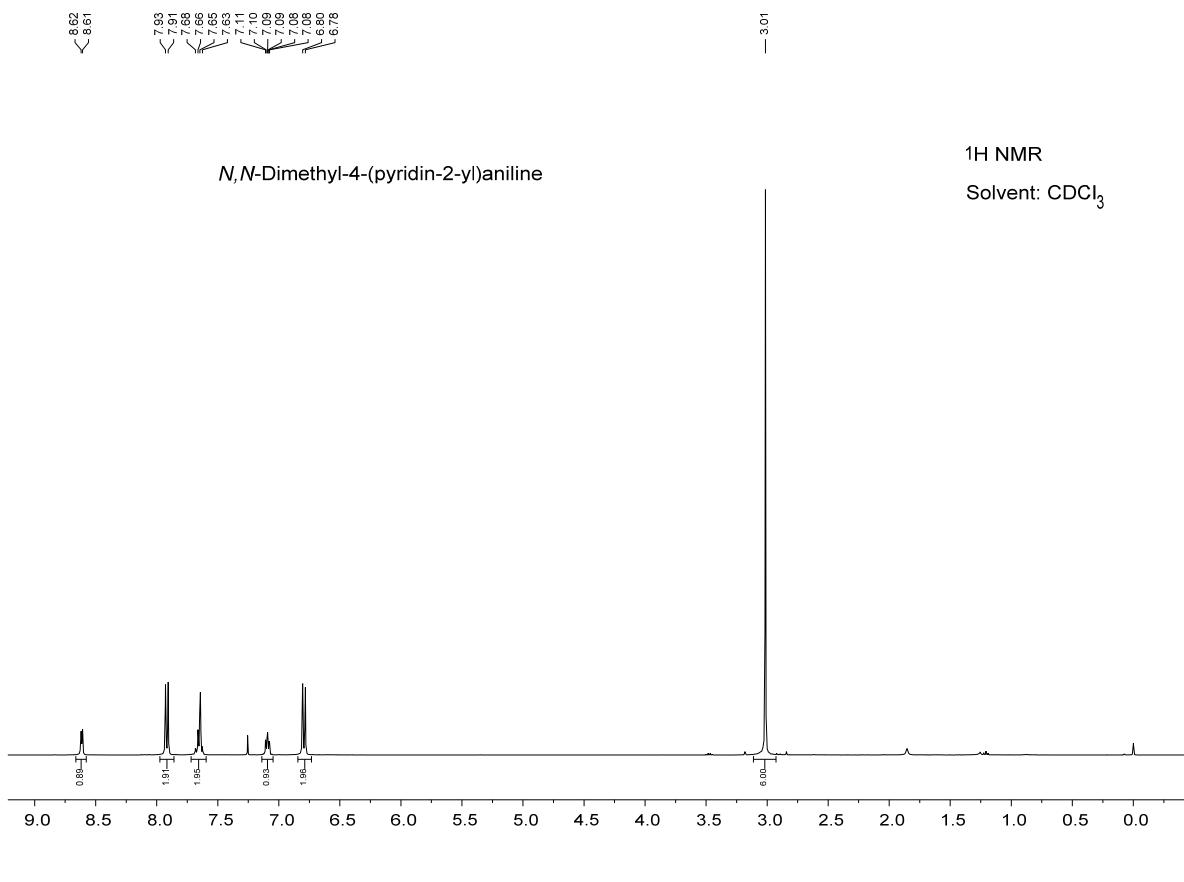
(15) 2-*p*-Tolylpyridine



(16) 2-(4-Methoxyphenyl)pyridine



(17) *N,N*-Dimethyl-4-(pyridin-2-yl)aniline



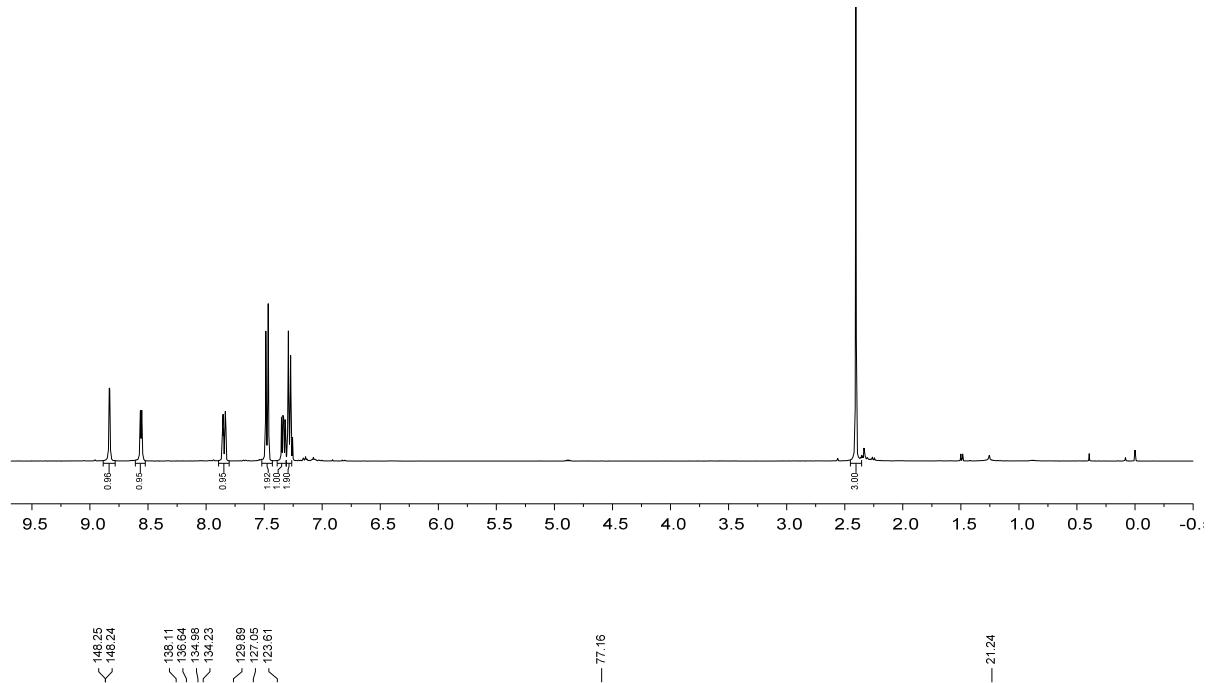
(18) 3-(*p*-Tolyl)pyridine



¹H NMR

3-(*p*-Tolyl)pyridine

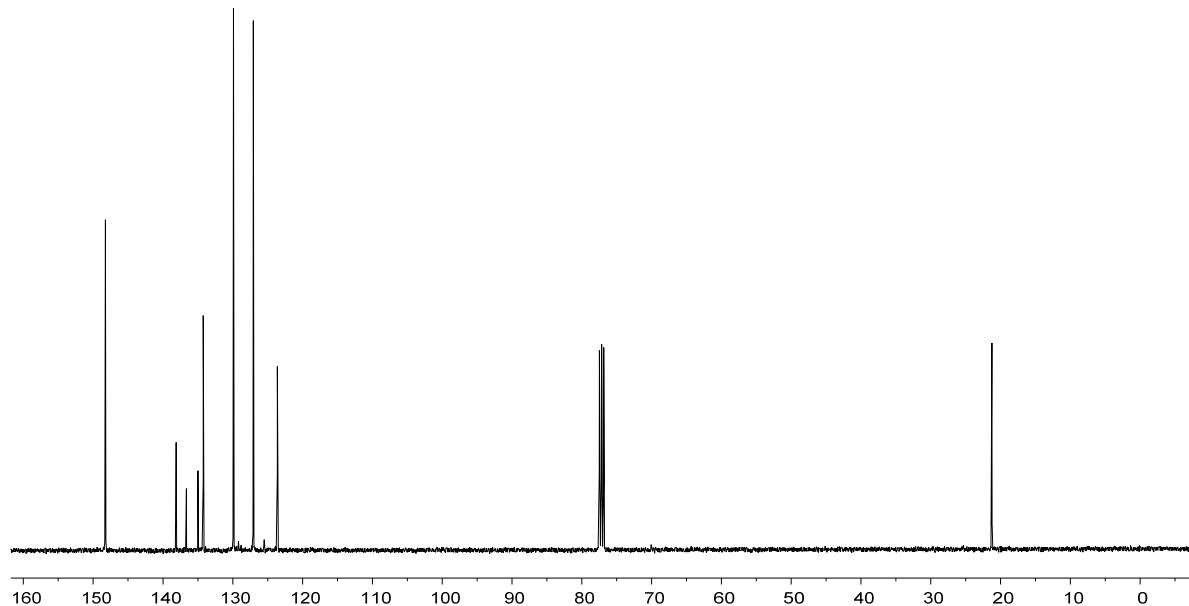
Solvent: CDCl₃



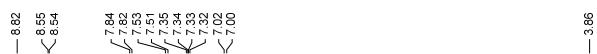
3-(*p*-Tolyl)pyridine

