Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Preparation and in vitro bioactivity evaluation of N-heterocyclic linked dihomooxacalix[4]arene derivatives

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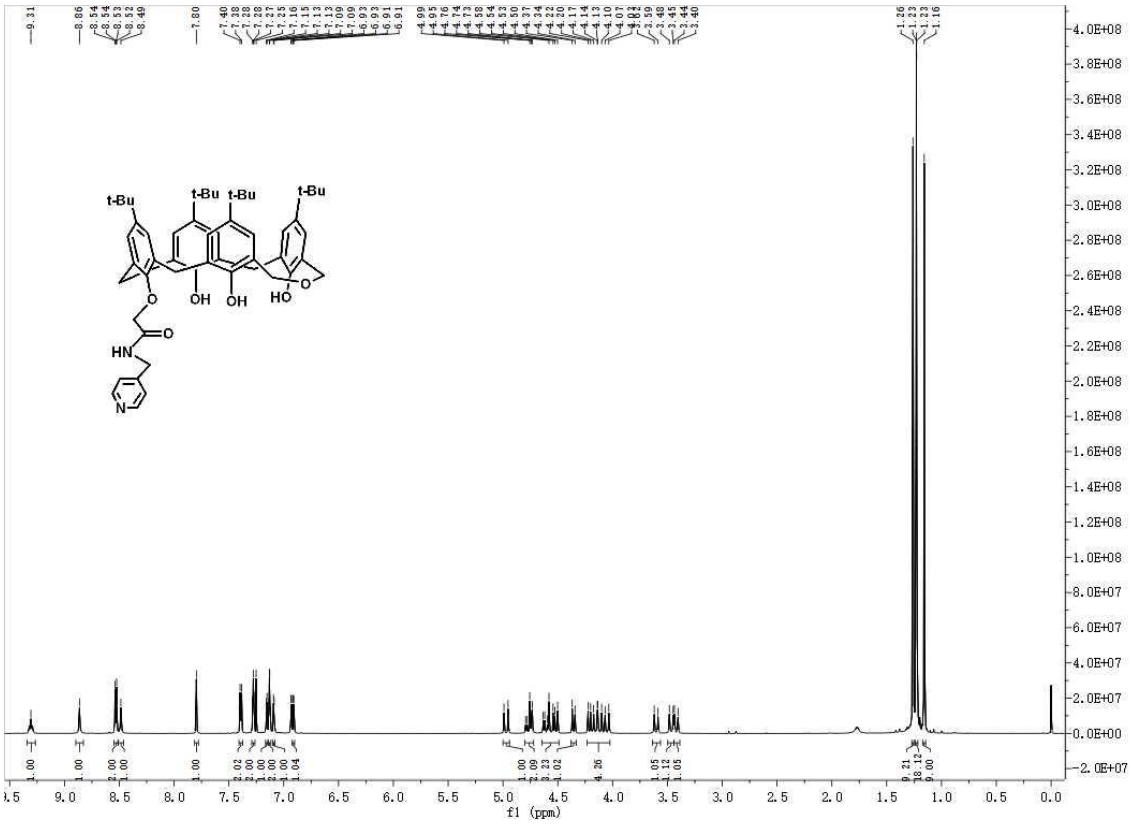
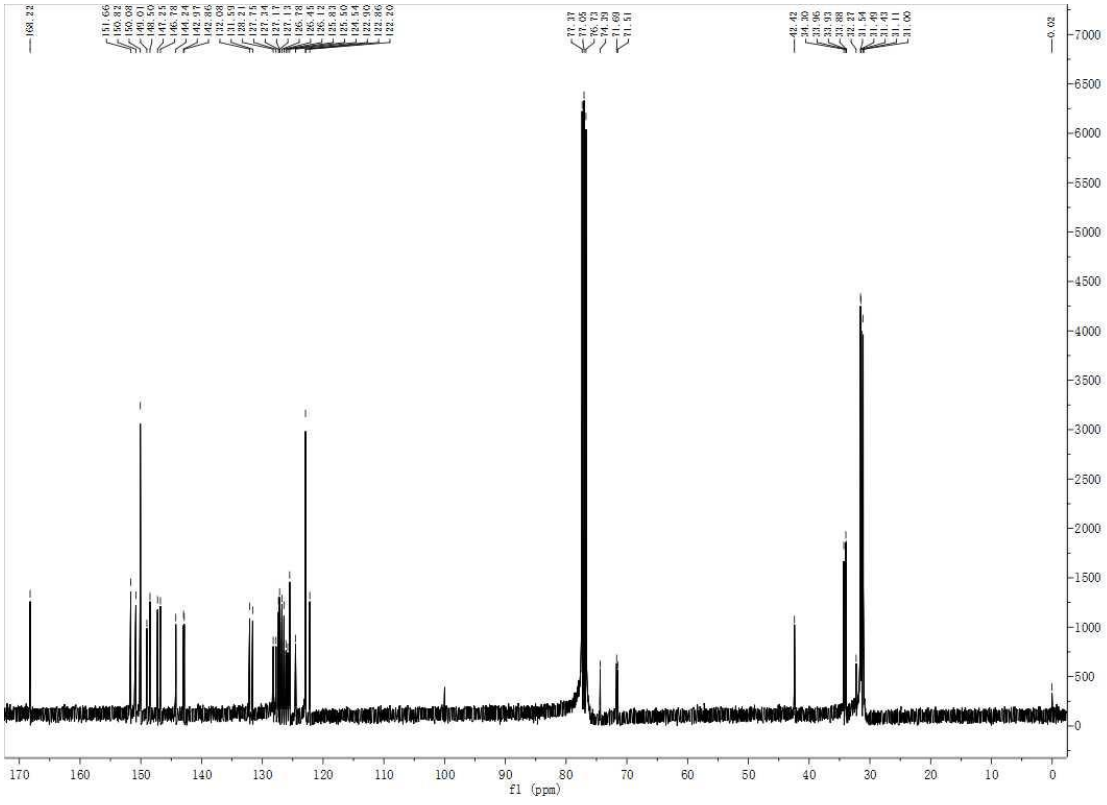
The supporting information provides the ^{1}H NMR, ^{13}C NMR and HRMS spectra ofl compounds **4a-4n**. All compounds were dissolved in $CDCl_3$ or DMSO-*d*6 and the ^{1}H and ^{13}C NMR spectra were recorded at 400 MHz on a Bruker AV-400 spectrometer. HRMS data were obtained using a (UHR-TOF) maXis 4G instrument.

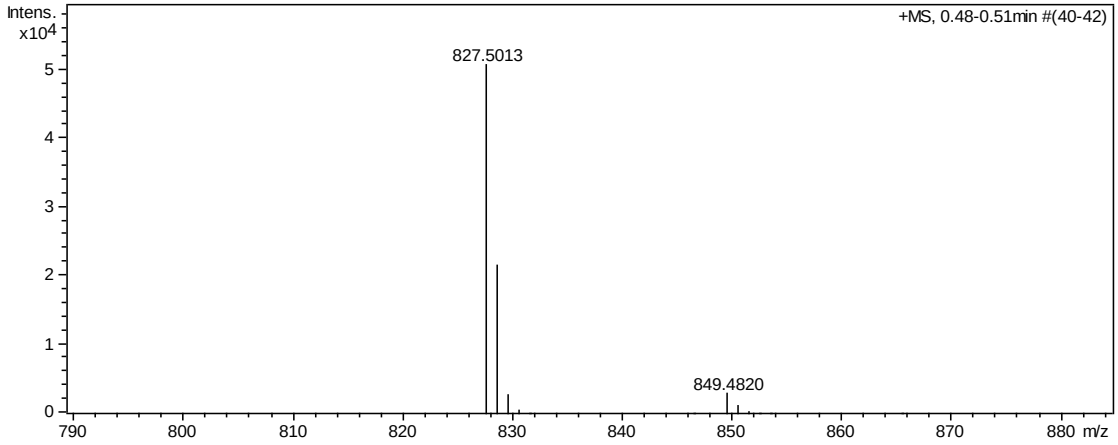
^{1}H NMR **of 4a**



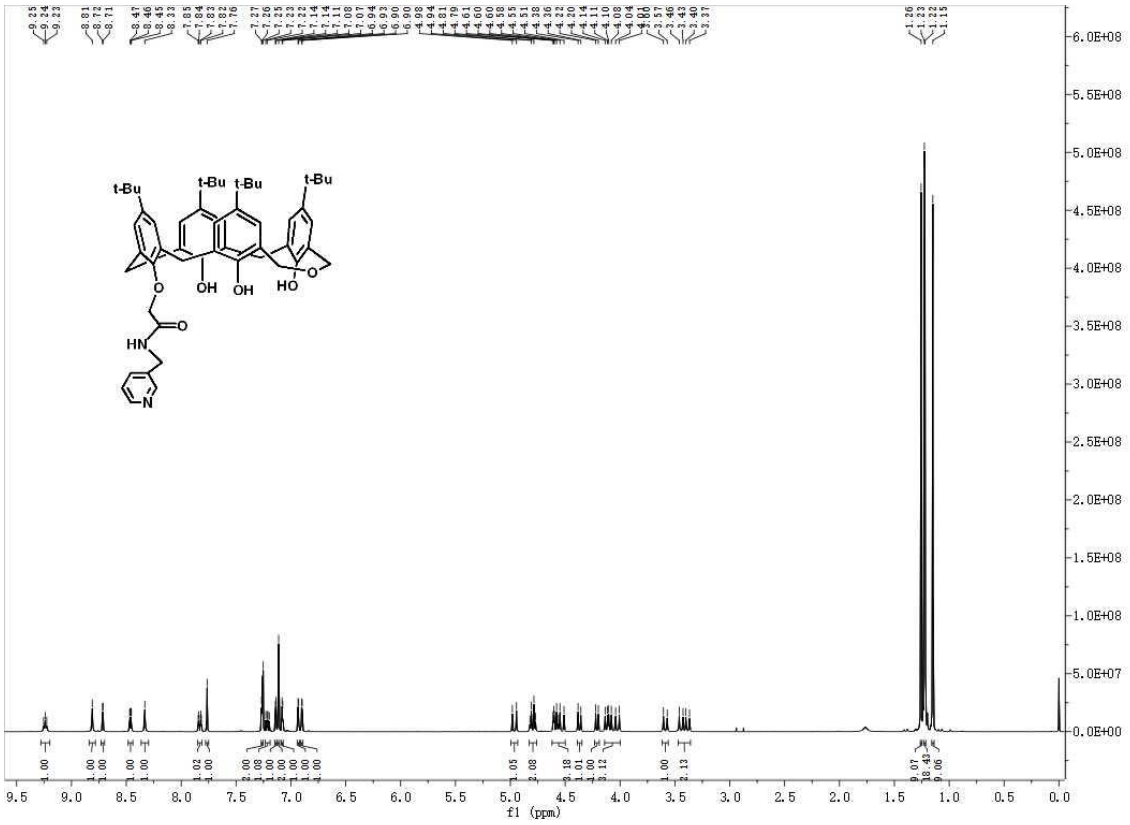
^{13}C NMR of **4a**



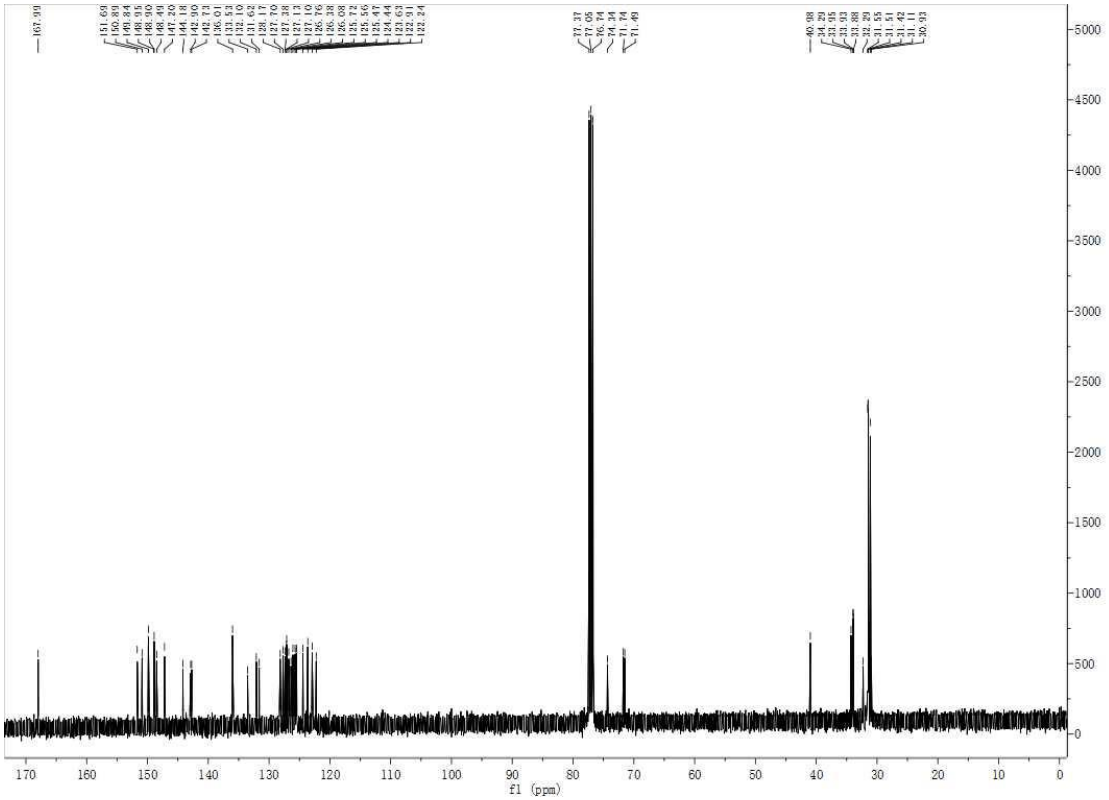
HRMS of **4a**


Intens.
x10^4
+MS, 0.48-0.51min #(40-42)
827.5013
849.4820
0
1
2
3
4
5
790
800
810
820
830
840
850
860
870
880
m/z

