

Supporting Information

Metal-free Propargylation/*aza*-Annulation Approach to Substituted β -Carbolines and Evaluation of their Photophysical Properties

Chada Raji Reddy,^{*, a, c} Mounika Aila,^{a, c} Puppala Sathish,^{a, c} Madoori Mrinalini,^{b, c} Lingamallu Giribabu,^{b, c} Seelam Prasanthkumar,^{b, c}
and René Grée^d

^aDepartment of Organic Synthesis & Process Chemistry, CSIR-Indian Institute of Chemical Technology (CSIR-IICT), Hyderabad 500007, India

^bDepartment of Polymers & Functional Materials, CSIR-Indian Institute of Chemical Technology (CSIR-IICT), Hyderabad 500007, India

^cAcademy of Scientific and Innovative Research (AcSIR), Ghaziabad 201 002, India

^dUniversity of Rennes, CNRS, Institut des Sciences Chimiques de Rennes (ISCR), UMR 6226, F-35000 Rennes, France

E-mail: rajireddy@iict.res.in

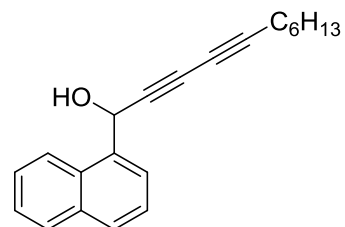
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SUBBA RAO-M0009

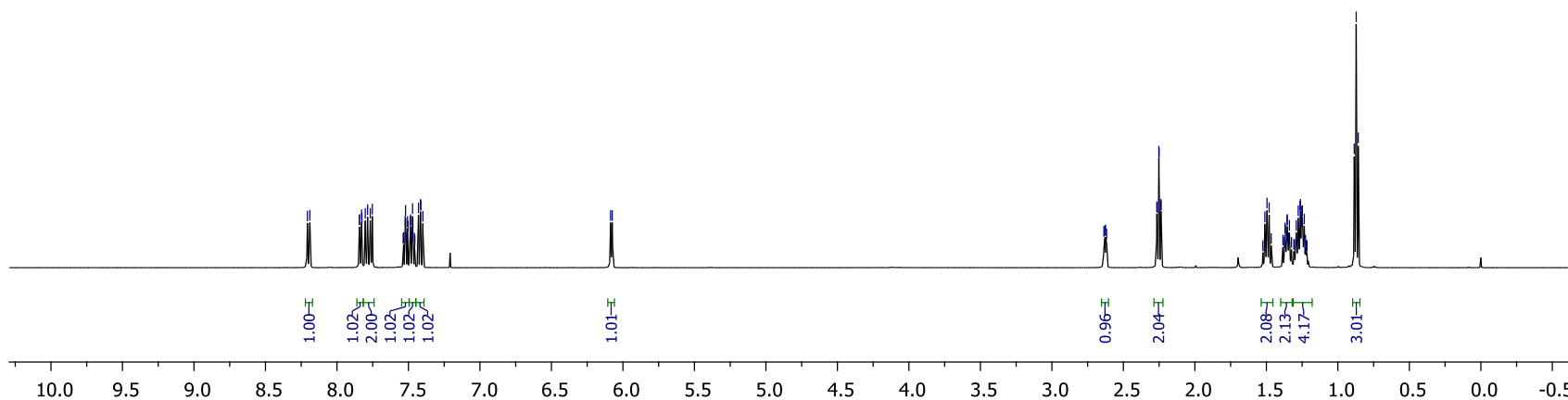
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7.84
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7.83
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7.52
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7.43
7.42
7.41
6.69
6.07

2.64
2.63
2.62
2.62
2.25
2.25
2.24
2.24
1.50
1.48
1.28
1.26
1.26
0.87
0.86



21

¹H, 500 MHz, CDCl₃



SUBBA RAO-M0009

134.96
133.94
130.37
129.48
128.70
126.53
125.91
125.19
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123.74