¹³C NMR

Solvent: CDCl₃



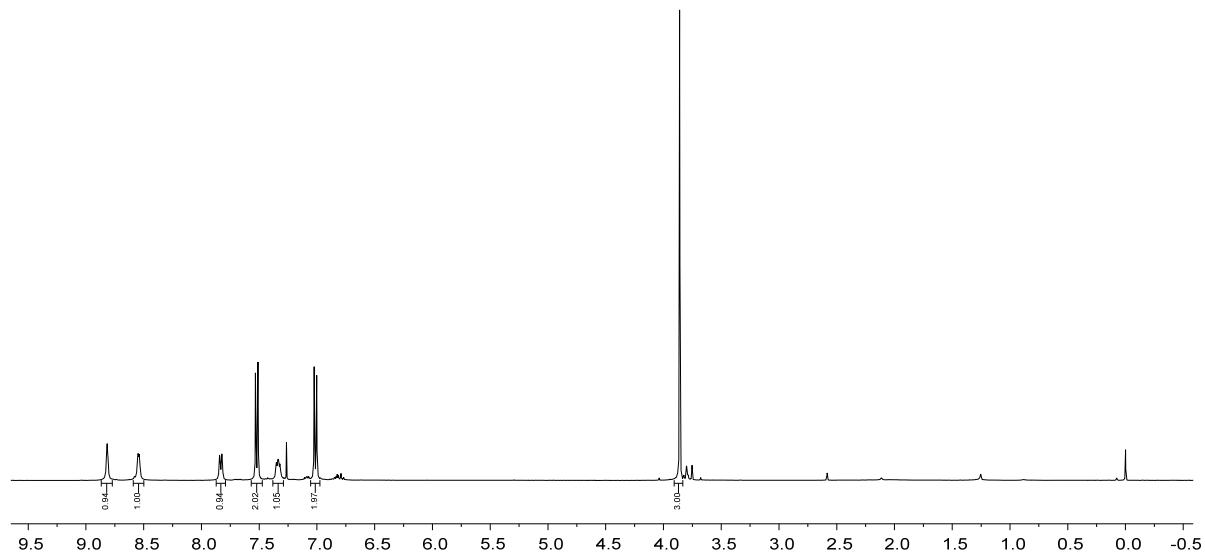
(19) 3-(4-Methoxyphenyl)pyridine



3-(4-Methoxyphenyl)pyridine

¹H NMR

Solvent: CDCl₃



— 159.85
— 147.98
— 147.66

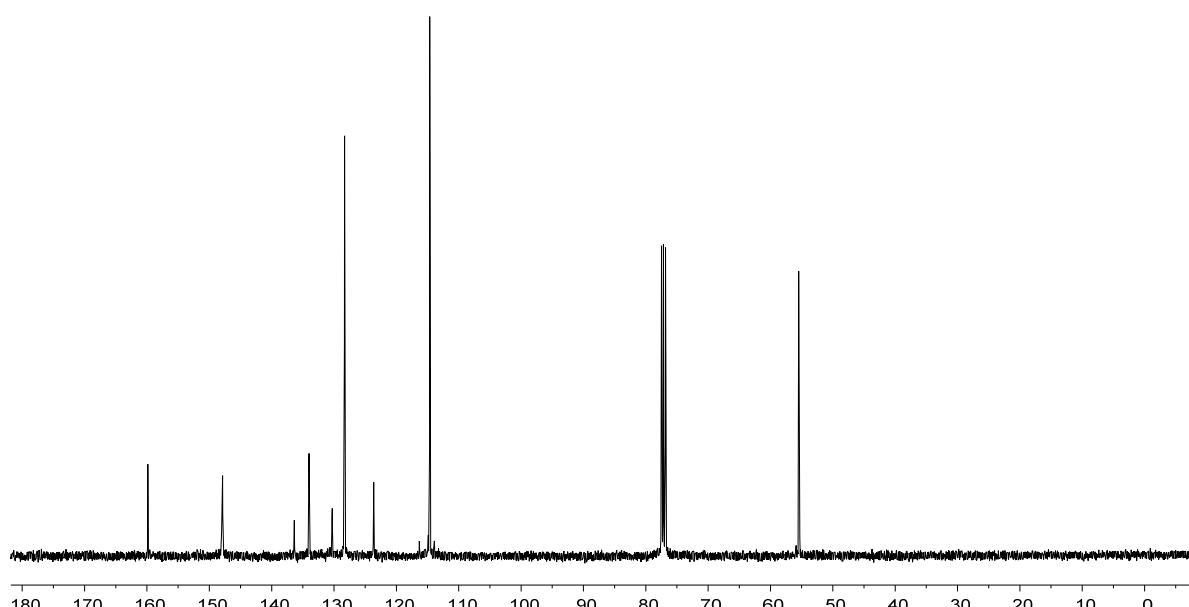
— 136.37
— 134.00
— 130.28
— 128.51
— 123.63

— 114.64

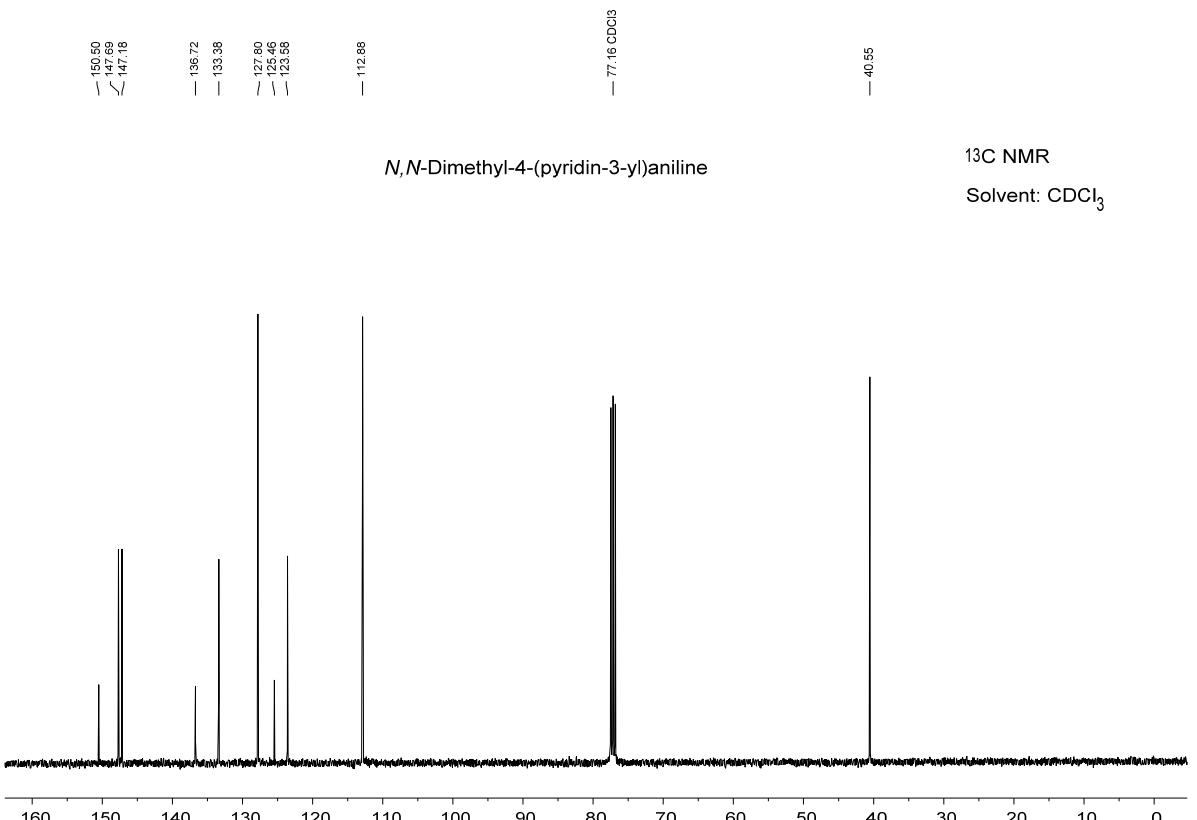
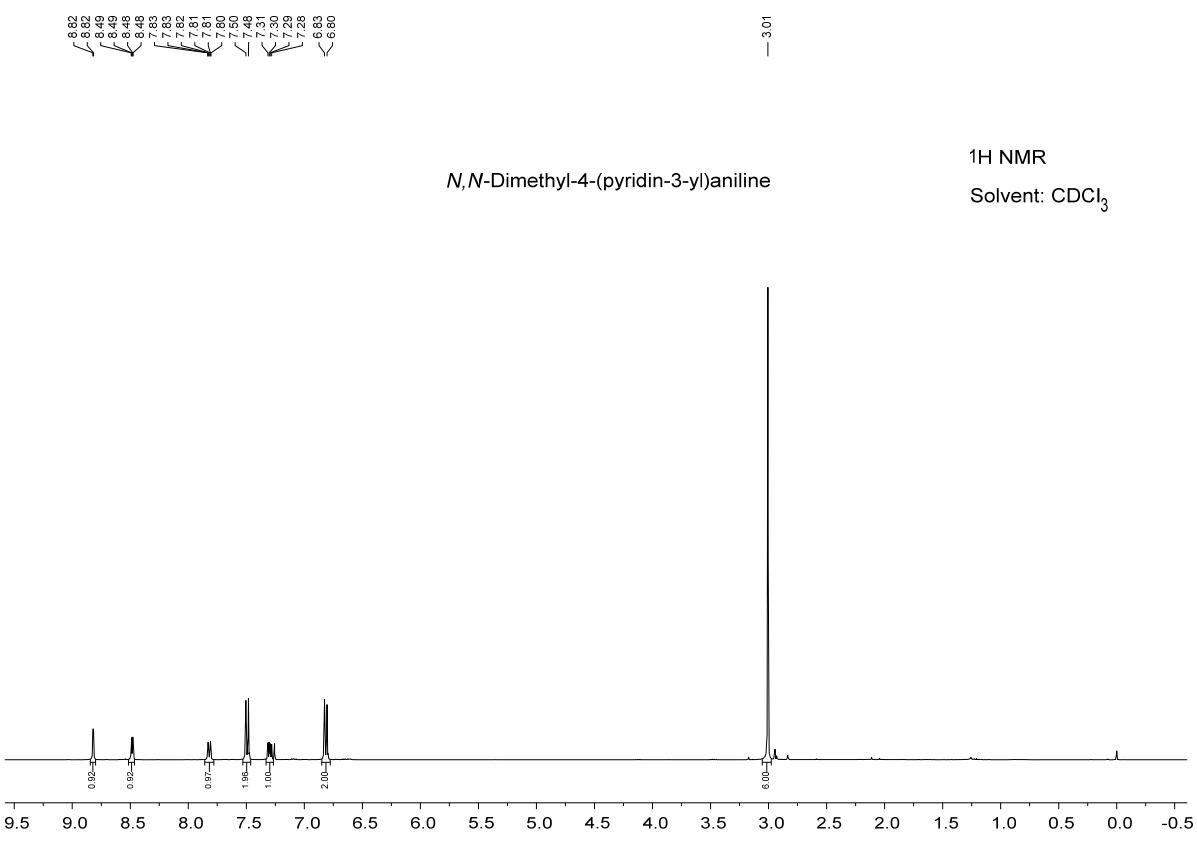
— 77.16 CDCl₃

