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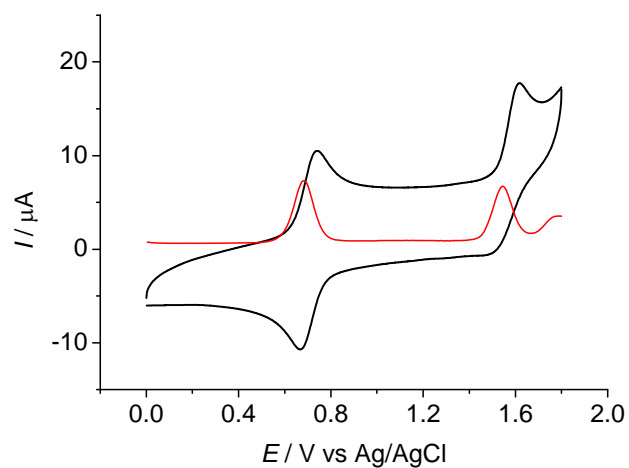
**Cyclometalated Ruthenium(II) Complexes with  
Bis(benzimidazolyl)benzene for Dye-Sensitized Solar Cells**

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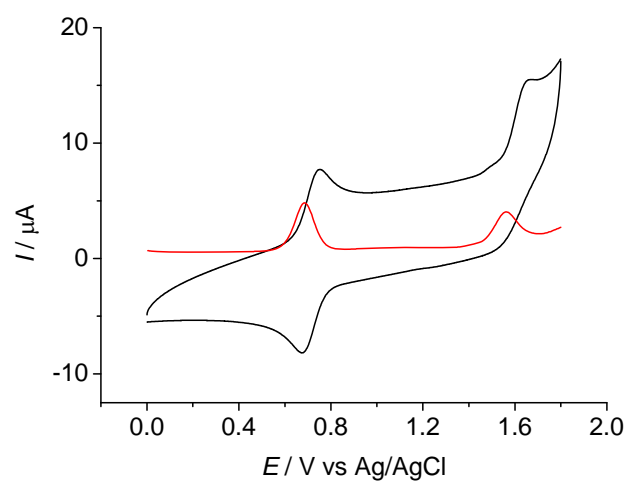
*Yuan Lin,\* and Jiannian Yao*

Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Photochemistry, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China.

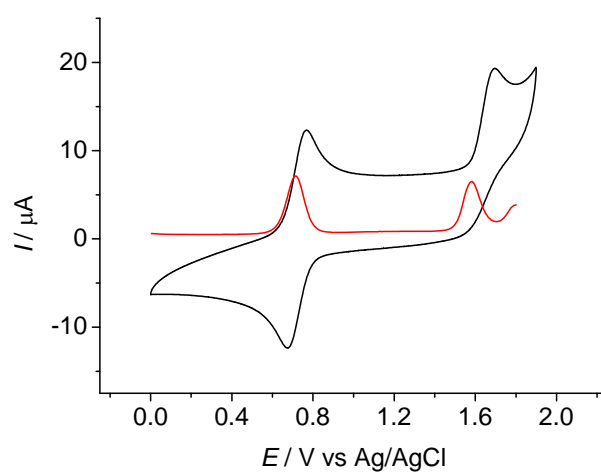
\*Email: [zhongyuwu@iccas.ac.cn](mailto:zhongyuwu@iccas.ac.cn) (Y.-W.Z.); [linyuan@iccas.ac.cn](mailto:linyuan@iccas.ac.cn) (Y.L.)



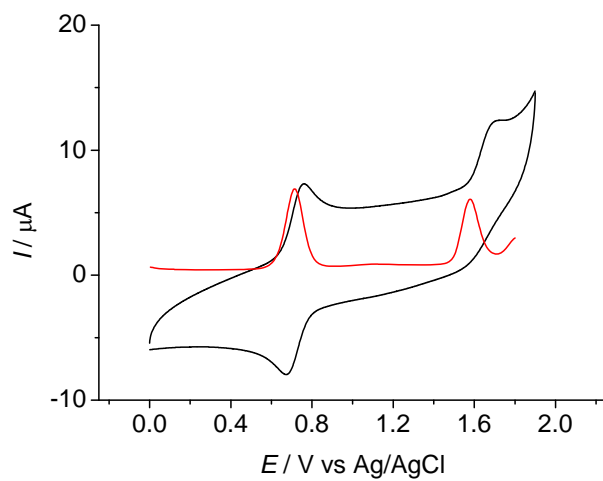
**Figure S1.** CV and DPV of **1a** in acetonitrile.



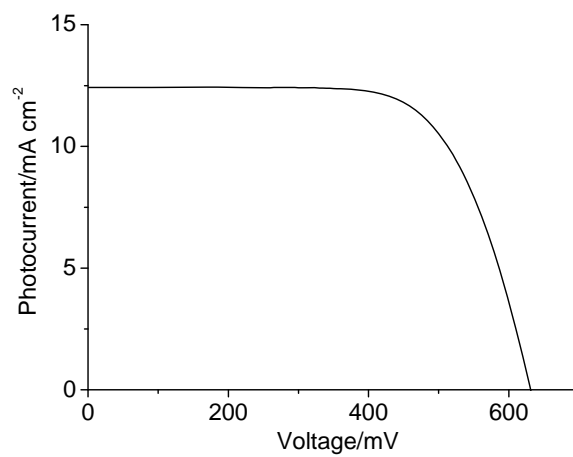
**Figure S2.** CV and DPV of **3a** in acetonitrile.



**Figure S3.** CV and DPV of **4a** in acetonitrile.

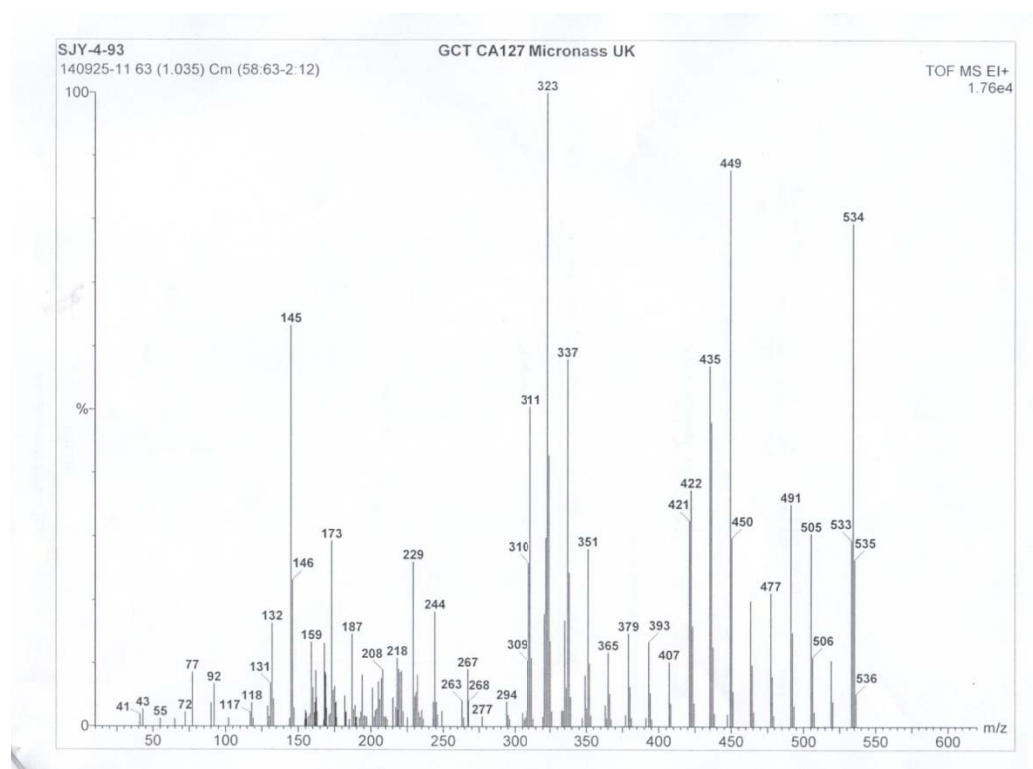
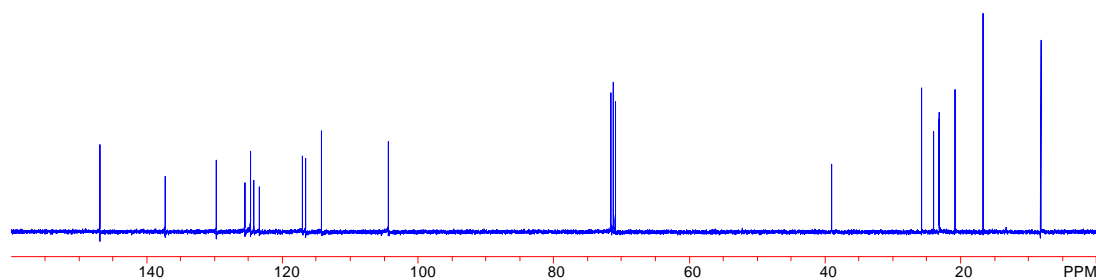
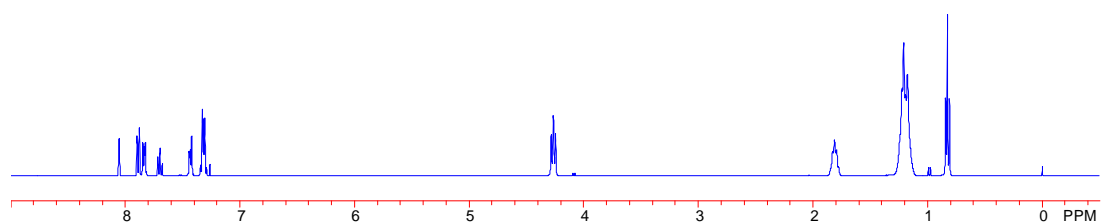