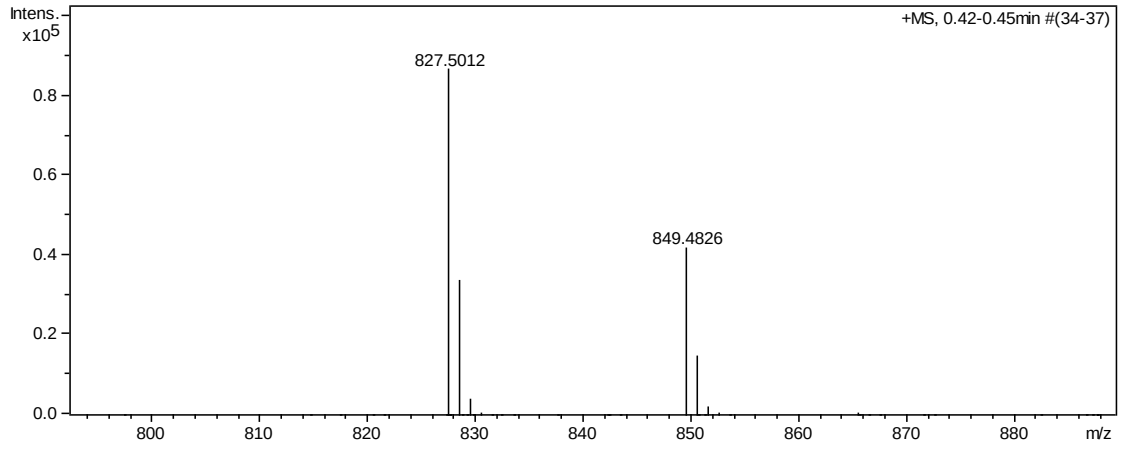
^{1}H NMR of **4b**



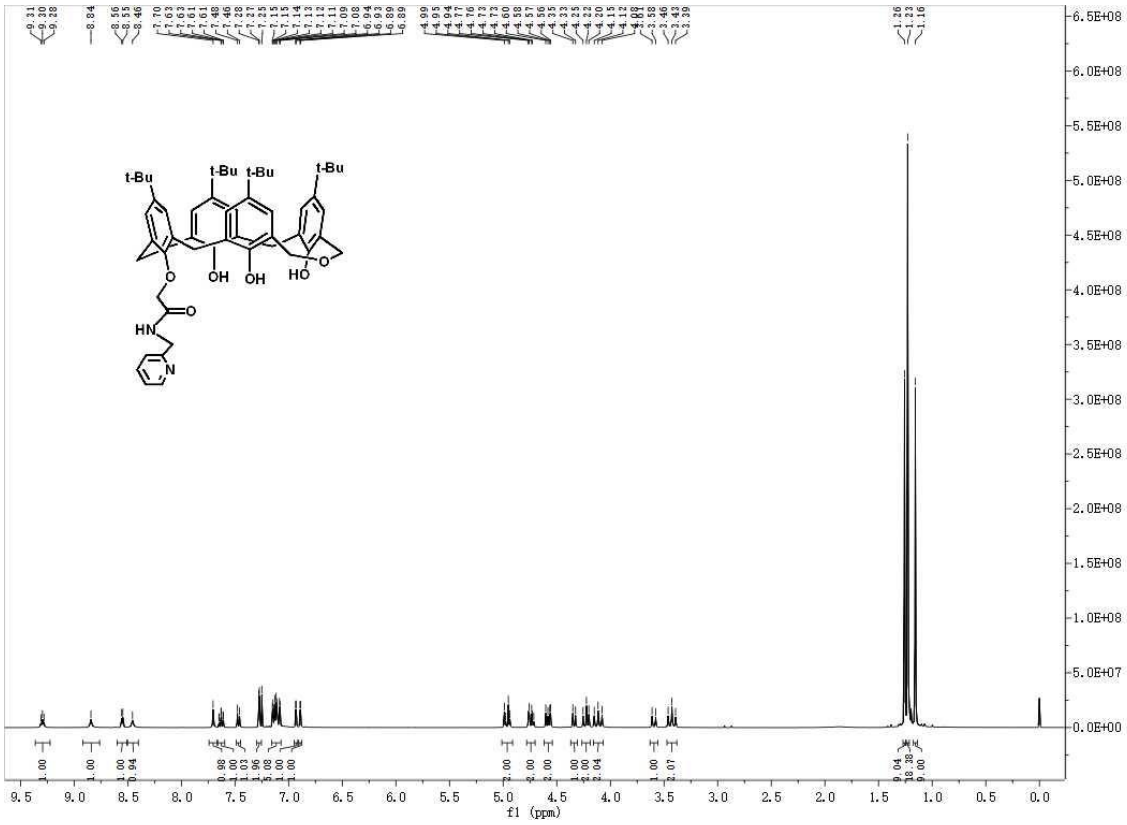
^{13}C NMR of **4b**



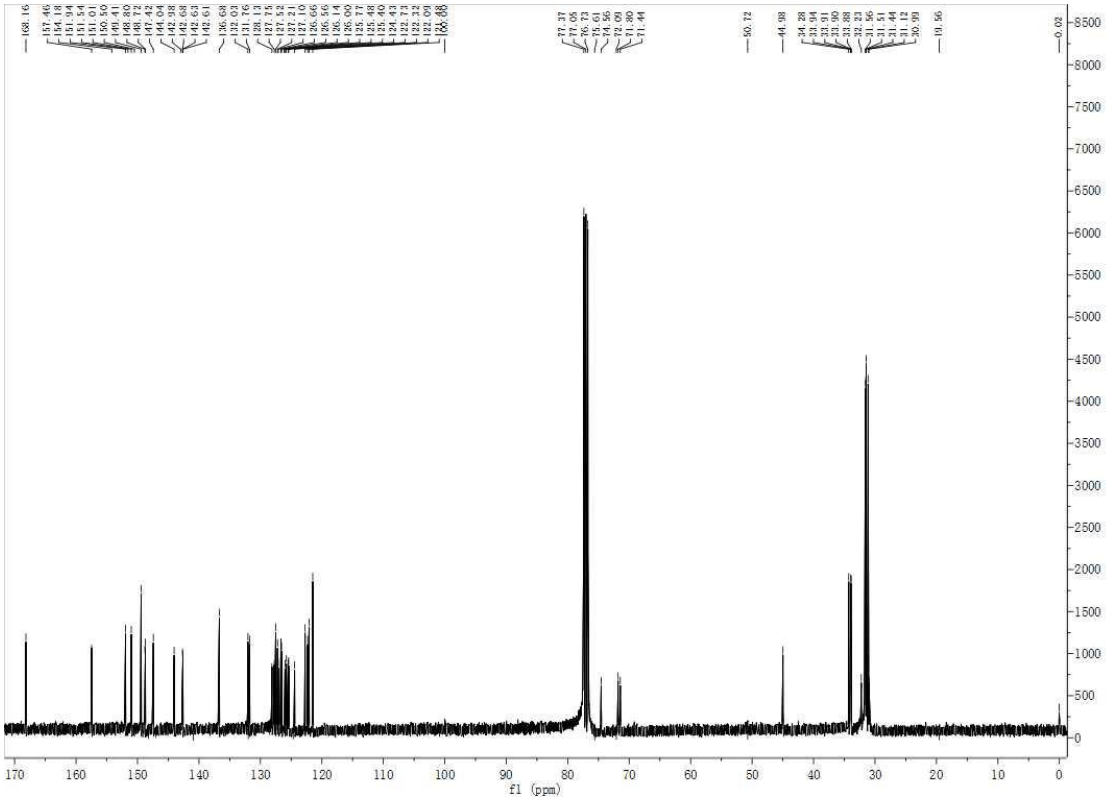
HRMS of **4b**


Intens.
x10^5
+MS, 0.42-0.45min #(34-37)
827.5012
849.4826
0.8
0.6
0.4
0.2
0.0
800
810
820
830
840
850
860
870
880
m/z