¹³C NMR

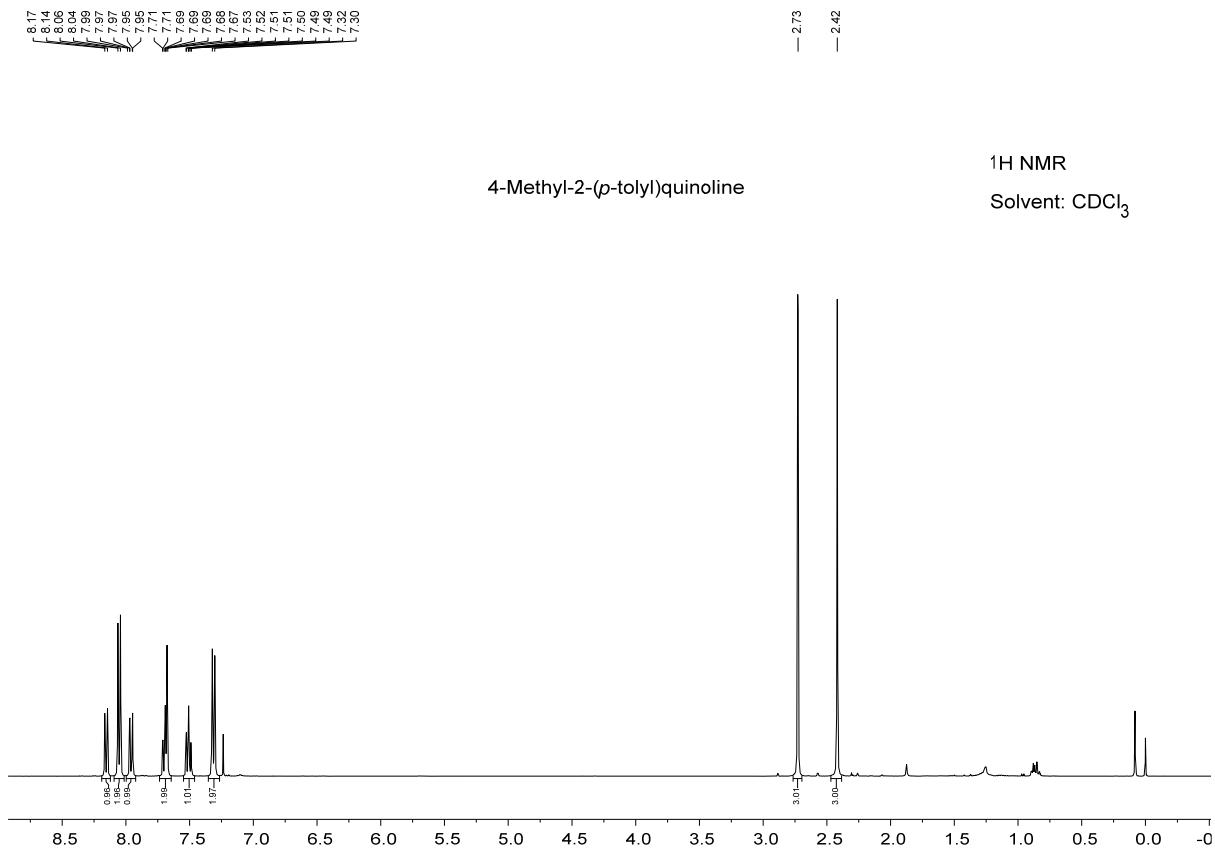
Solvent: CDCl₃



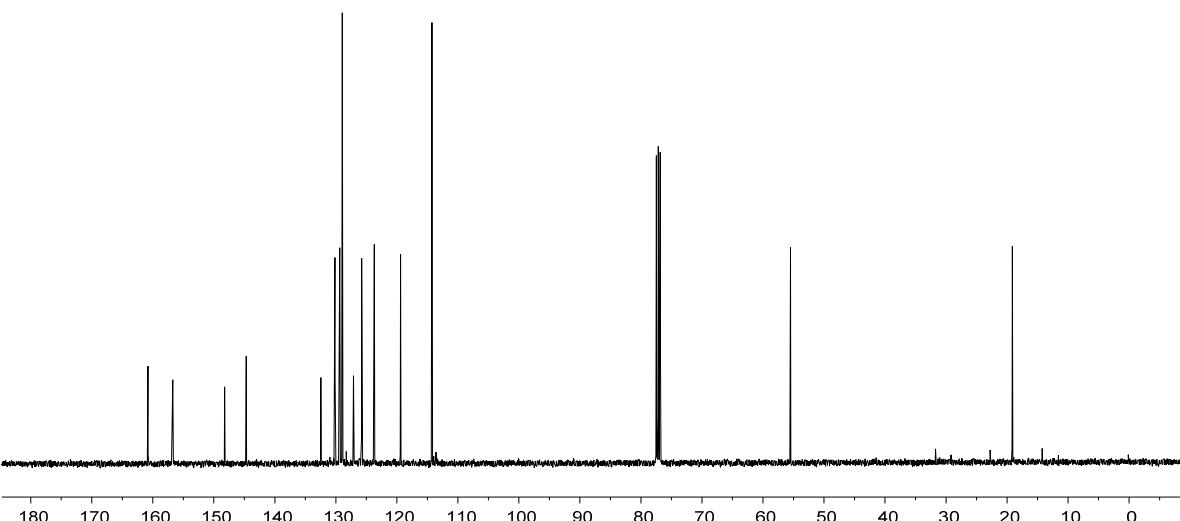
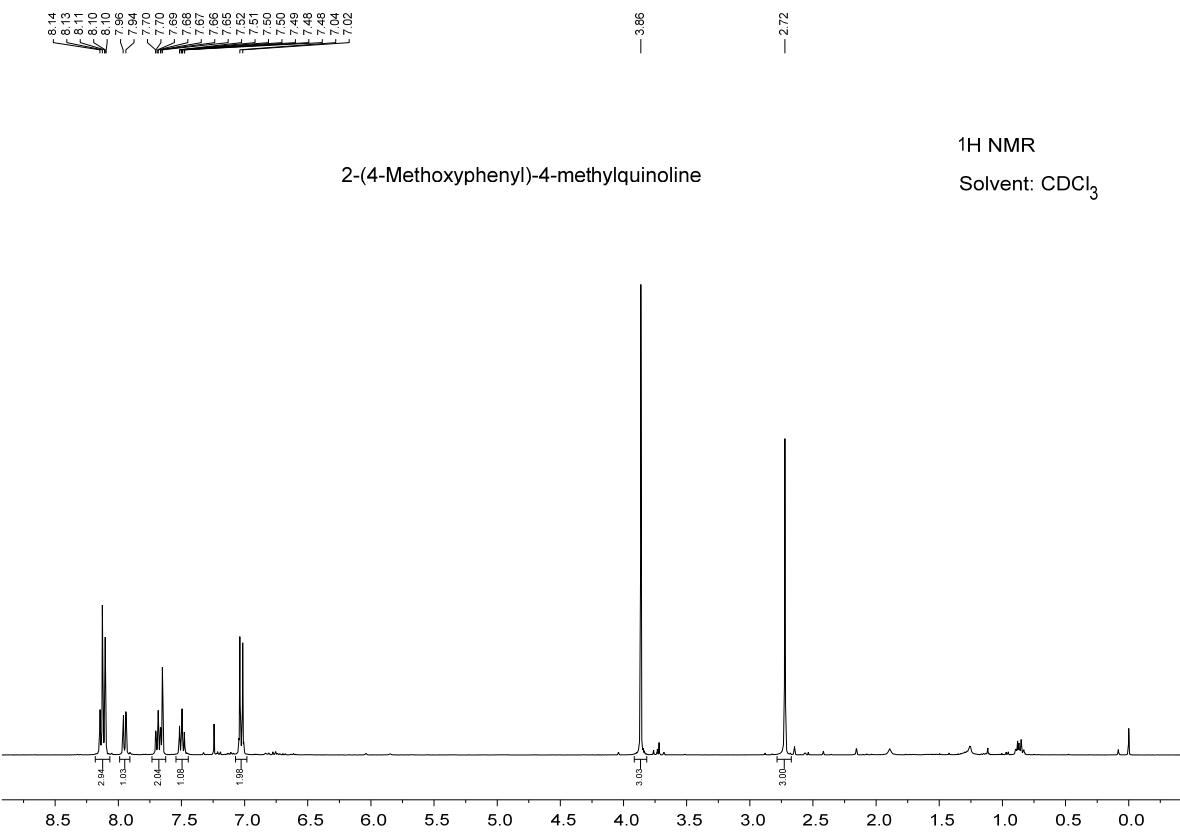
(20) *N,N*-Dimethyl-4-(pyridin-3-yl)aniline



