

Electronic Supplementary Information

Small Organic Molecules with Tailored Structures: Initiators in Transition-Metal-Free C–H Arylation of Unactivated Arenes

Zhenghui Liu^{a,*}, Peng Wang^{b,c}, Yu Chen^d, Zhenzhong Yan^a, Suqing Chen^a,
Wenjun Chen^e, Tiancheng Mu^{e,*}

^a School of Pharmaceutical and Materials Engineering, Taizhou University, Taizhou
318000, Zhejiang, China

^b Beijing National Laboratory for Molecular Sciences, CAS Research/Education Center
for Excellence in Molecular Sciences, Institute of Chemistry, Chinese Academy of
Sciences, Beijing 100190, China

^c Key Laboratory of Green Chemical Media and Reactions, Ministry of Education,
School of Chemistry and Chemical Engineering, Henan Normal University, Xinxiang
453007, Henan, China

^d Department of Chemistry and Material Science, Langfang Normal University,
Langfang 065000, Hebei, China

^e Department of Chemistry, Renmin University of China, Beijing 100872, China

* Corresponding author.

Table of Contents

1.	Result of kinetic isotope experiment	S3
2.	FT-IR spectra of pure SOM and SOM with tBuOK	S4
3.	Information for GC analysis	S5
4.	NMR spectra of products	S6-S39

1. Result of kinetic isotope experiment

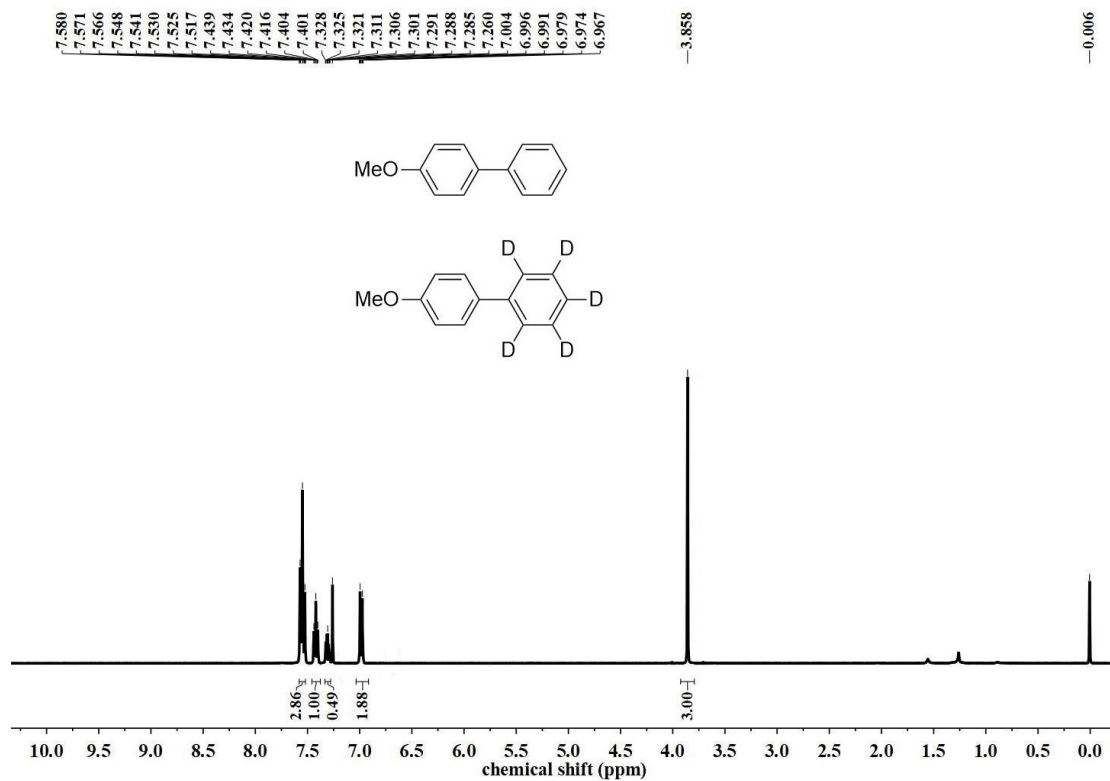


Figure S1 NMR spectrum of kinetic isotope experiment

2. FT-IR spectra of pure SOM and SOM with tBuOK

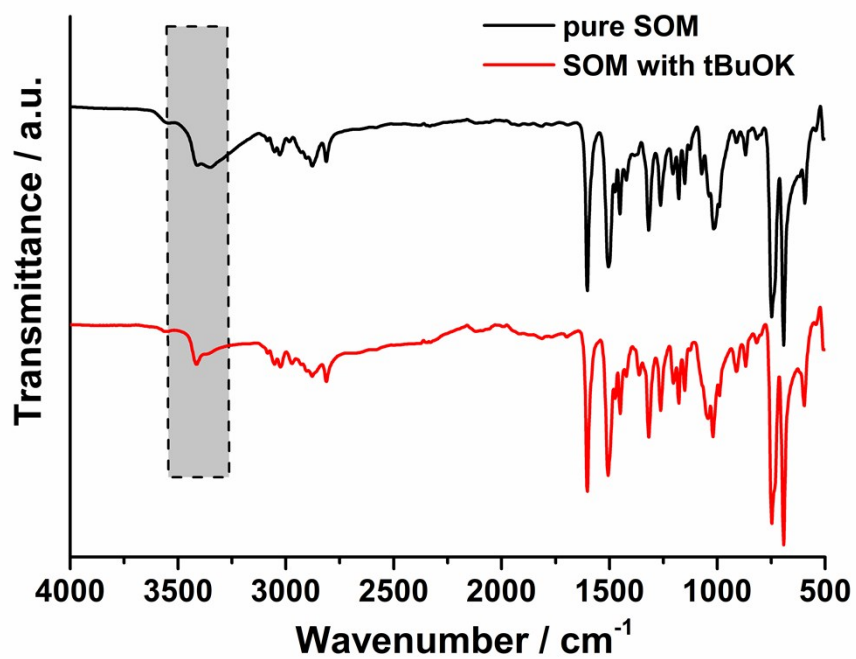


Figure S2 FT-IR spectra of pure SOM and SOM with tBuOK

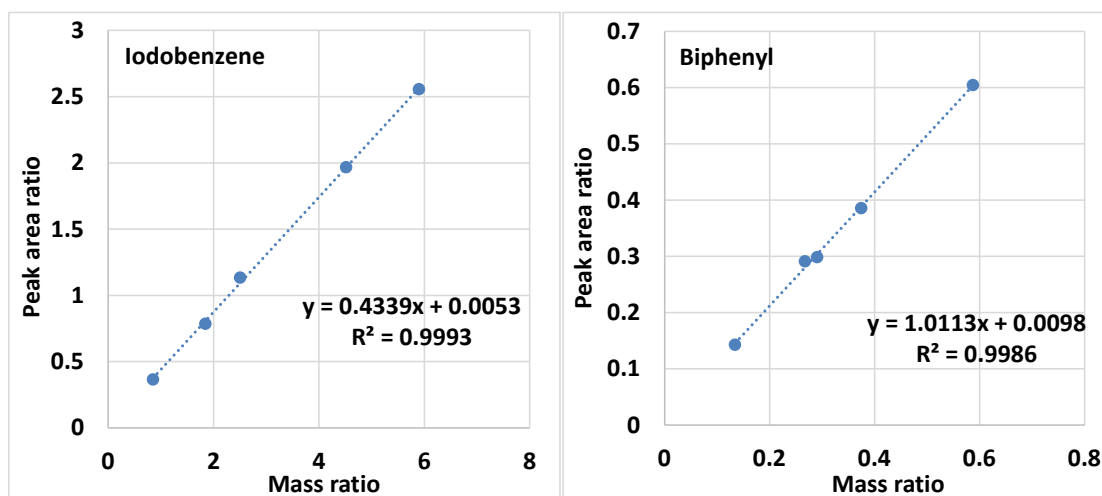
3. Information for GC analysis

The yields of the product biphenyl of each reaction were determined by GC using dodecane as the internal standard and calculated through the calibration curves as shown below.

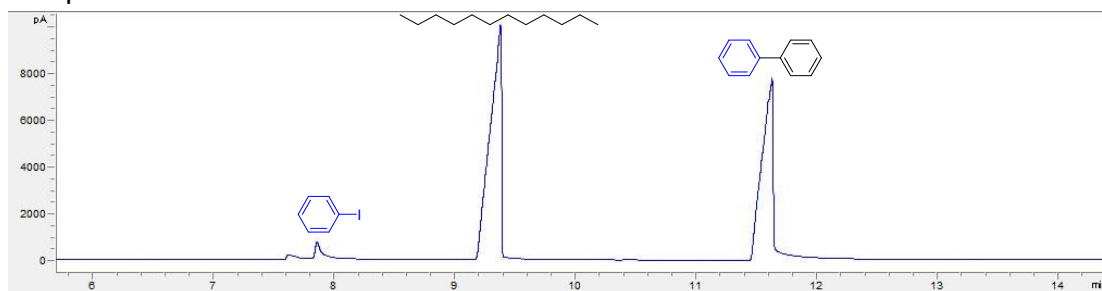
Calibration Curve

Standard Solution	iodobenzene/g	dodecane/g
1	0.0624	0.0488
2	0.1289	0.0502
3	0.2231	0.0491
4	0.3471	0.0509
5	0.4696	0.0502

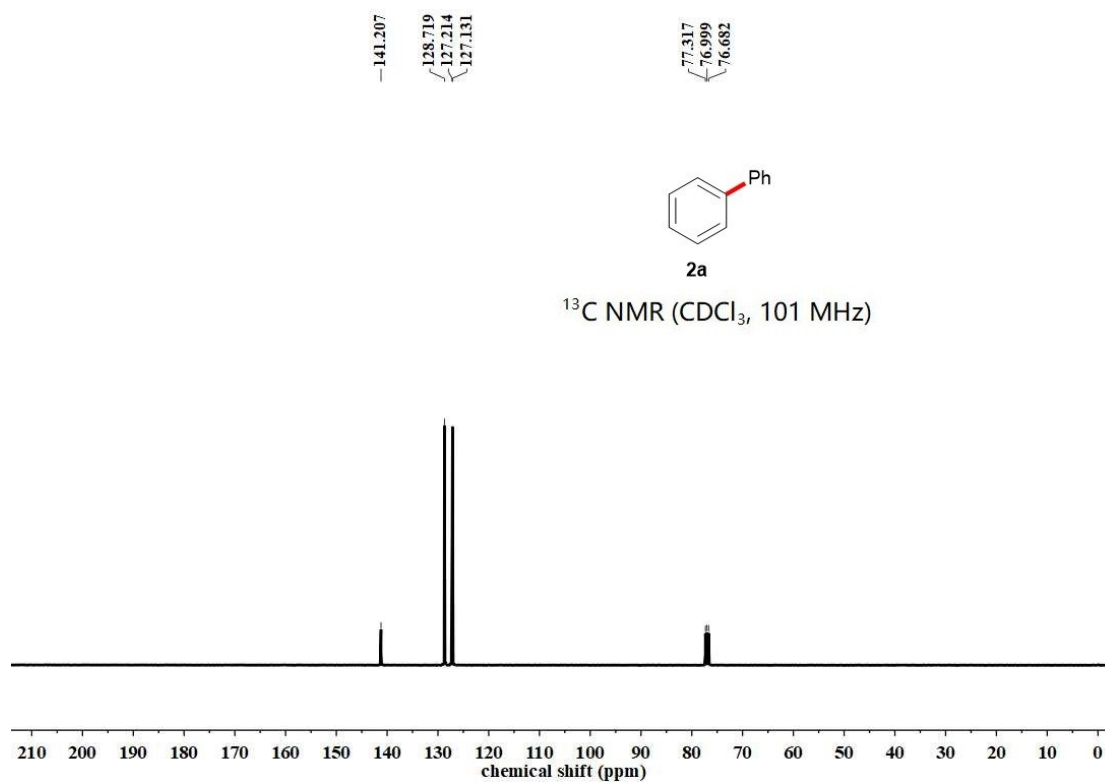
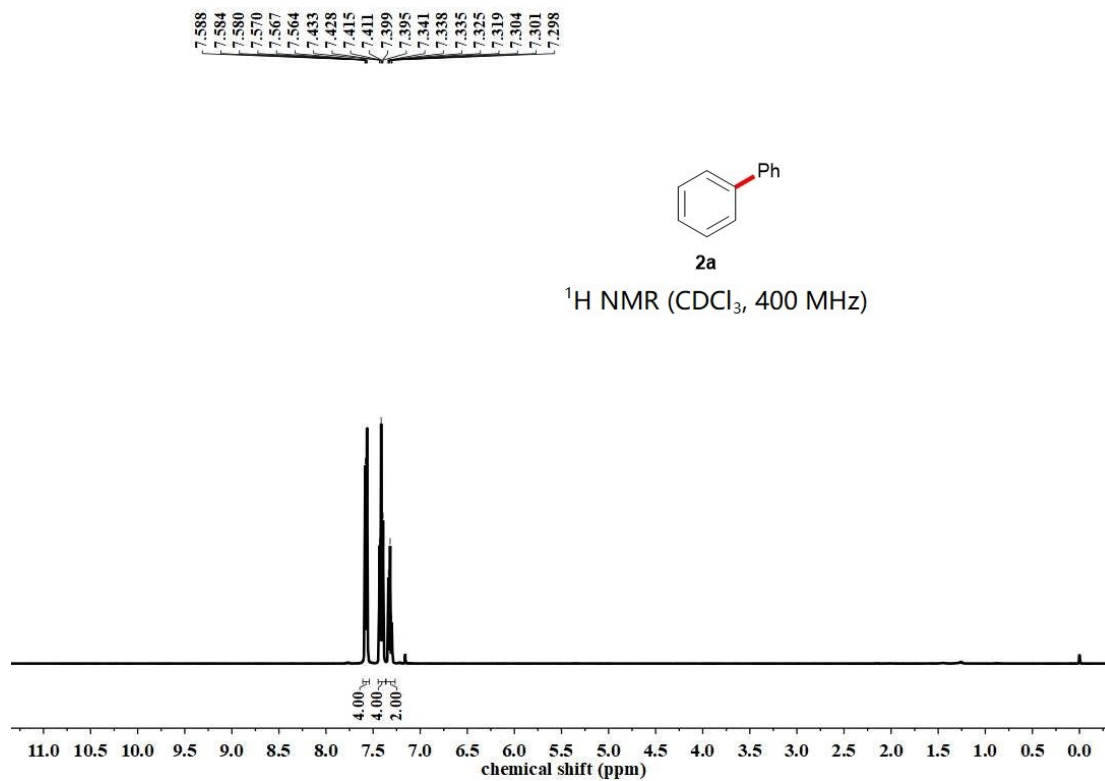
Standard Solution	biphenyl/g	dodecane/g
1	0.0100	0.0745
2	0.0213	0.0796
3	0.0266	0.0710
4	0.0313	0.1077
5	0.0466	0.0793

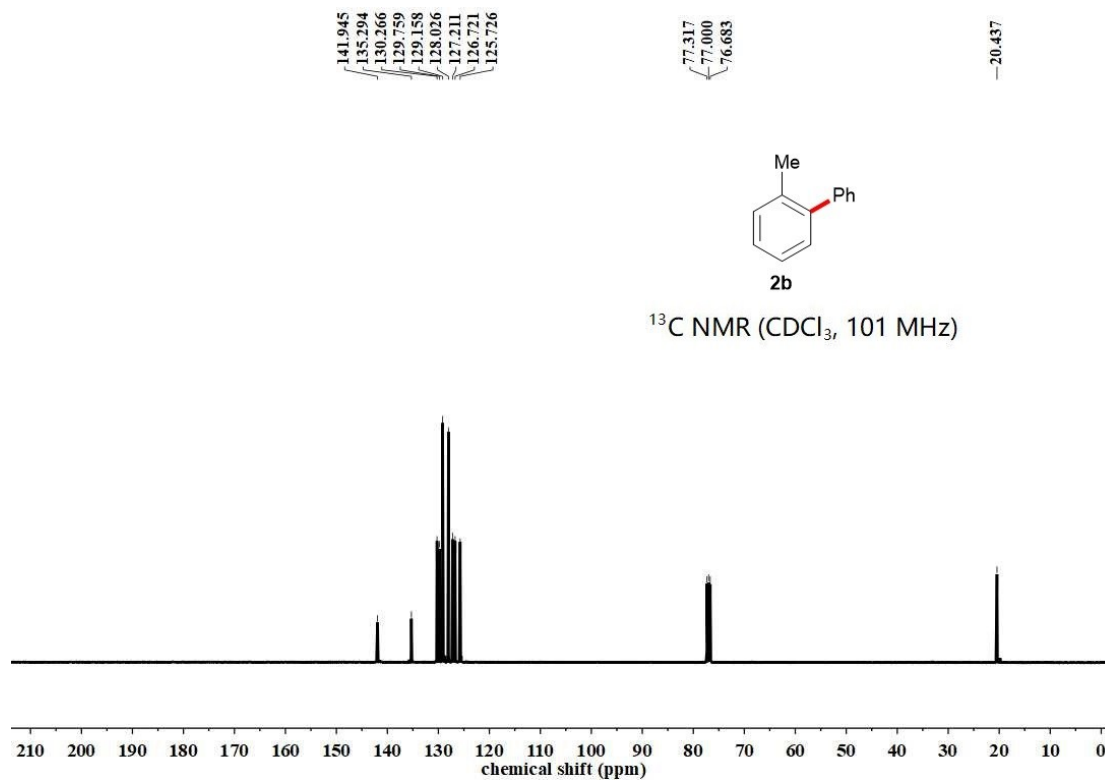
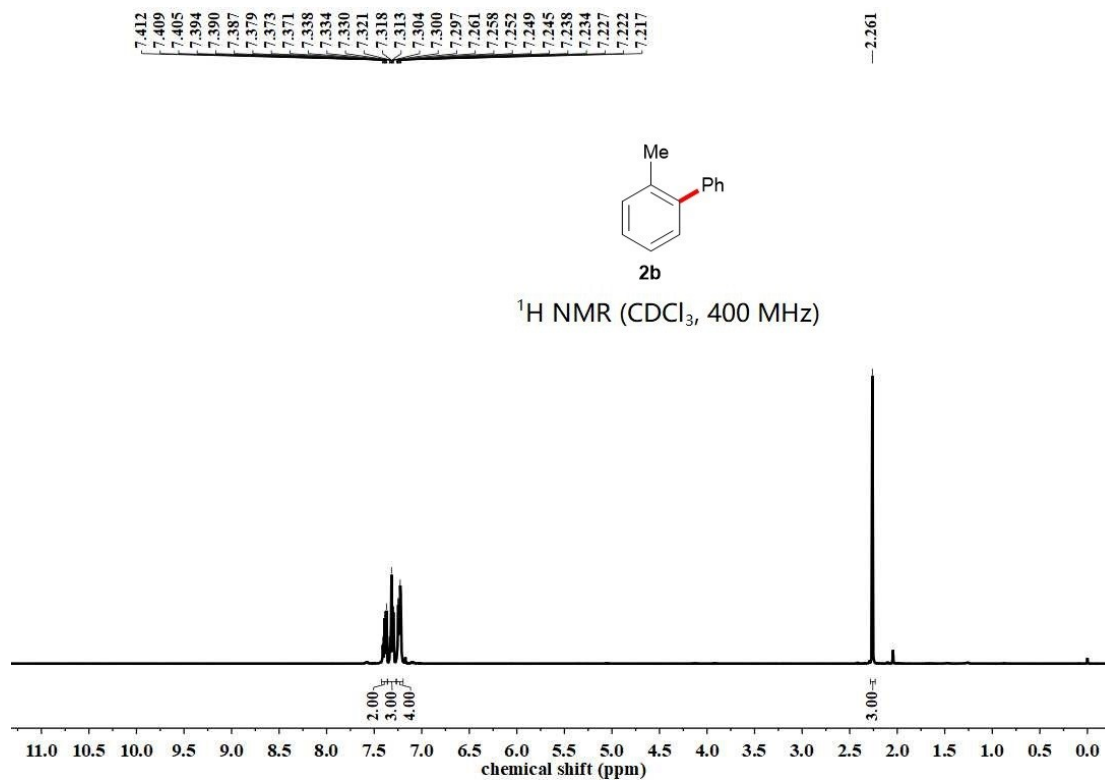