82.86

74.42

72.39

64.40

63.28

31.22

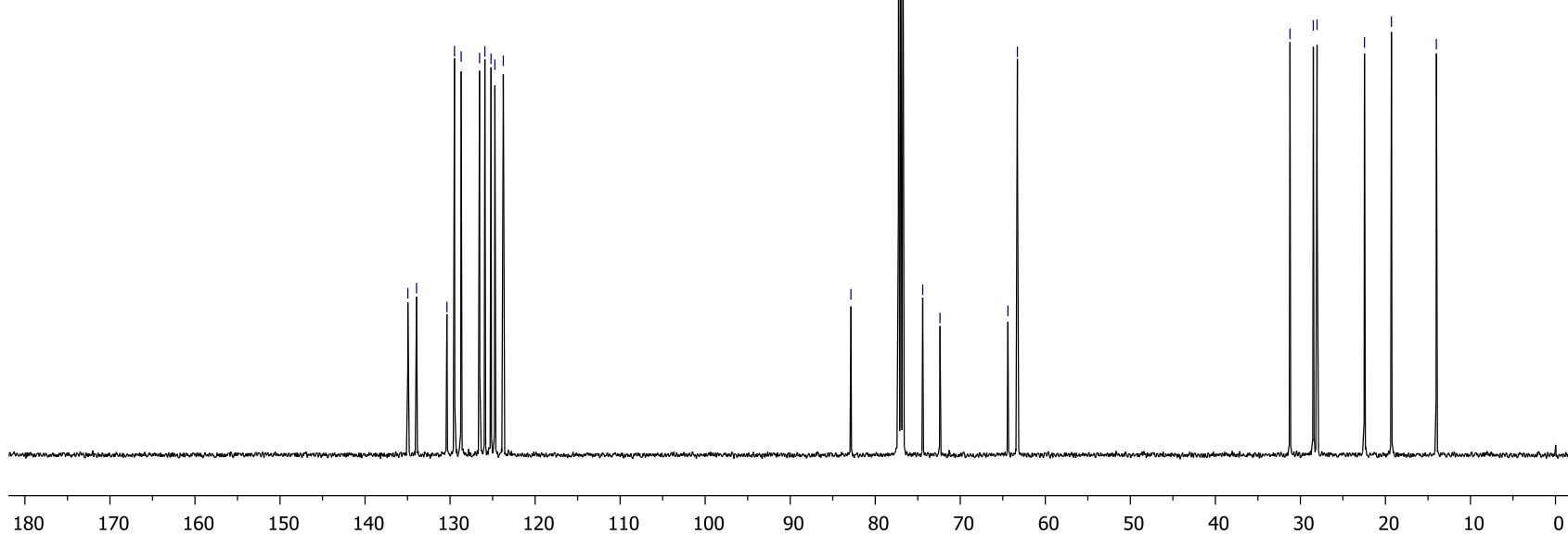
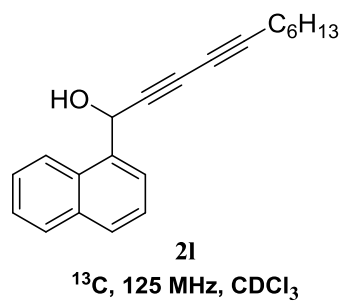
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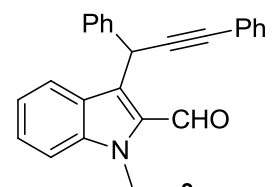
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22.46