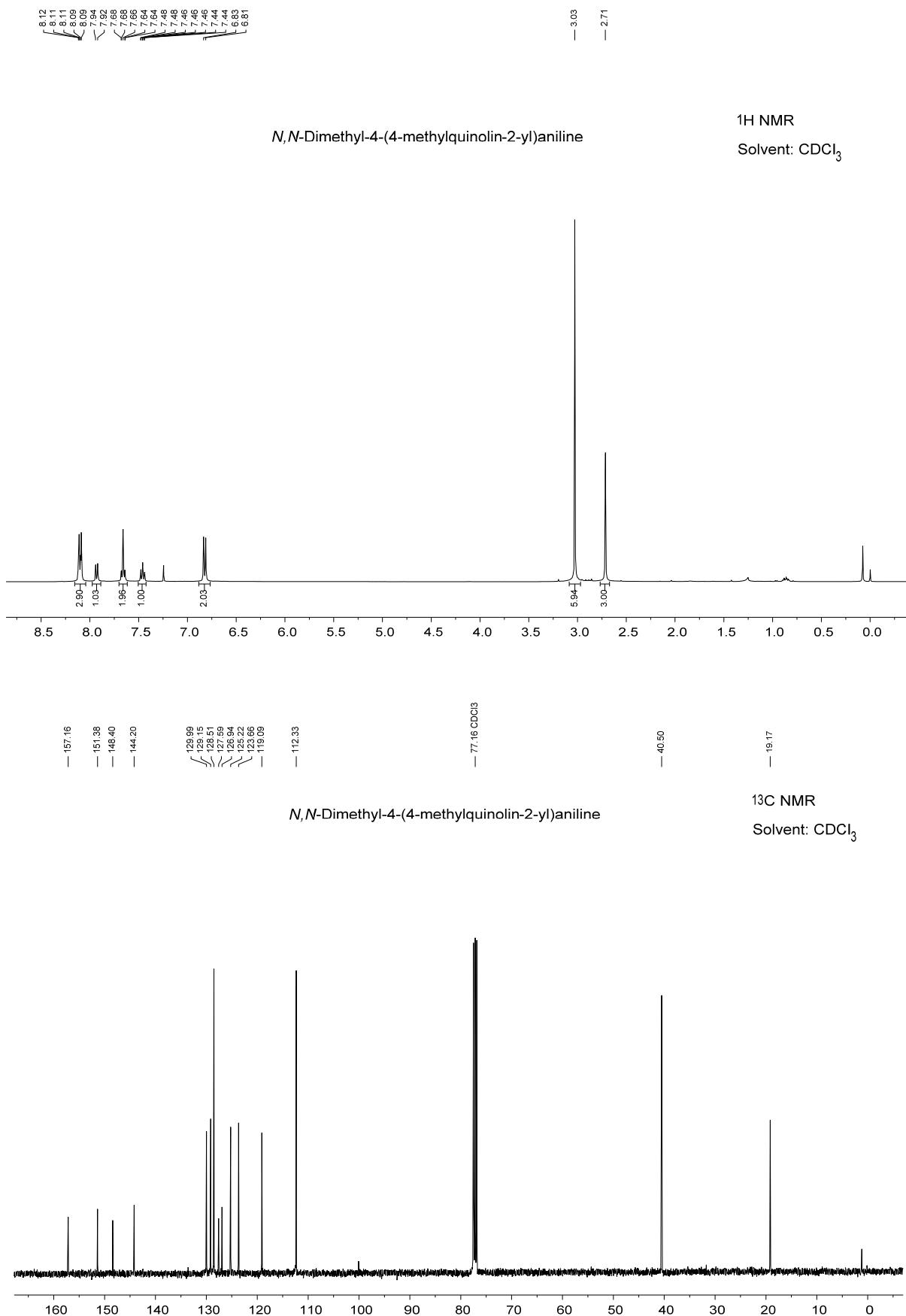
(21) 4-Methyl-2-(*p*-tolyl)quinoline



(22) 2-(4-Methoxyphenyl)-4-methylquinoline



(23) *N,N*-Dimethyl-4-(4-methylquinolin-2-yl)aniline



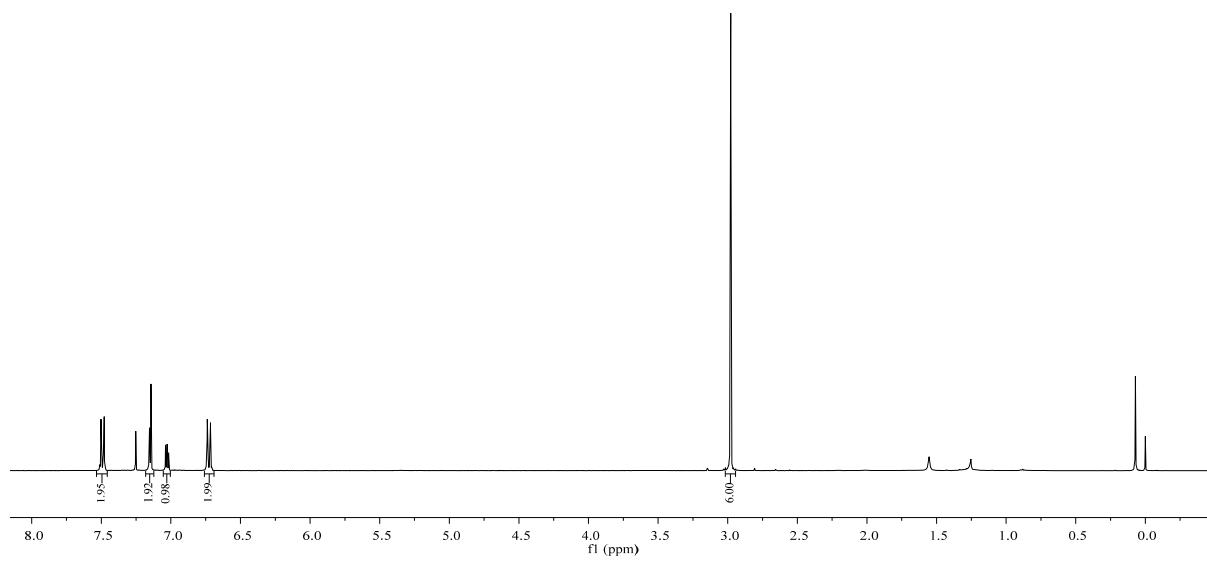
(24) *N,N*-dimethyl-4-(thiophen-2-yl)aniline

> 7.50
— 7.48
— 7.15
— 7.15
— 7.04
— 7.03
— 7.02
— 6.74
— 6.72

— 2.98

N,N-dimethyl-4-(thiophen-2-yl)aniline

¹H NMR (CDCl_3)

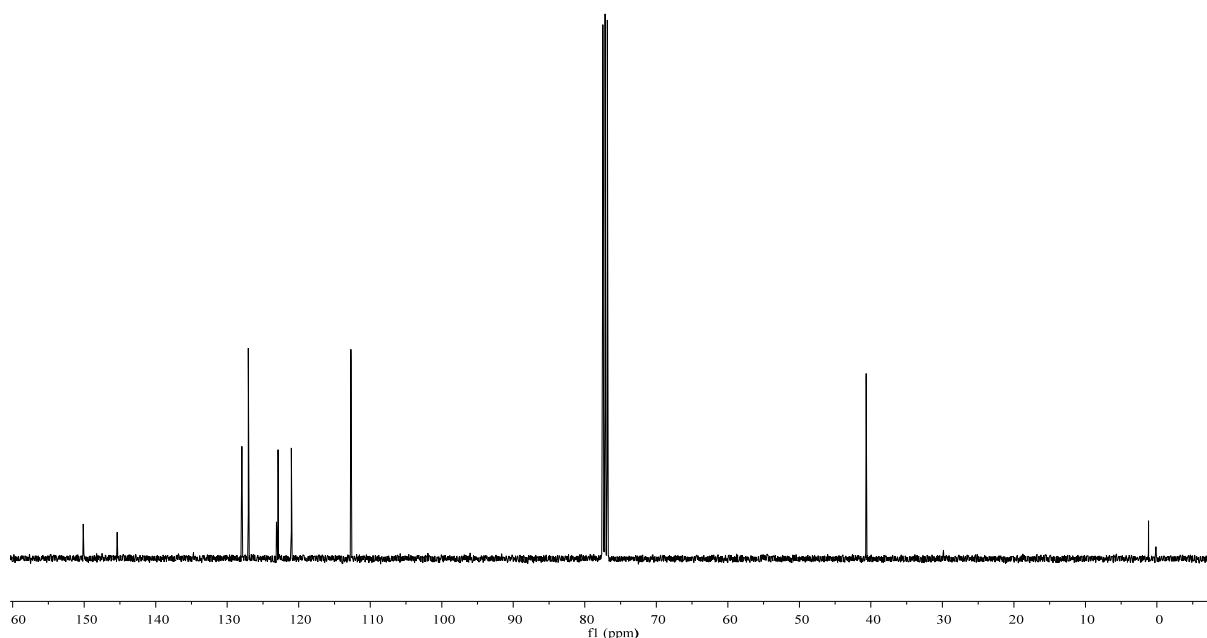


— 150.12
— 148.39
— 127.95
— 127.05
— 123.30
— 123.10
— 122.89
— 121.03
— 112.70

— 40.65

N,N-dimethyl-4-(thiophen-2-yl)aniline

¹³C NMR (CDCl_3)