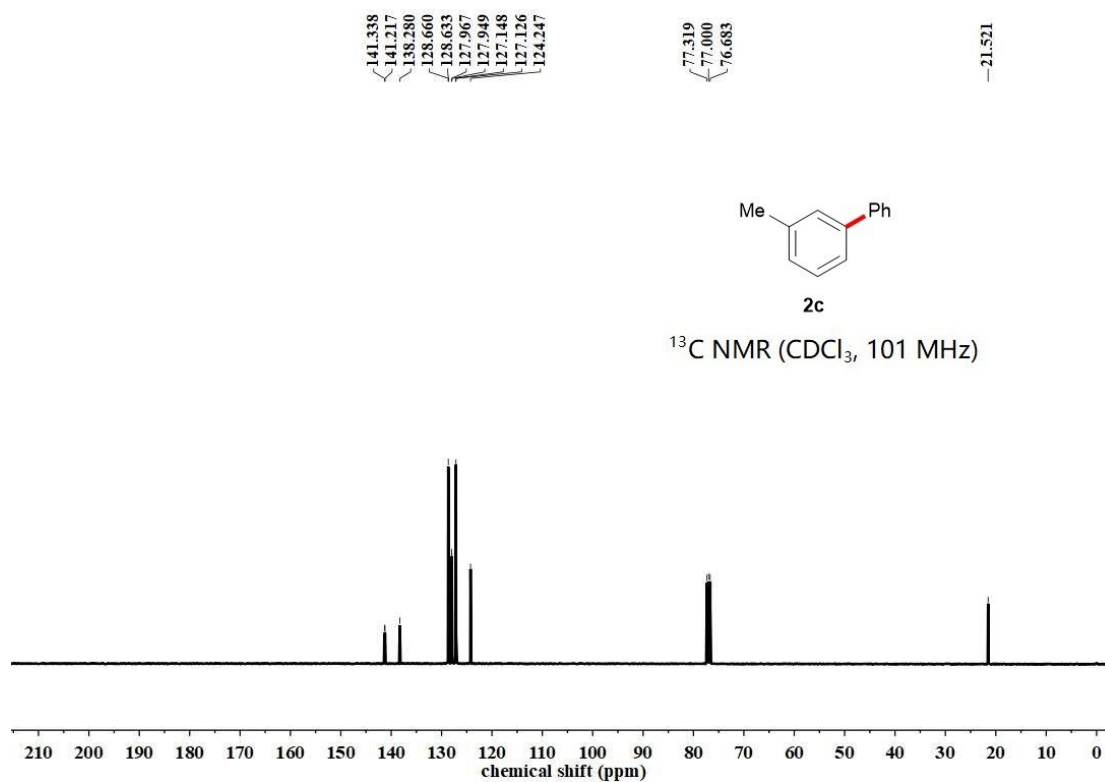
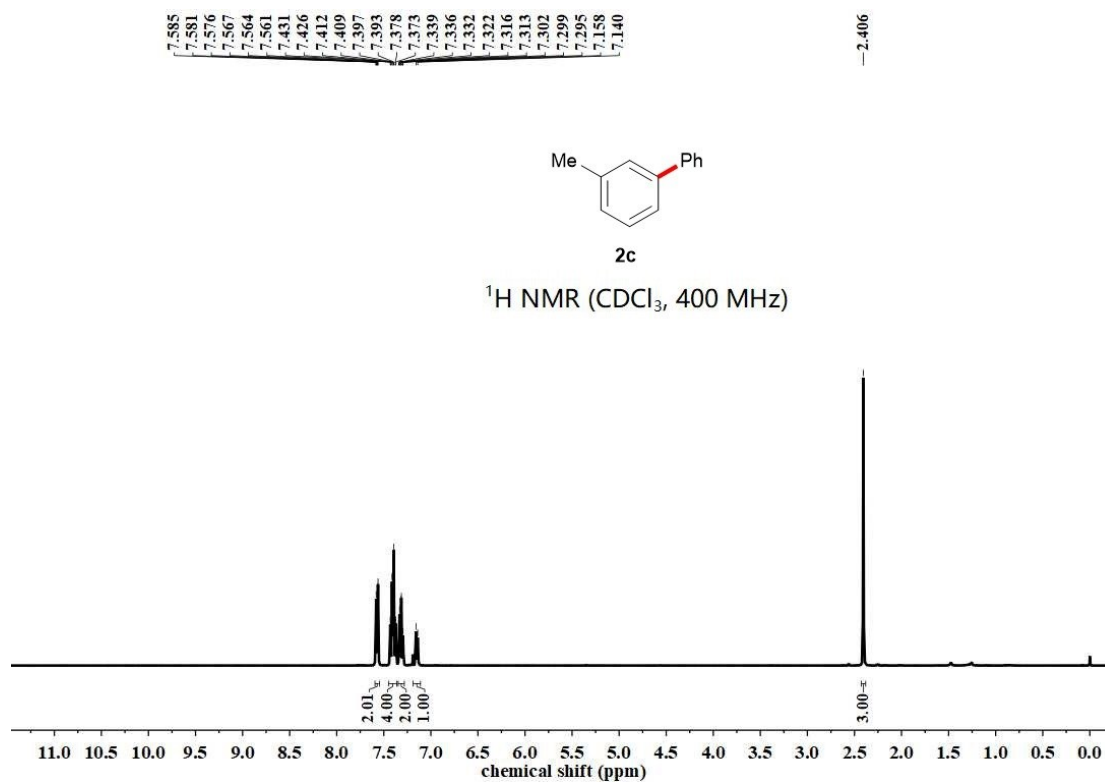
GC spectra

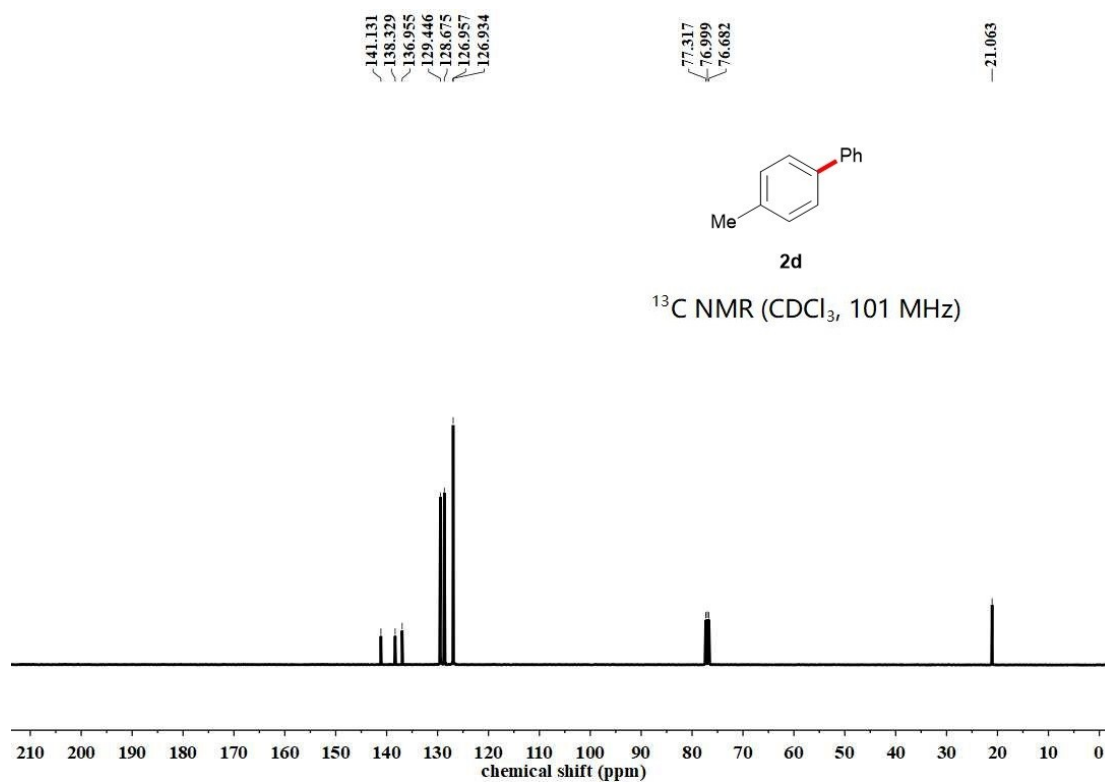
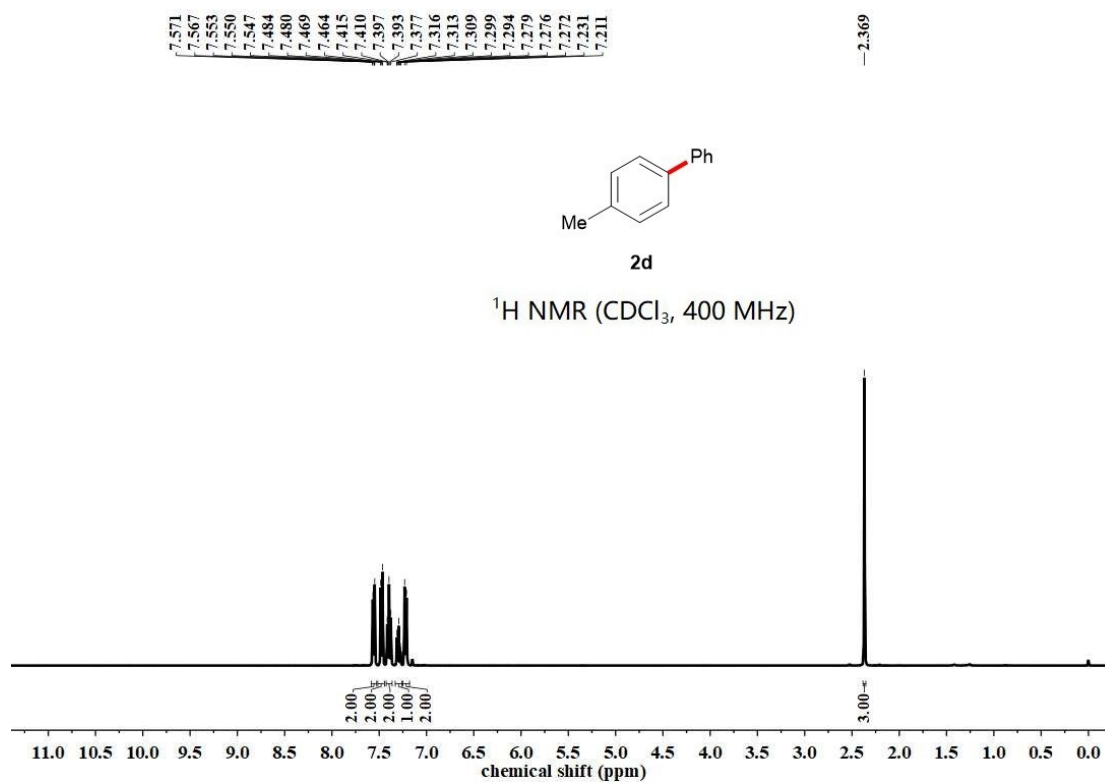


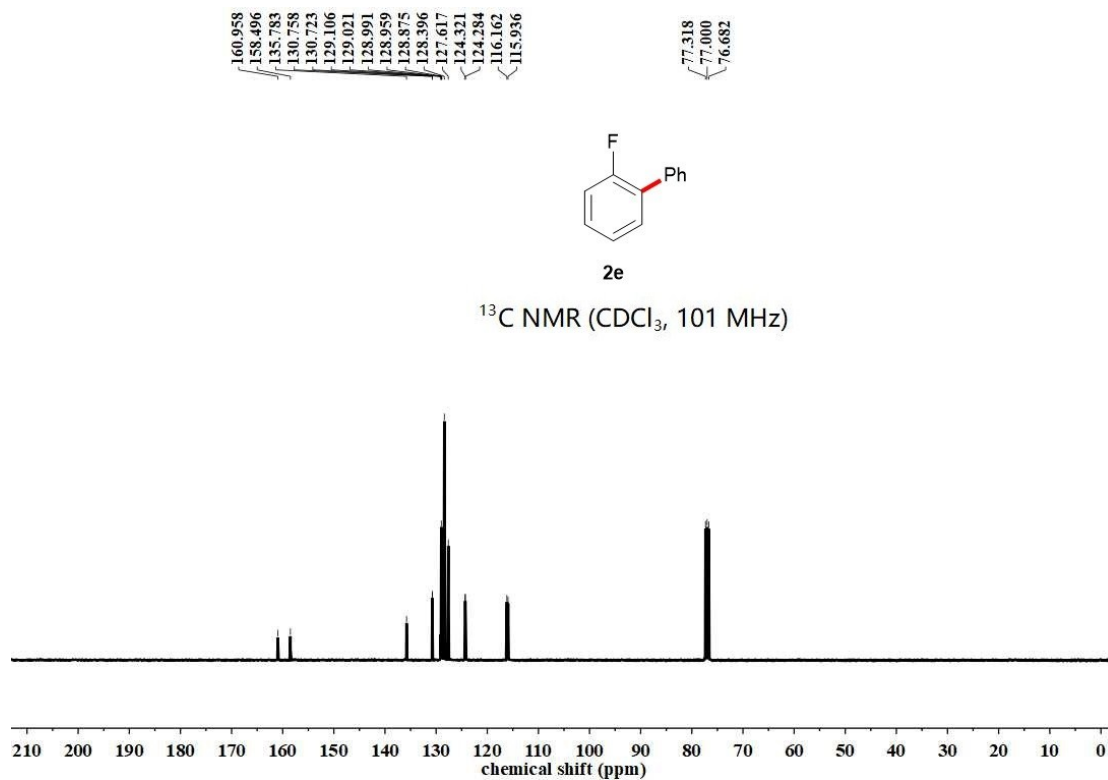
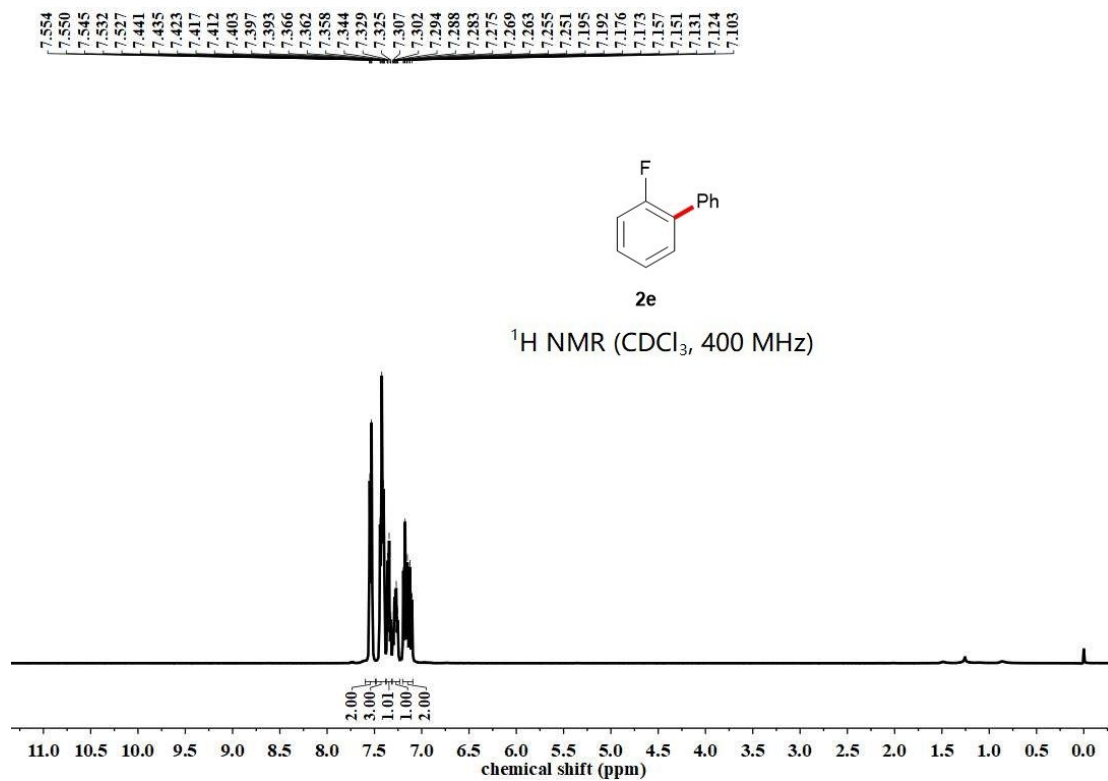
4. NMR spectra of products

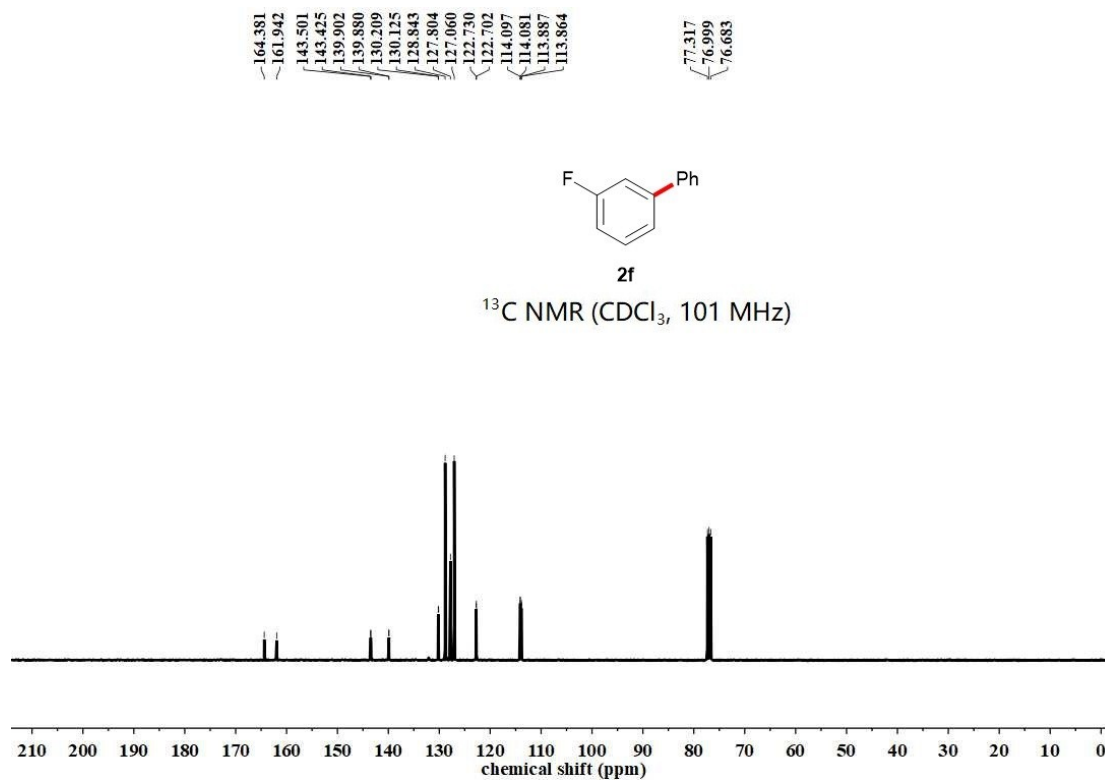
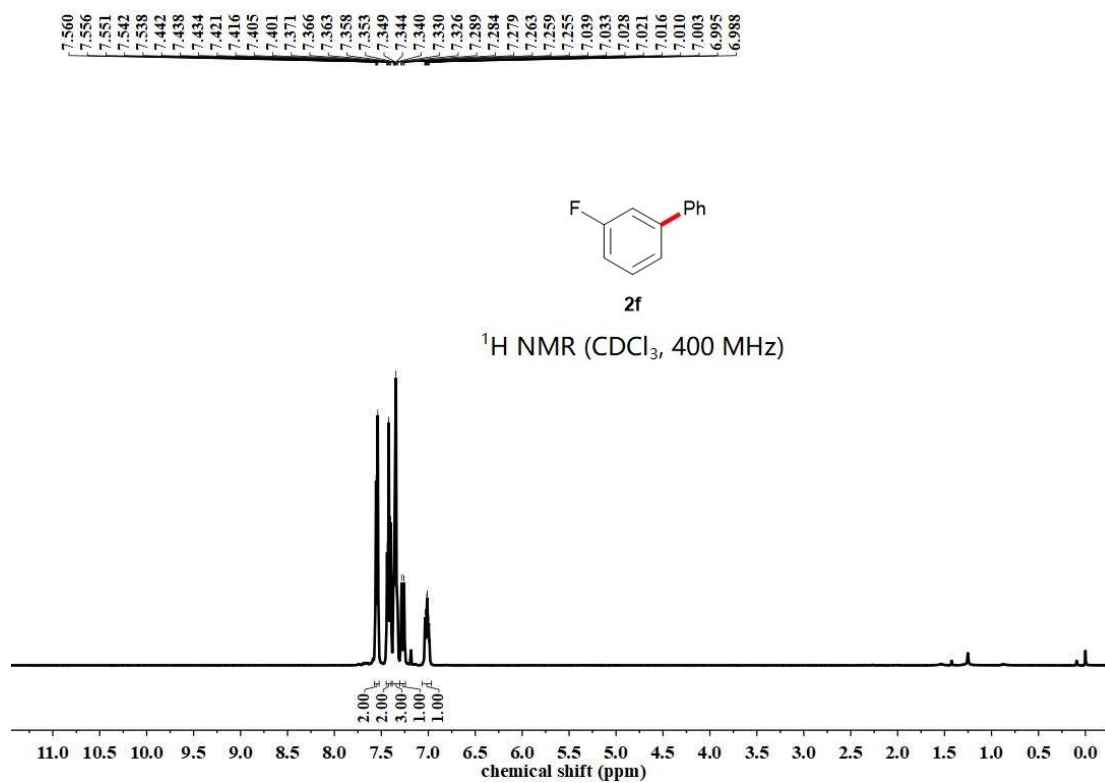