19.30

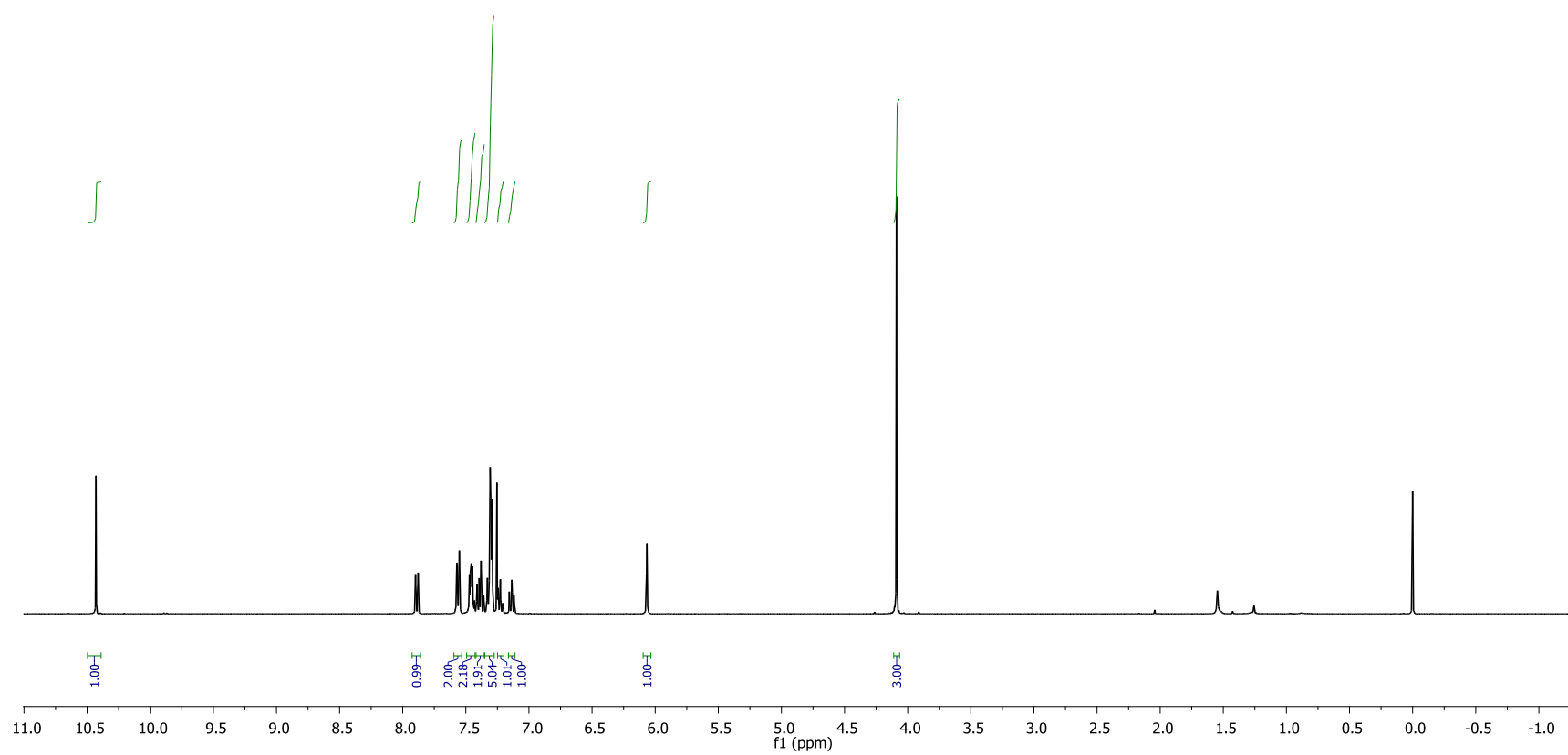