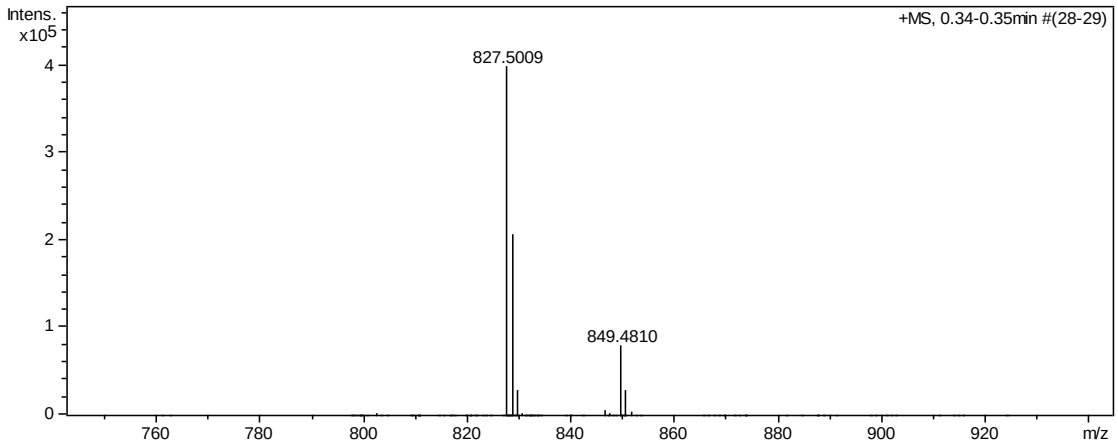
^{1}H NMR of **4c**



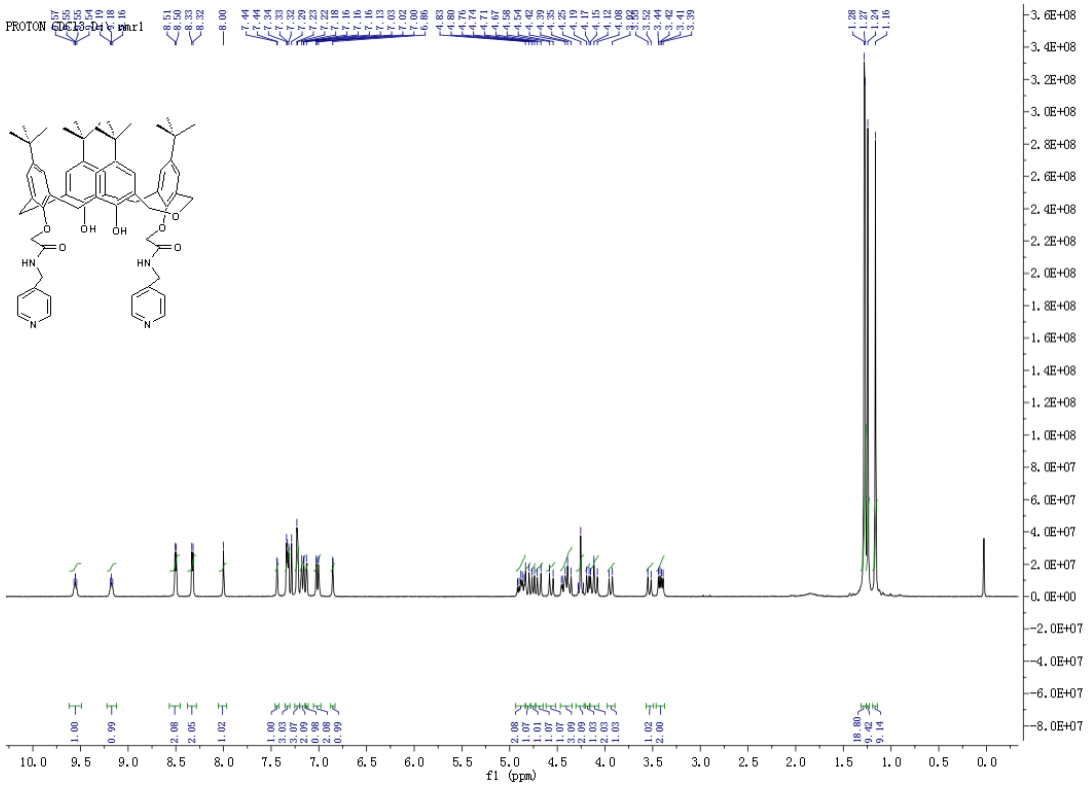
^{13}C NMR of **4c**



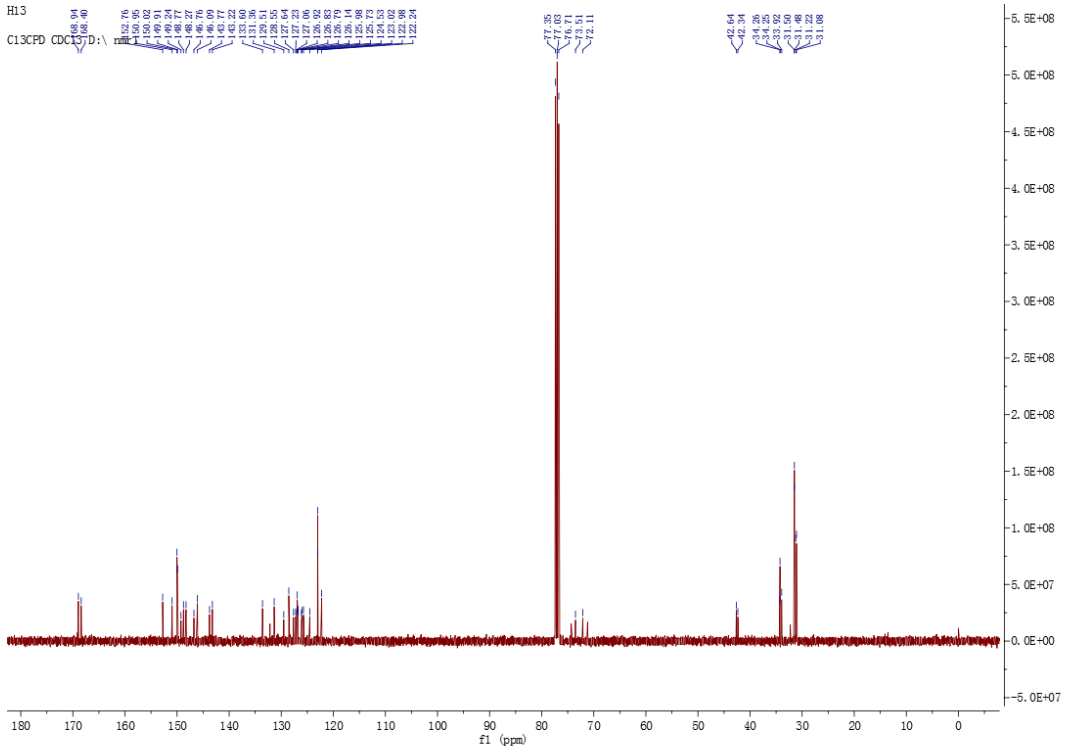
HRMS of **4c**


Intens.
x10^5
+MS, 0.34-0.35min #(28-29)
827.5009
849.4810
4
3
2
1
0
760
780
800
820
840
860
880
900
920
m/z

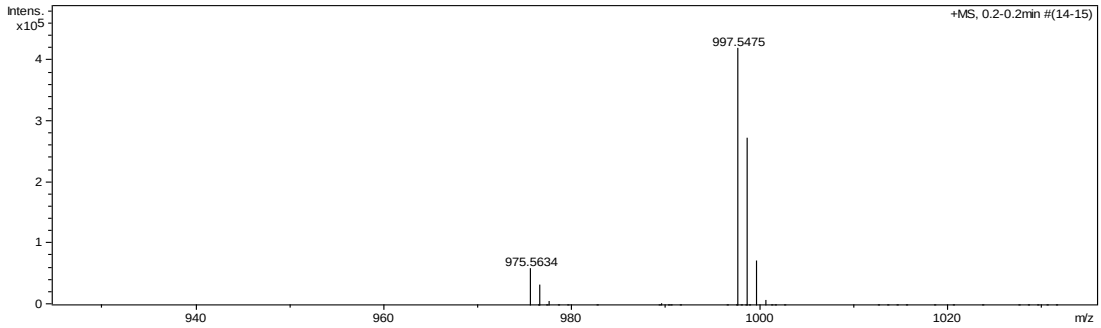
^{1}H NMR of **4d**



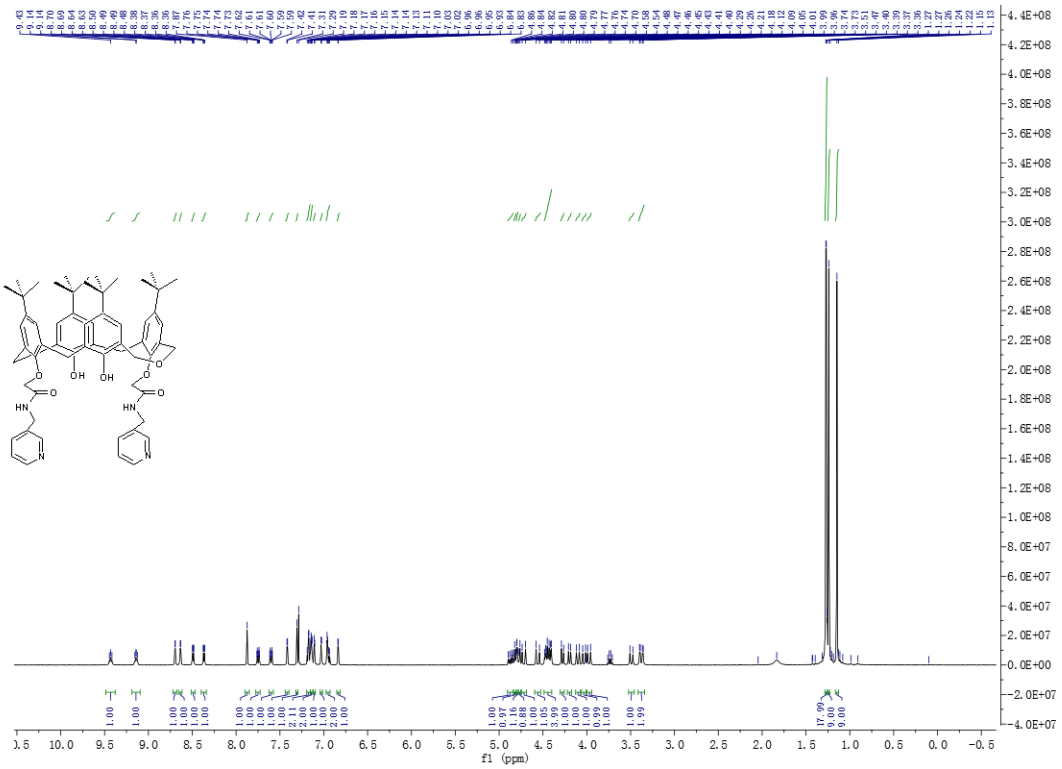
^{13}C NMR of **4d**



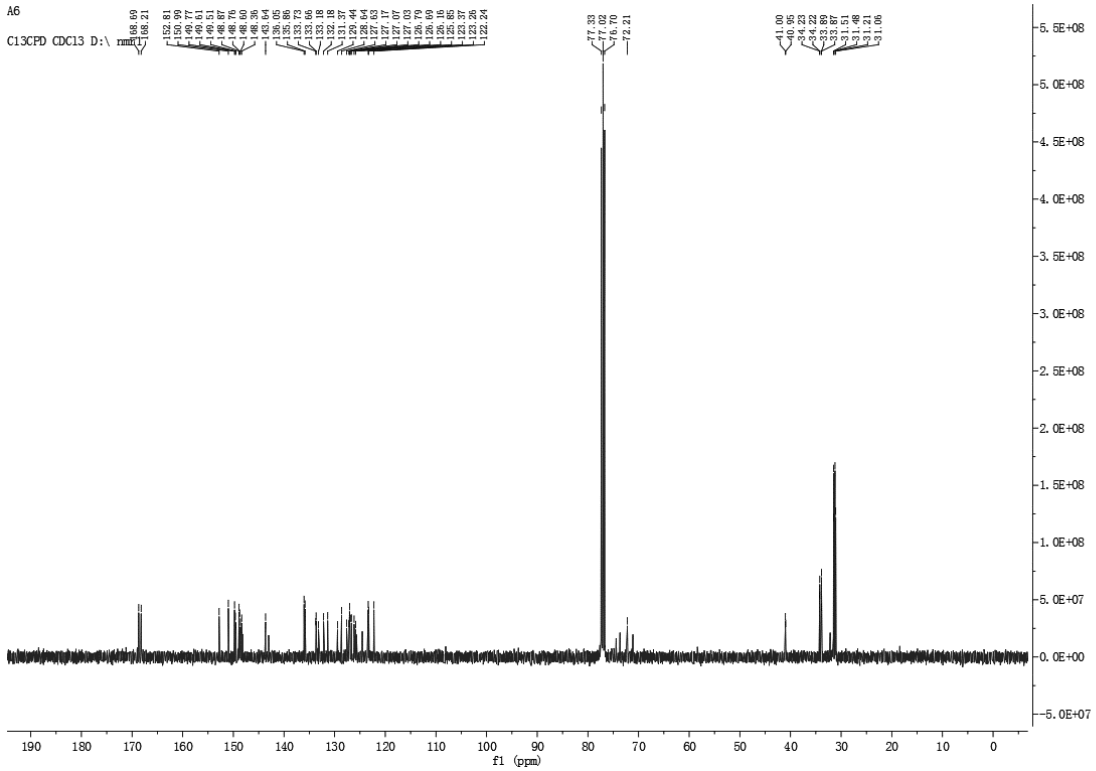
HRMS of **4d**


Intens.
x10^5
+MS, 0.2-0.2min #(14-15)
997.5475
975.5634
4
3
2
1
0
940
960
980
1000
1020
m/z