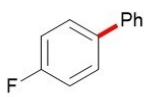






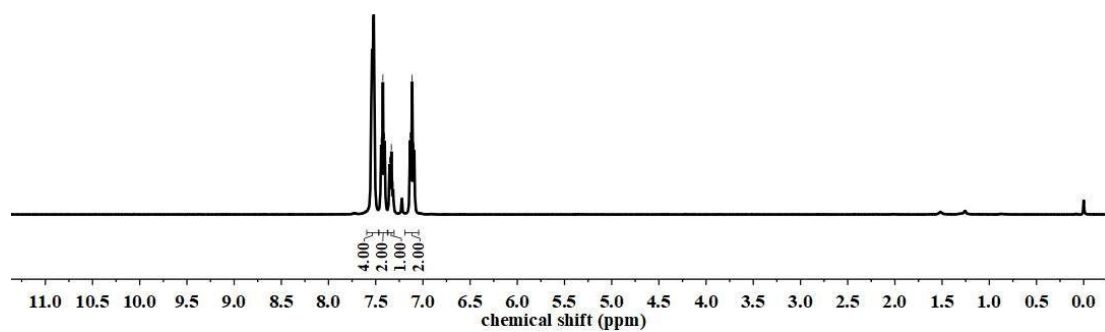


7.542
7.537
7.526
7.519
7.443
7.424
7.405
7.353
7.334
7.316
7.115
7.114
7.093

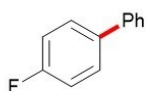


2g

$^1\text{H NMR}$ (CDCl_3 , 400 MHz)

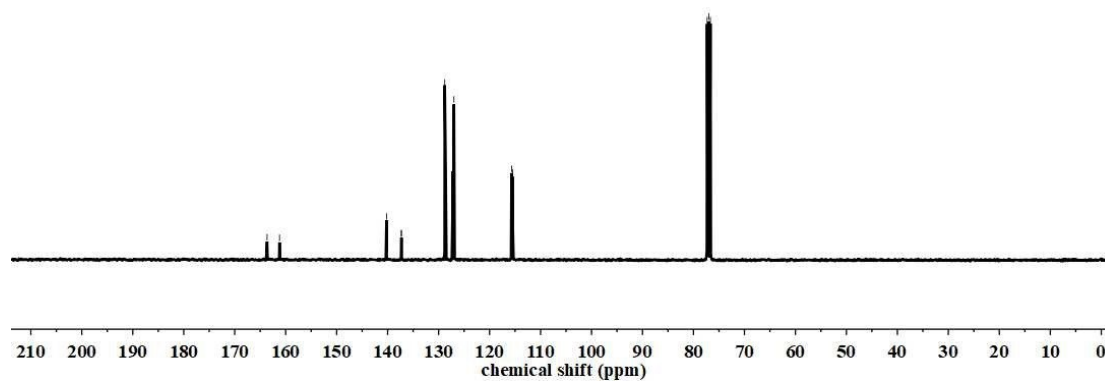


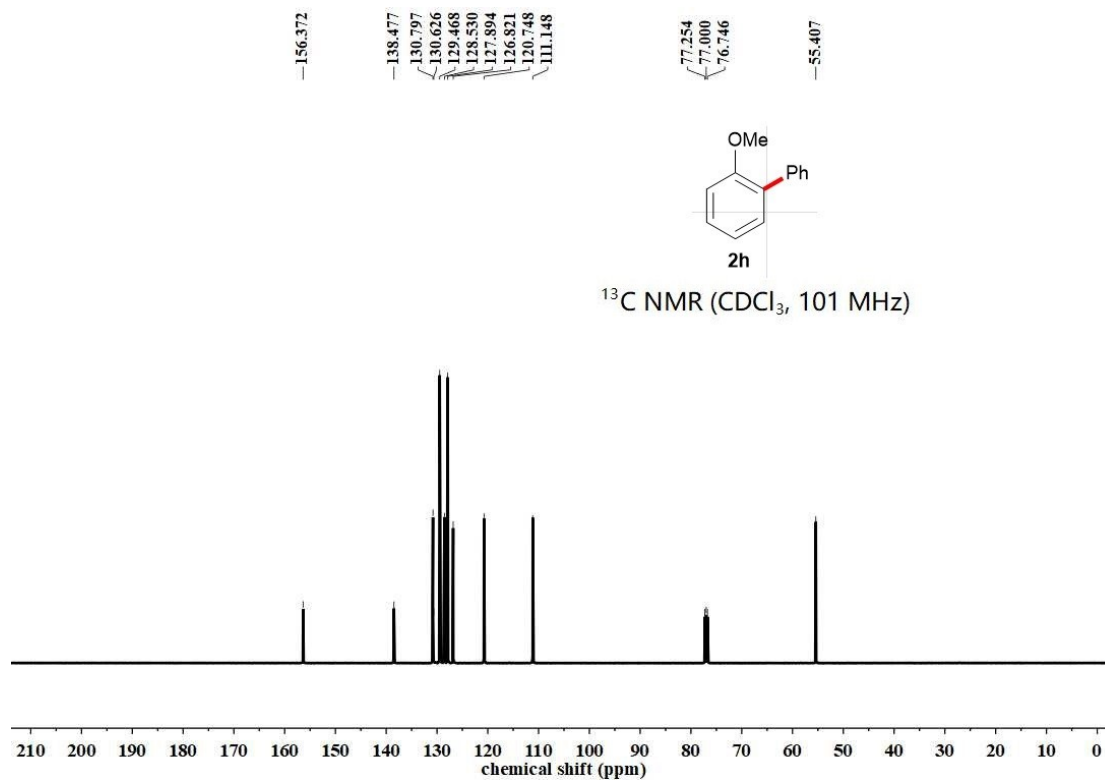
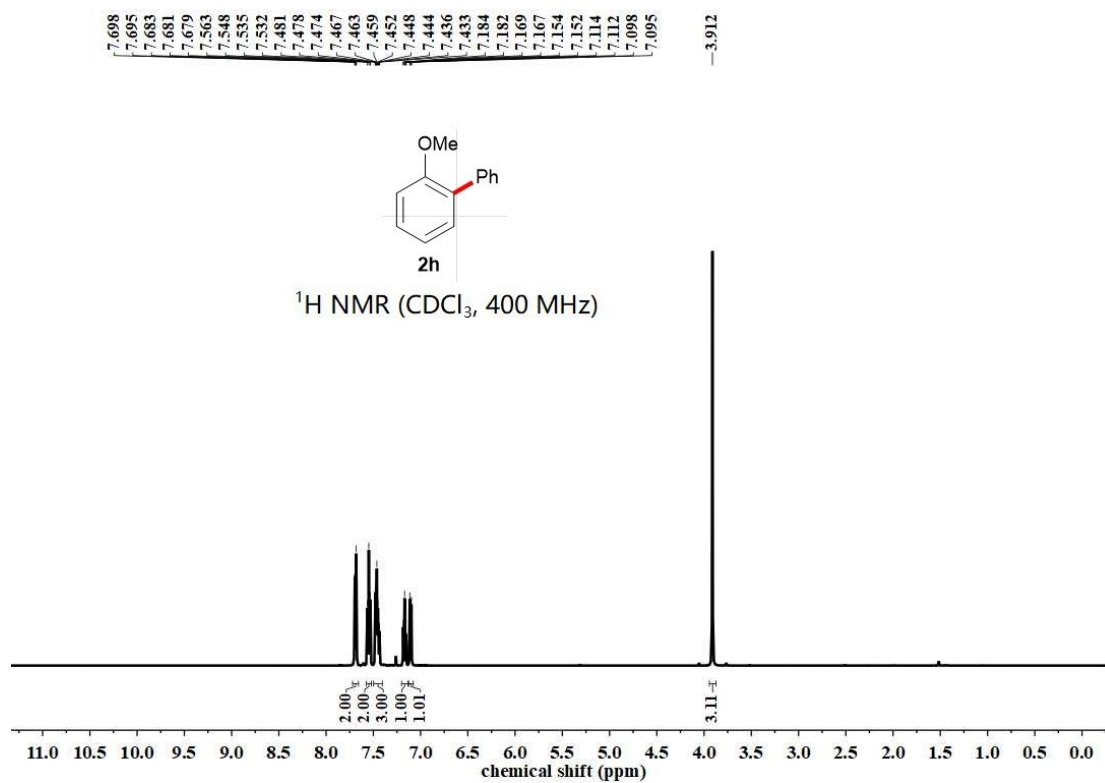
163.658
161.212
140.225
137.323
137.291
128.793
128.696
128.616
127.231
126.993
115.689
115.476
77.318
77.001
76.683

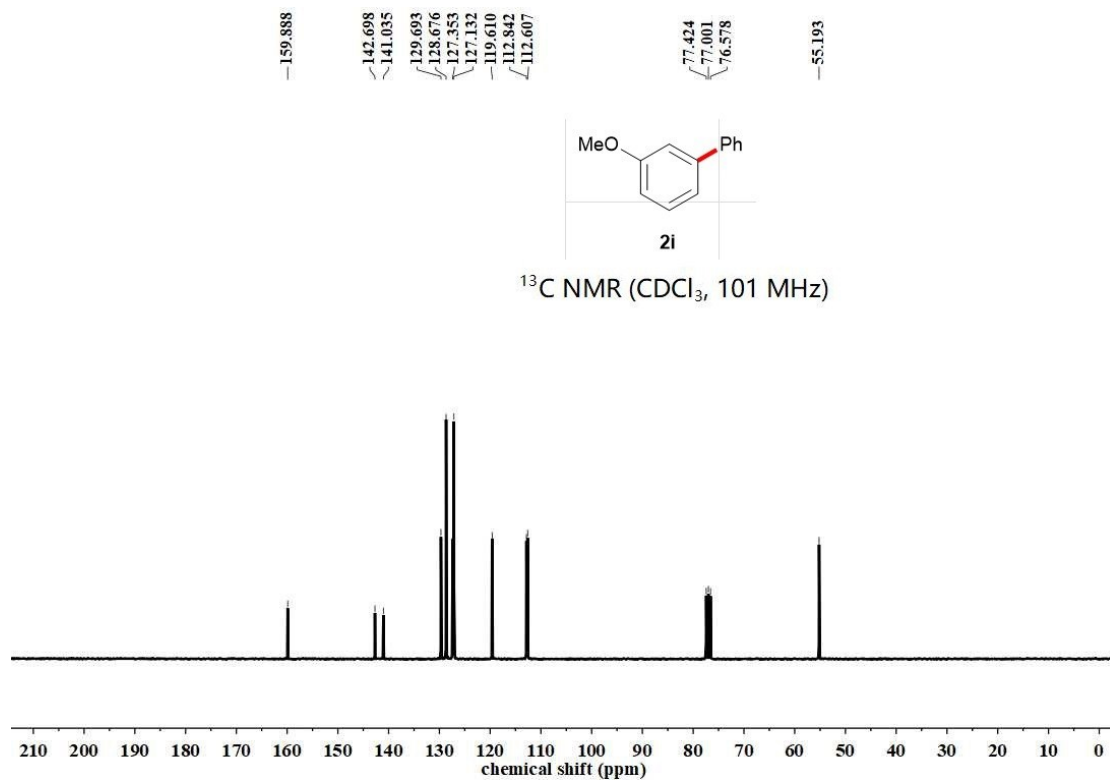
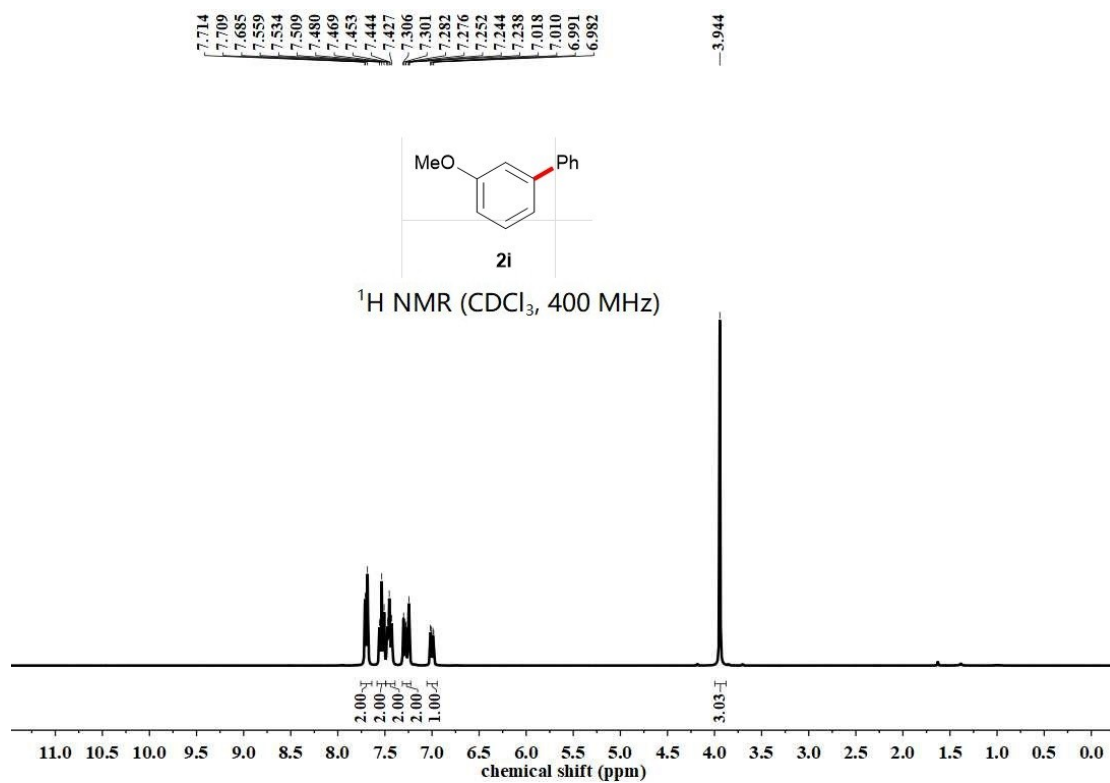


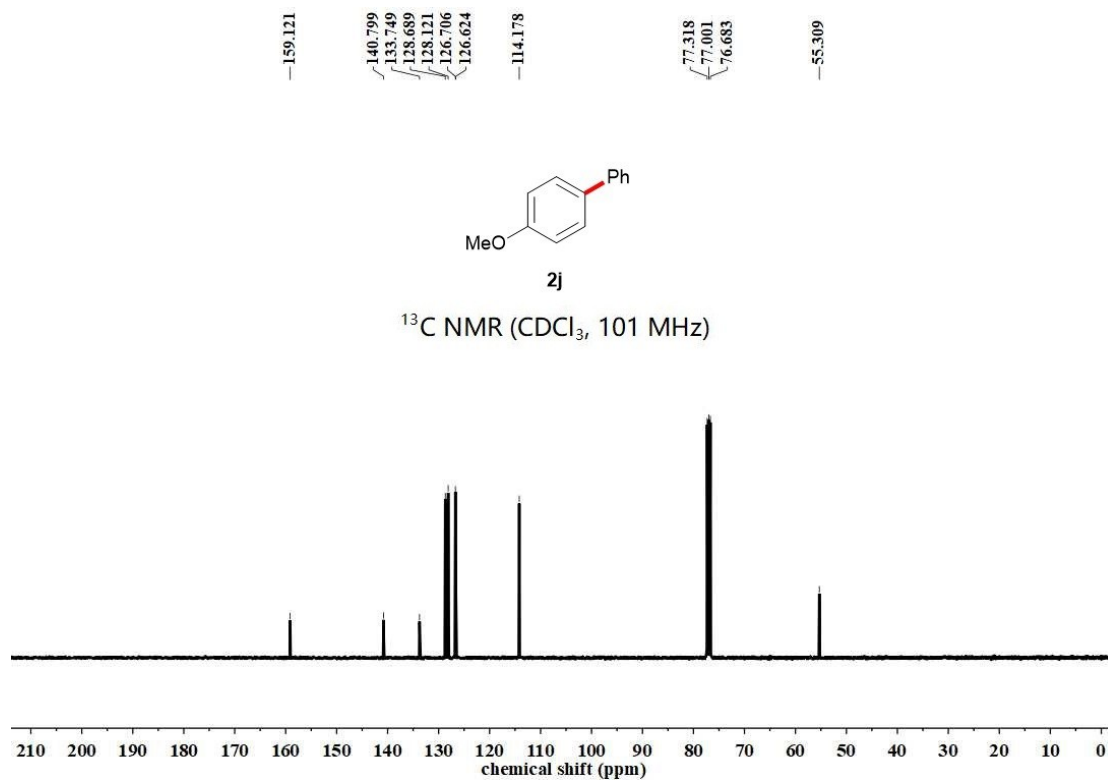
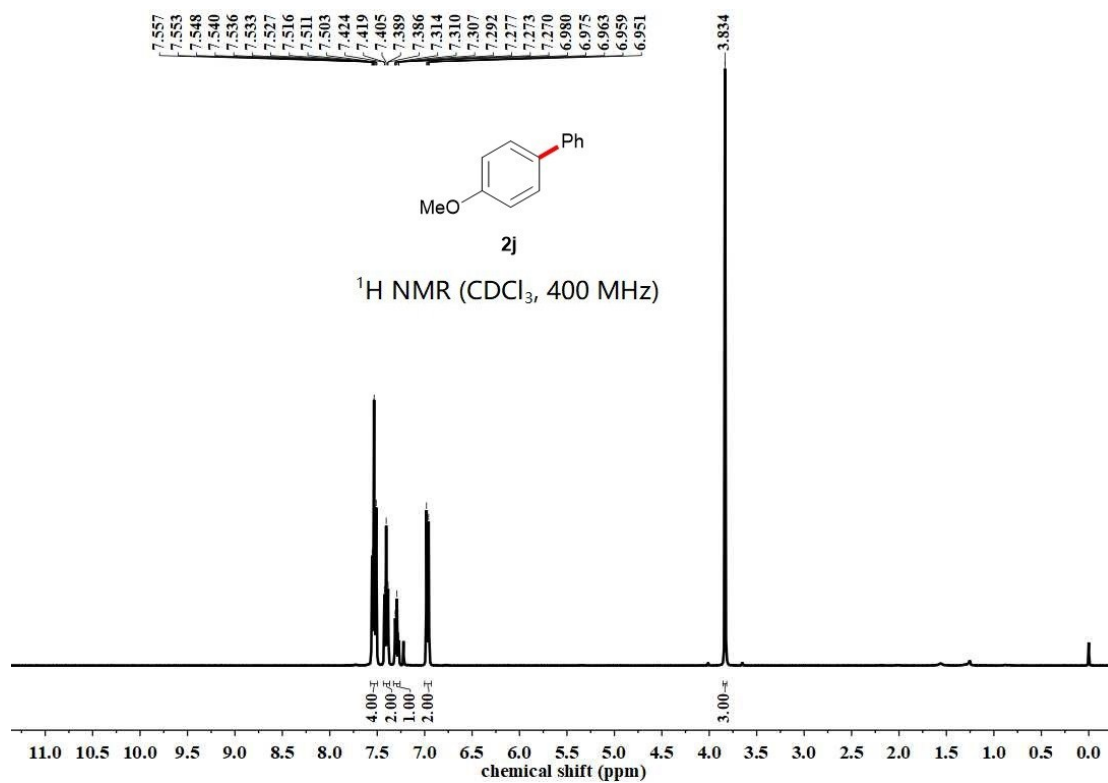
2g