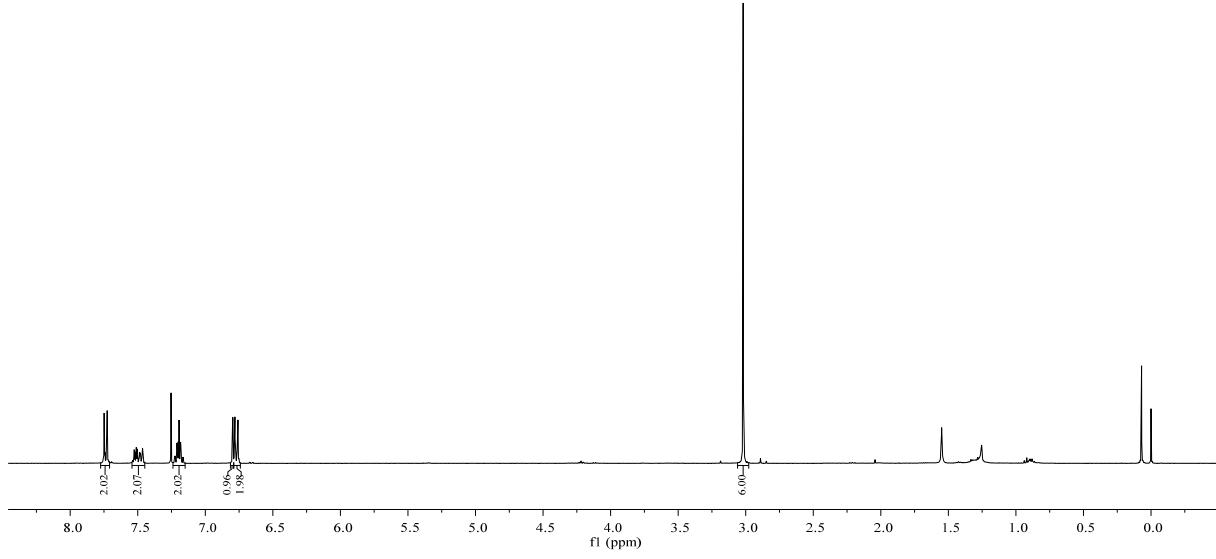


(25) 4-(benzofuran-2-yl)-*N,N*-dimethylaniline

7.75
7.73
7.53
7.53
7.52
7.51
7.51
7.50
7.49
7.49
7.48
7.48
7.47
7.46
7.46
7.46
7.46
7.46
7.46
7.46
7.46
7.46
7.45
7.41
7.30
7.29
7.29
7.22
7.22
7.22
7.19
7.19
7.18
7.18
7.16
7.16
6.80
6.78
6.76

4-(benzofuran-2-yl)*N,N*-dimethylaniline

^1H NMR (CDCl_3)



157.17
154.67
150.71

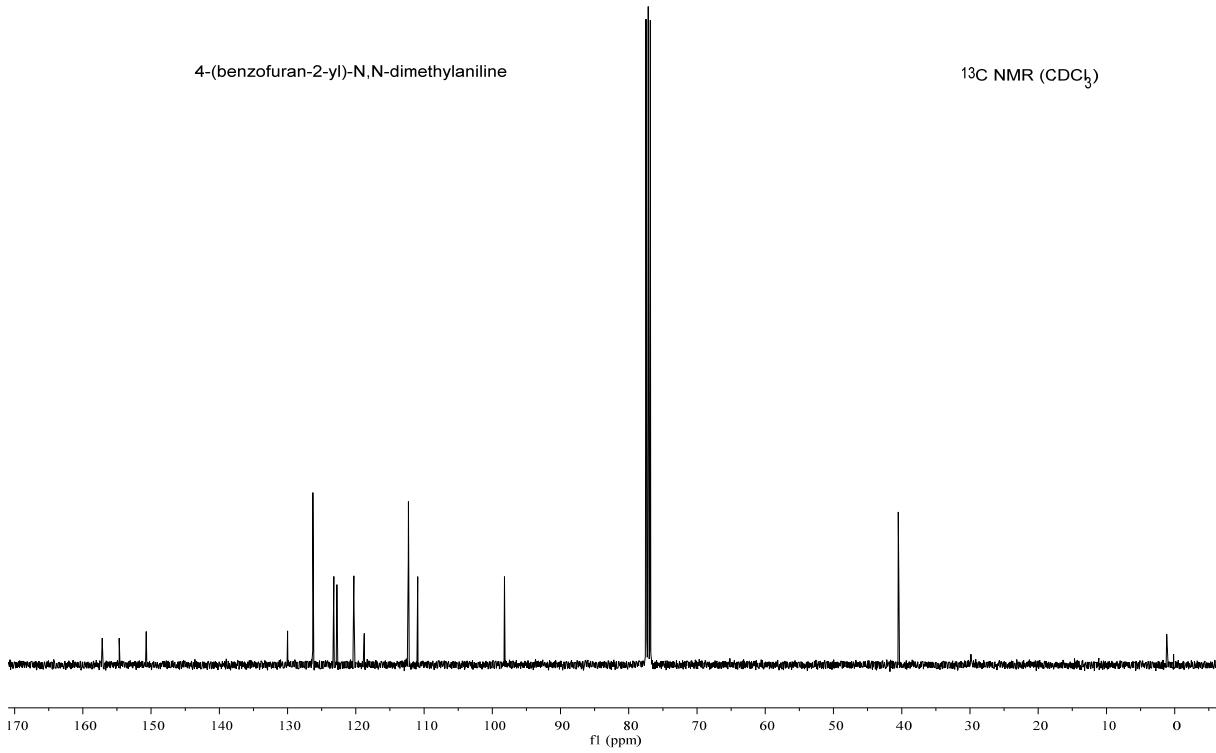
129.99
129.29
129.29
122.77
122.77
120.29
120.29
118.77
118.77