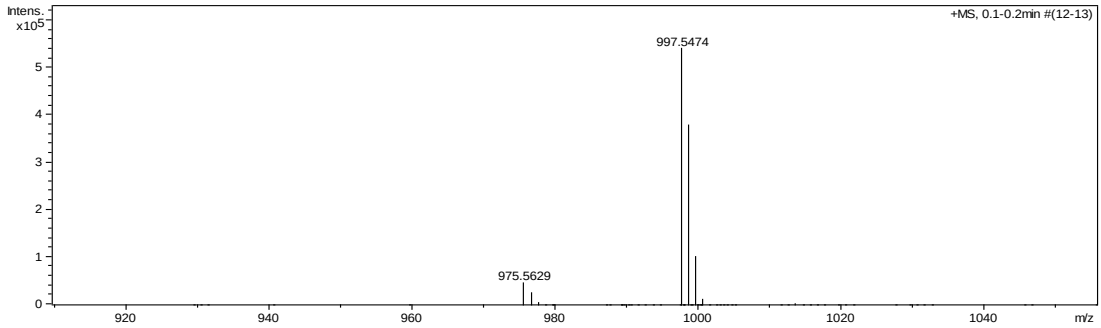
^{1}H NMR of **4e**



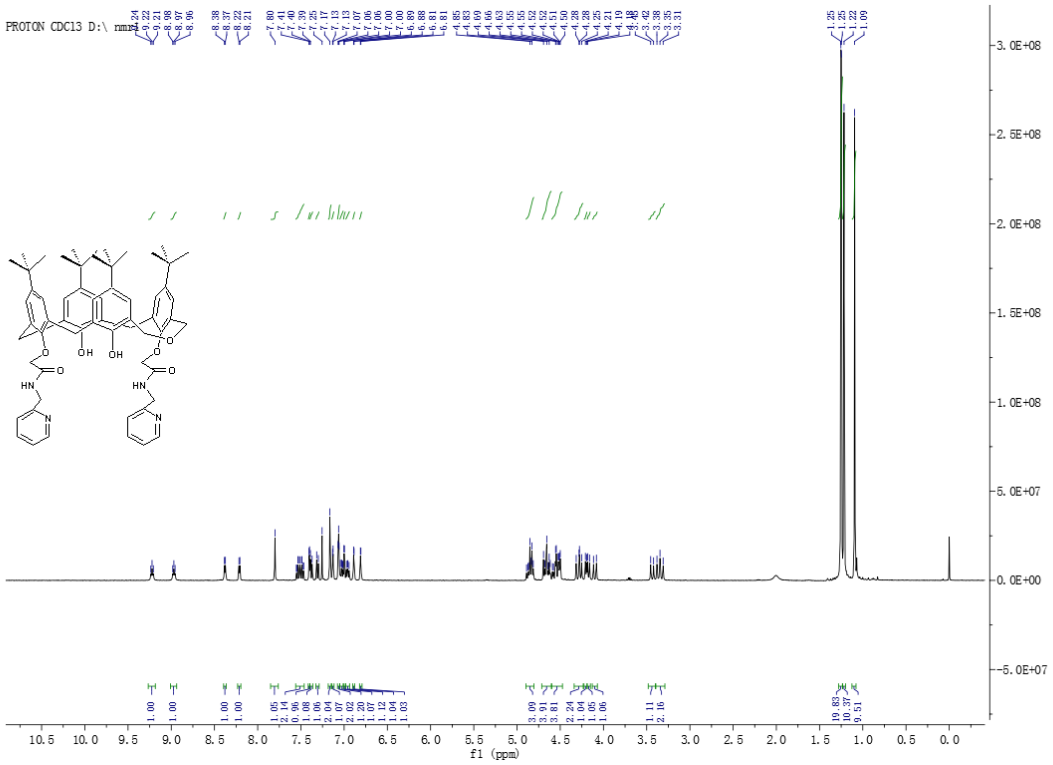
^{13}C NMR of **4e**



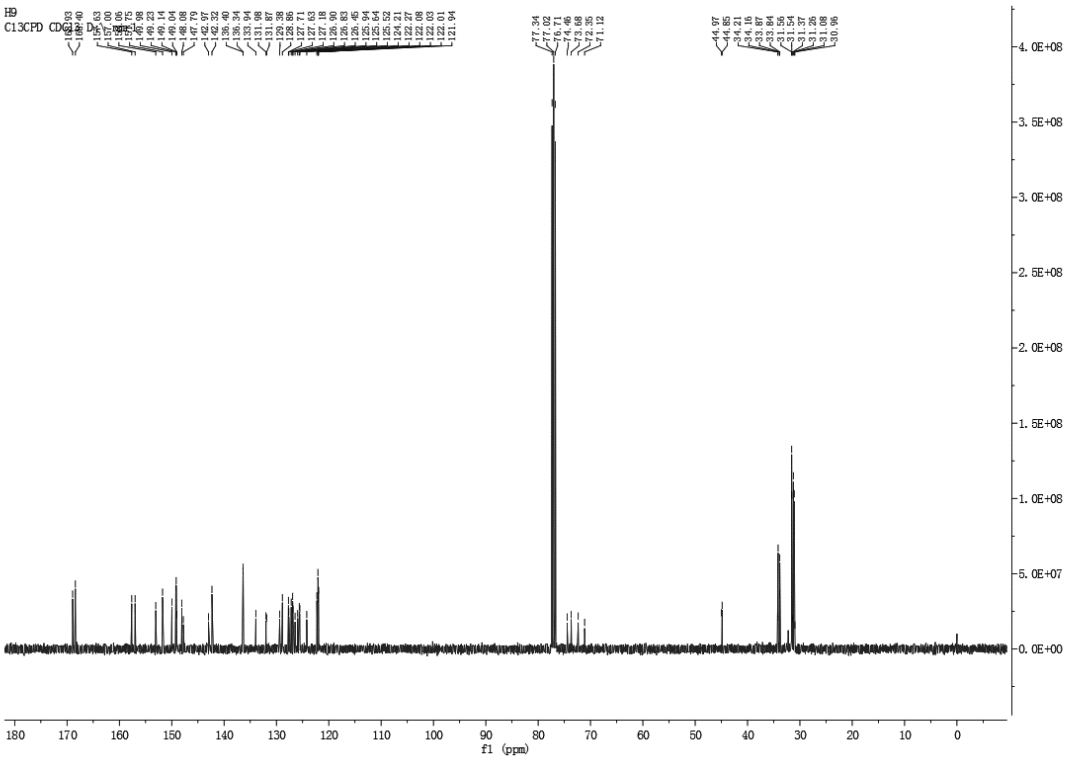
HRMS of **4e**


Intens.
x10^5
+MS, 0.1-0.2min #(12-13)
997.5474
975.5629
0
1
2
3
4
5
920
940
960
980
1000
1020
1040
m/z

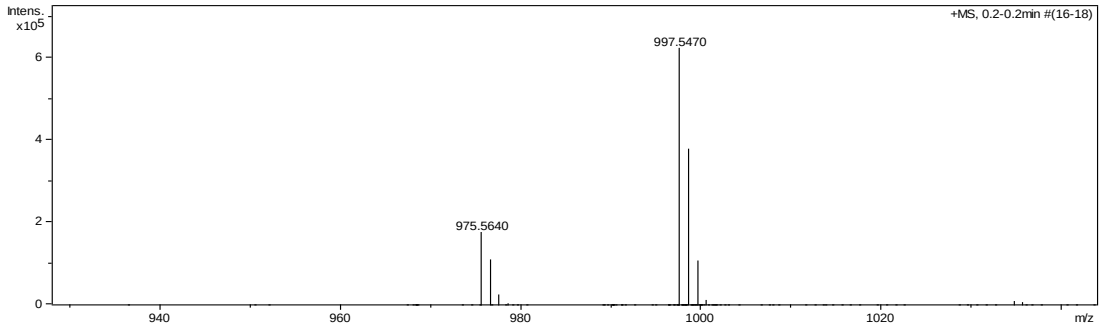
^{1}H NMR of **4f**



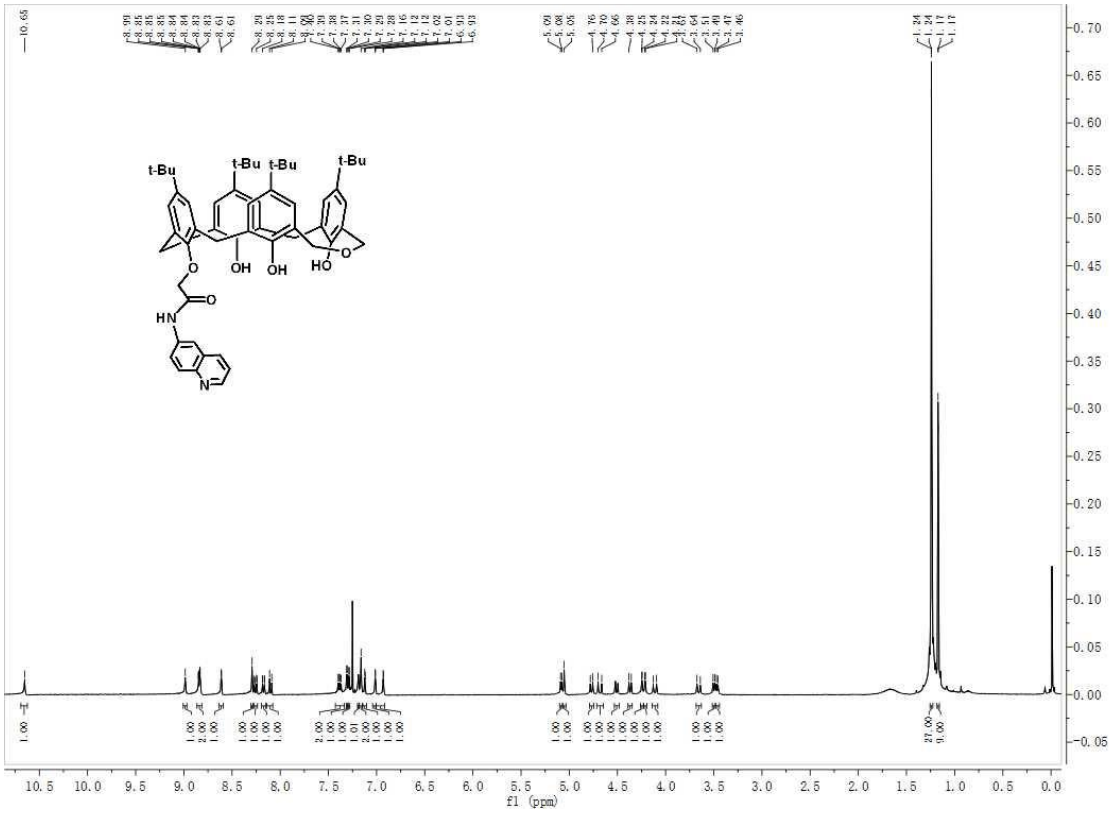
^{13}C NMR of **4f**



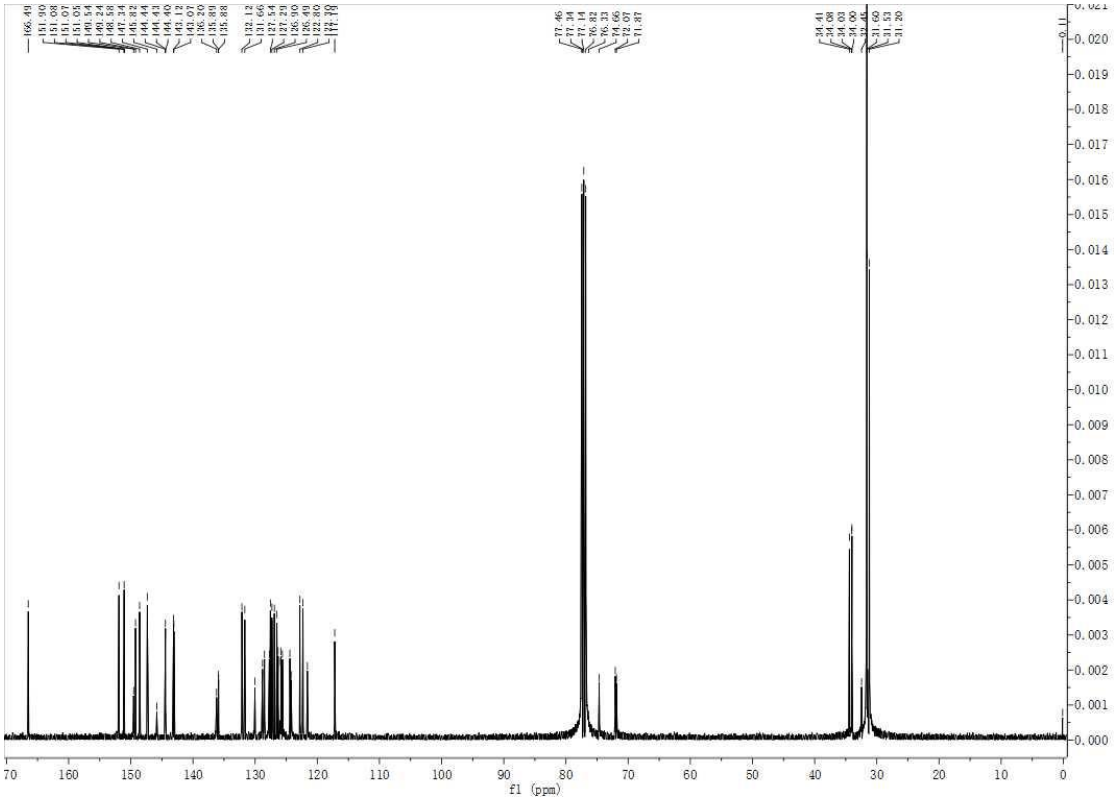
HRMS of **4f**


Intens.
x10^5
+MS, 0.2-0.2min #(16-18)
997.5470
975.5640
6
4
2
0
940
960
980
1000
1020
m/z