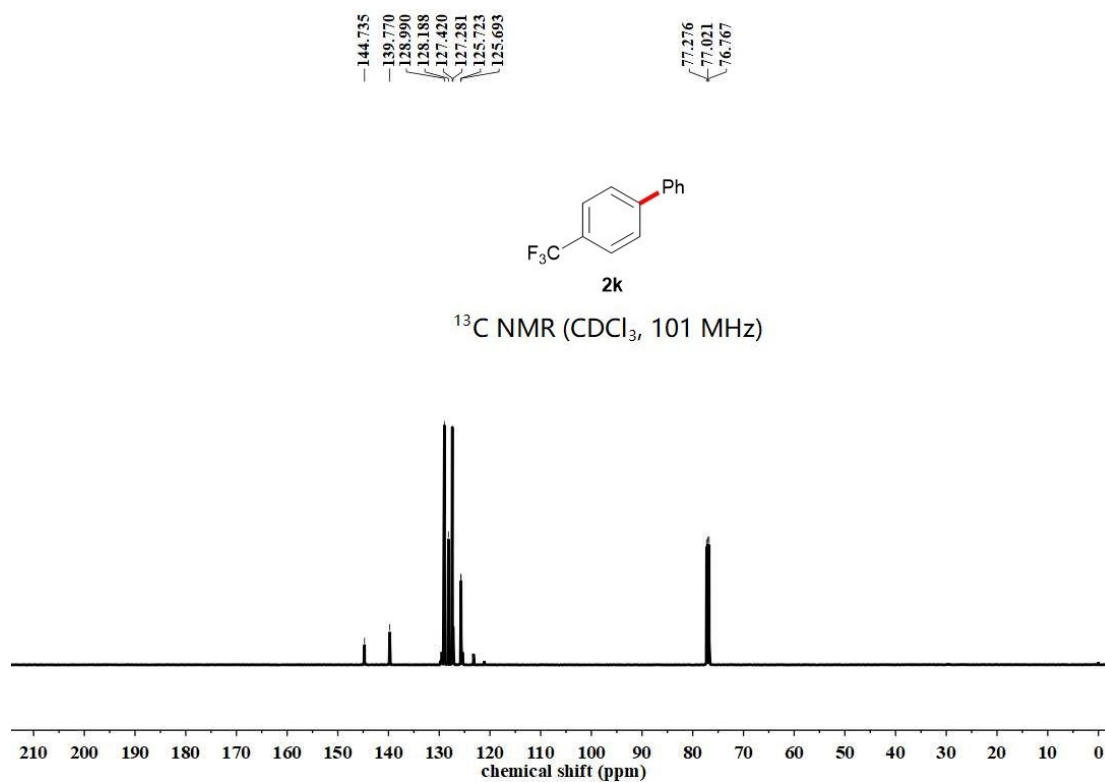
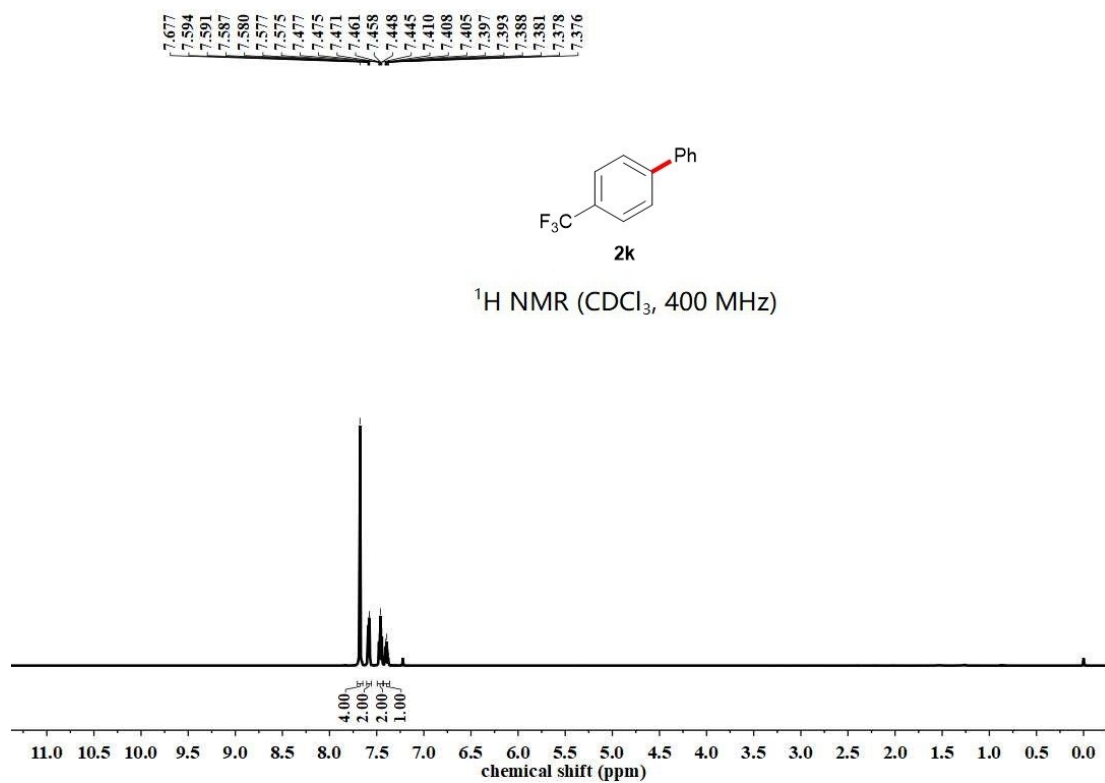
$^{13}\text{C NMR}$ (CDCl_3 , 101 MHz)



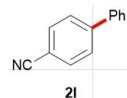




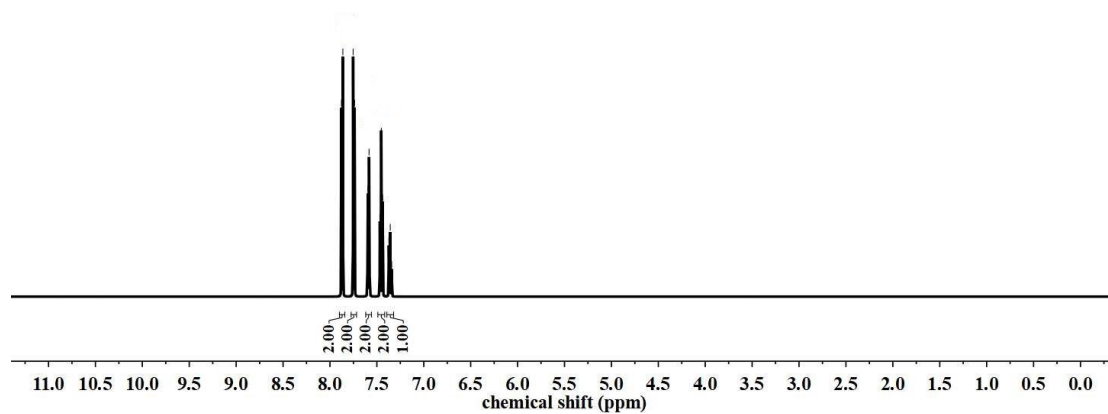




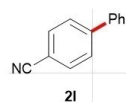
7.881
7.878
7.875
7.865
7.863
7.859
7.757
7.753
7.751
7.741
7.738
7.735
7.601
7.598
7.595
7.592
7.586
7.583
7.580
7.576
7.472
7.469
7.468
7.465
7.457
7.456
7.454
7.453
7.451
7.441
7.439
7.438
7.435
7.375
7.369
7.362
7.359
7.357
7.356
7.353
7.346
7.343
7.339



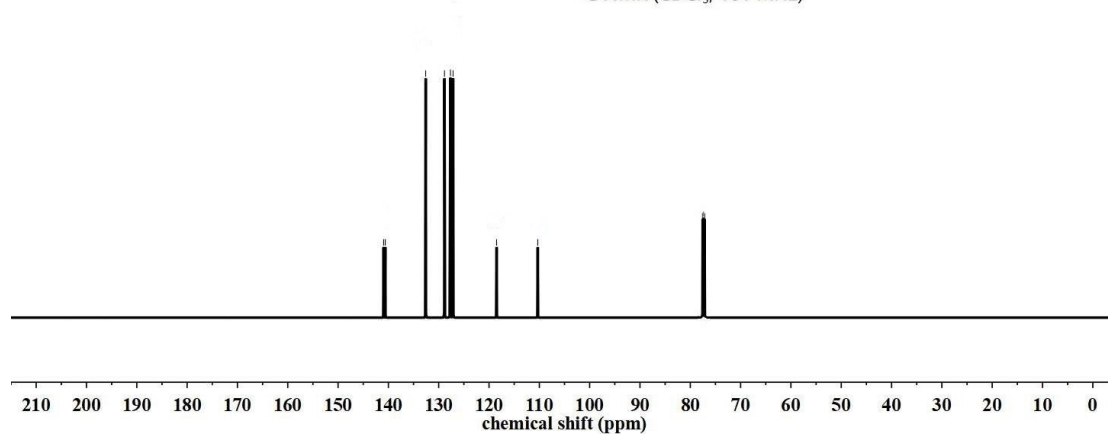
$^1\text{H NMR}$ (CDCl_3 , 400 MHz)

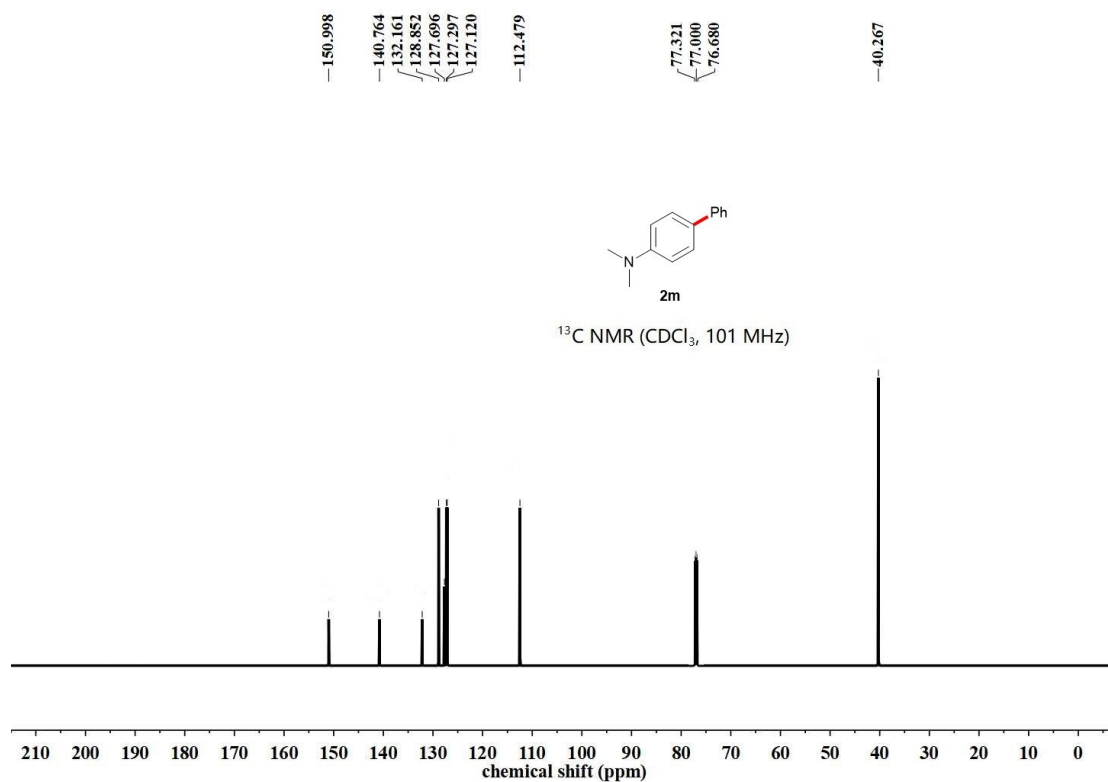
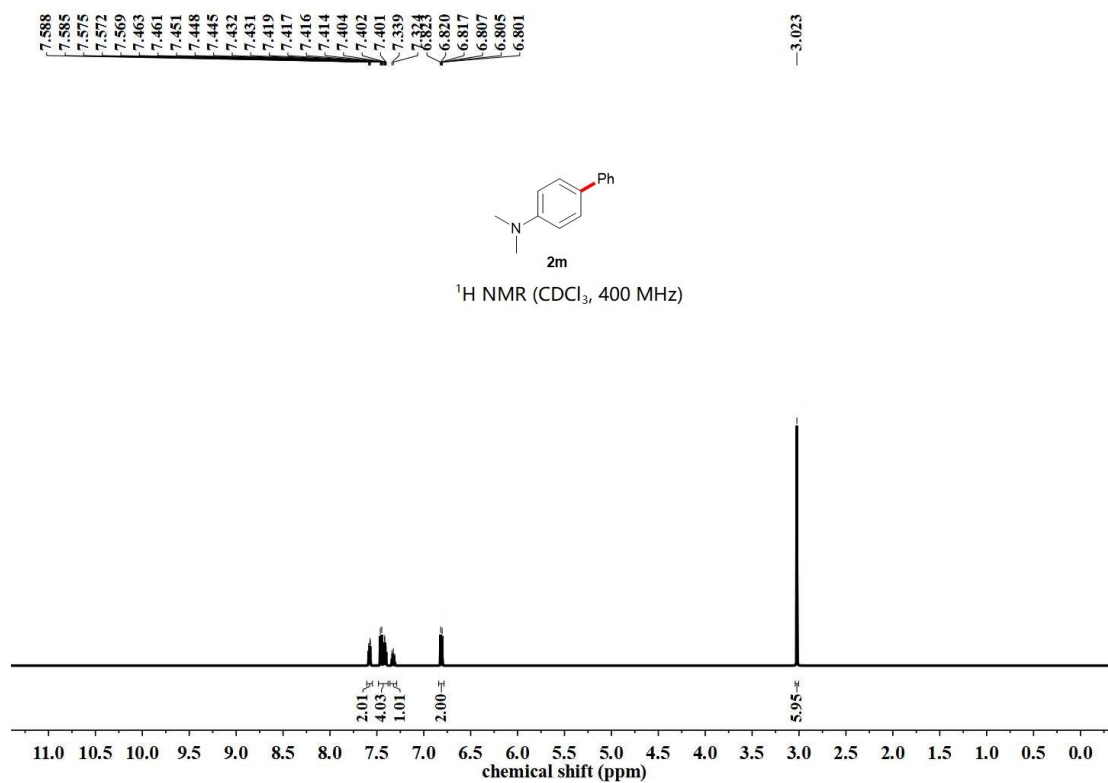


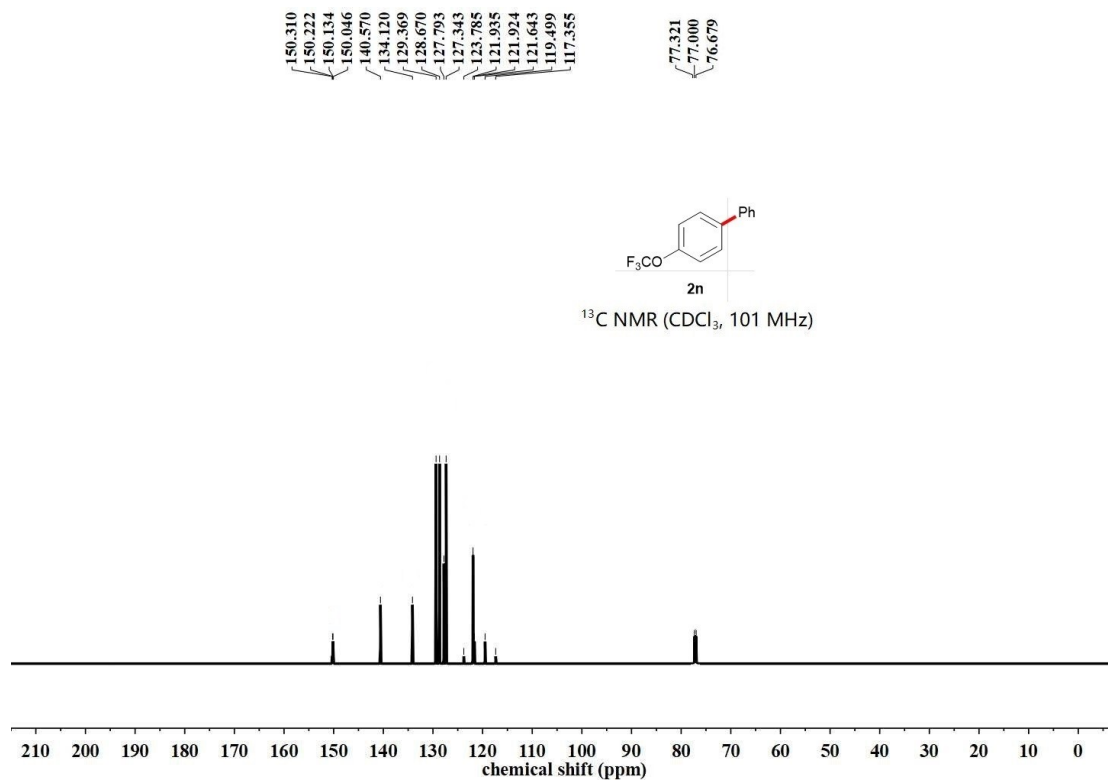
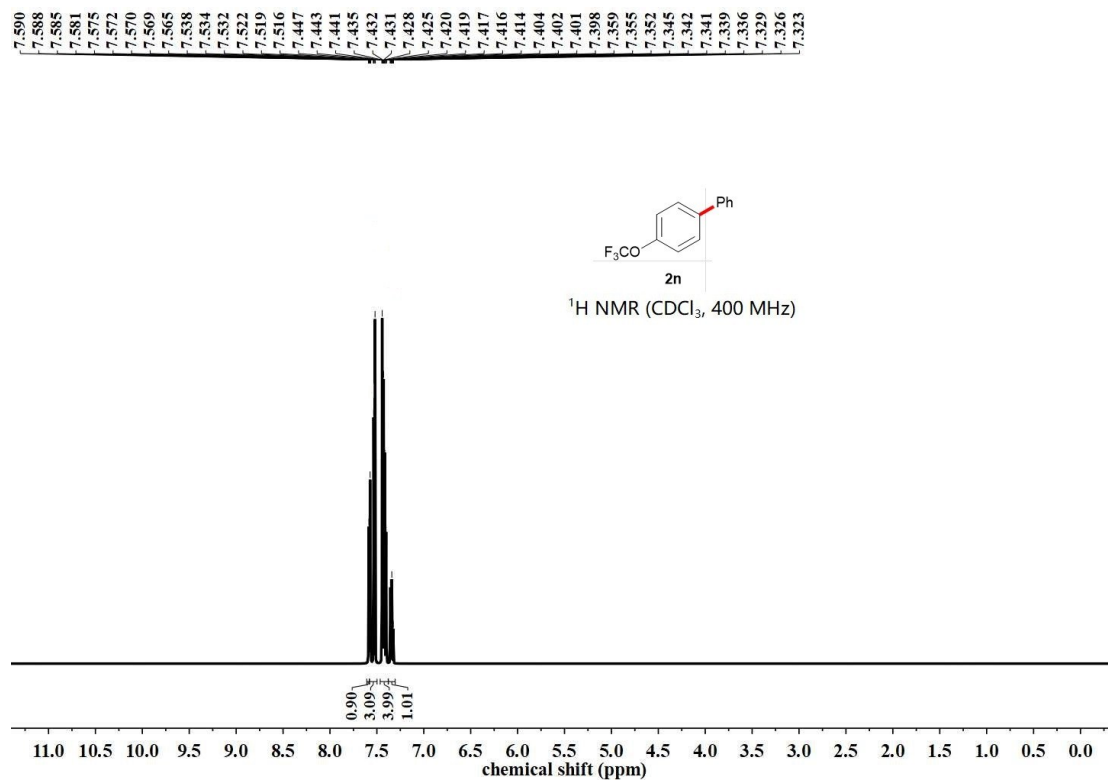
140.945
140.617
132.581
128.852
127.741
127.663
127.144
118.490
110.314
77.318
77.001
76.681