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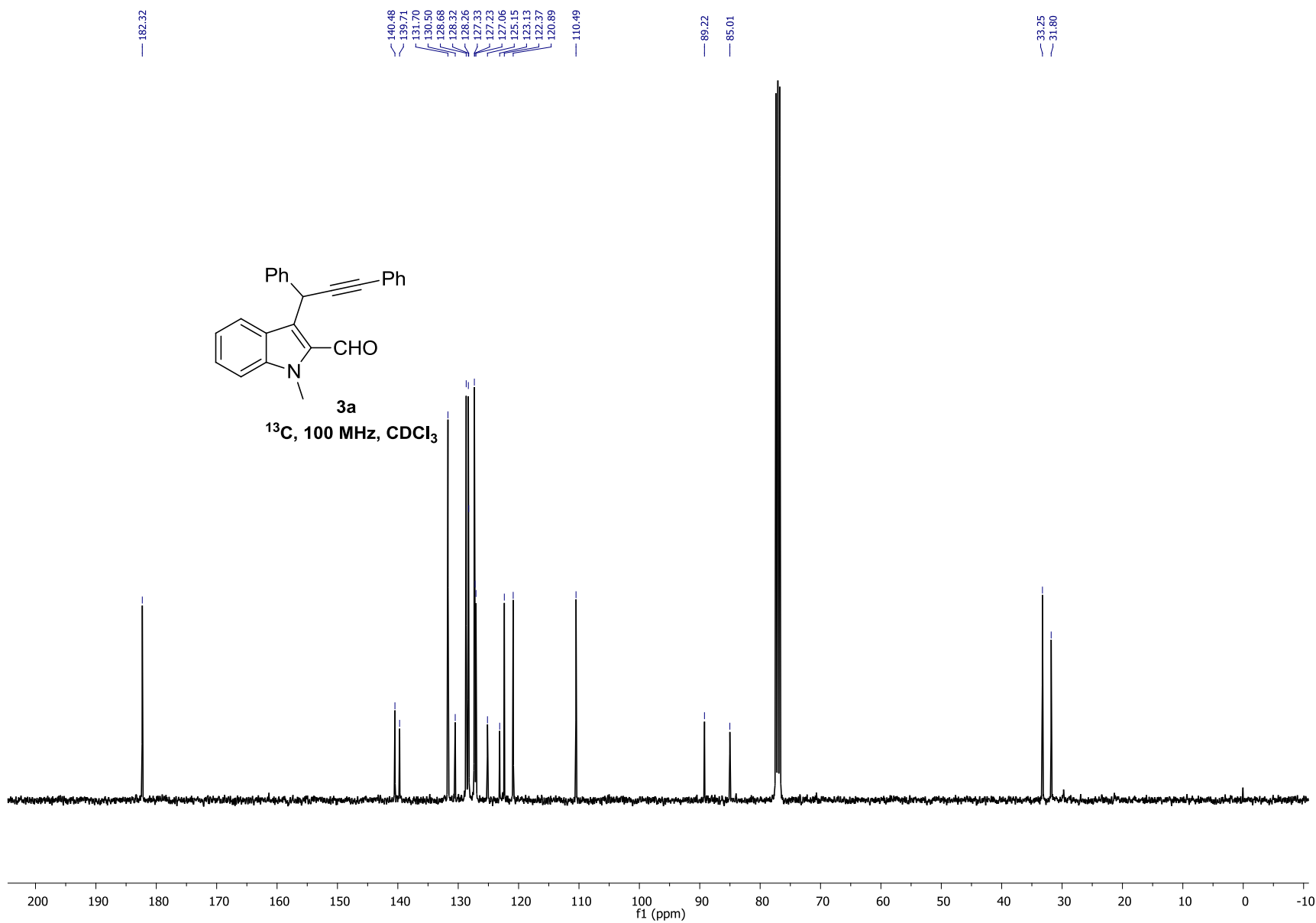