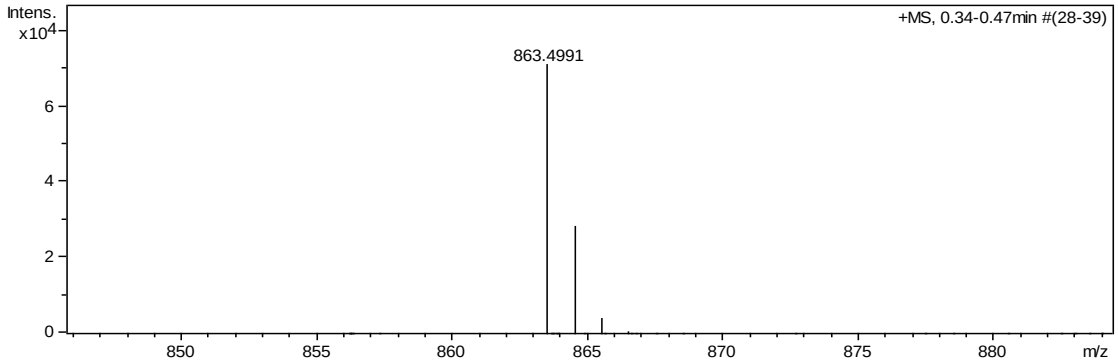
^{1}H NMR of **4g**



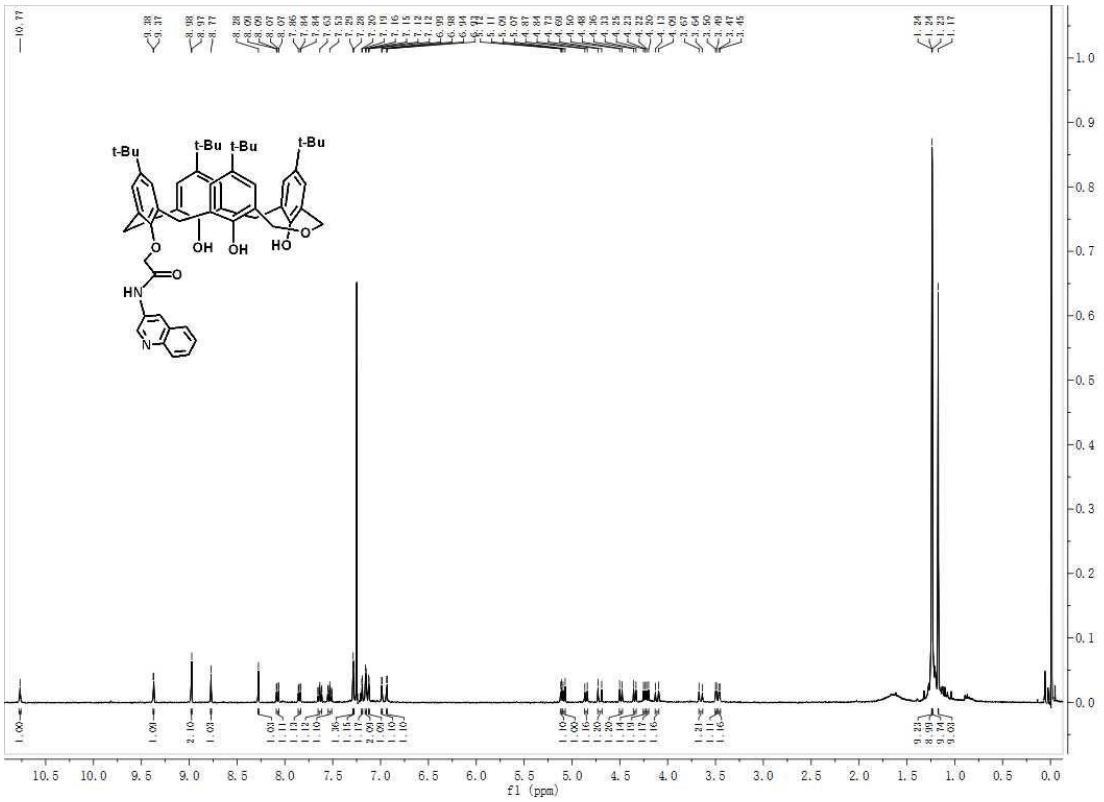
^{13}C NMR of **4g**



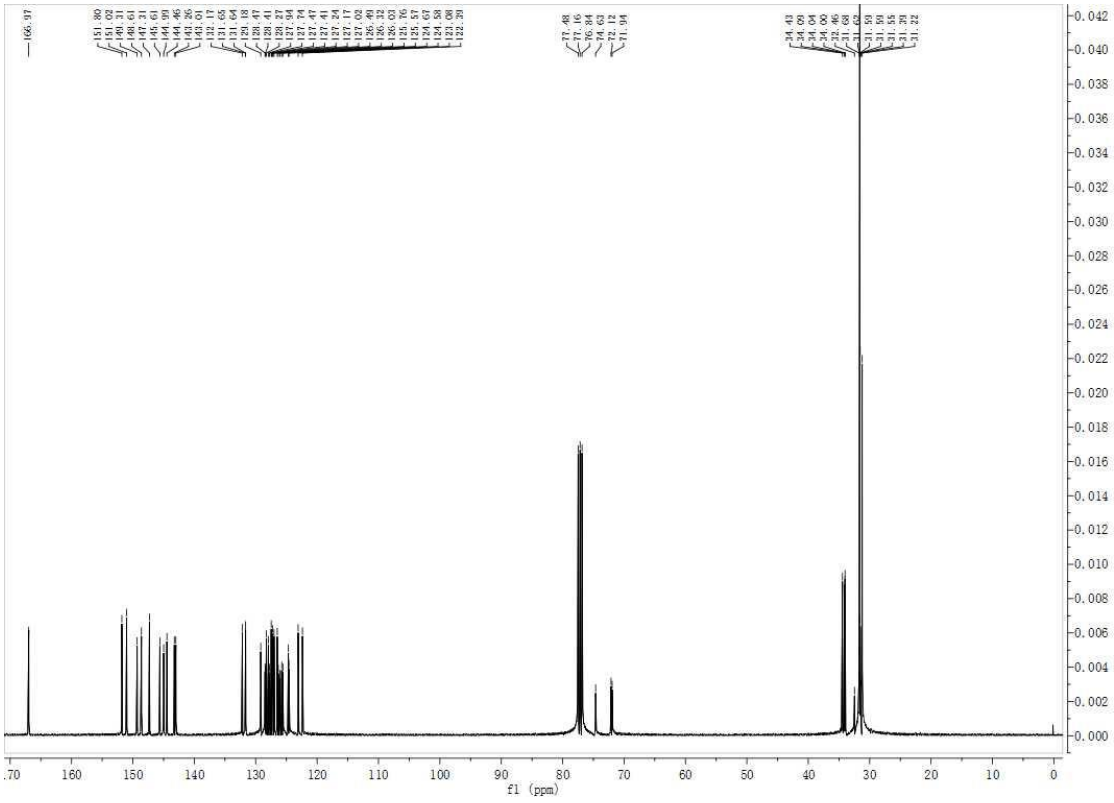
HRMS of **4g**


Intens.
x10^4
+MS, 0.34-0.47min #(28-39)
863.4991
6
4
2
0
850
855
860
865
870
875
880
m/z

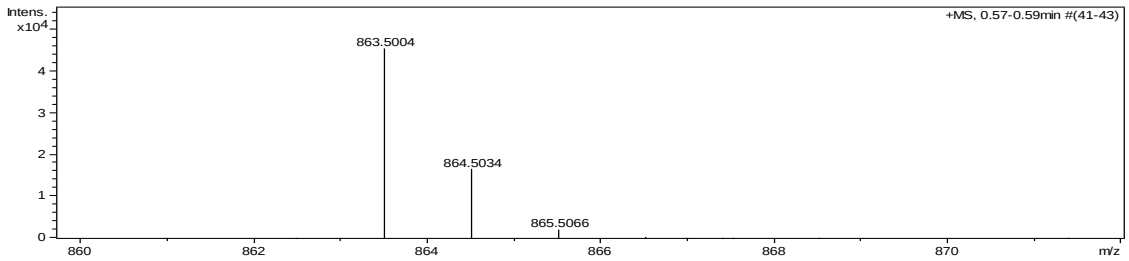
^{1}H NMR of **4h**



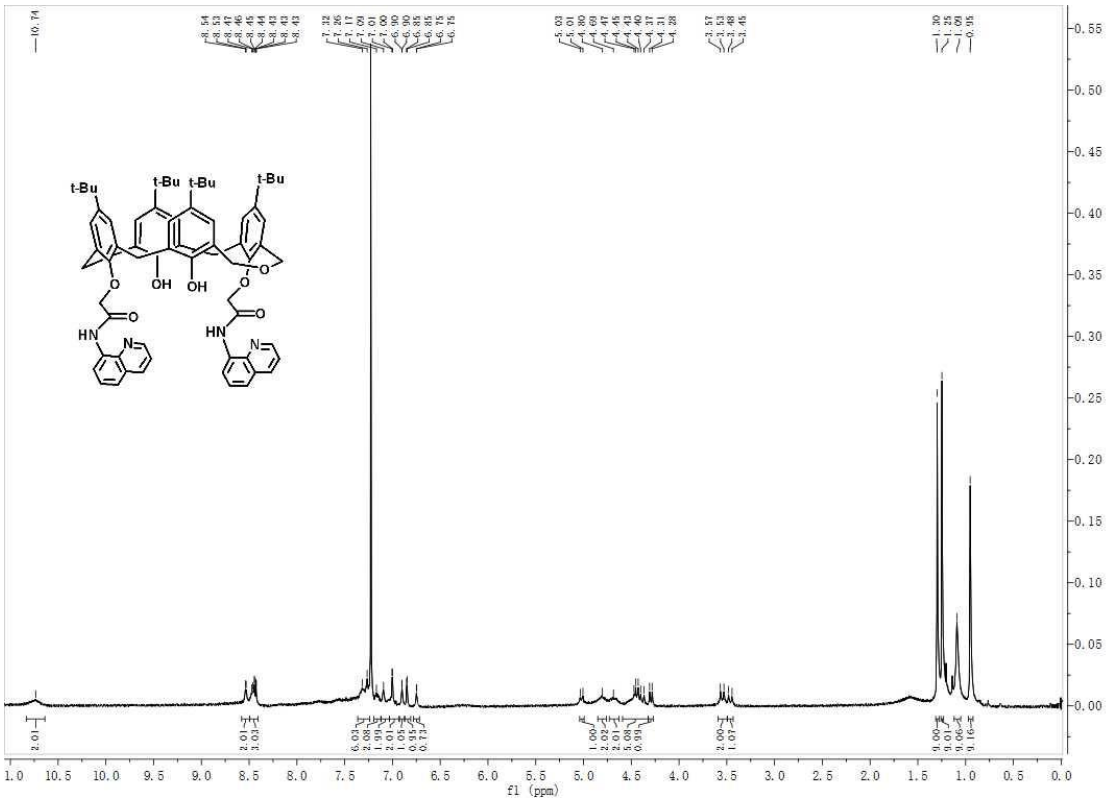
^{13}C NMRof **4h**



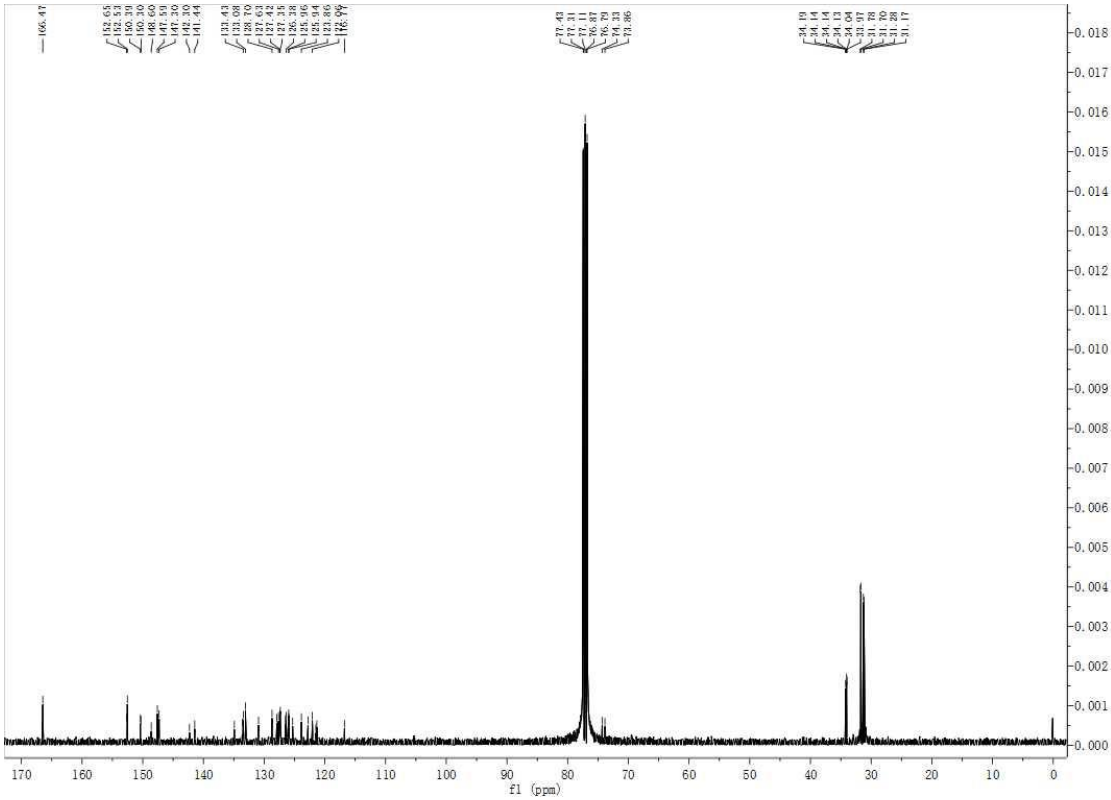
HRMS of **4h**


Intens.
x10^4
+MS, 0.57-0.59min #(41-43)
863.5004
864.5034
865.5066
0
1
2
3
4
860
862
864
866
868
870
m/z