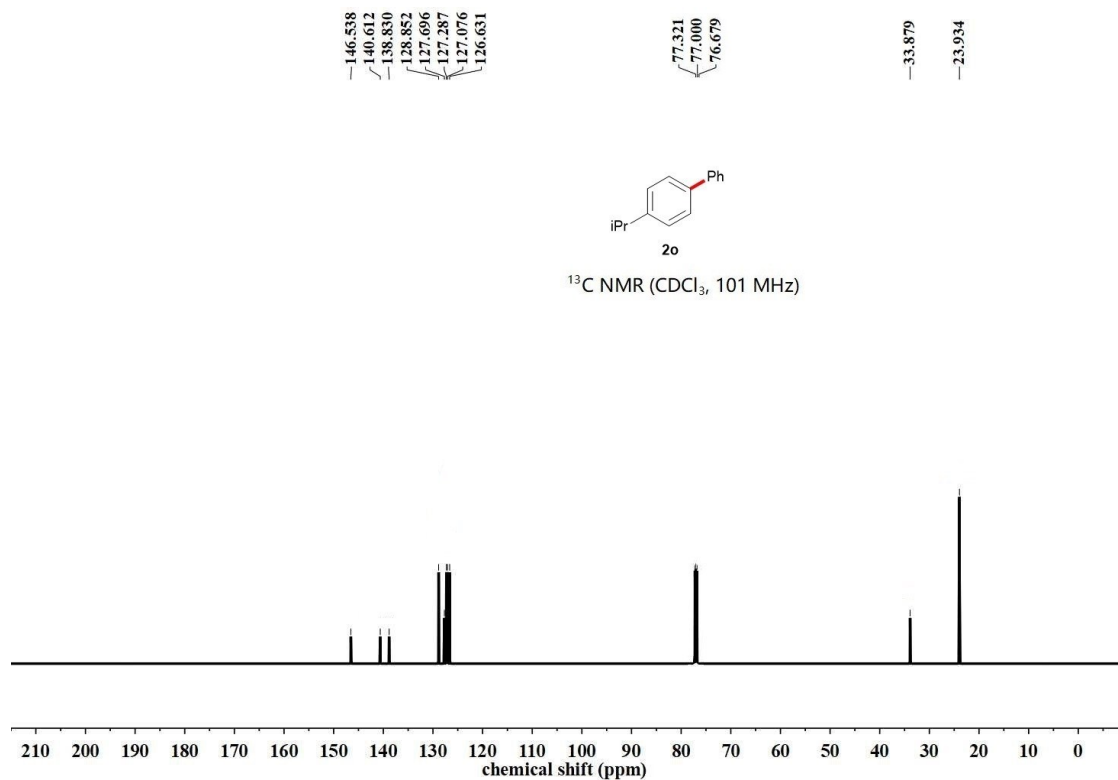
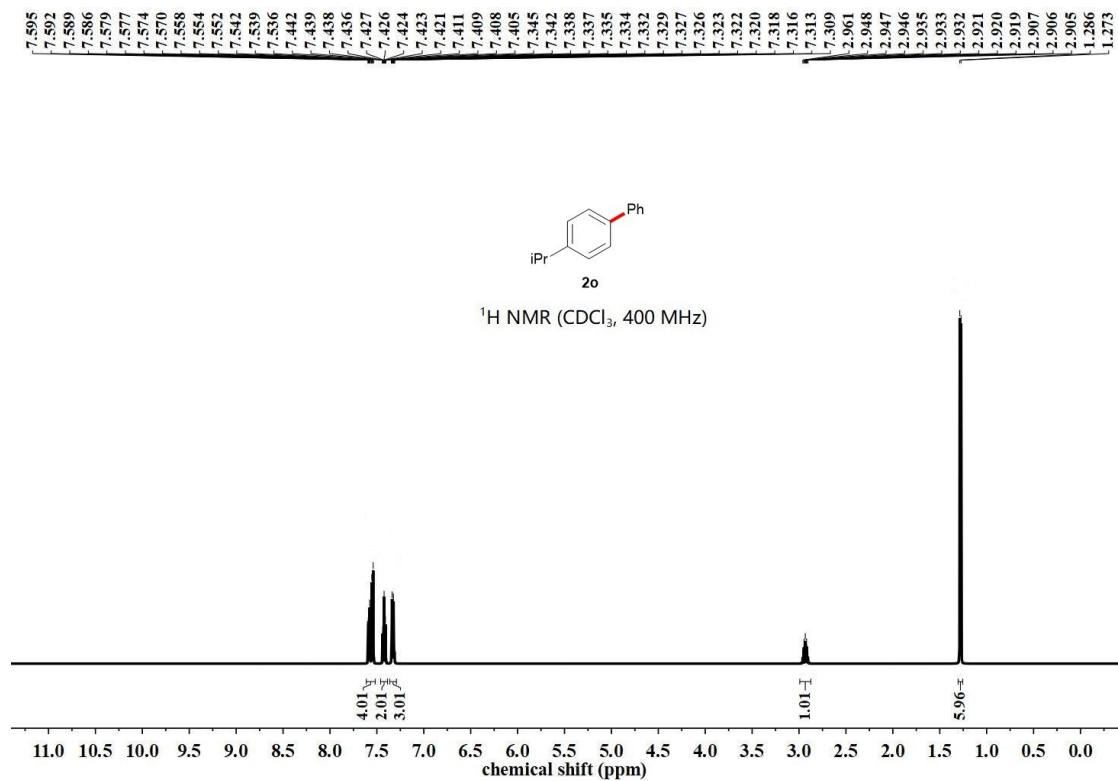


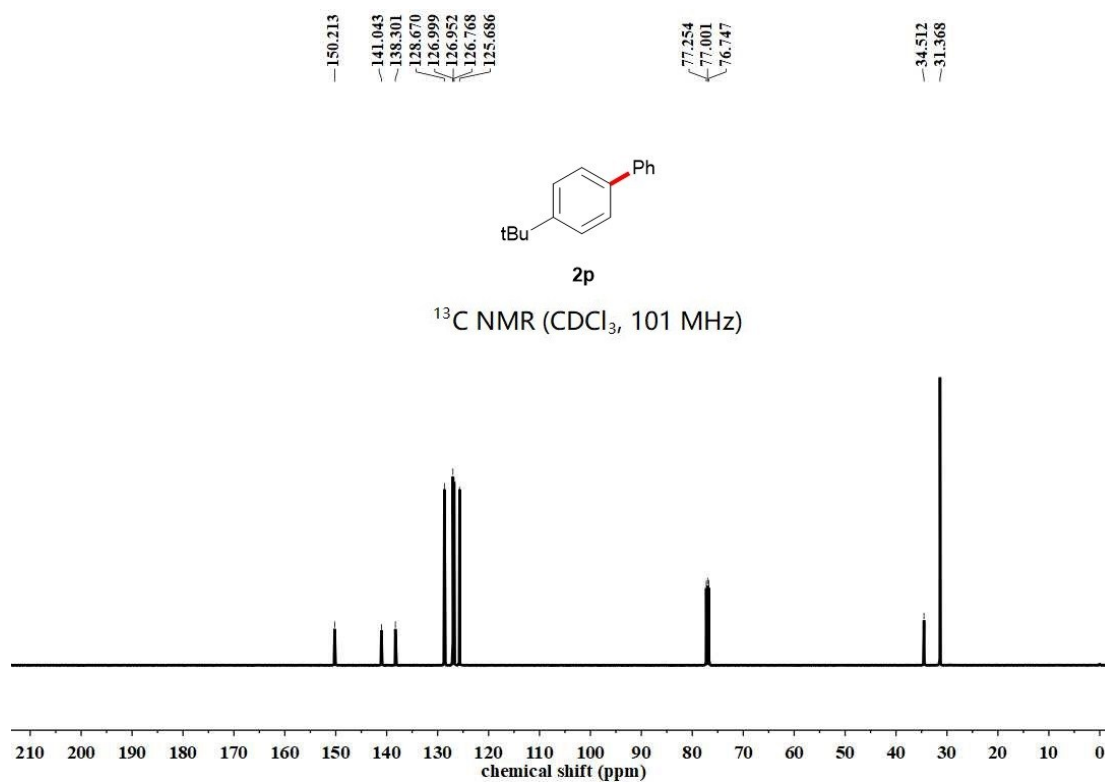
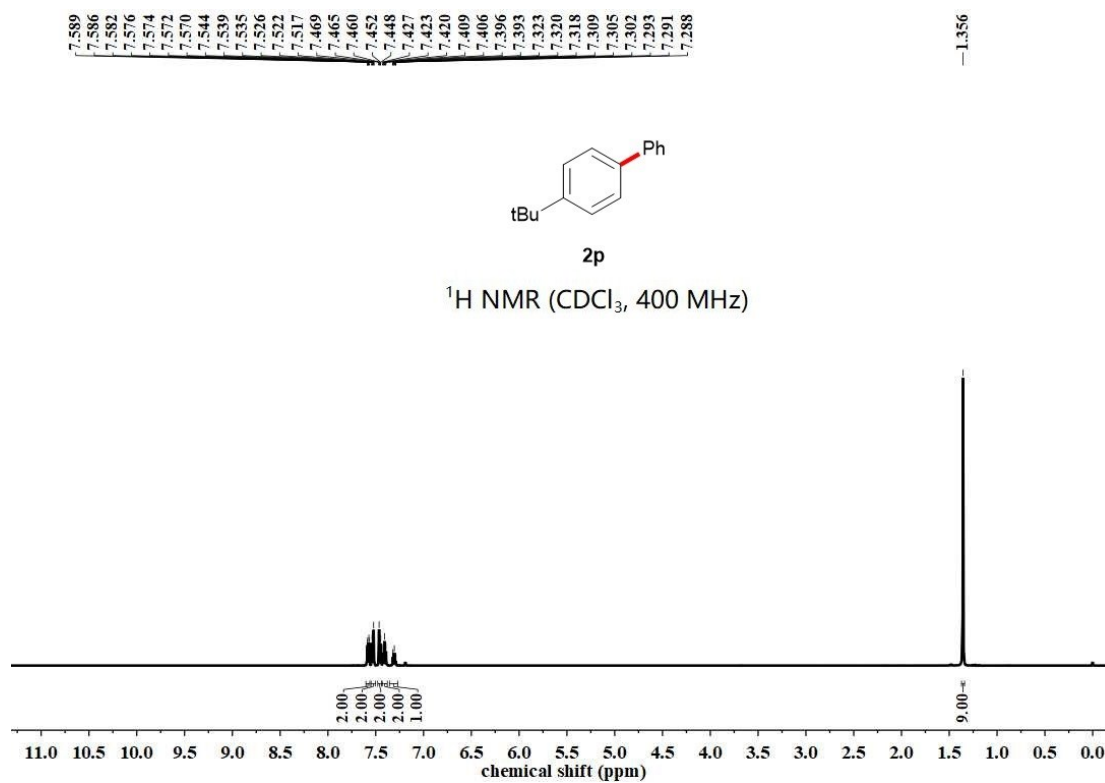
$^{13}\text{C NMR}$ (CDCl_3 , 101 MHz)

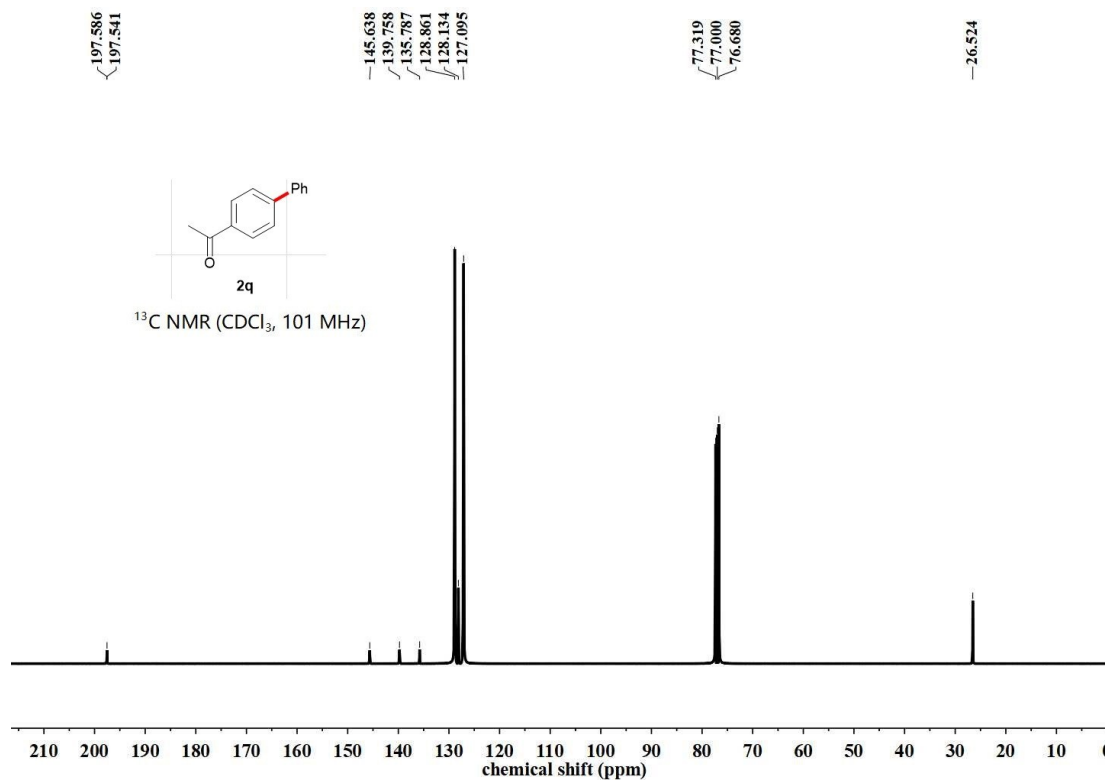
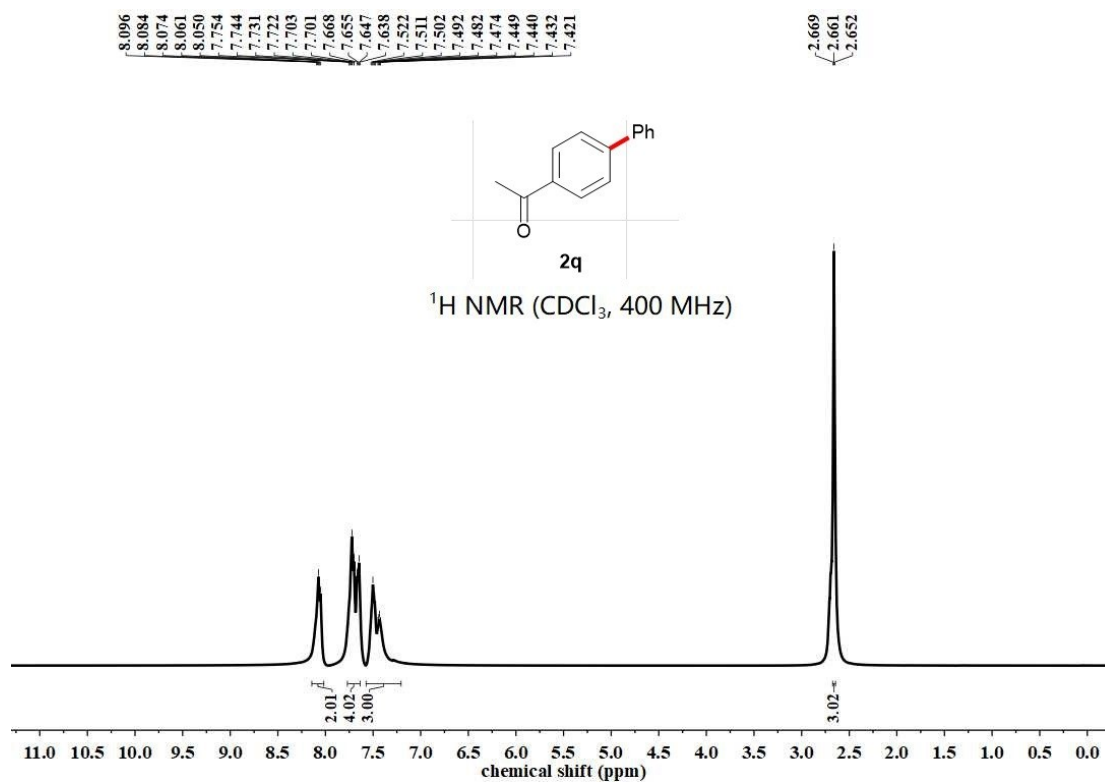


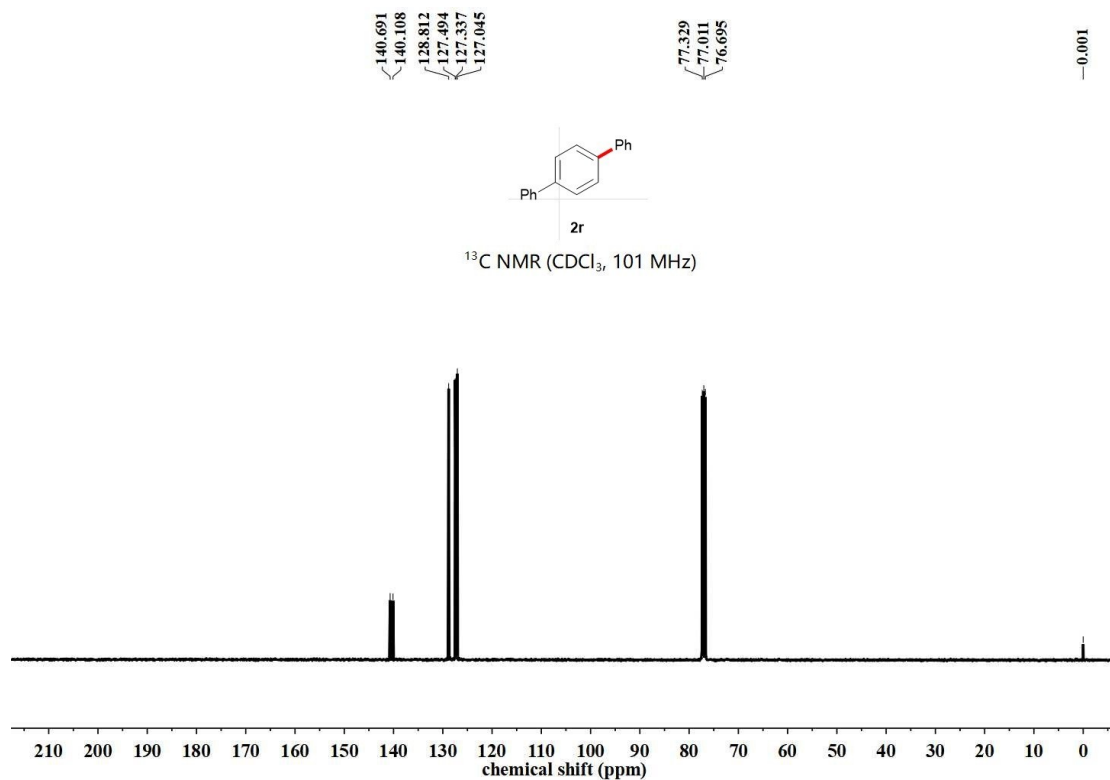
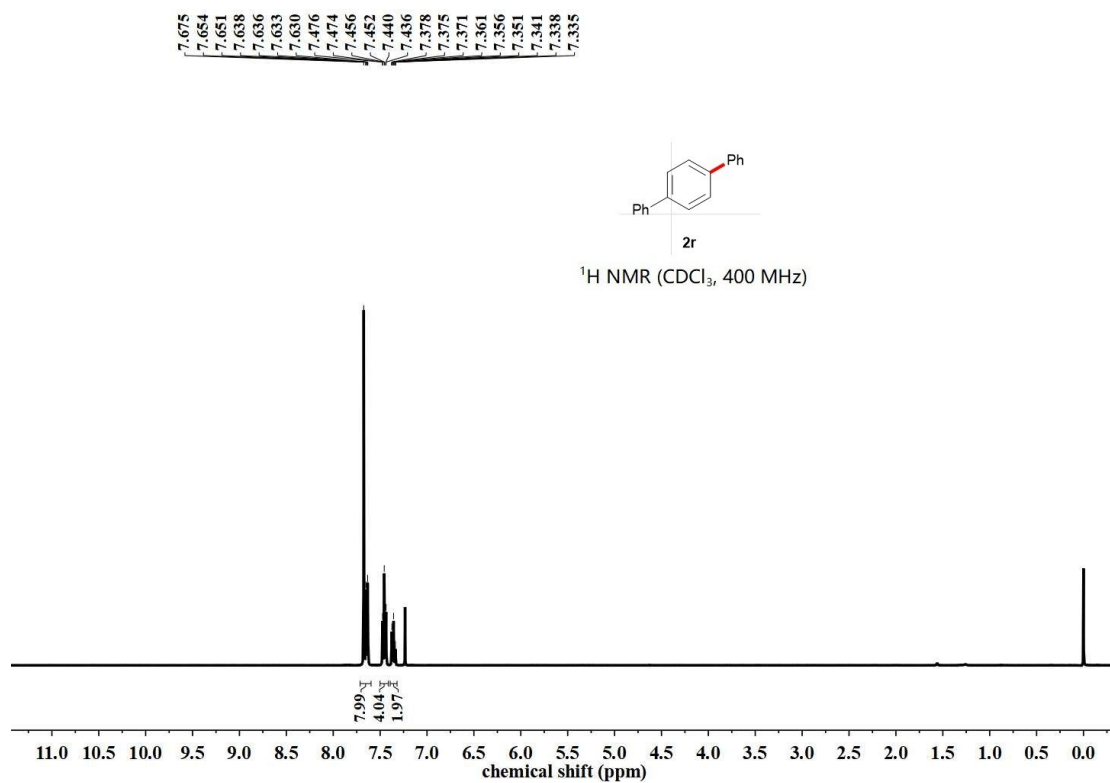