12.30
110.92

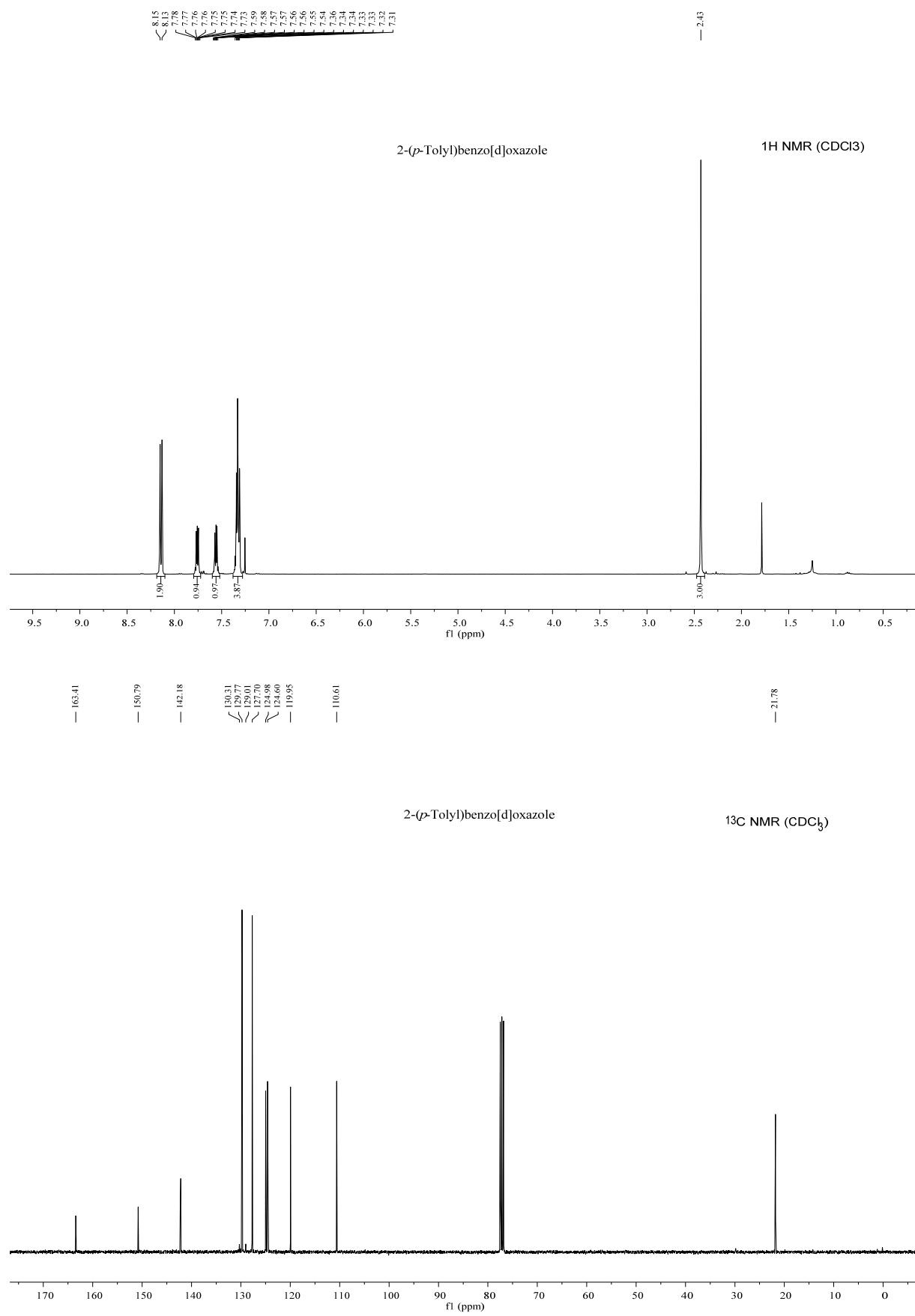
40.50

4-(benzofuran-2-yl)-*N,N*-dimethylaniline

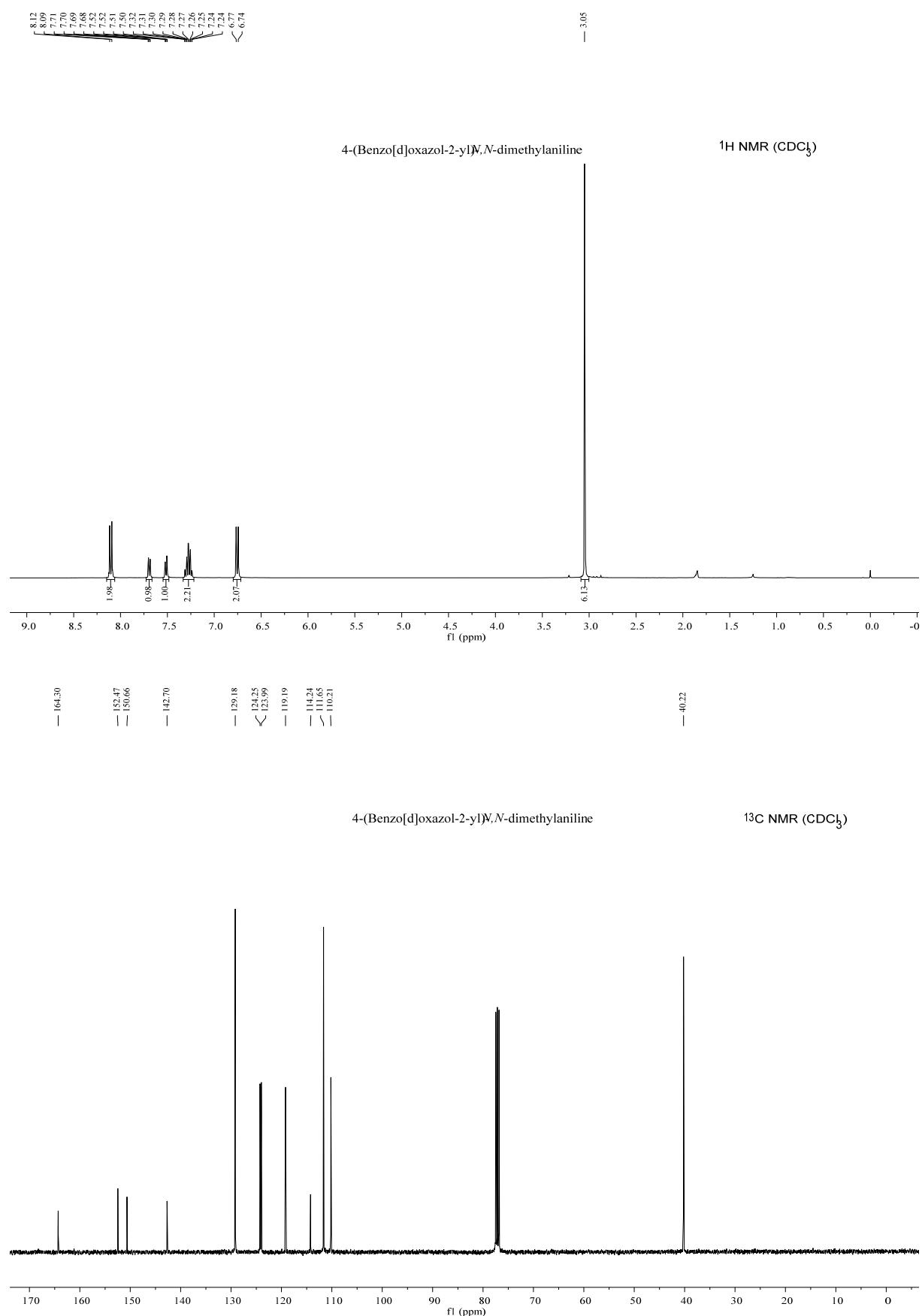
^{13}C NMR (CDCl_3)