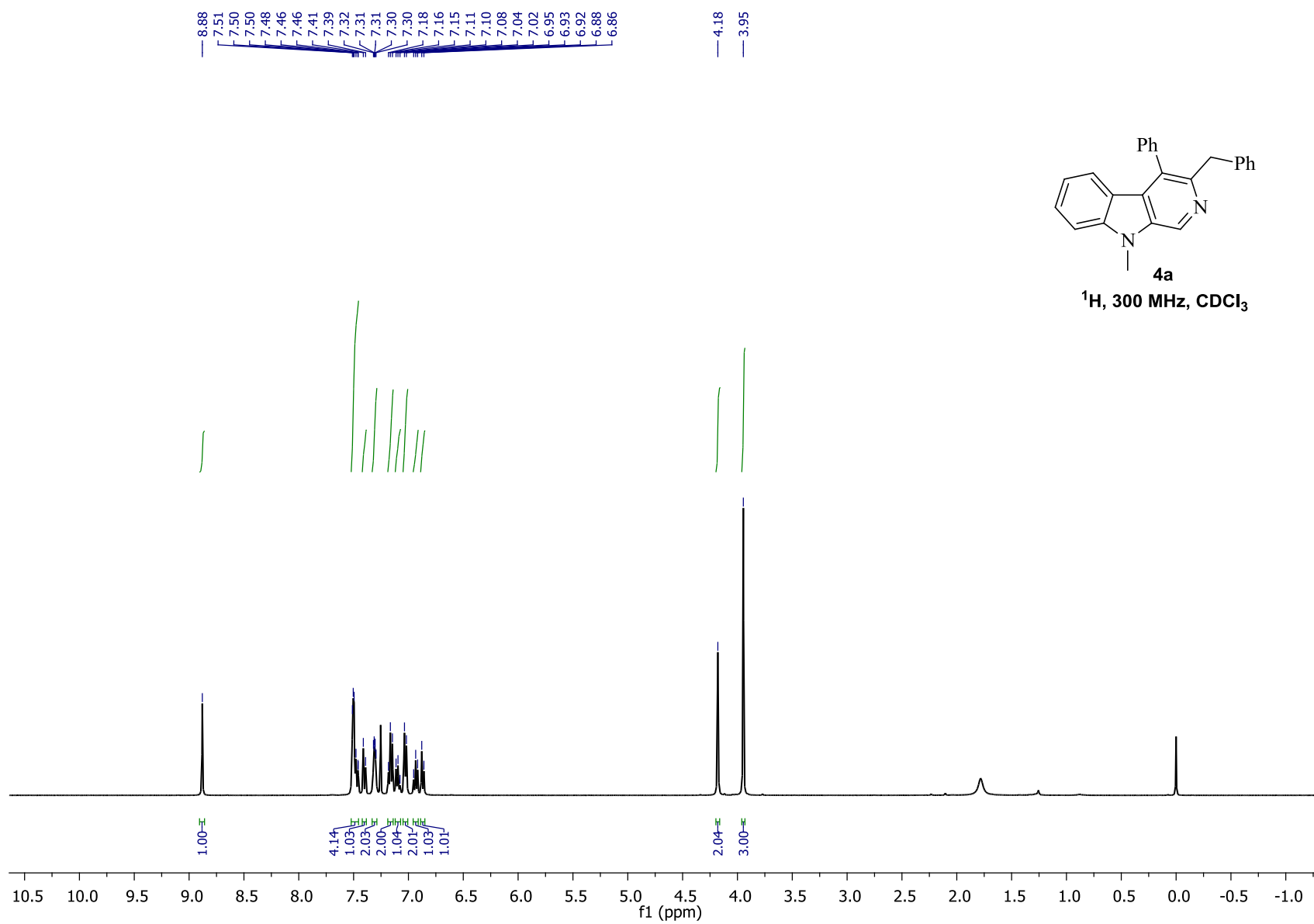


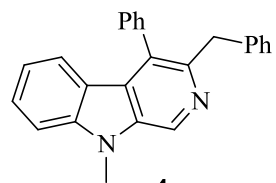