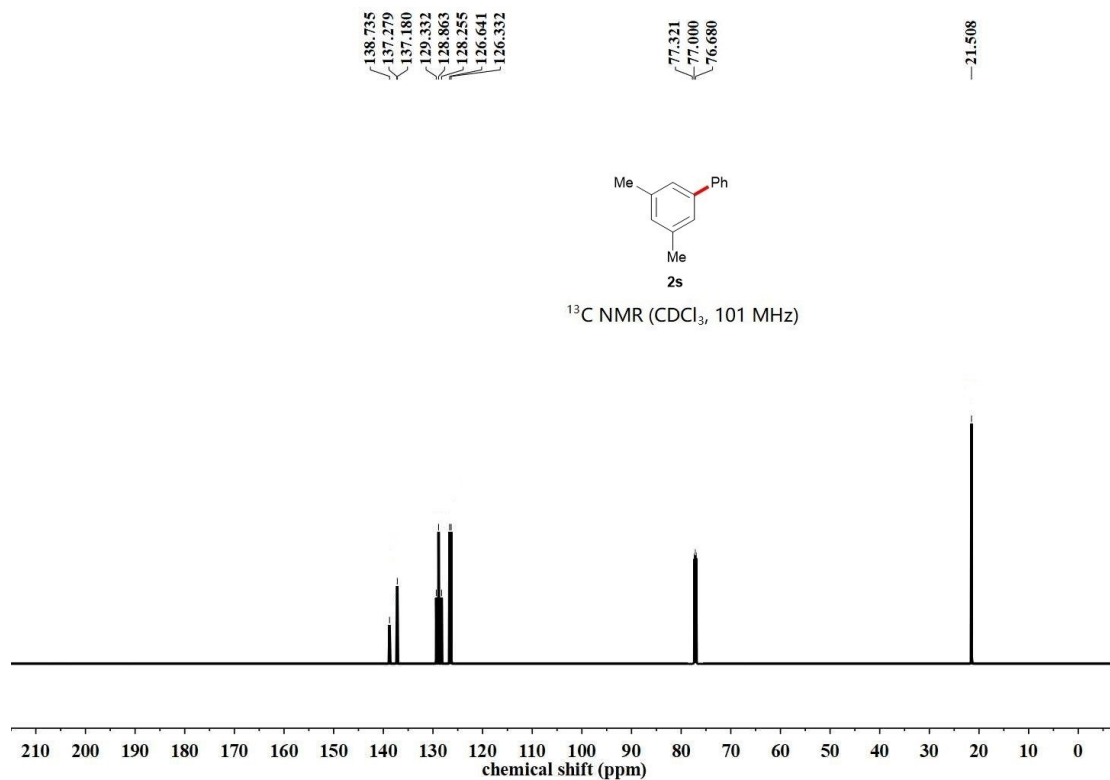
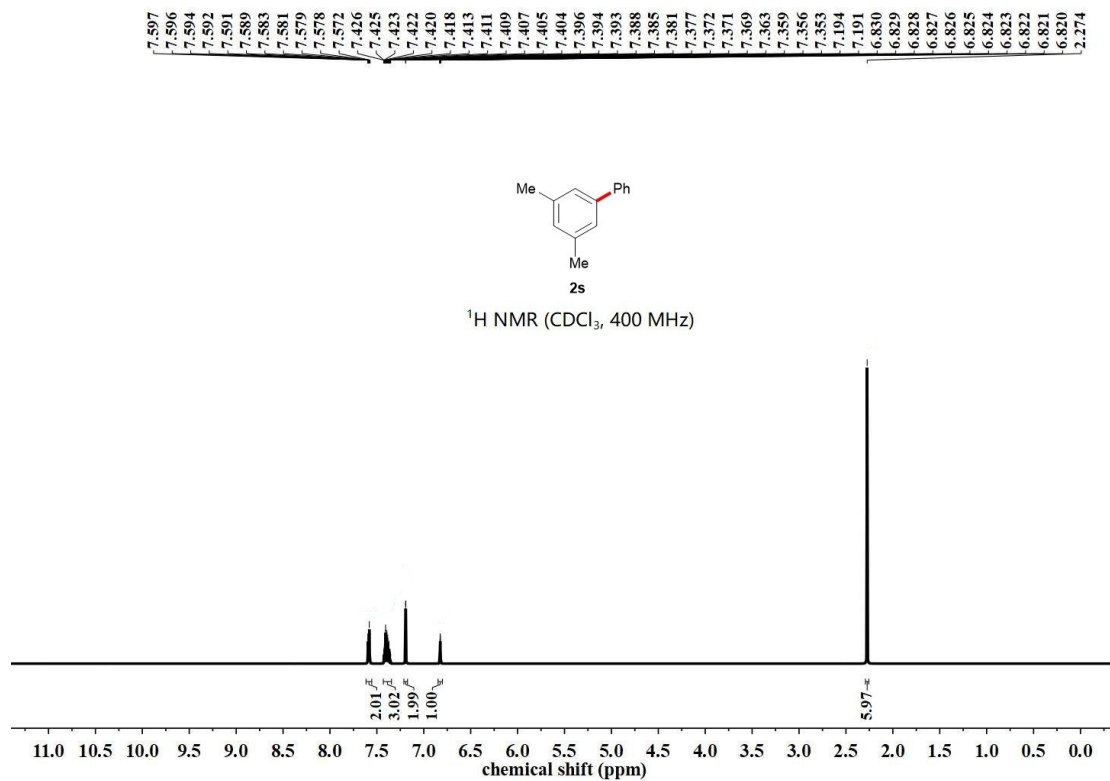




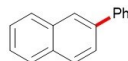






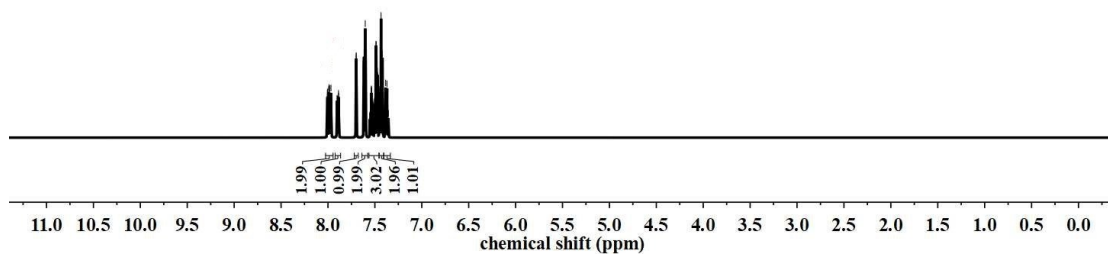


8.008
8.007
8.006
8.005
8.004
7.993
7.992
7.990
7.989
7.984
7.983
7.969
7.968
7.967
7.963
7.901
7.888
7.886
7.772
7.701
7.700
7.698
7.697
7.695
7.618
7.616
7.615
7.605
7.603
7.601
7.600
7.540
7.539
7.536
7.535
7.524
7.503
7.501
7.500
7.490
7.489
7.486
7.475
7.474
7.472
7.471
7.450
7.449
7.448
7.435
7.434
7.432
7.422
7.420
7.419
7.385
7.372
7.371
7.369



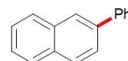
2t

¹H NMR (CDCl₃, 400 MHz)



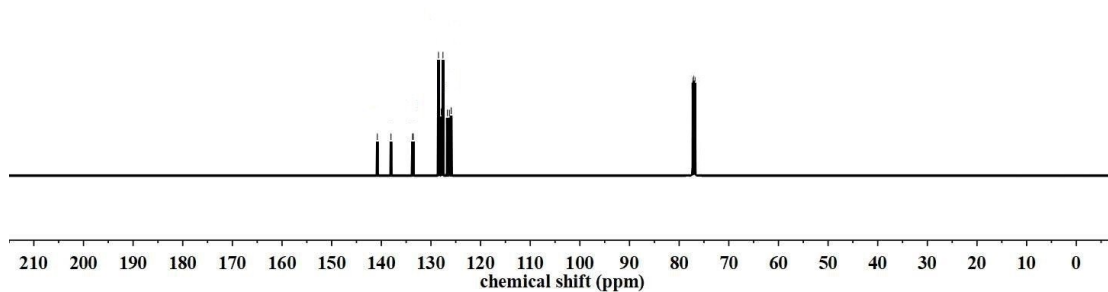
140.810
138.054
133.712
133.563
128.476
128.289
127.913
127.862
127.799
127.581
126.706
126.290
125.943
125.912

77.318
77.001
76.681

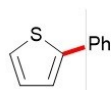


2t

¹³C NMR (CDCl₃, 101 MHz)

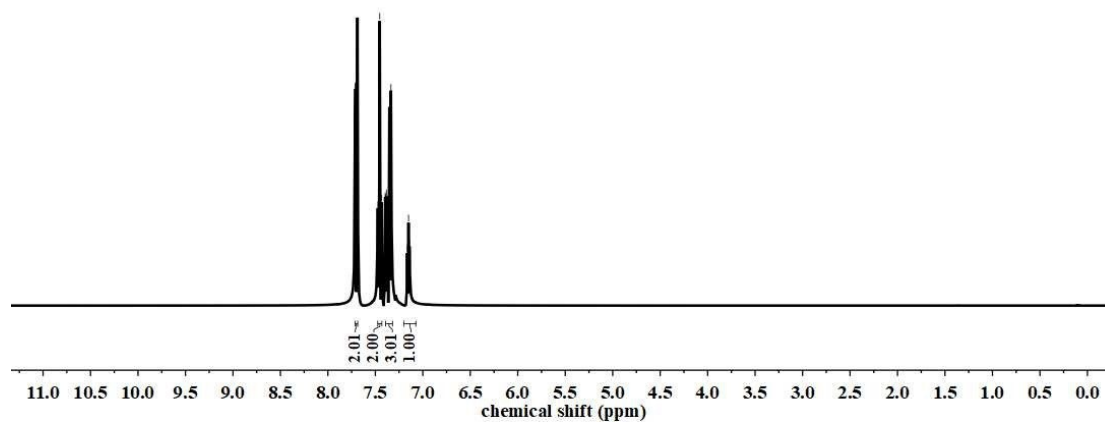


7.712
7.709
7.691
7.688
7.476
7.473
7.453
7.433
7.396
7.393
7.387
7.384
7.353
7.349
7.335
7.164
7.154
7.151
7.140



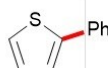
2u

$^1\text{H NMR}$ (CDCl_3 , 400 MHz)



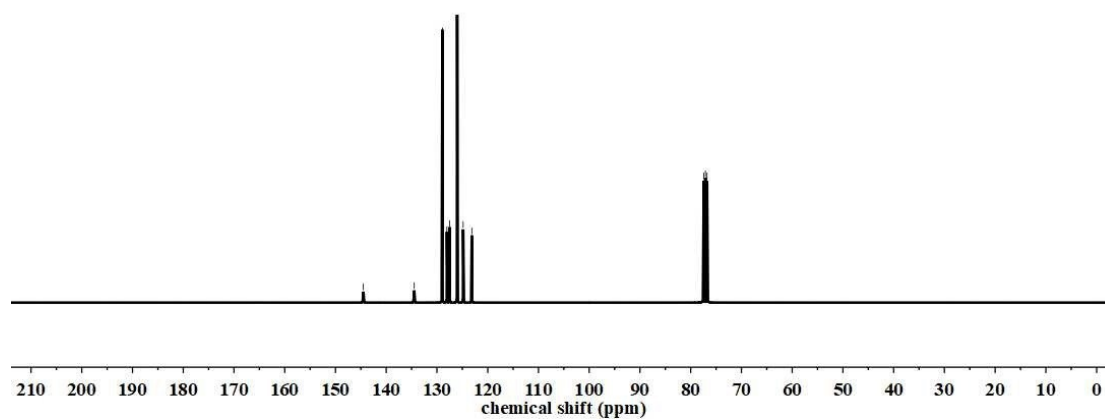
144.503
134.487
128.933
128.043
127.506
126.021
124.841
123.134

77.416
77.097
76.778



2u

$^{13}\text{C NMR}$ (CDCl_3 , 101 MHz)

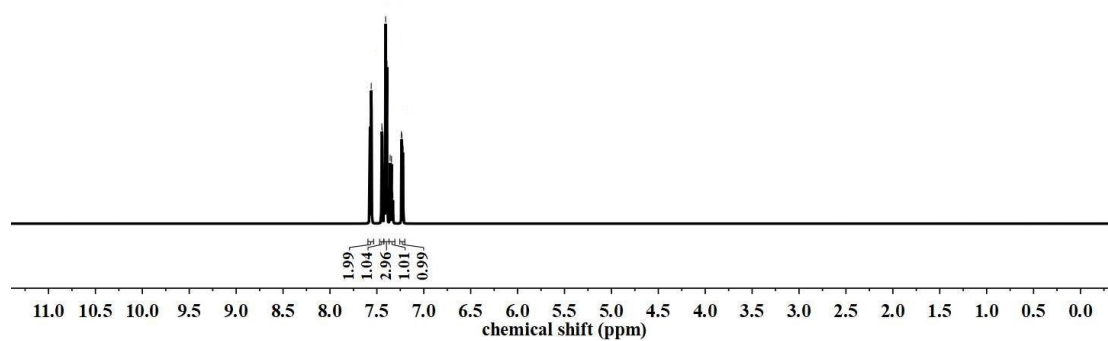


7.577
7.576
7.574
7.572
7.569
7.562
7.560
7.558
7.557
7.553
7.452
7.449
7.447
7.444
7.425
7.423
7.422
7.421
7.419
7.412
7.410
7.408
7.407
7.405
7.397
7.395
7.393
7.392
7.388
7.362
7.358
7.355
7.349
7.345
7.344
7.343
7.339
7.332
7.329
7.326
7.238
7.235
7.223
7.220



2v

^1H NMR (CDCl_3 , 400 MHz)

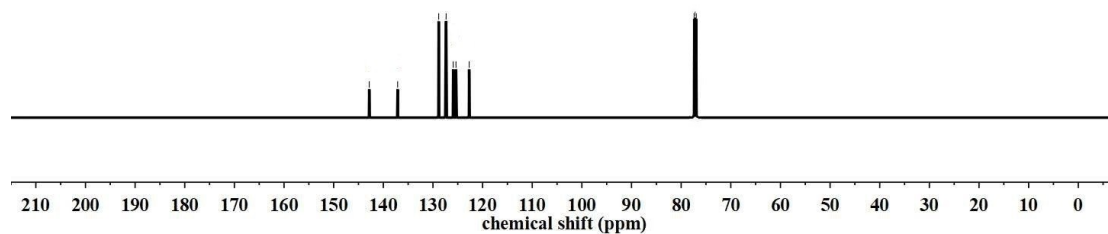


142.832
137.115
128.838
127.455
127.347
125.918
125.355
122.707
77.321
77.000
76.680

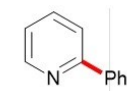


2v

^{13}C NMR (CDCl_3 , 101 MHz)

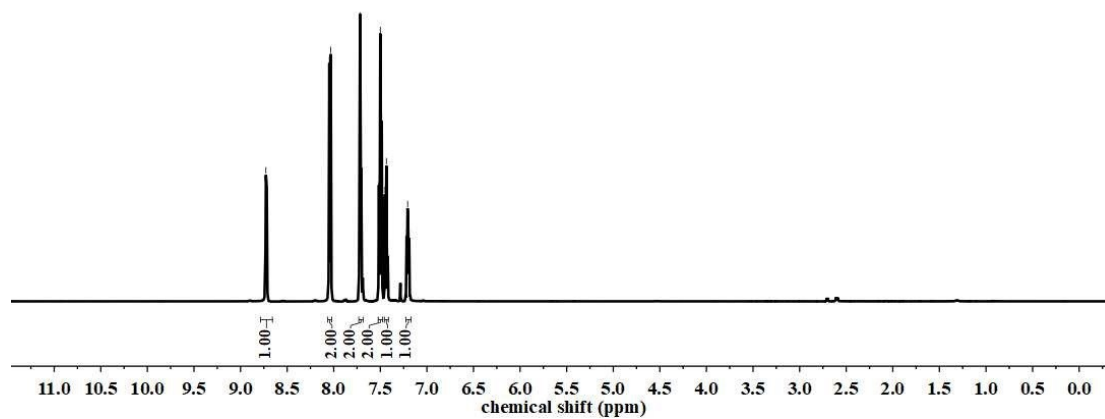


8.731
8.728
8.725
8.721
8.718
8.716
8.050
8.047
8.036
8.032
8.030
7.718
7.715
7.710
7.706
7.702
7.515
7.511
7.501
7.497
7.488
7.485
7.452
7.449
7.447
7.439
7.435
7.430
7.423
7.420
7.217
7.212
7.207
7.202
7.200
7.196
7.190



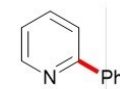
2w

$^1\text{H NMR}$ (CDCl_3 , 400 MHz)



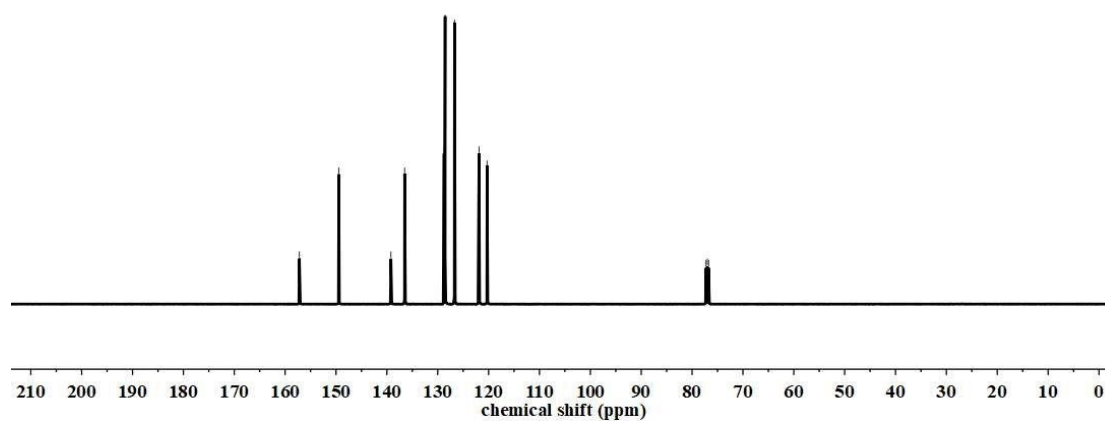
-157.195
-149.456
-139.199
-136.508
-128.753
-128.548
-126.706
-121.885
-120.304