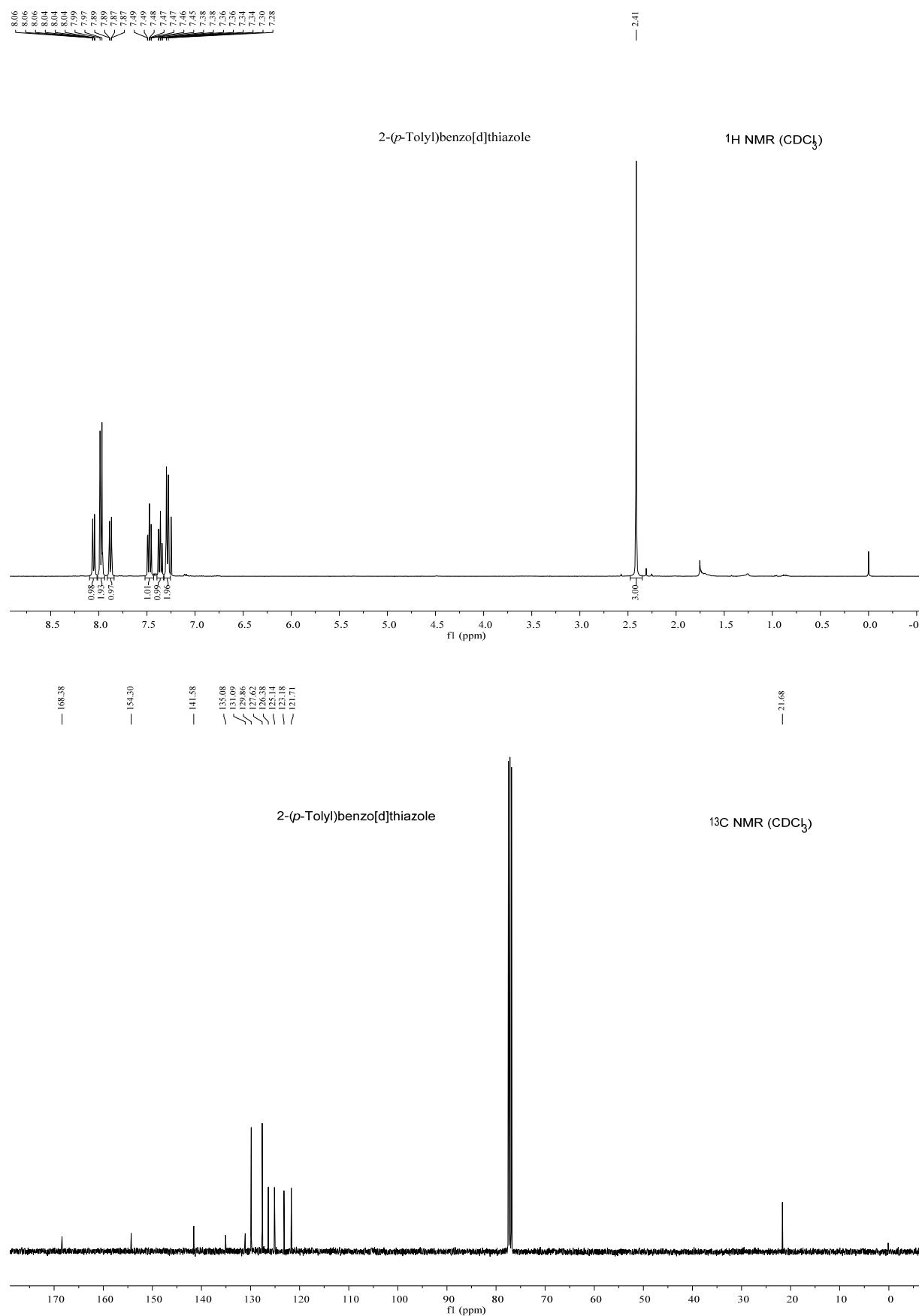
(26) 2-(*p*-Tolyl)benzo[*d*]oxazole



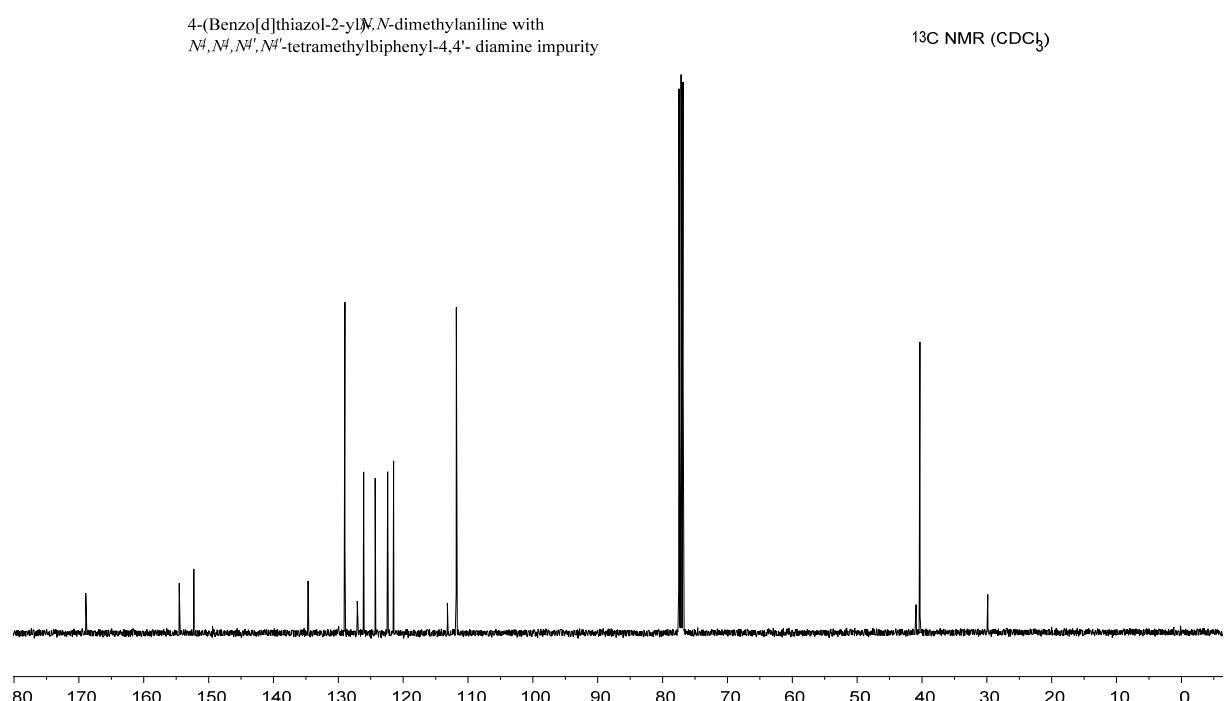
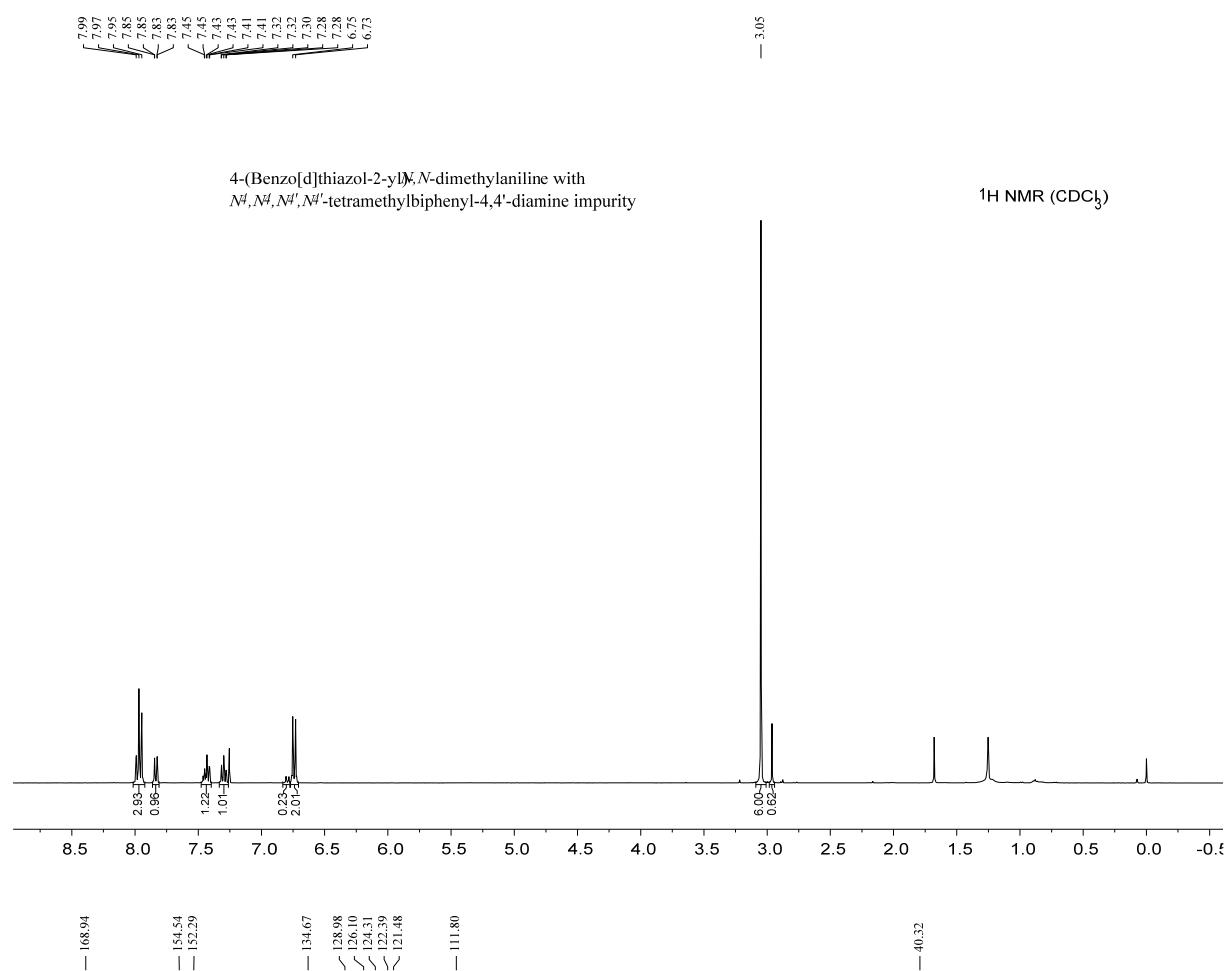
(27) 4-(Benzo[*d*]oxazol-2-yl)-*N,N*-dimethylaniline



(28) 2-(*p*-tolyl)benzo[*d*]thiazole



(29) 4-(Benzo[*d*]thiazol-2-yl)-*N,N*-dimethylaniline with *N⁴,N⁴',N⁴',N⁴'-tetramethylbiphenyl-4,4'-diamine impurity*