3a

¹H, 400 MHz, CDCl₃

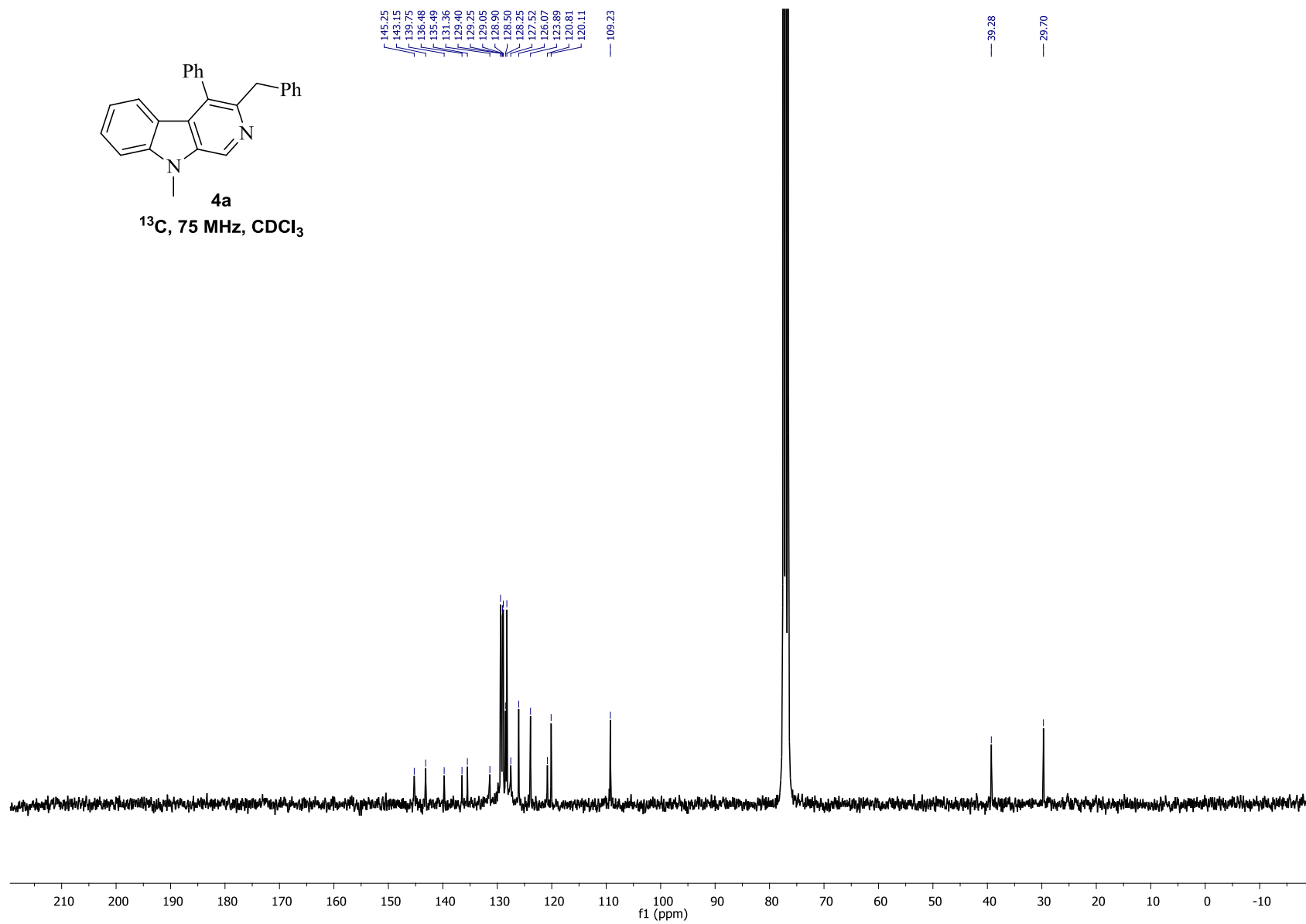