**Figure S4.** CV and DPV of **5a** in acetonitrile.

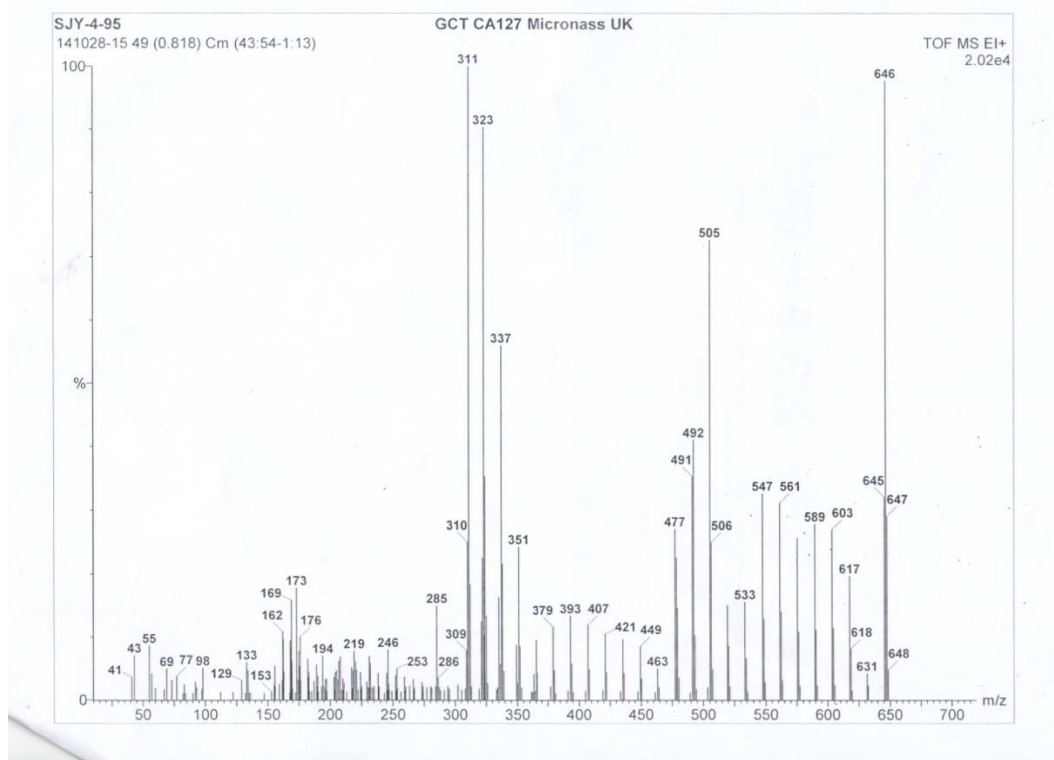
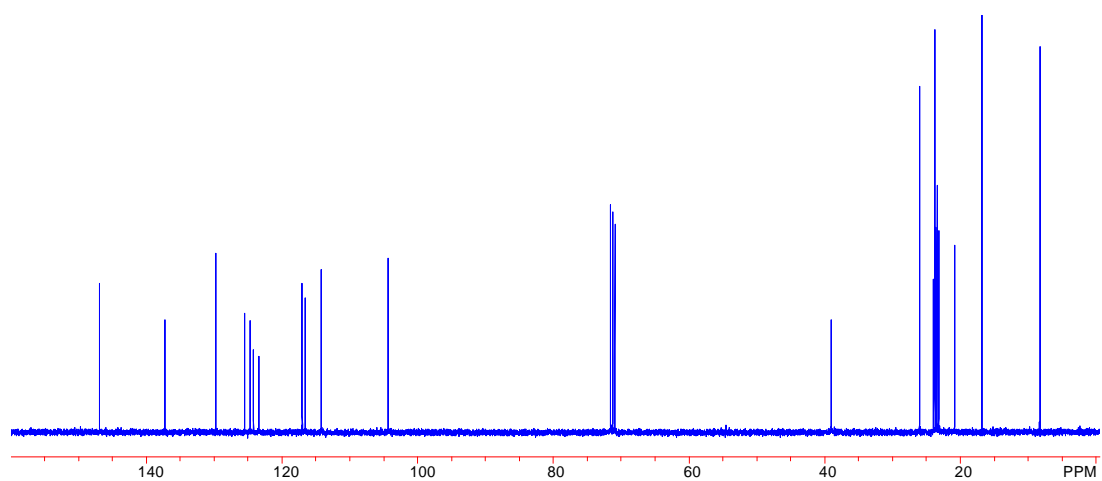
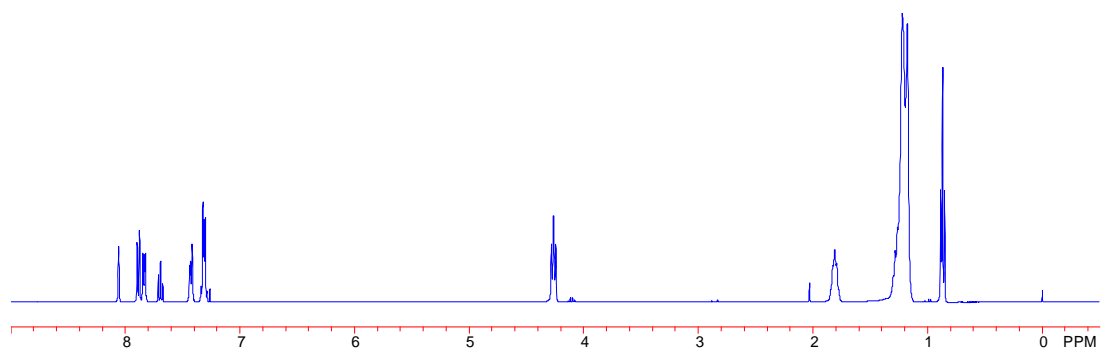