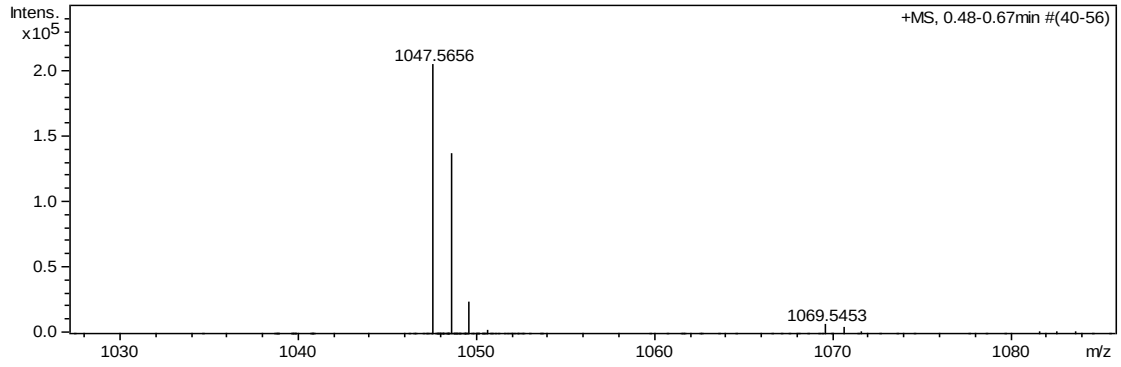
^{1}H NMR of **4i**



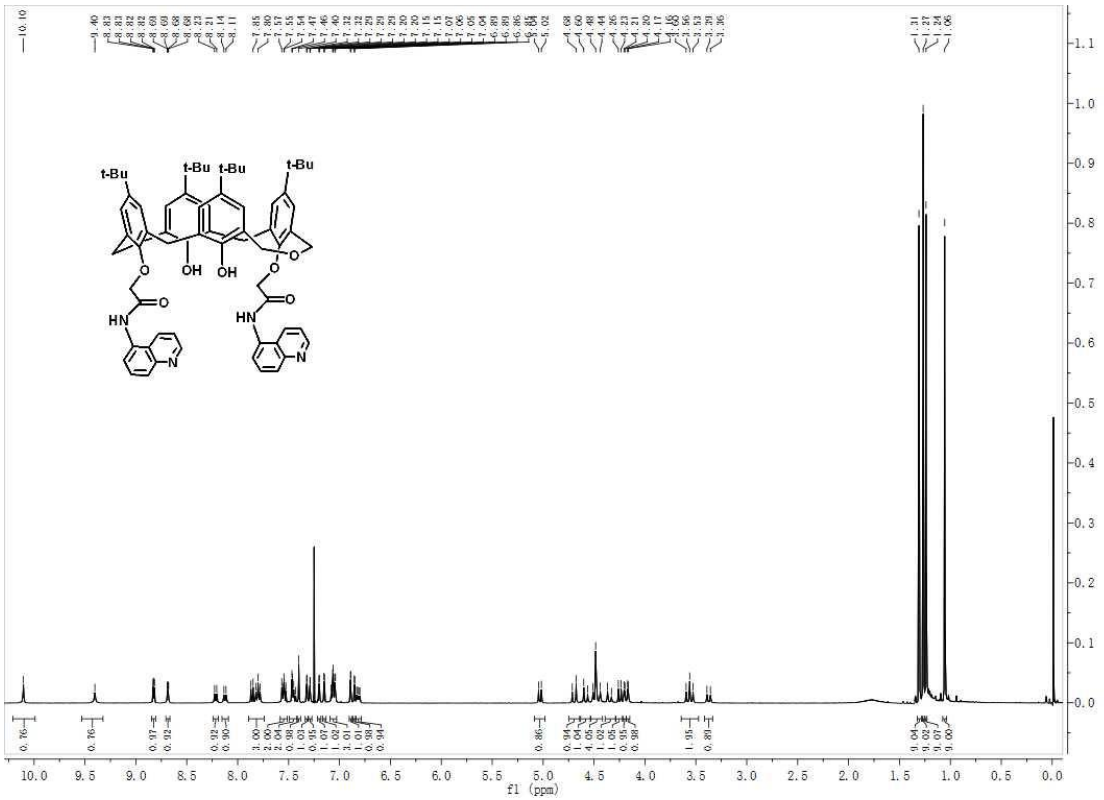
^{13}C NMR of **4i**



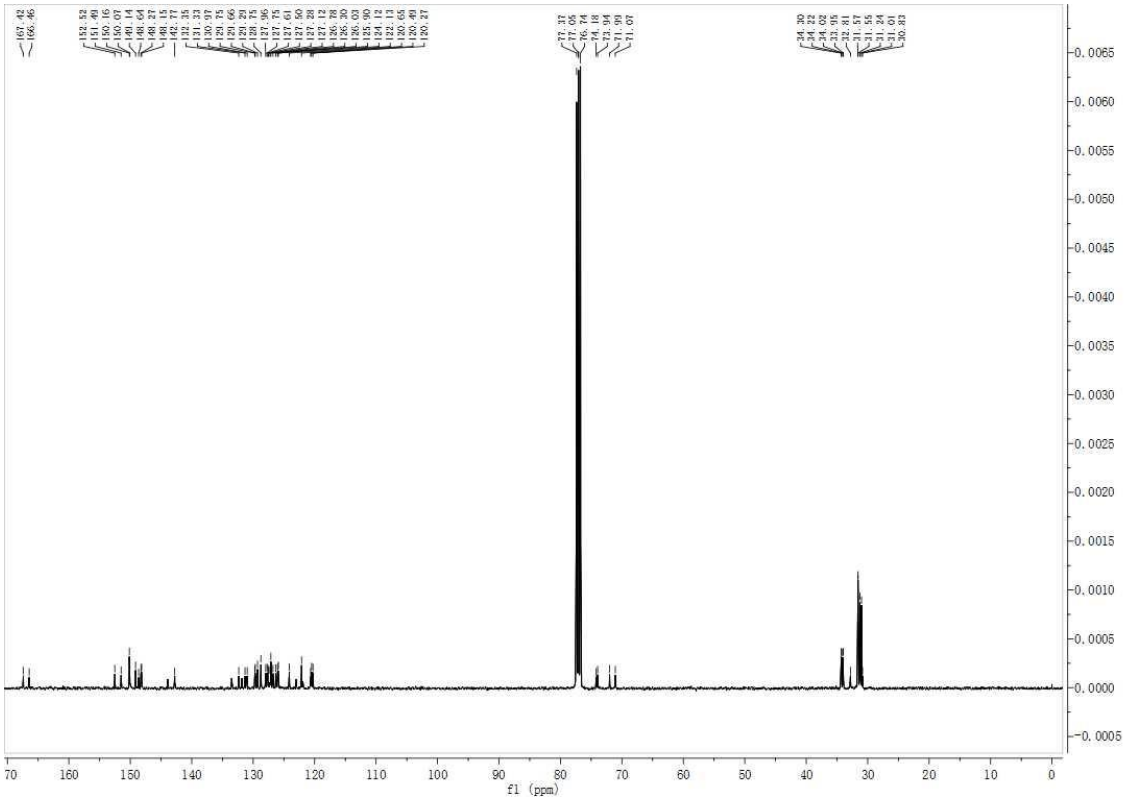
HRMS of **4i**


Intens.
x10^5
+MS, 0.48-0.67min #(40-56)
1047.5656
1069.5453
2.0
1.5
1.0
0.5
0.0
1030
1040
1050
1060
1070
1080
m/z