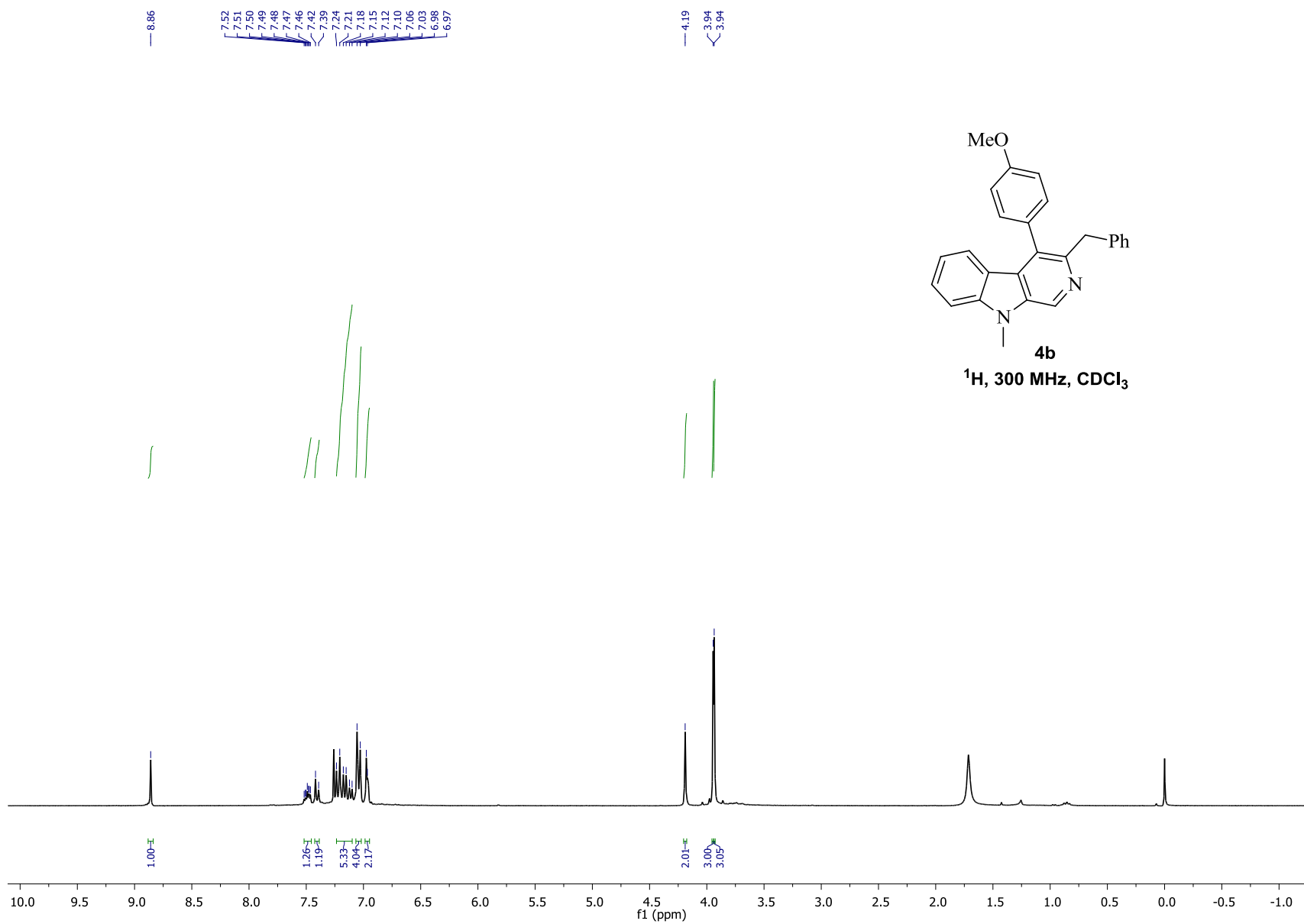


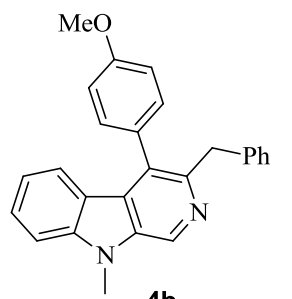