**Figure S5.** Photocurrent density-voltage characteristic of the device using N3 sensitizers.

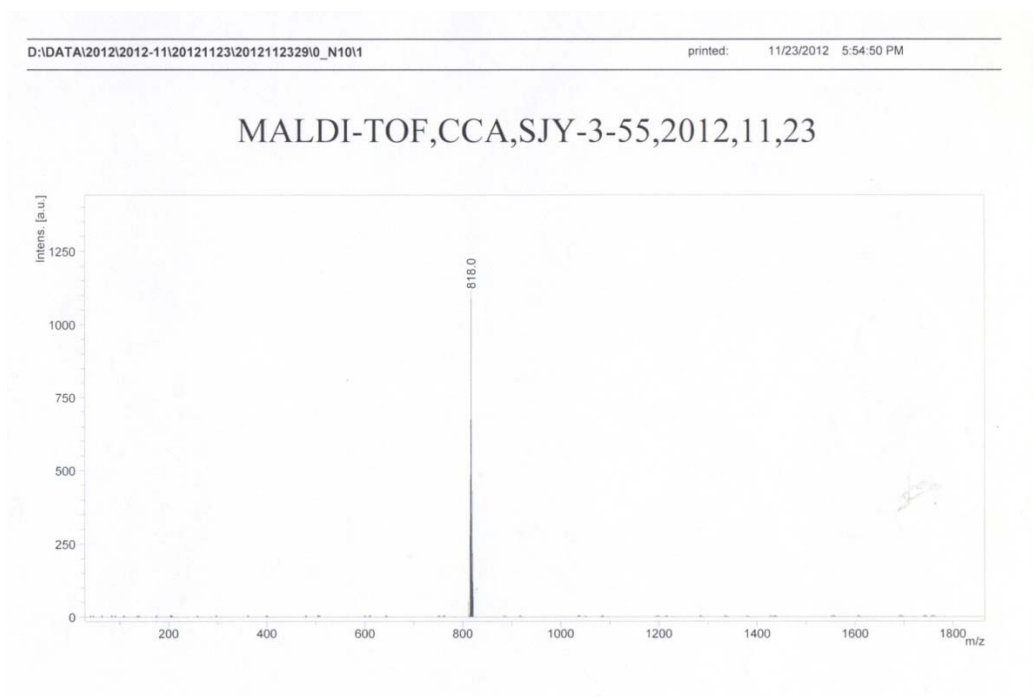
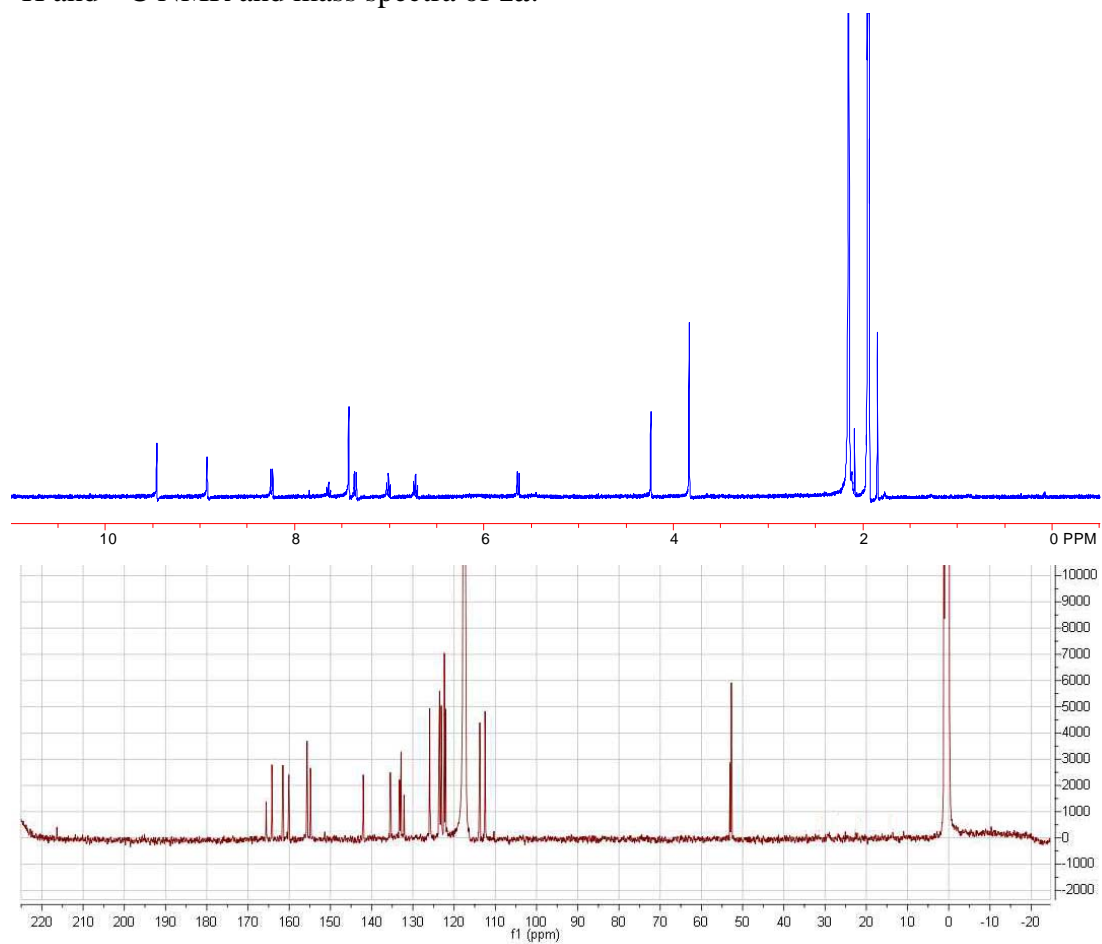
$^1\text{H}$  and  $^{13}\text{C}$  NMR and mass spectra of **L4**:



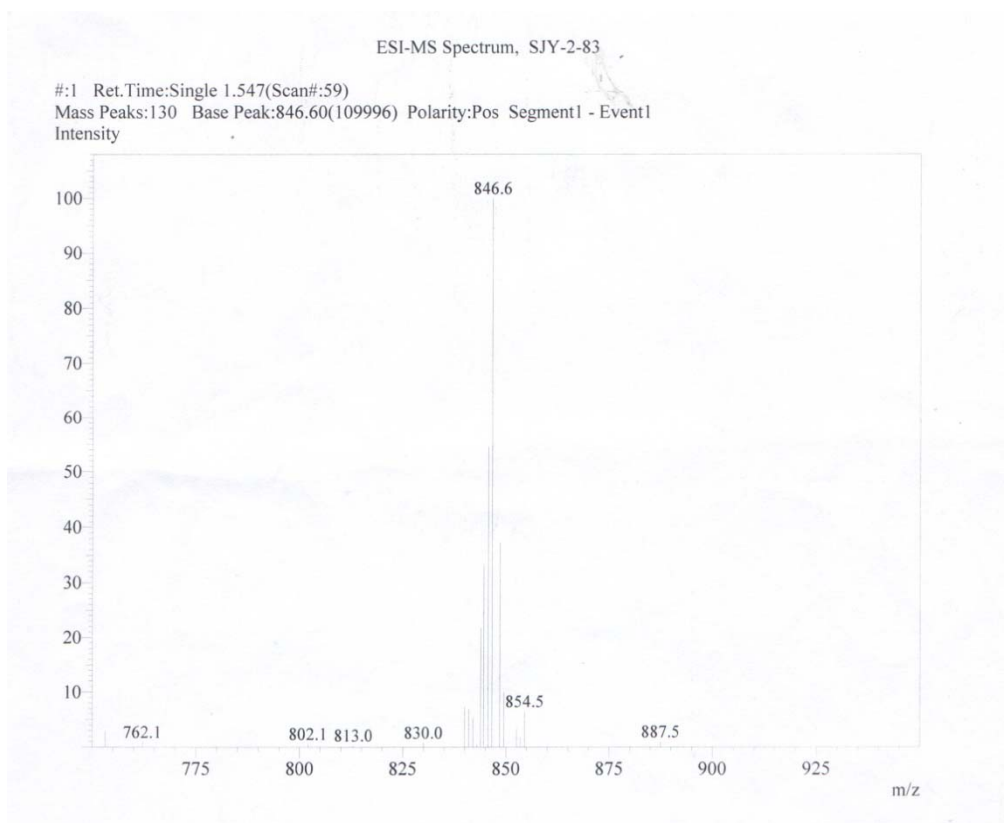
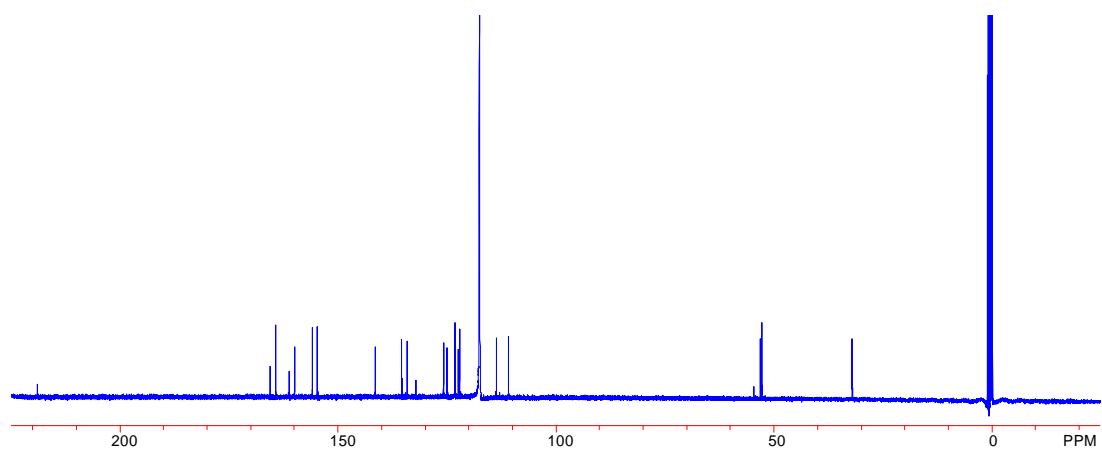
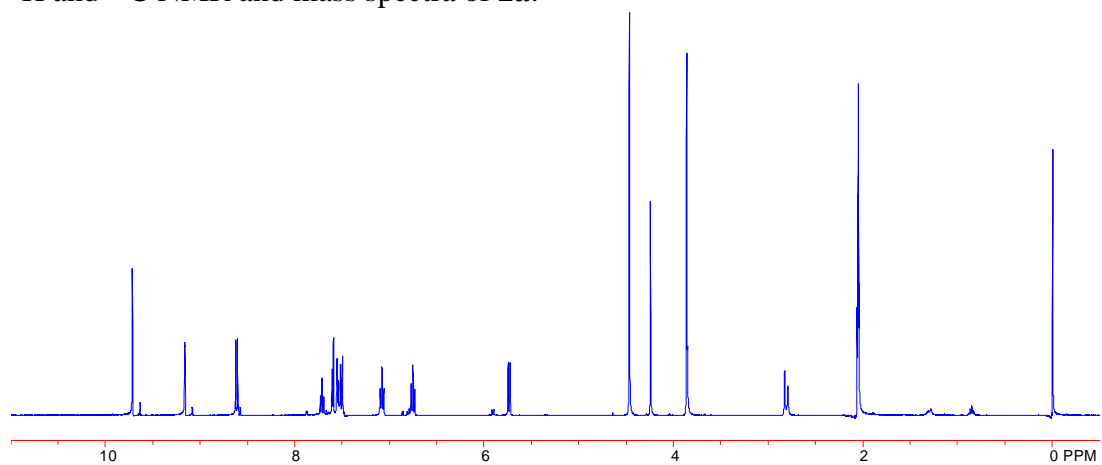
$^1\text{H}$  and  $^{13}\text{C}$  NMR and mass spectra of **L5**:



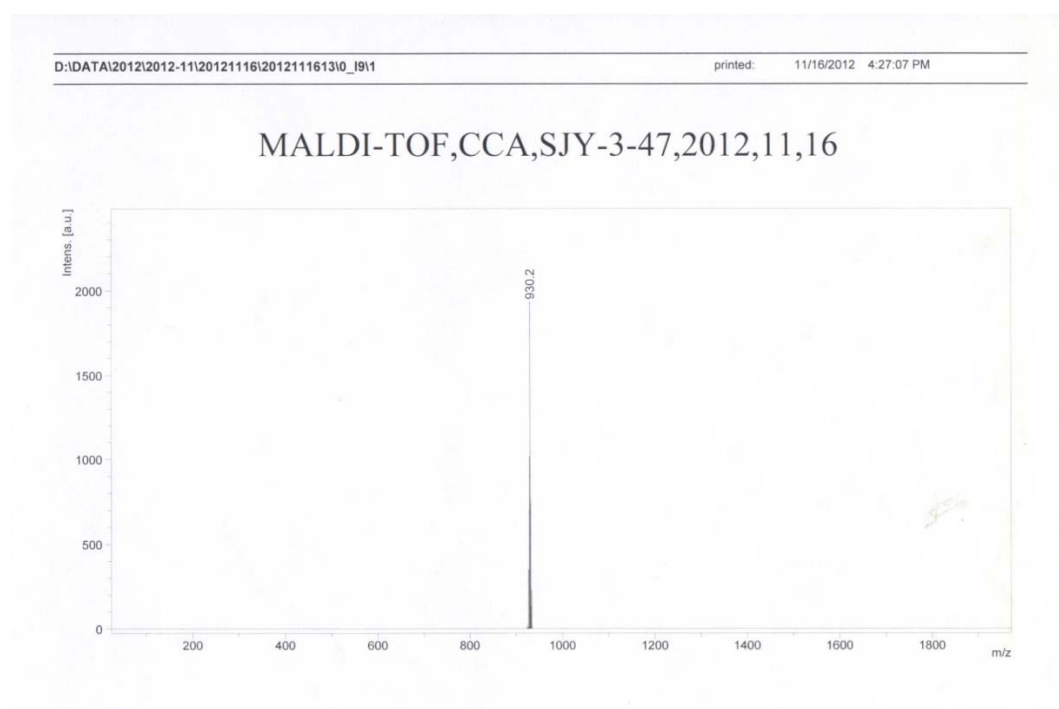
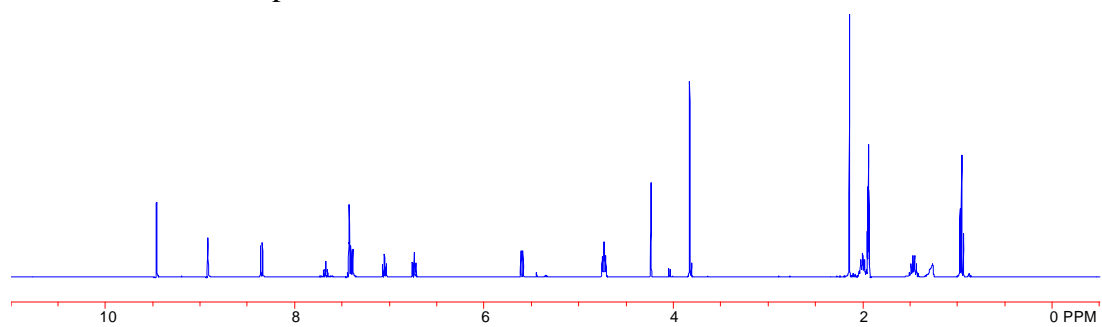
$^1\text{H}$  and  $^{13}\text{C}$  NMR and mass spectra of **1a**:



$^1\text{H}$  and  $^{13}\text{C}$  NMR and mass spectra of **2a**:

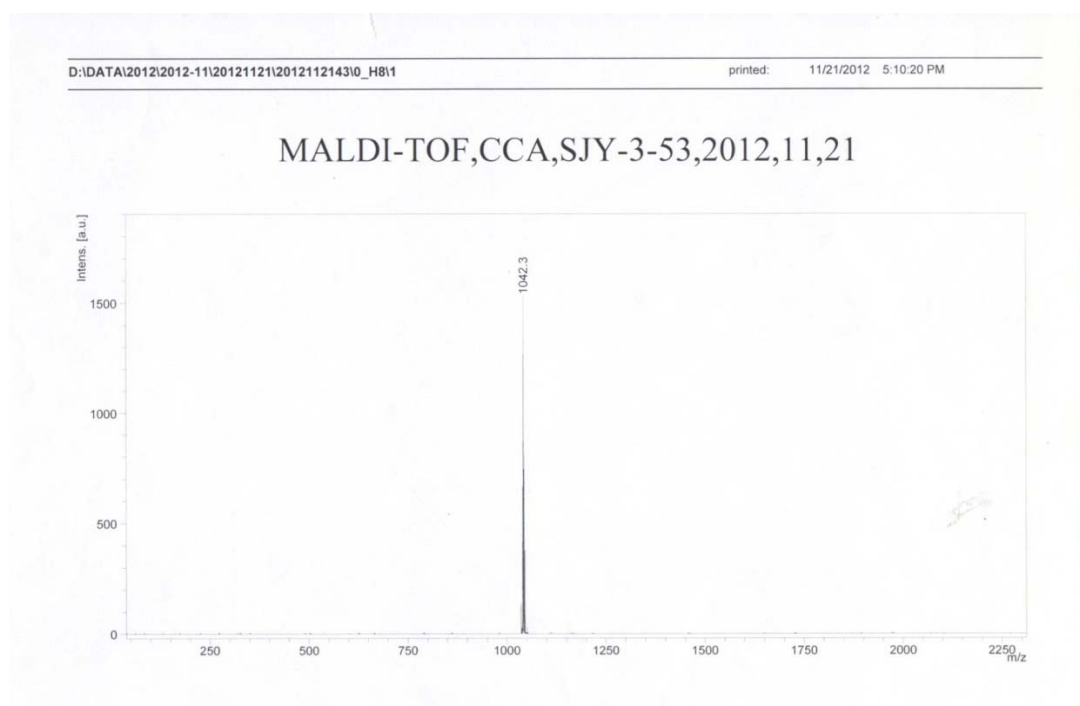
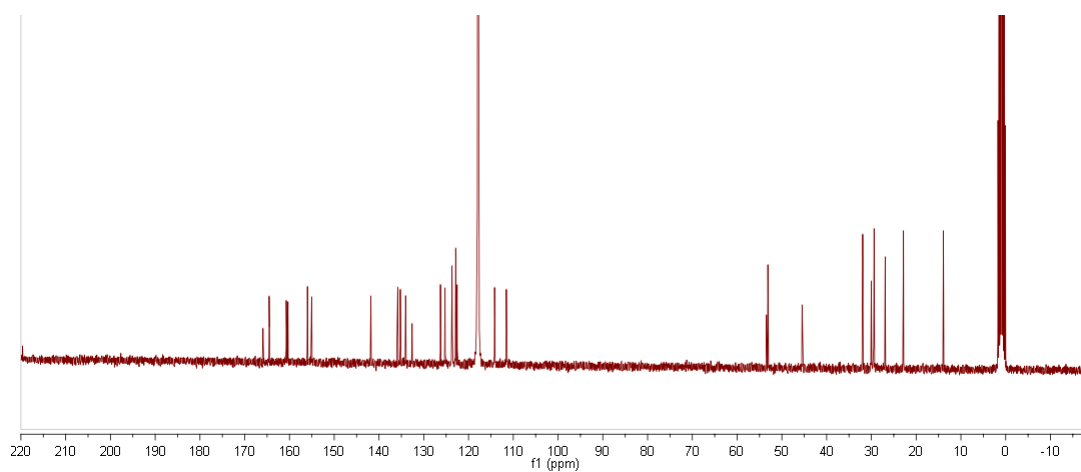
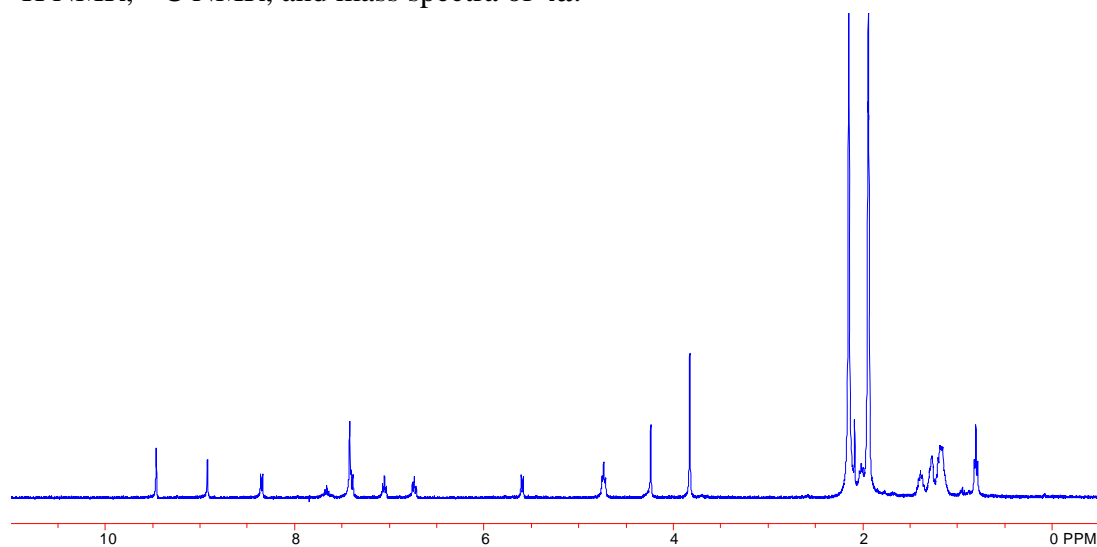


$^1\text{H}$  NMR and mass spectra of **3a**:

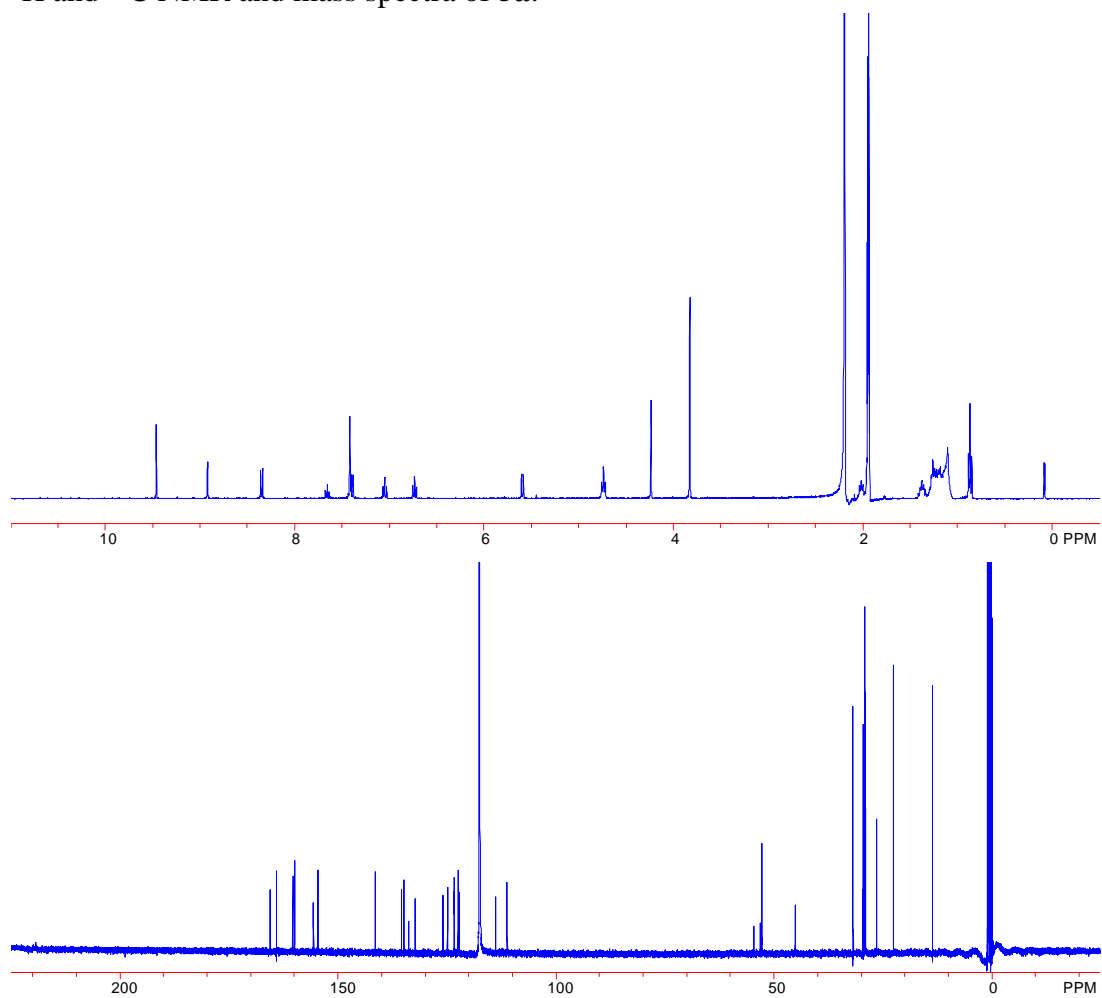




$^1\text{H}$  NMR,  $^{13}\text{C}$  NMR, and mass spectra of **4a**:



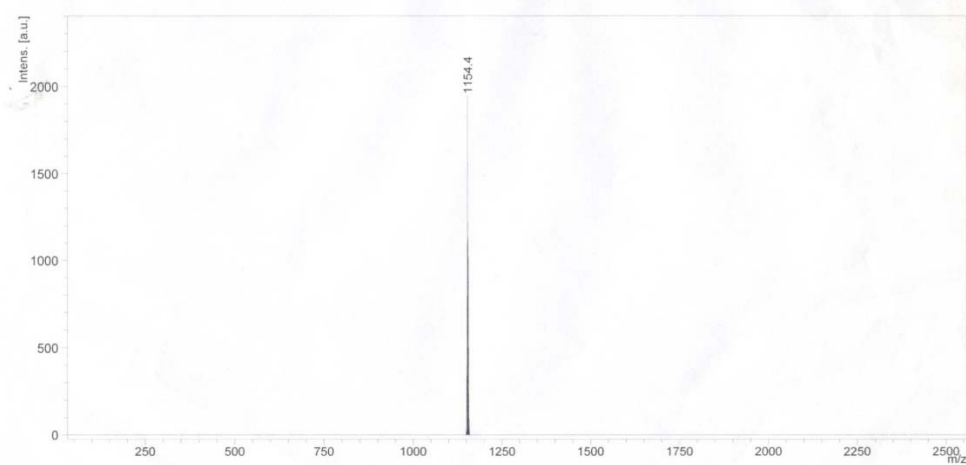
$^1\text{H}$  and  $^{13}\text{C}$  NMR and mass spectra of **5a**:



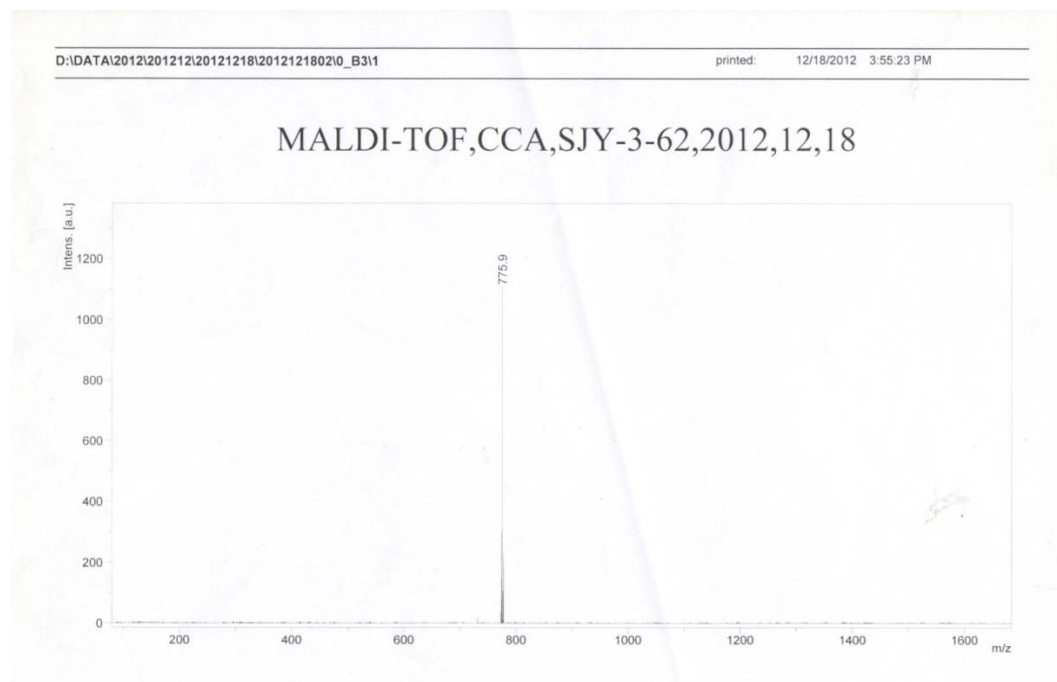
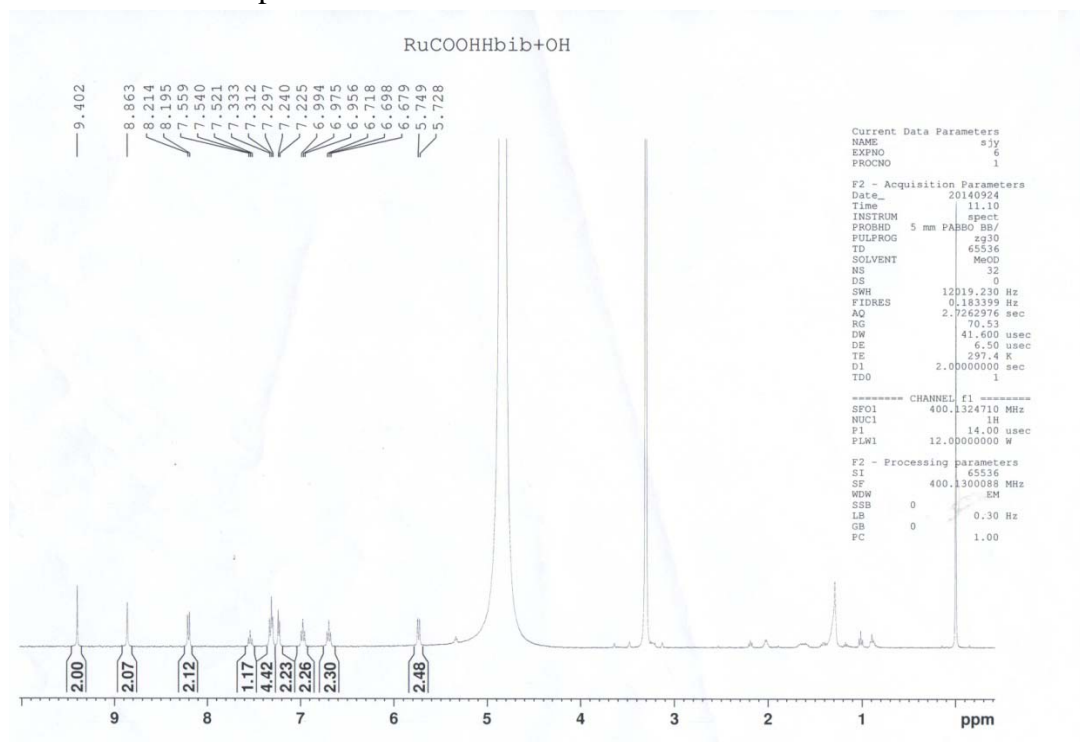
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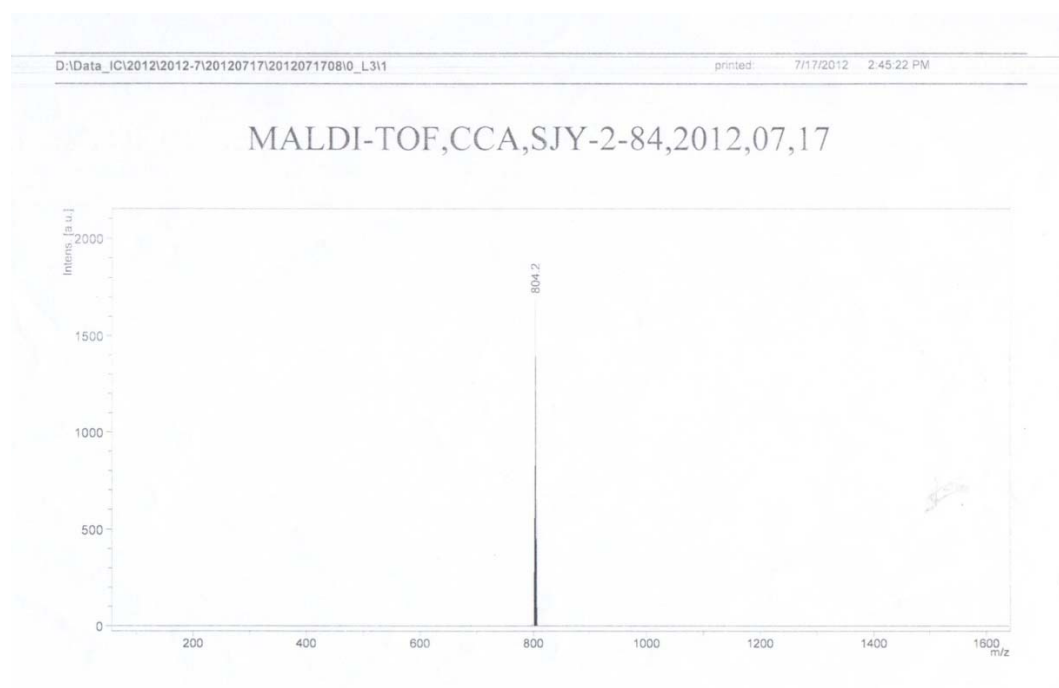
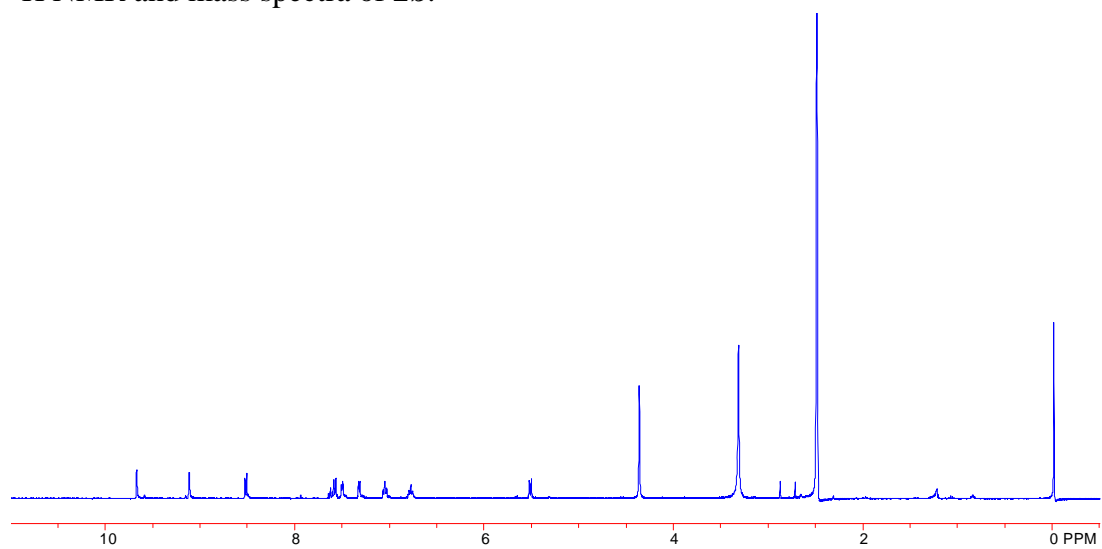
MALDI-TOF,CCA,SJY,2012,10,26