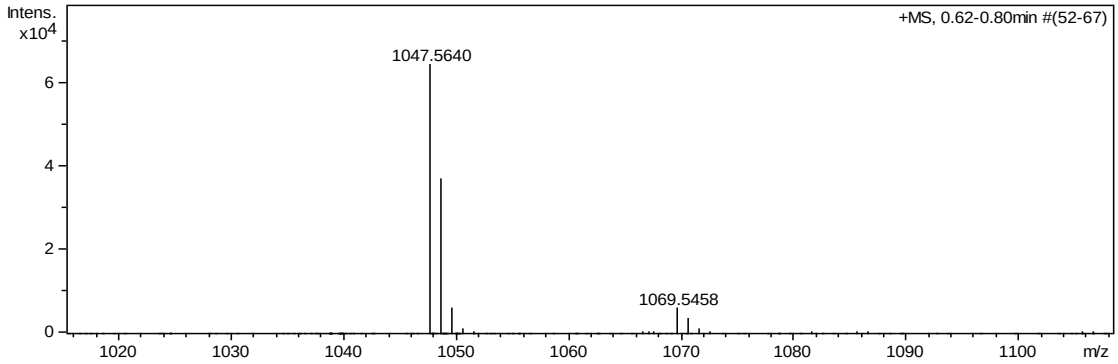
^{1}H NMR of **4j**



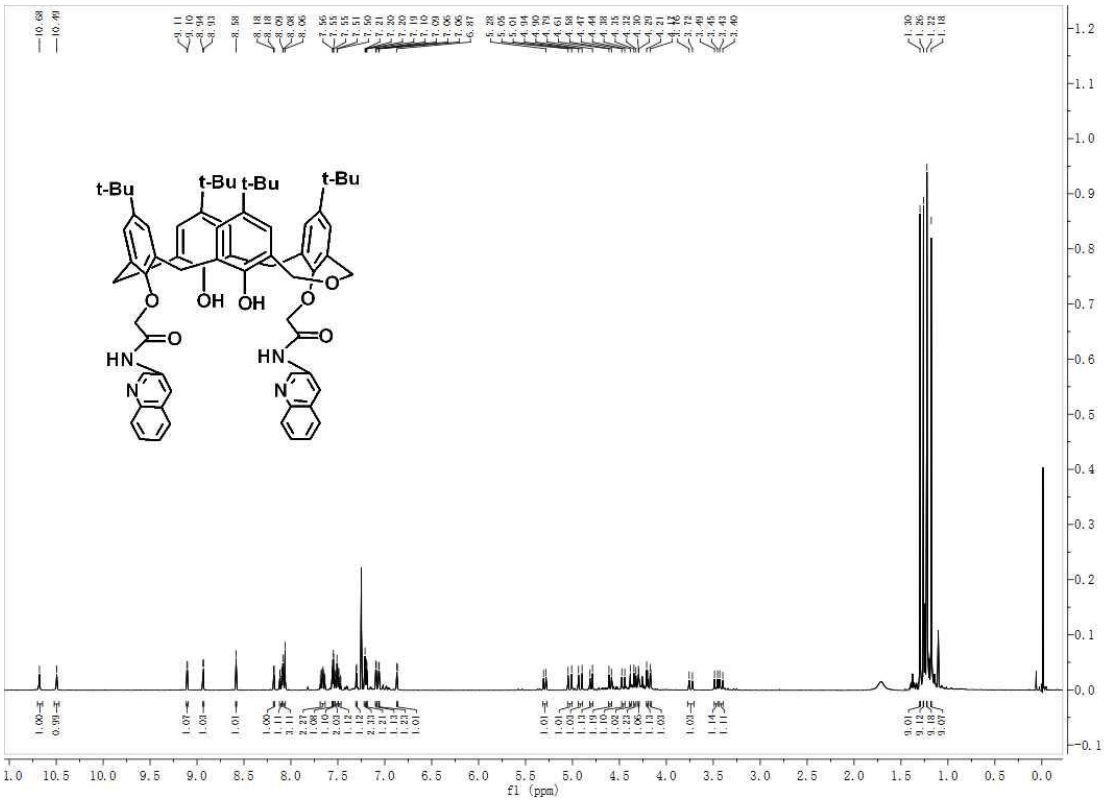
^{13}C NMR of **4j**



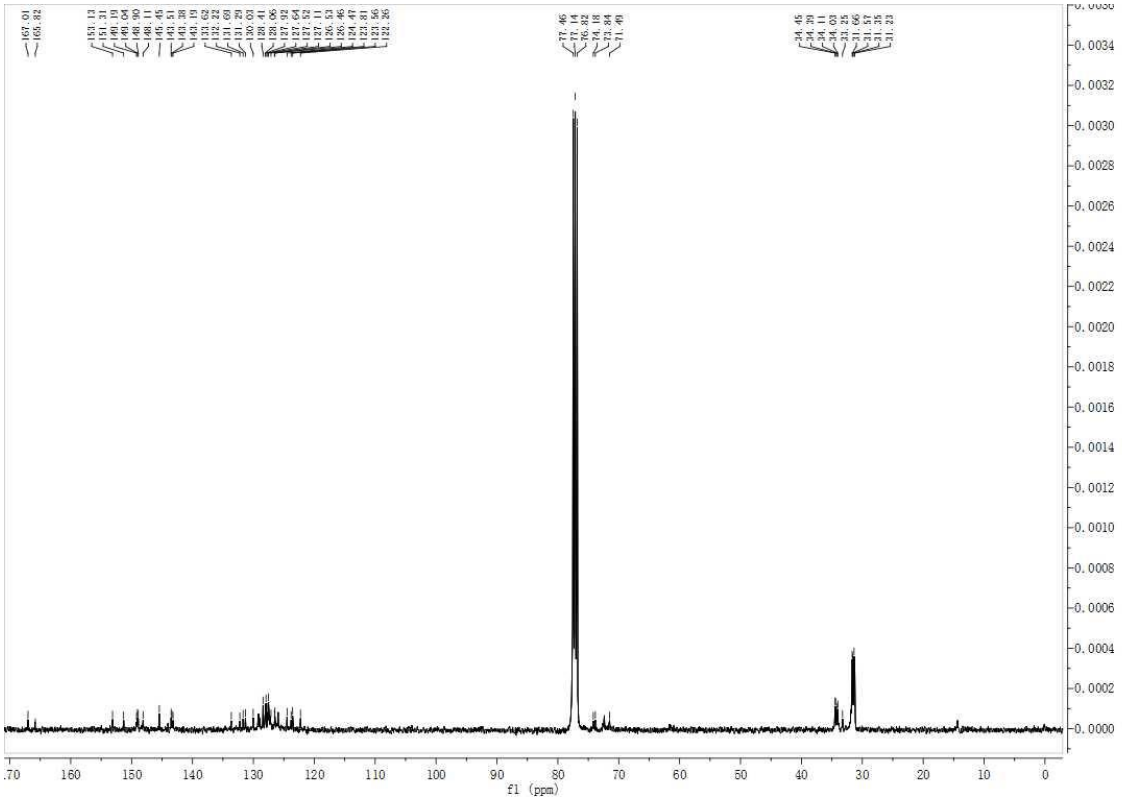
HRMS of **4j**


Intens.
x10^4
+MS, 0.62-0.80min #(52-67)
1047.5640
1069.5458
6
4
2
0
1020
1030
1040
1050
1060
1070
1080
1090
1100
m/z

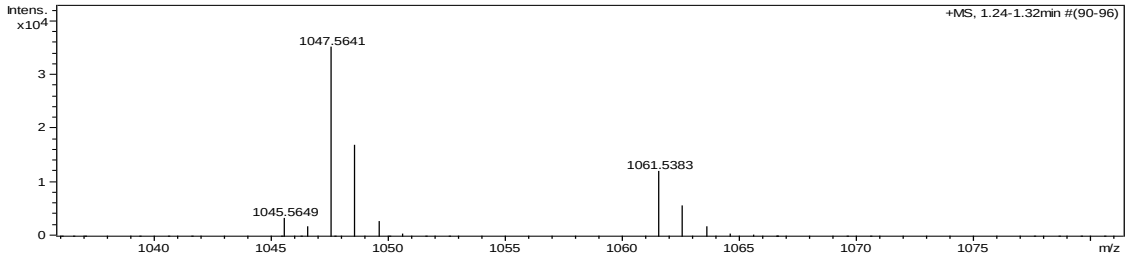
^{1}H NMR of **4k**



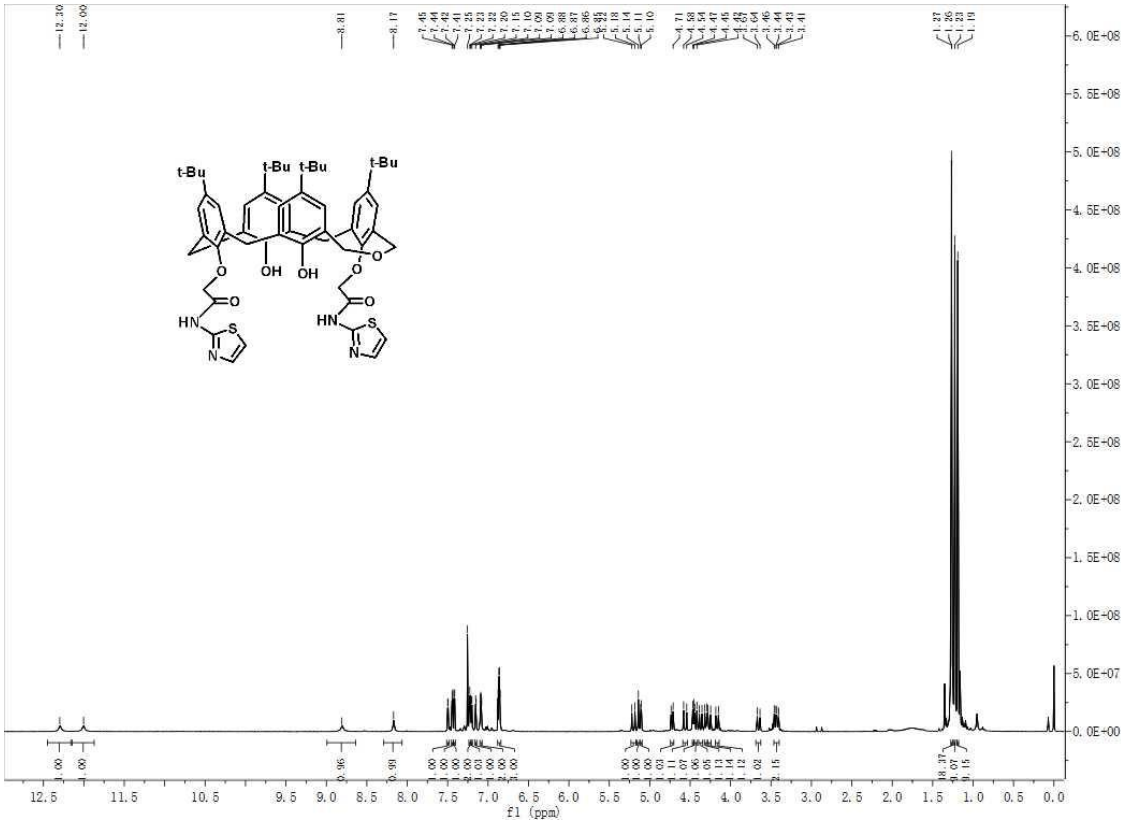
^{13}C NMR of **4k**



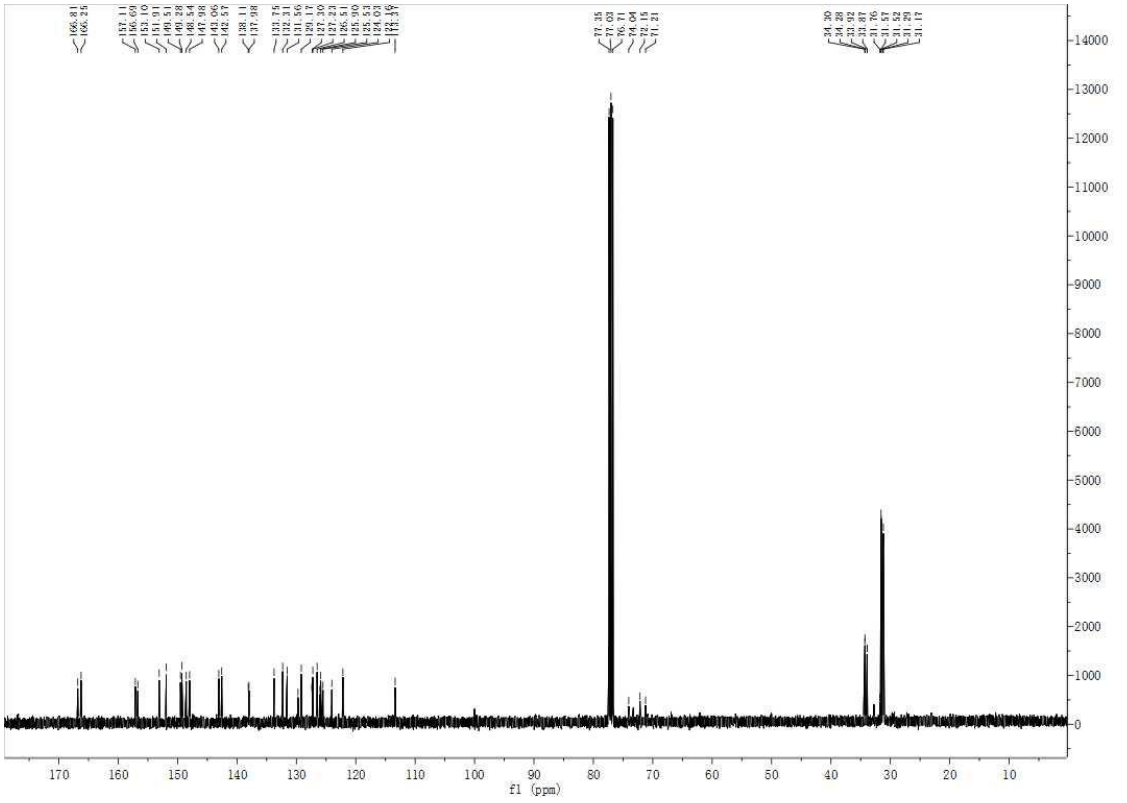
HRMS of **4k**


Intens.
x10^4
+MS, 1.24-1.32min #(90-96)
1047.5641
1061.5383
1045.5649
0
1
2
3
1040
1045
1050
1055
1060
1065
1070
1075
m/z