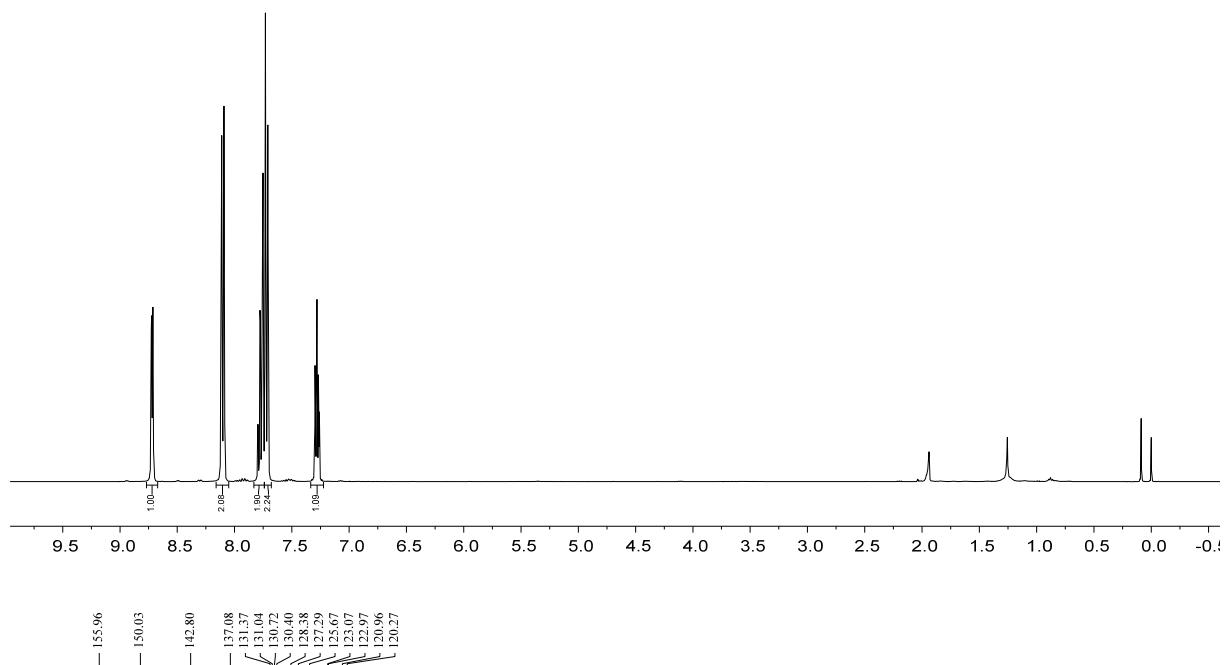


(30) 2-(4-(trifluoromethyl)phenyl)pyridine



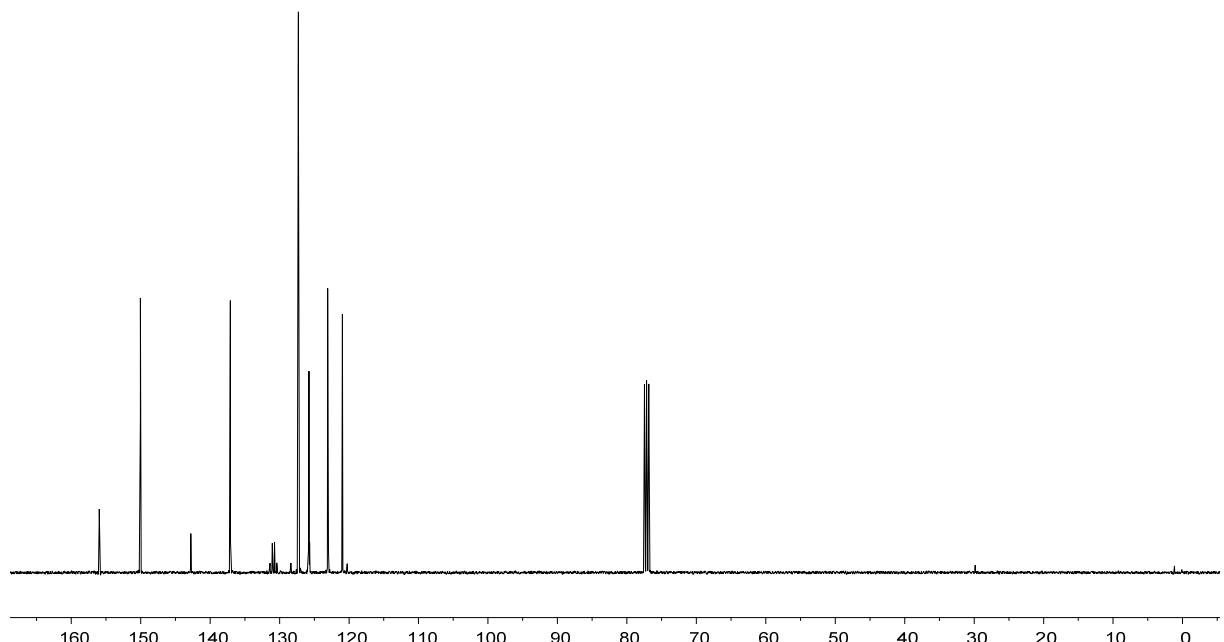
2-(4-(trifluoromethyl)phenyl)pyridine

¹H NMR (CDCl_3)



2-(4-(trifluoromethyl)phenyl)pyridine

¹³C NMR (CDCl_3)

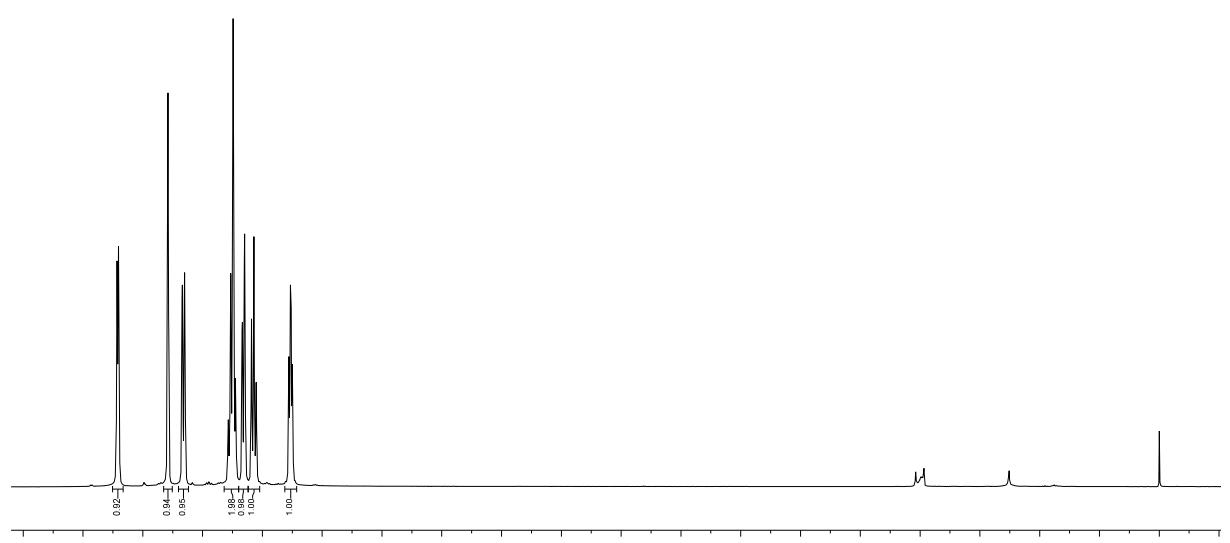


(31) 2-(3-(Trifluoromethyl)phenyl)pyridine



2-(3-(trifluoromethyl)phenyl)pyridine

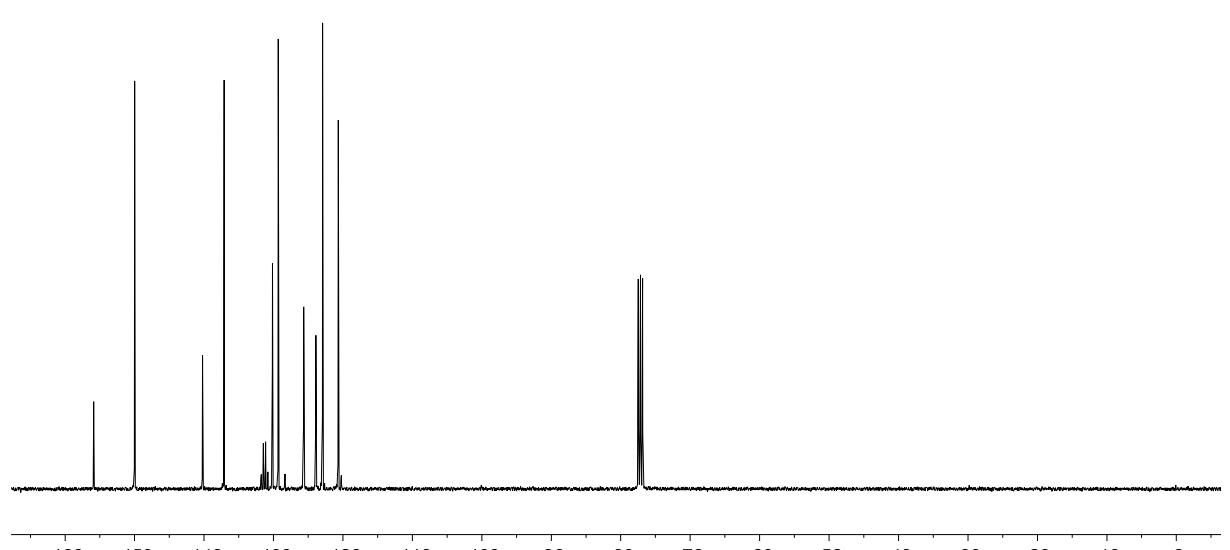
^1H NMR (CDCl_3)



— 155.89
— 149.98
— 140.22
— 137.09
— 131.77
— 131.45
— 131.12
— 130.80
— 130.52
— 129.52
— 128.35
— 125.68
— 125.64
— 125.60
— 125.57
— 123.94
— 123.90
— 123.86
— 123.83
— 122.93
— 120.68
— 120.25

2-(3-(trifluoromethyl)phenyl)pyridine

^{13}C NMR (CDCl_3)

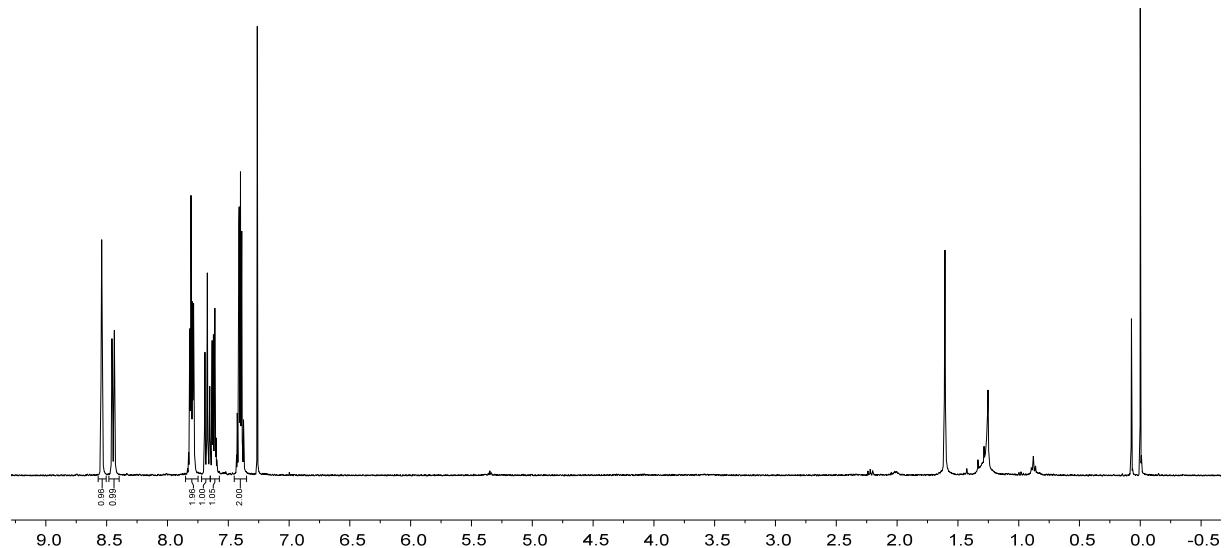


(32) 2-(3-(Trifluoromethyl)phenyl)benzo[d]oxazole



2-(3-(Trifluoromethyl)phenyl)benzo[d]oxazole

¹H NMR (CDCl₃)



2-(3-(trifluoromethyl)phenyl)benzo[d]oxazole

¹³C NMR (CDCl₃)