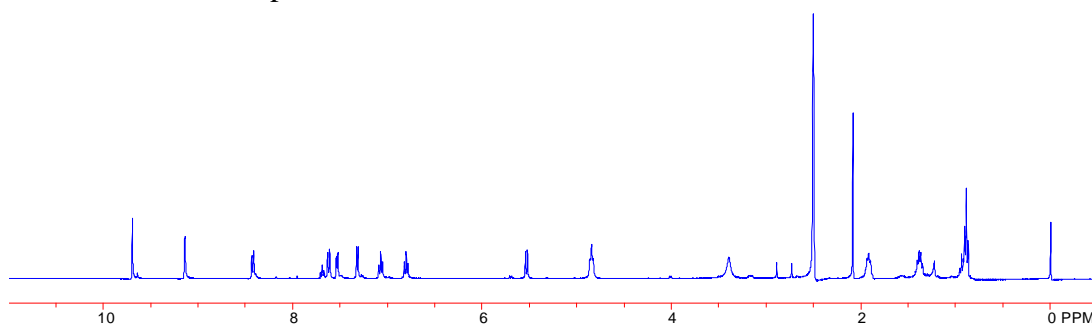
# <sup>1</sup>H NMR and mass spectra of **1b**:



$^1\text{H}$  NMR and mass spectra of **2b**:



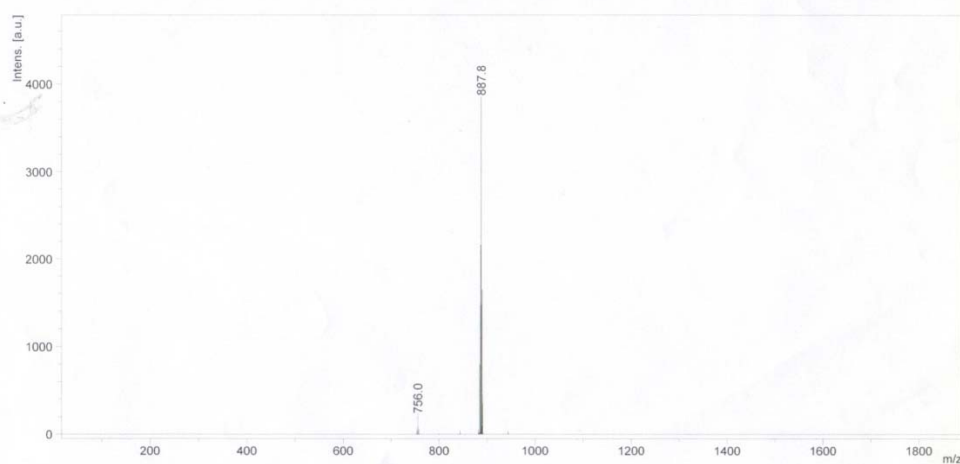
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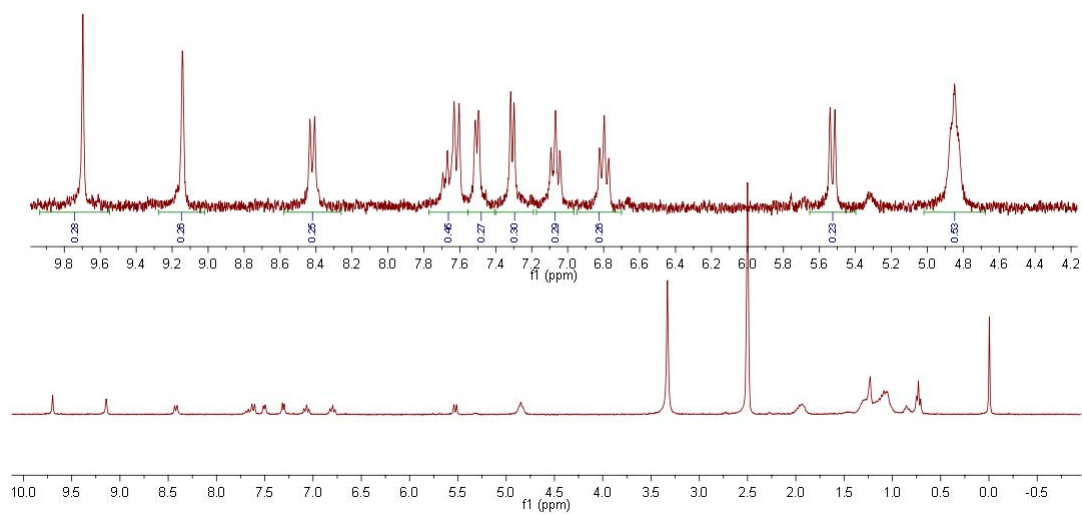
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MALDI-TOF,CCA,SJY-61,2012,12,17