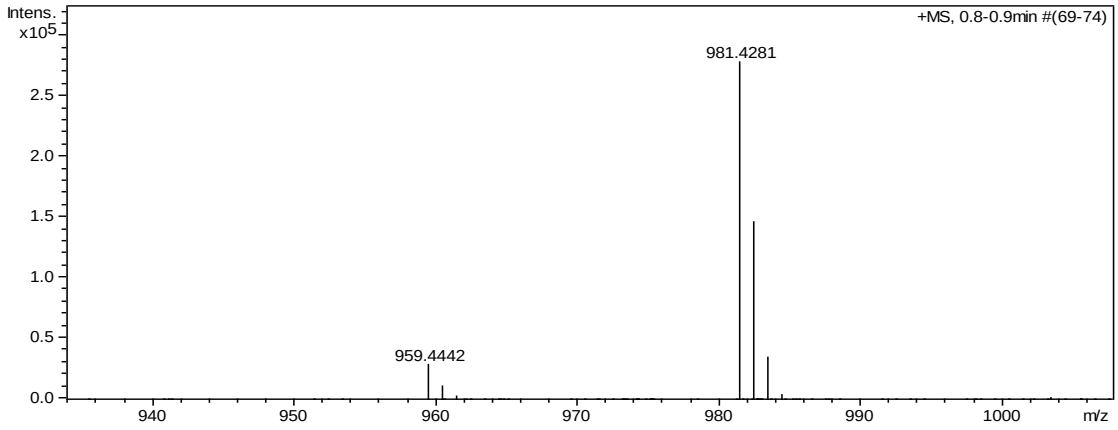
^{1}H NMR of **4l**



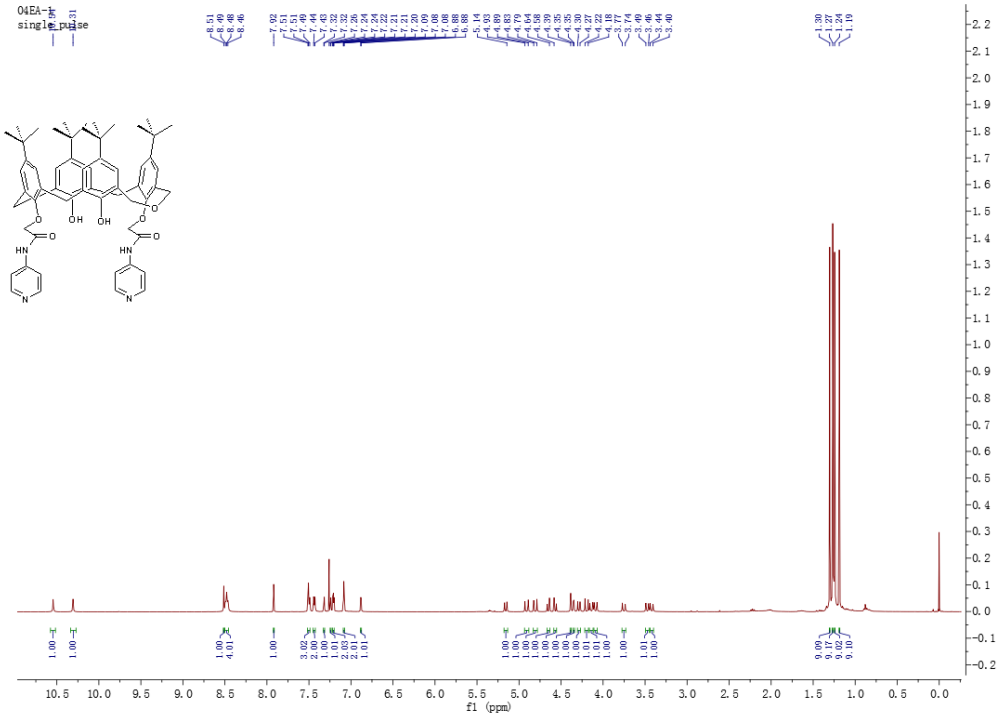
^{13}C NMR of **4l**



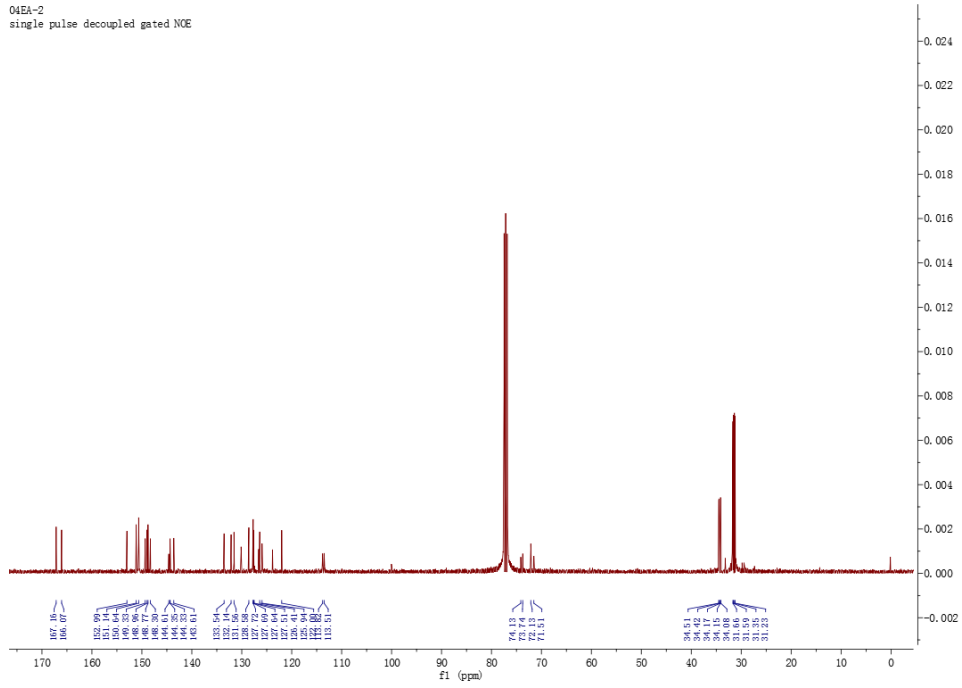
HRMS of **4l**


Intens.
x10^5
+MS, 0.8-0.9min #(69-74)
981.4281
959.4442
2.5
2.0
1.5
1.0
0.5
0.0
940
950
960
970
980
990
1000
m/z

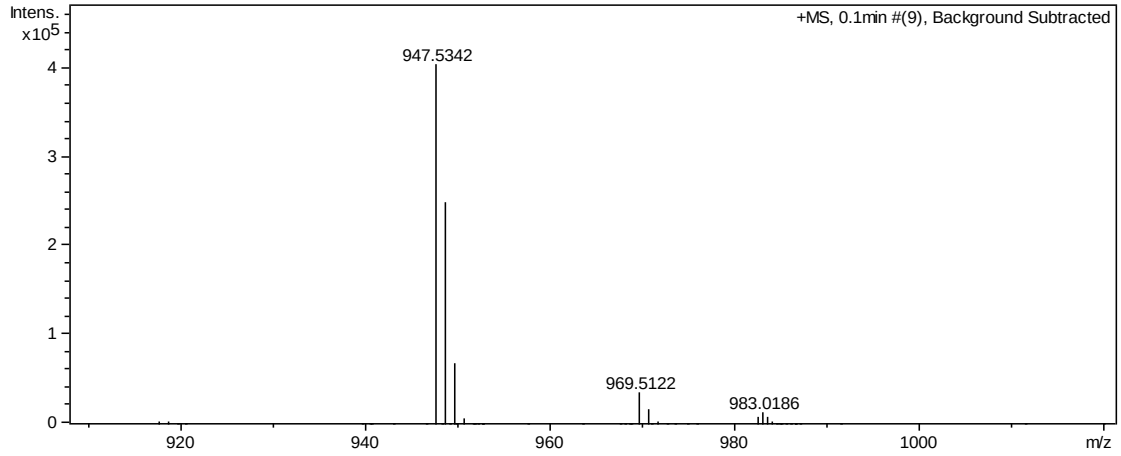
^{1}H NMR of **4m**



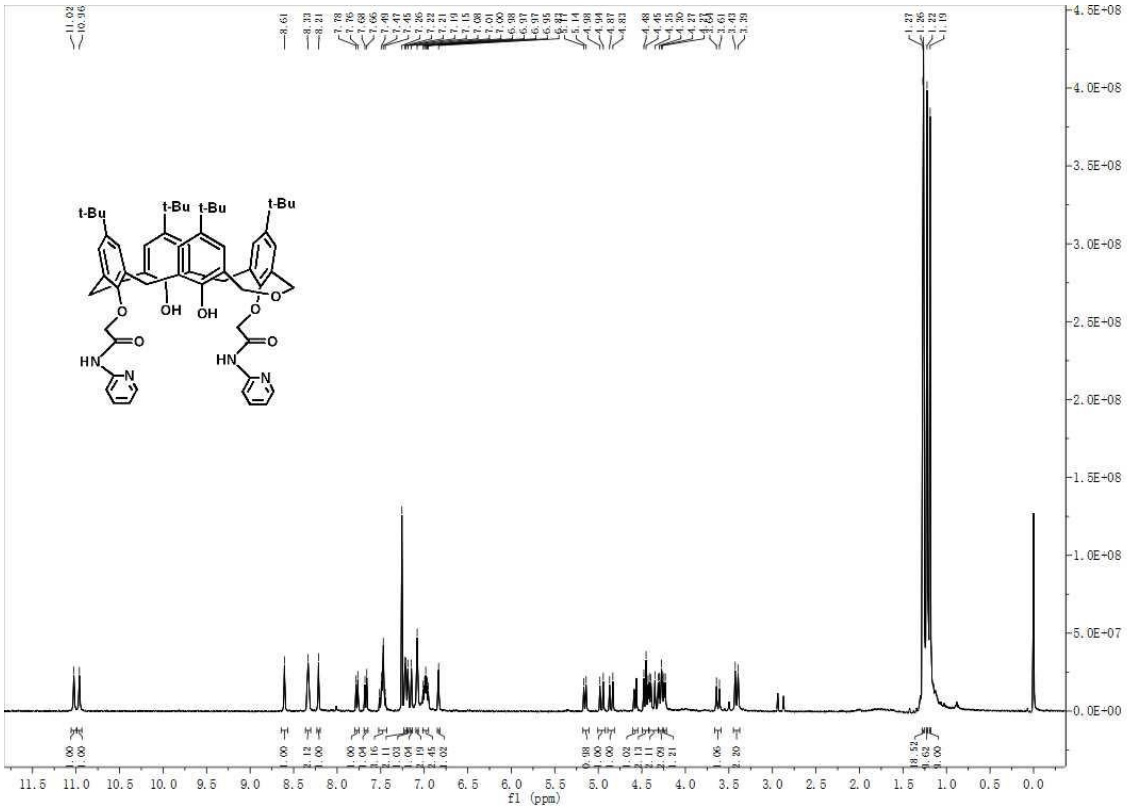
^{13}C NMR of **4m**



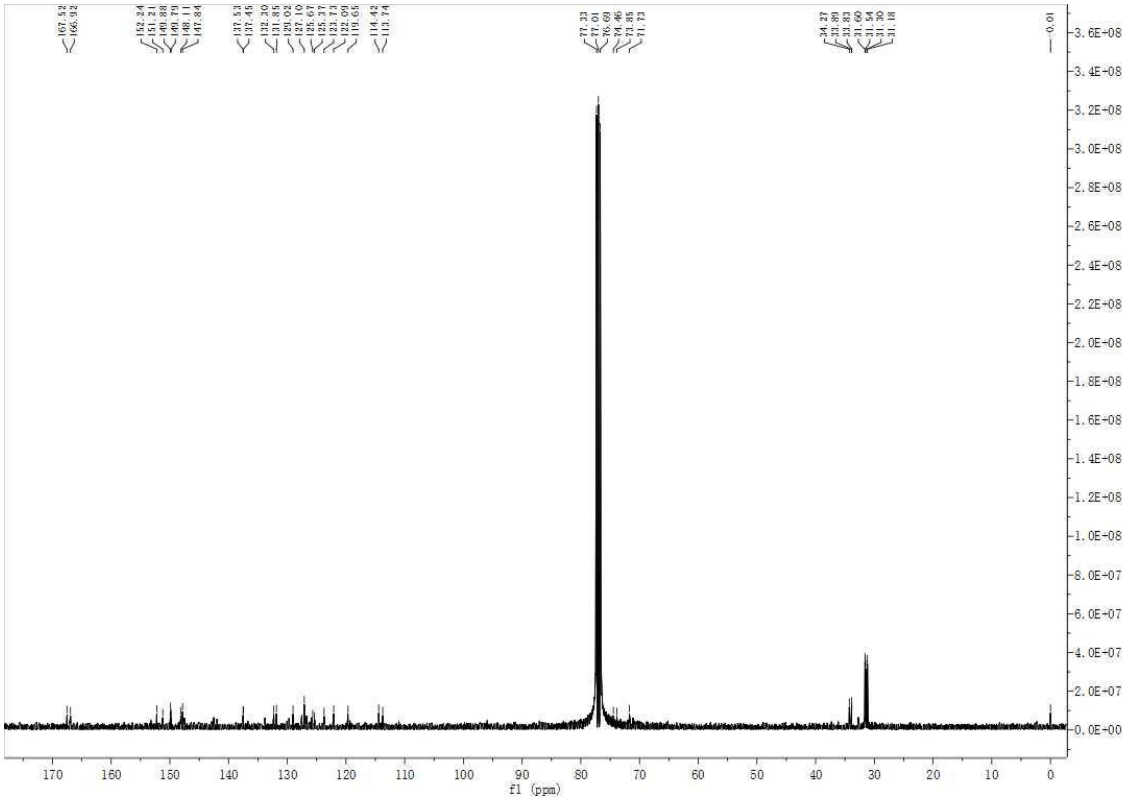
HRMS of **4m**


Intens.
x10^5
+MS, 0.1min #(9), Background Subtracted
947.5342
969.5122
983.0186
0
1
2
3
4
920
940
960
980
1000
m/z

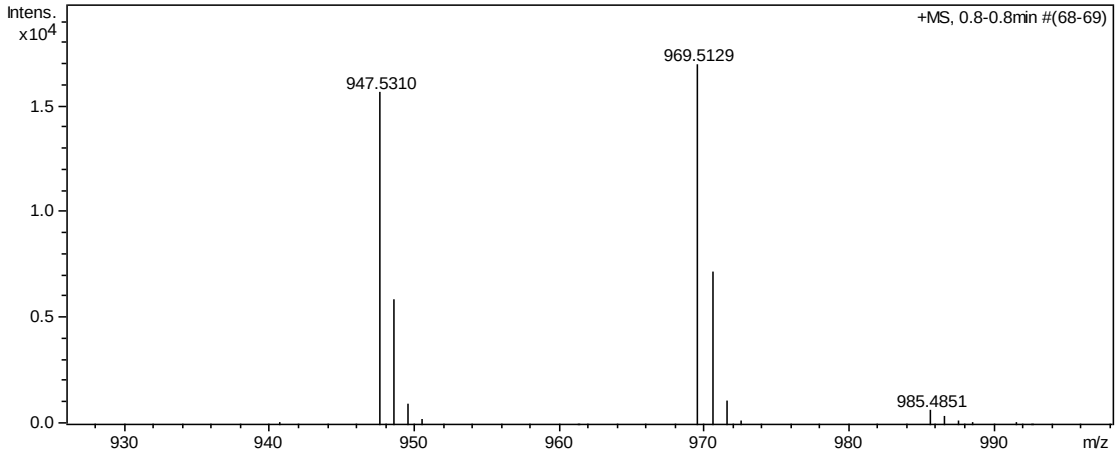
^{1}H NMR of **4n**



^{13}C NMR of **4n**



HRMS of **4n**


Intens.
x10^4
+MS, 0.8-0.8min #(68-69)
947.5310
969.5129
985.4851
1.5
1.0
0.5
0.0
930
940
950
960
970
980
990
m/z