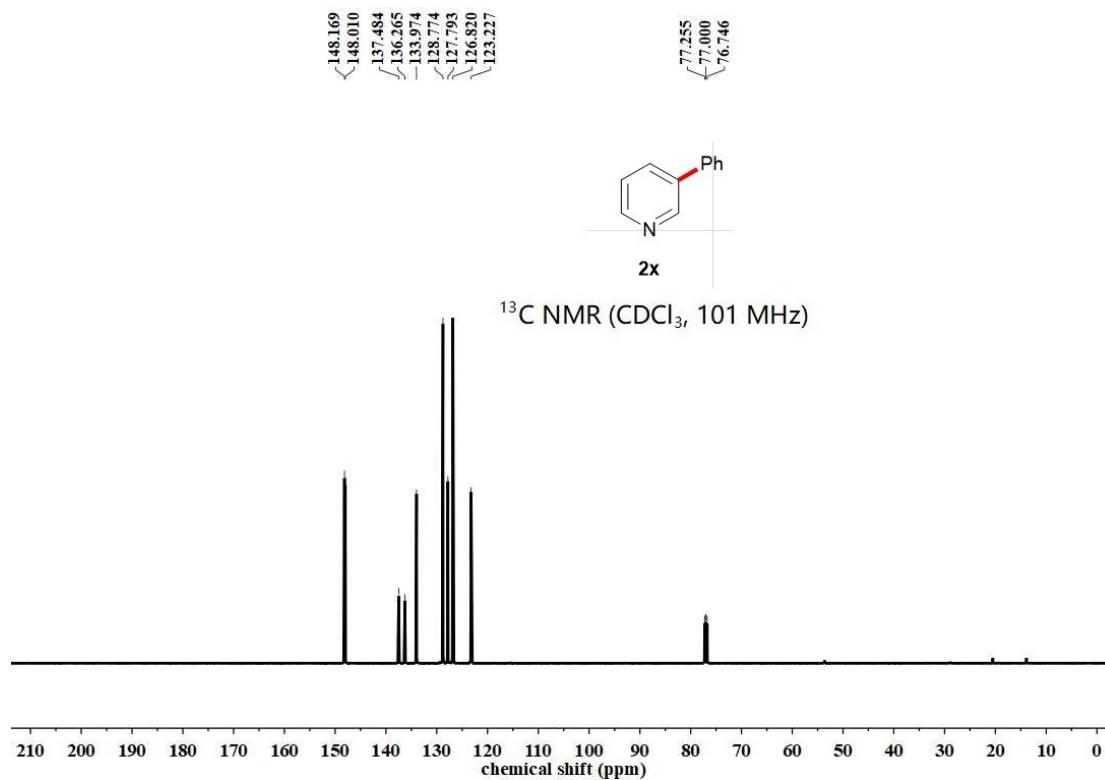
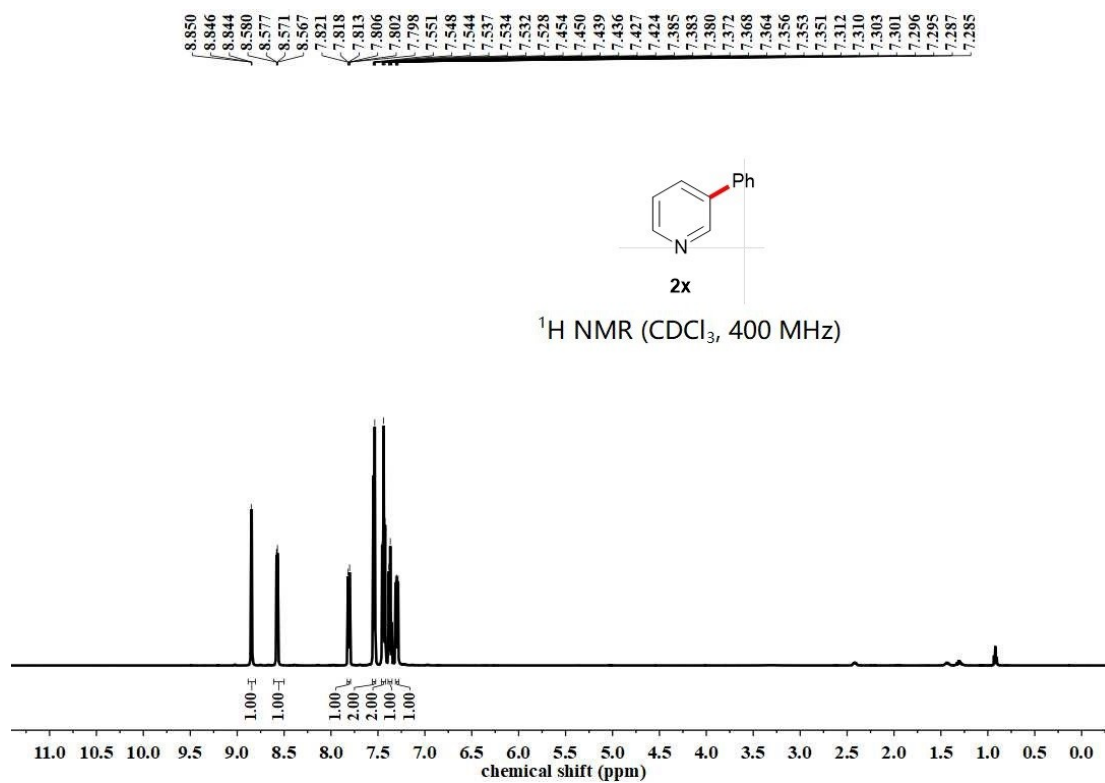
77.255
77.000
76.746



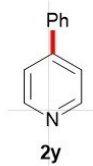
2w

$^{13}\text{C NMR}$ (CDCl_3 , 101 MHz)

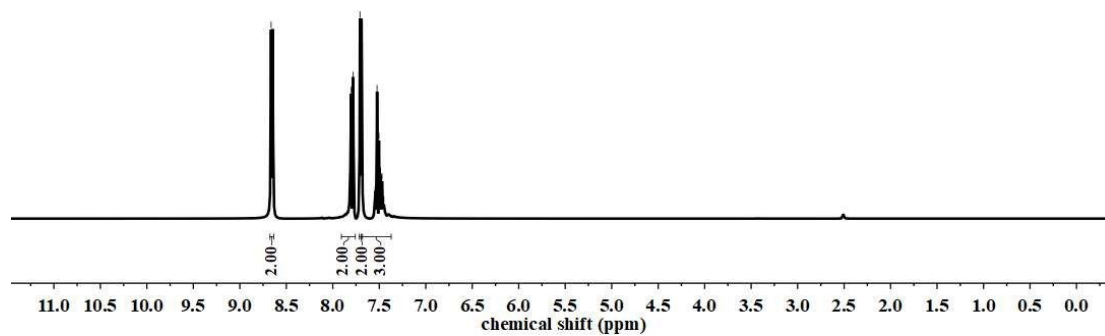




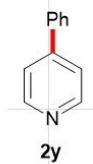
8.663
8.659
8.652
8.646
7.806
7.801
7.788
7.784
7.781
7.708
7.703
7.696
7.690
7.546
7.541
7.524
7.519
7.504
7.493
7.490
7.486
7.470
7.453
7.450



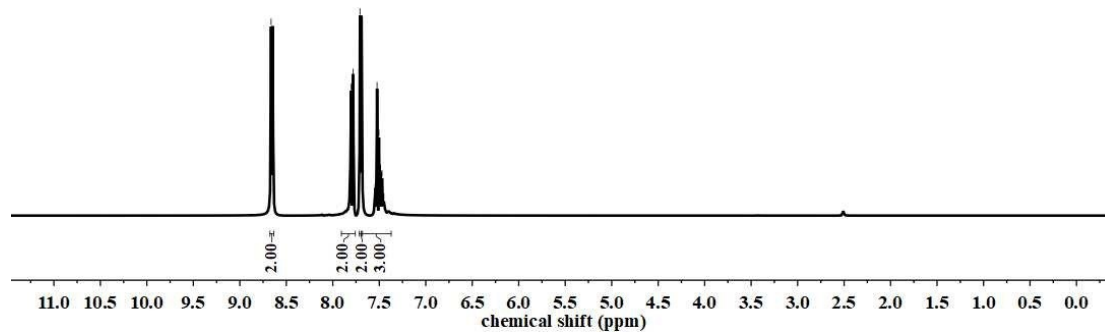
¹H NMR (DMSO-d₆, 400 MHz)

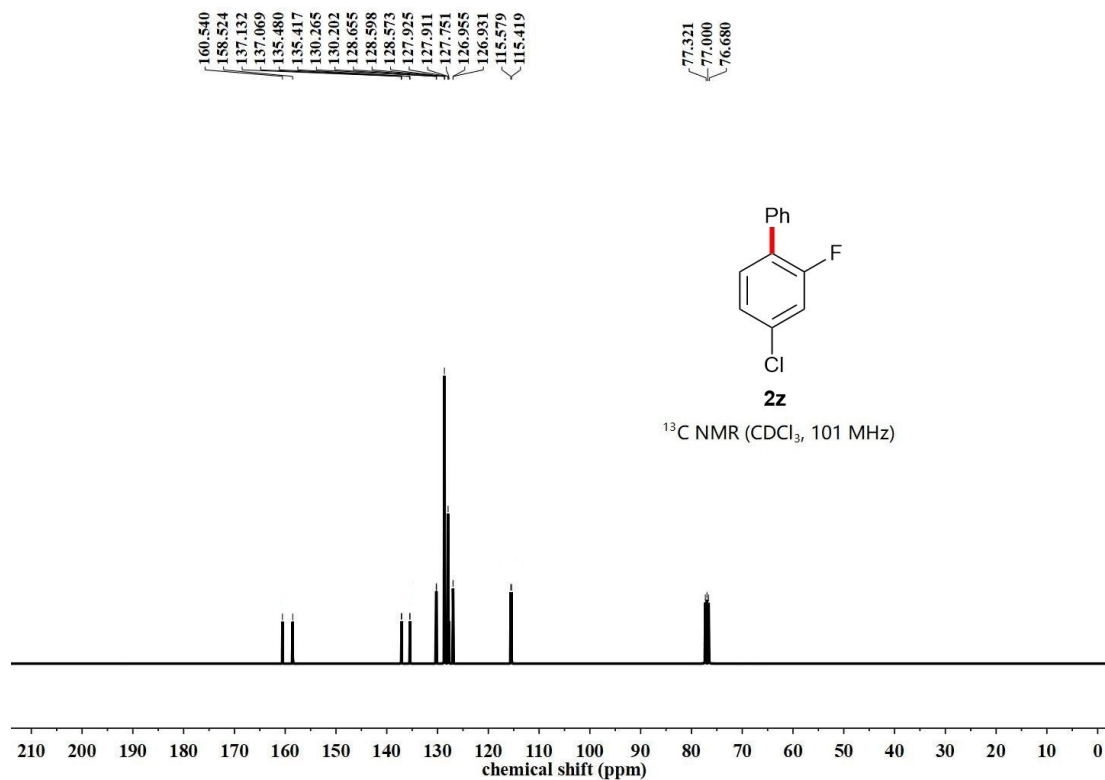
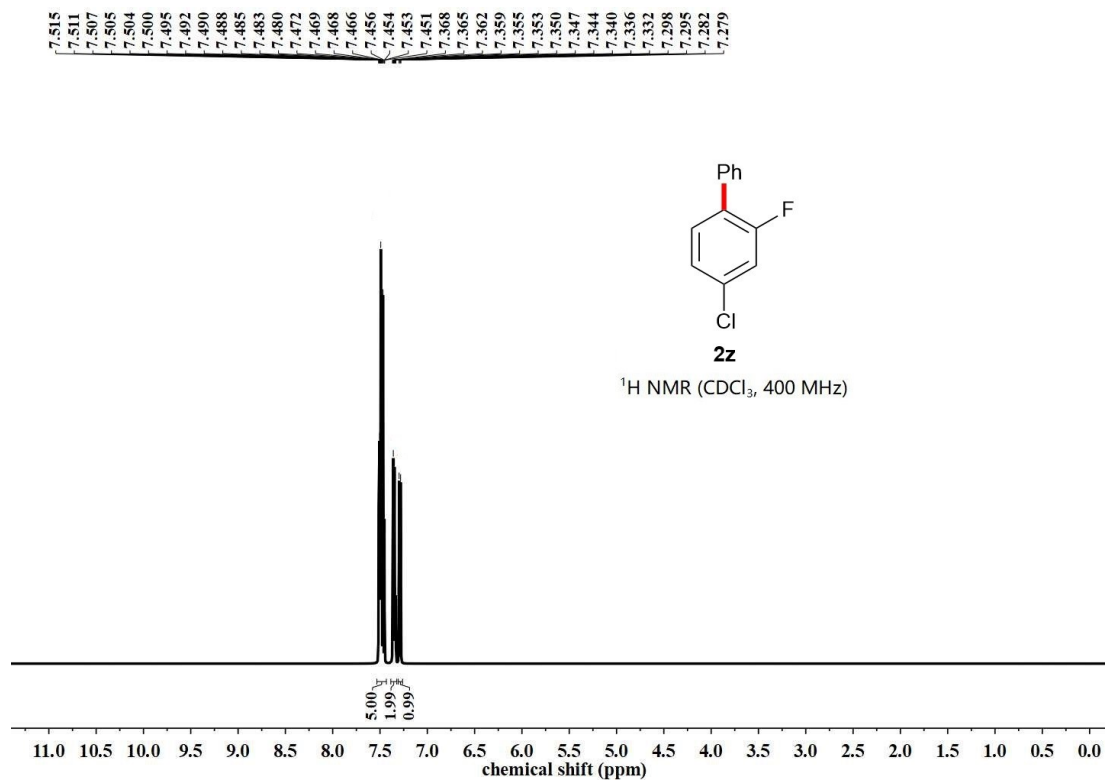


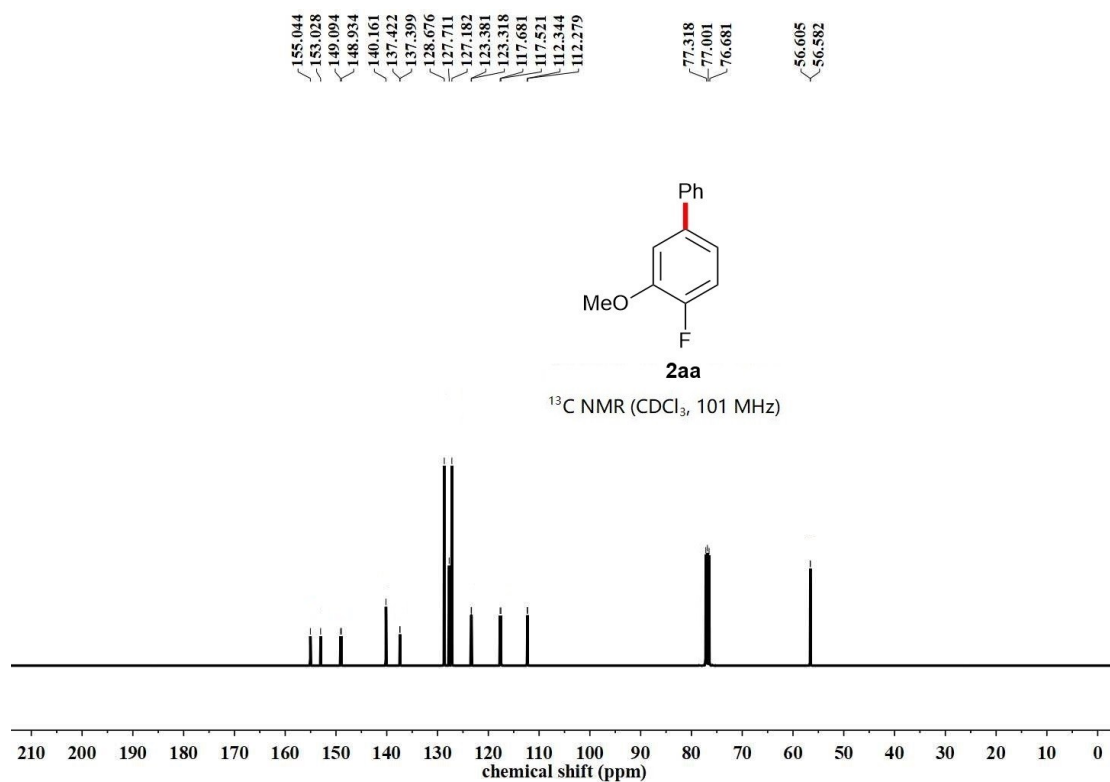
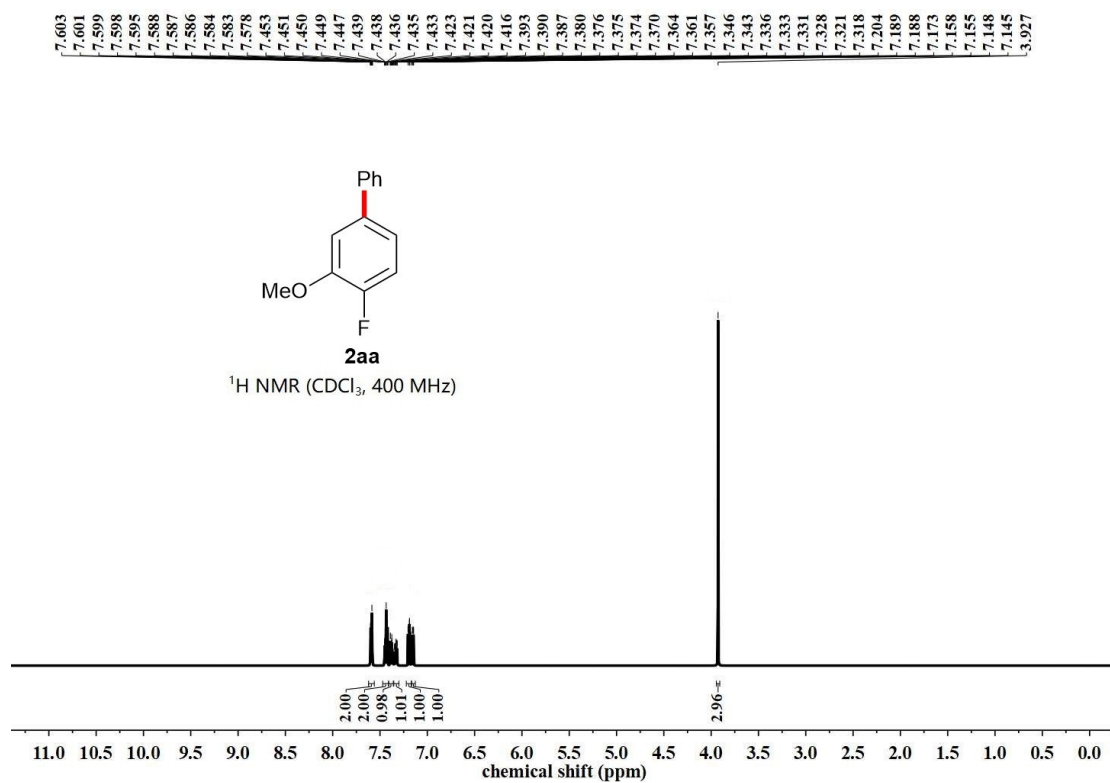
8.663
8.659
8.652
8.646
7.806
7.801
7.788
7.784
7.781
7.708
7.703
7.696
7.690
7.546
7.541
7.524
7.519
7.504
7.493
7.490
7.486
7.470
7.453
7.450

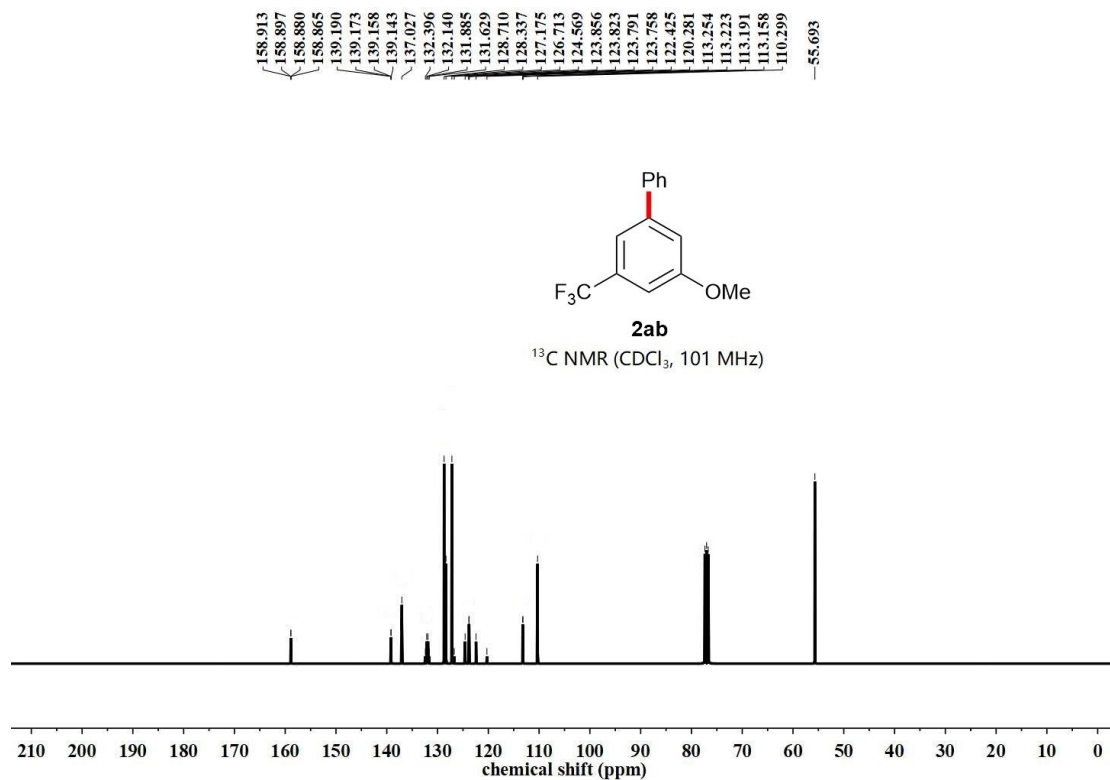
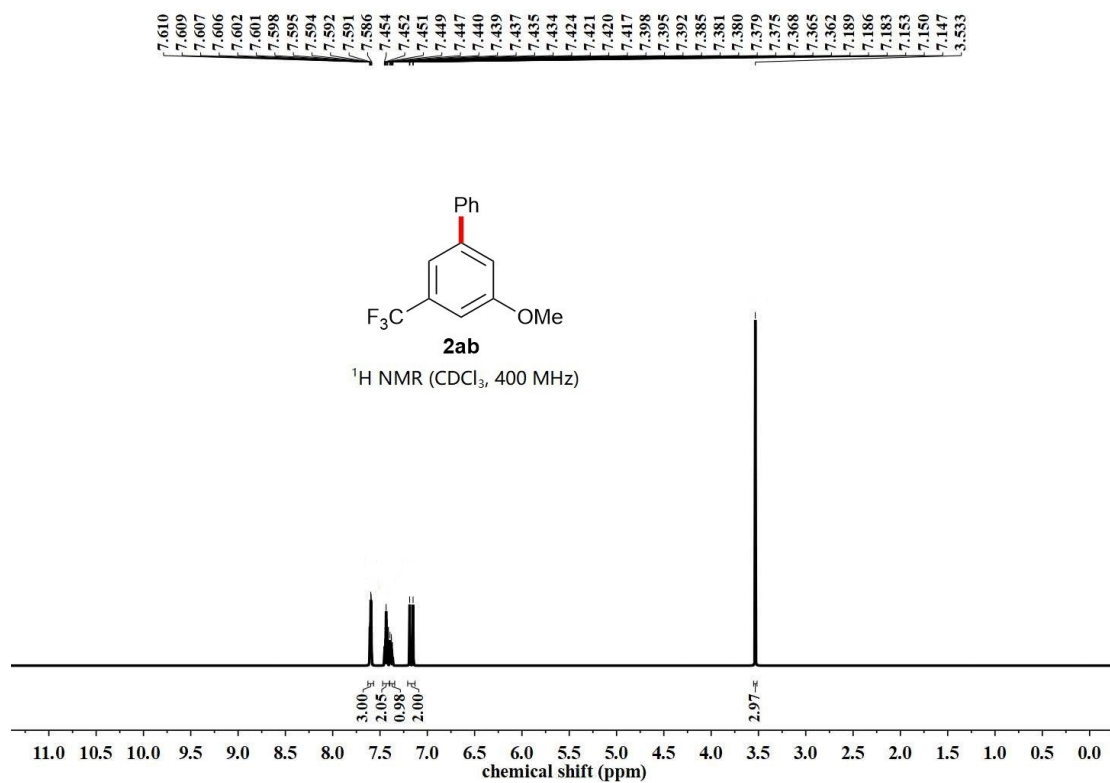