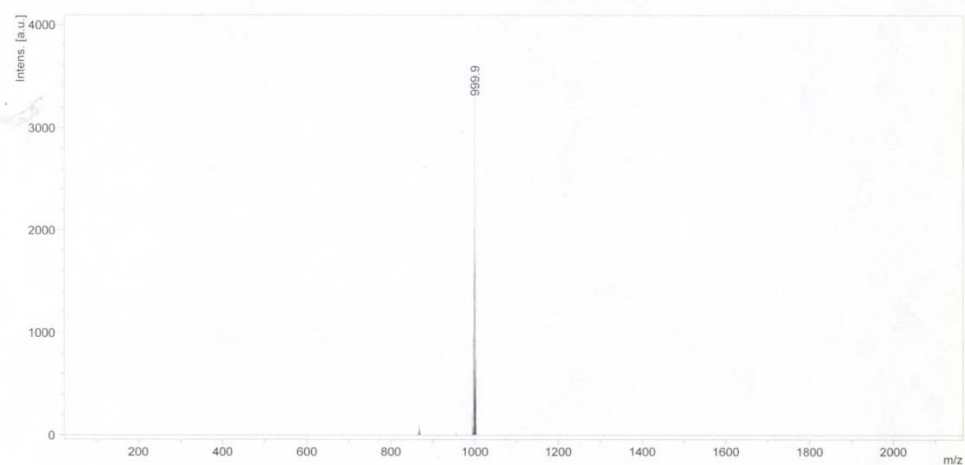
<sup>1</sup>H NMR and mass spectra of **4b**:



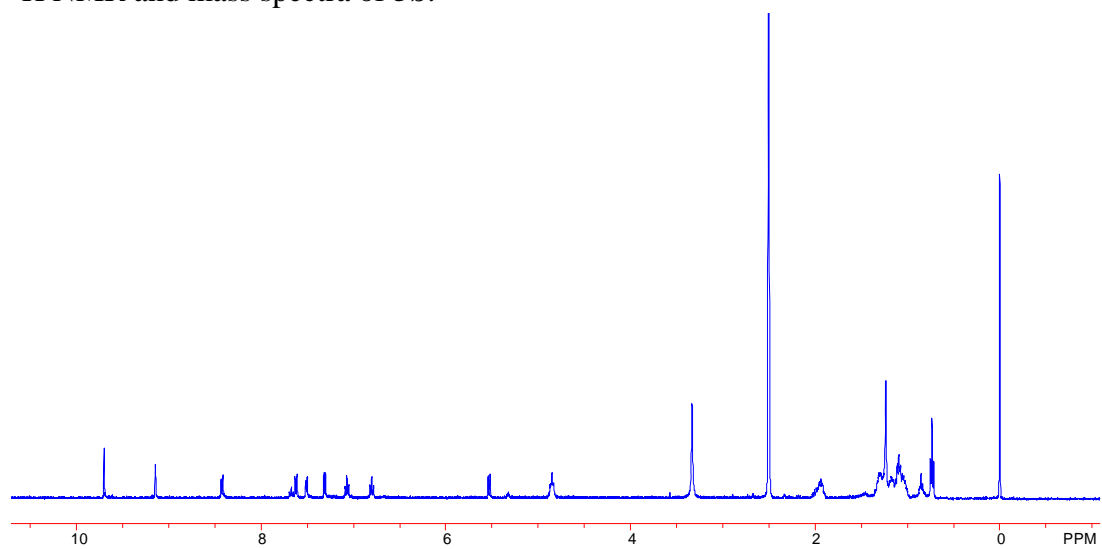
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MALDI-TOF,CCA,SJY-60,2012,12,17



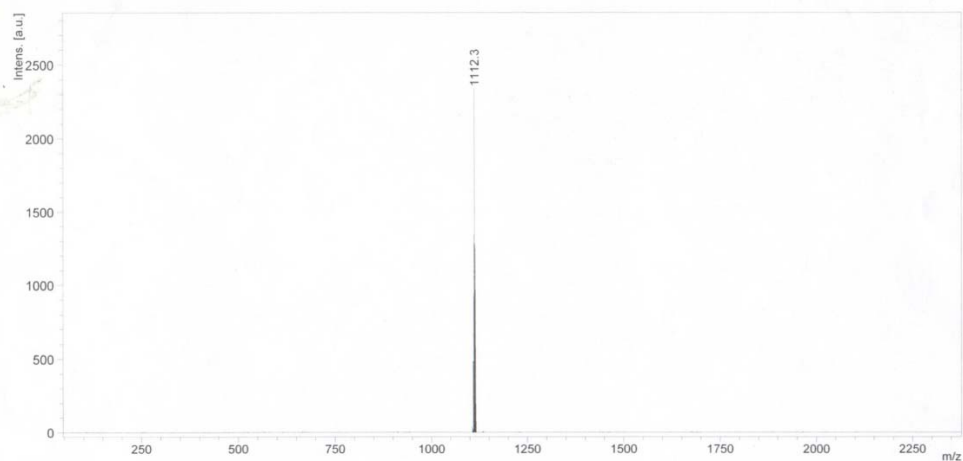
$^1\text{H}$  NMR and mass spectra of **5b**:



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MALDI-TOF,CCA,SJY-3-33,2012,10,31



Cartesian coordinates for the DFT-optimized structure of **2a<sup>+</sup>** by B3LYP:

Charge = 1 multiplicity = 1

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N	-4.93658612	0.59900400	2.04558454
N	-3.35079392	1.00050024	3.57678948
N	-5.01438133	-0.55281000	-1.97028896
N	-3.48921814	-1.02097776	-3.54330828
C	-5.56546582	0.94755720	3.22677243
C	-6.92439432	1.06870016	3.54662883
C	-7.25513560	1.44561396	4.84452641
C	-6.26037720	1.69854061	5.81119494
C	-4.90564818	1.58265405	5.50822419
C	-4.57550247	1.20422806	4.20393265
C	-2.04344668	1.14640712	4.20780880
C	-3.60916940	0.64008872	2.28076704
C	-2.70660098	0.31474499	1.18216844
C	-3.44346484	-0.00506539	0.01586410
C	-2.75216870	-0.35370732	-1.17009461
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C	-0.63980266	-0.05880326	-0.02343979
C	-1.30152646	0.28817347	1.15919831
C	-3.69673344	-0.64648869	-2.24214327
C	-2.20703937	-1.22332779	-4.20917216
C	-4.73809384	-1.17814970	-4.13523606
C	-5.11965849	-1.54735820	-5.42811284
C	-6.48594562	-1.60926529	-5.69269384
C	-7.44232264	-1.31289299	-4.69995118
C	-7.06040266	-0.94586081	-3.41327615
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H	-8.30070957	1.54759619	5.11992197
H	-6.55481883	1.99084718	6.81471323
H	-4.14846089	1.78076948	6.25974711
H	-1.46658162	1.93823106	3.72290232
H	-2.18953538	1.41336834	5.25371560
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H	-0.78909090	-0.64439913	-2.07781959
H	-0.70931898	0.52981149	2.03423057
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H	-6.81988906	-1.89277091	-6.68632875
H	-8.49842316	-1.37307182	-4.94593884



H	-7.79645477	-0.71892934	-2.65002292
H	-4.58995761	5.01719639	-1.37836562
C	-5.36065687	4.28444181	-1.17113656
C	-6.72108050	4.60229505	-1.23383284
C	-4.98718052	2.99706666	-0.80087065
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C	-7.75544856	-3.45060478	1.08290706
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O	-8.33199580	-6.29182949	1.01514090
C	-7.23994949	5.98755389	-1.50792368
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C	-11.75011628	0.12558095	0.26878073
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