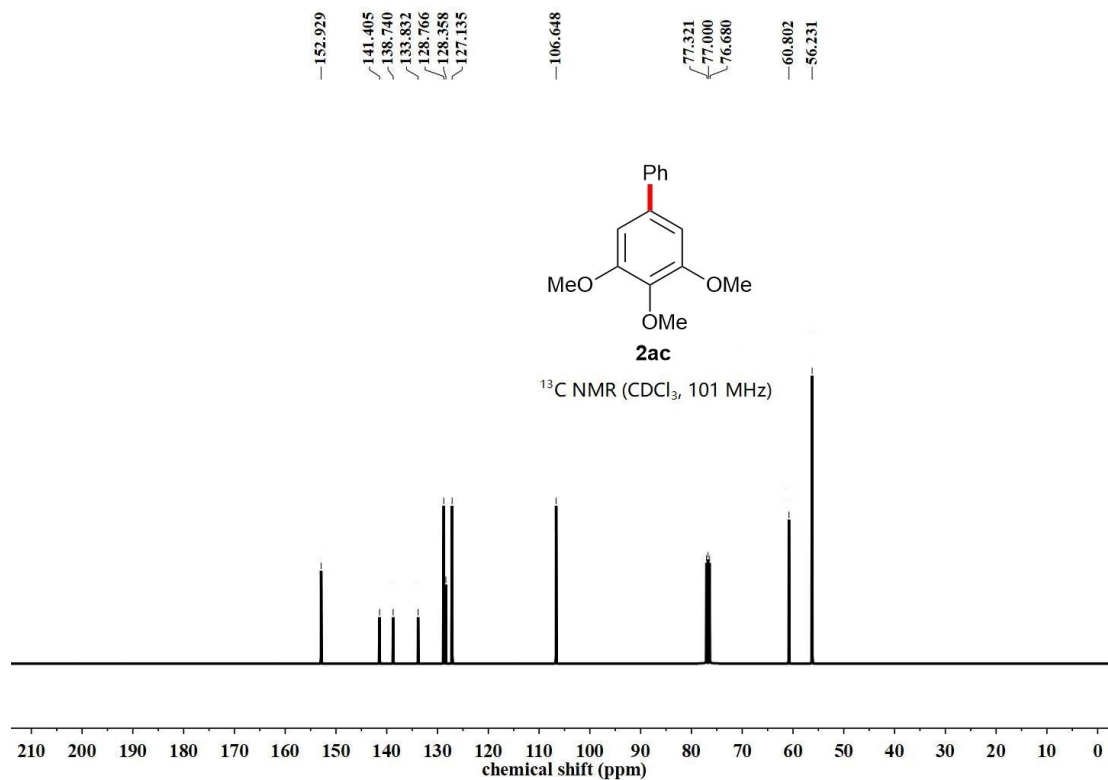
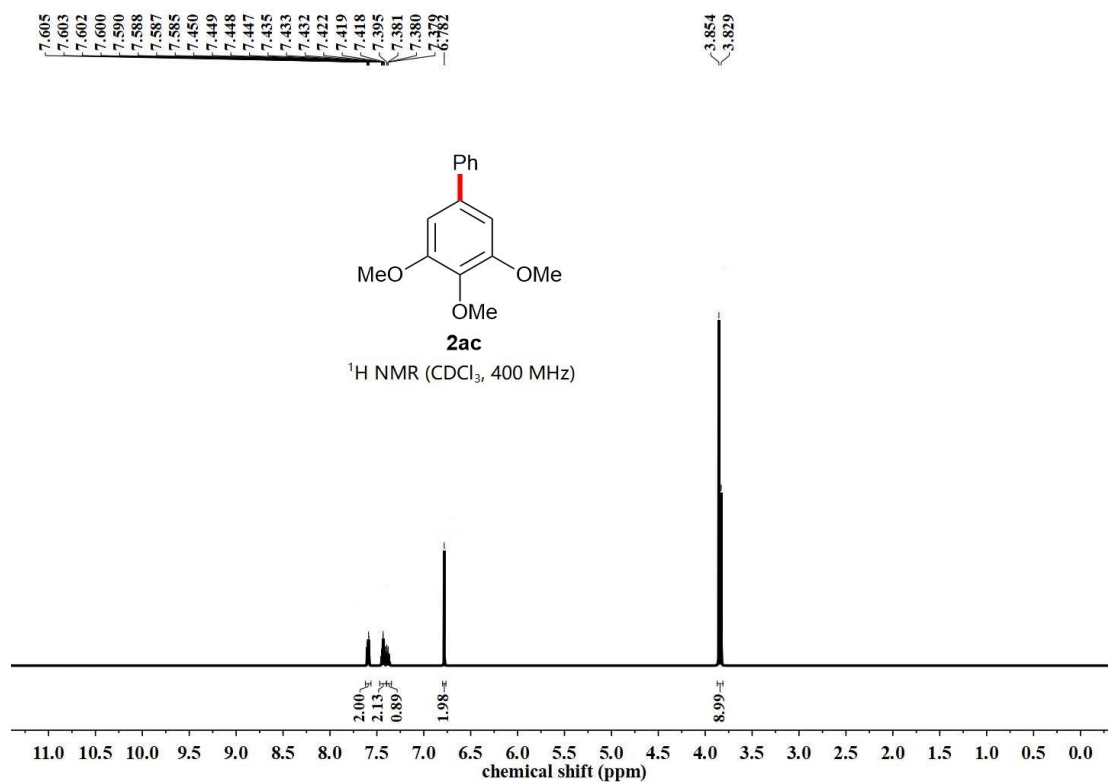
¹H NMR (DMSO-d₆, 400 MHz)

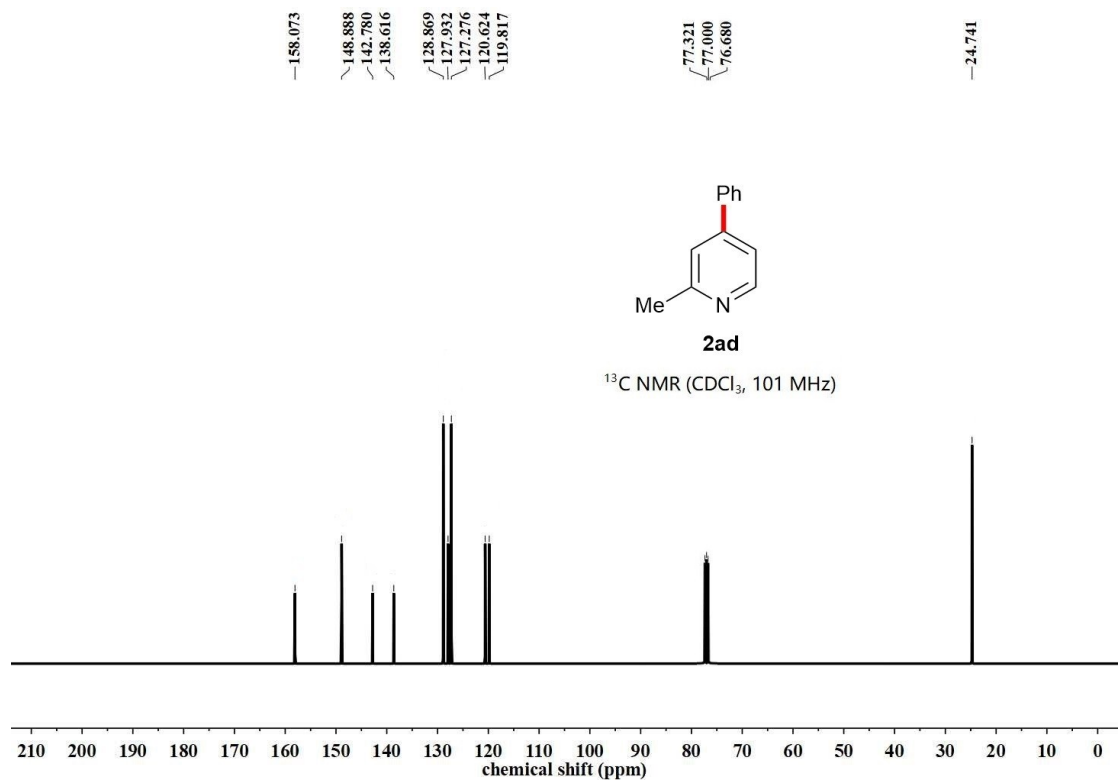
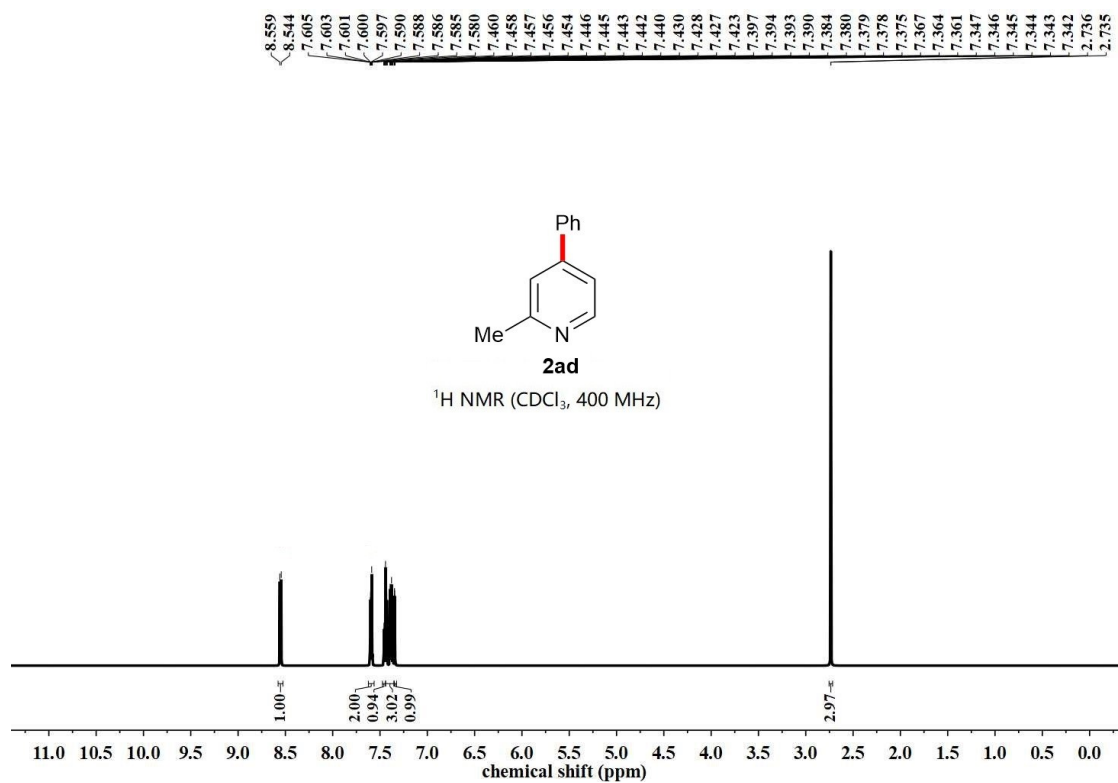


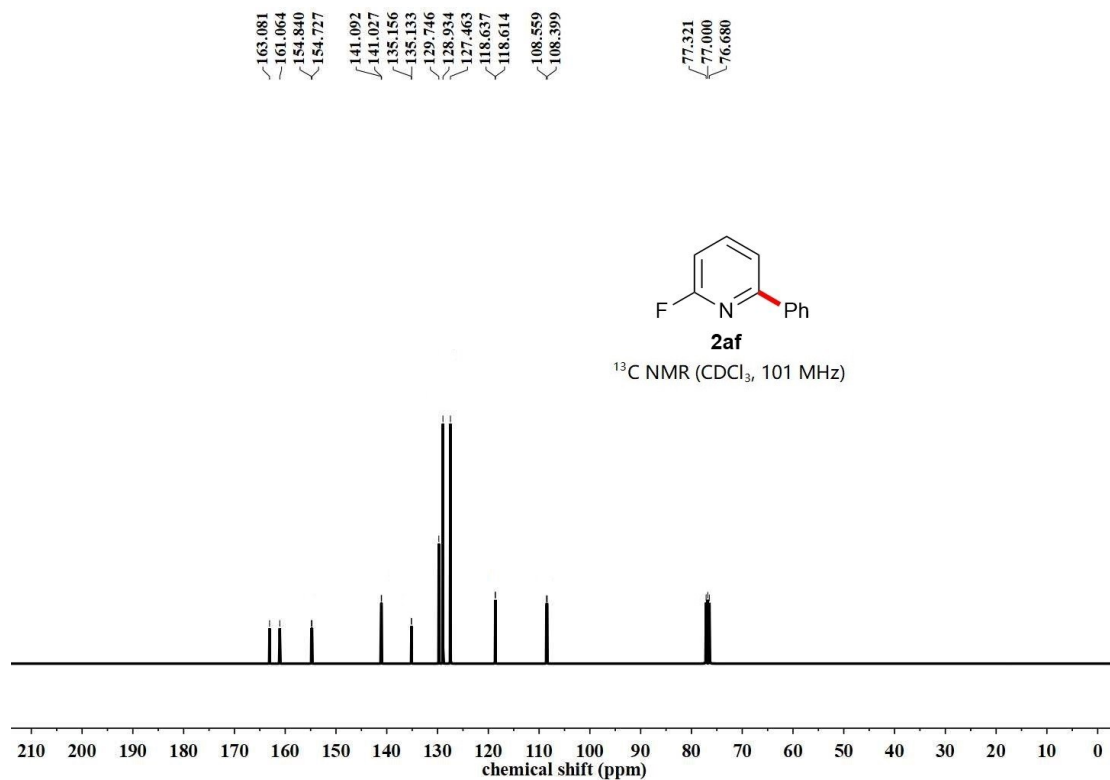
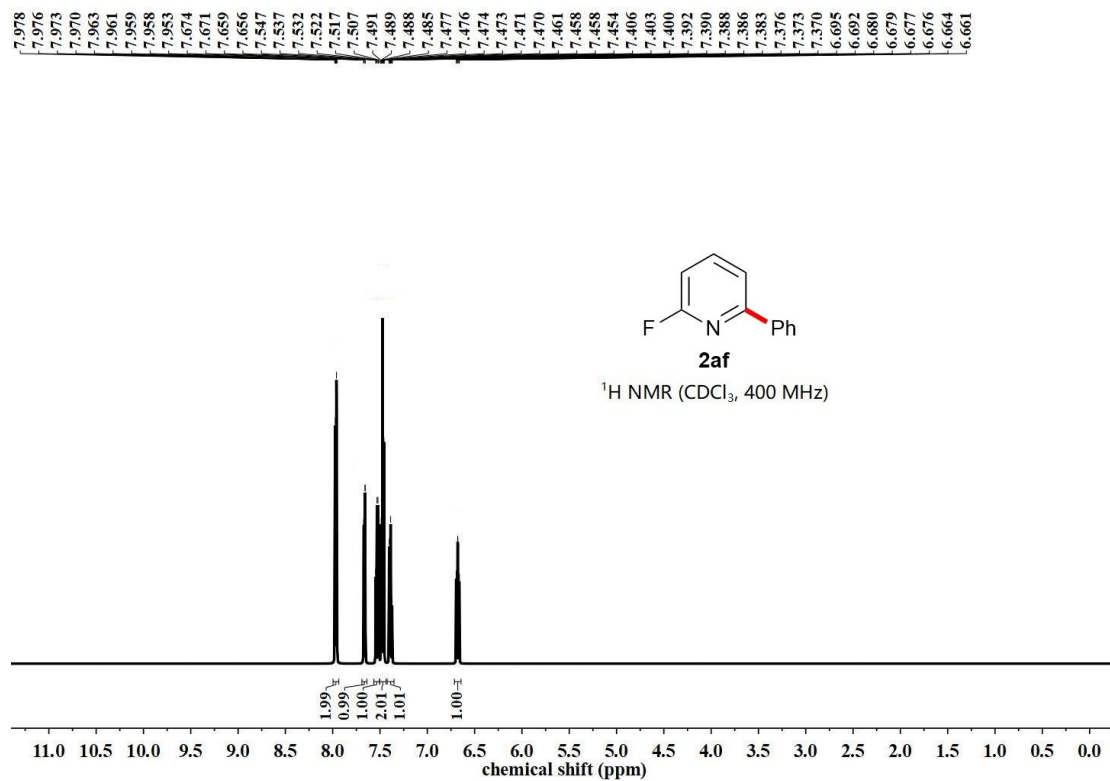




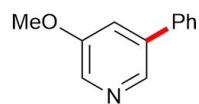






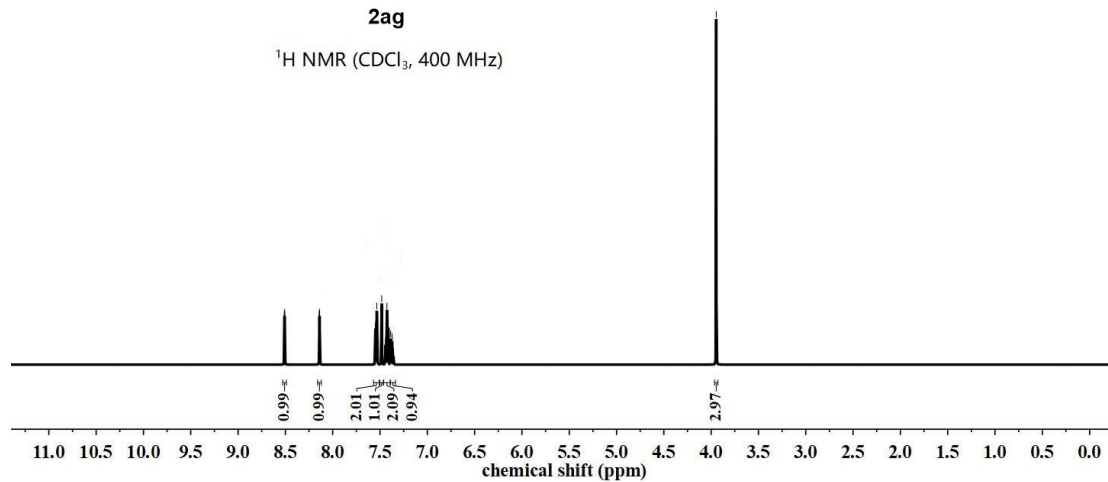


8.511
8.510
8.508
8.507
8.142
8.141
8.139
8.138
7.551
7.549
7.547
7.546
7.543
7.536
7.534
7.532
7.531
7.526
7.485
7.482
7.479
7.445
7.443
7.442
7.441
7.439
7.431
7.430
7.428
7.427
7.425
7.415
7.413
7.412
7.408
7.390
7.387
7.384
7.378
7.373
7.372
7.371
7.367
7.361
7.358
7.355
5.946

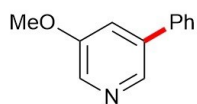


2ag

¹H NMR (CDCl₃, 400 MHz)



155.468
143.631
135.501
135.330
134.212
129.025
127.885
127.846
113.288
77.318
77.001
76.081
55.838



2ag

¹³C NMR (CDCl₃, 101 MHz)