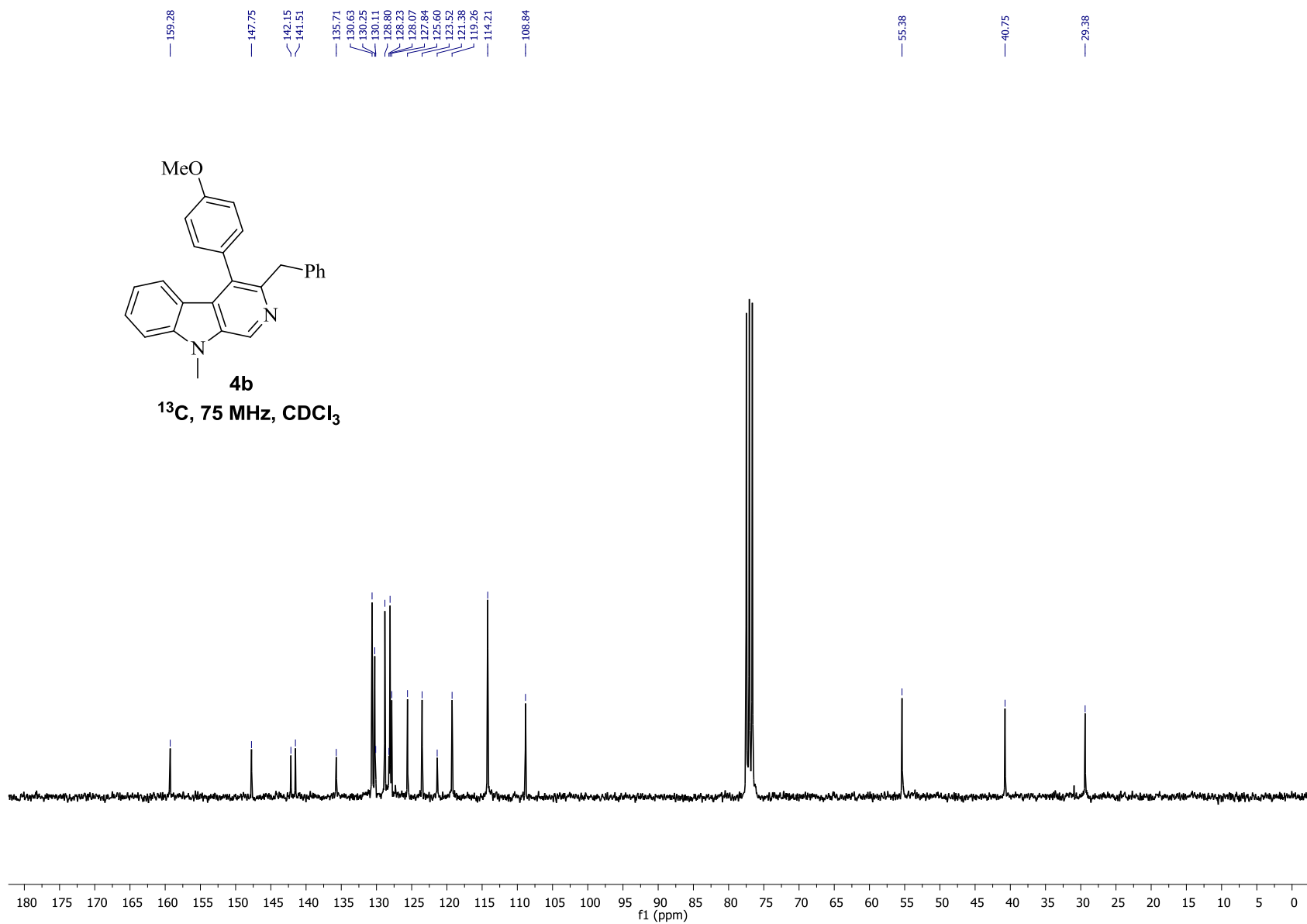
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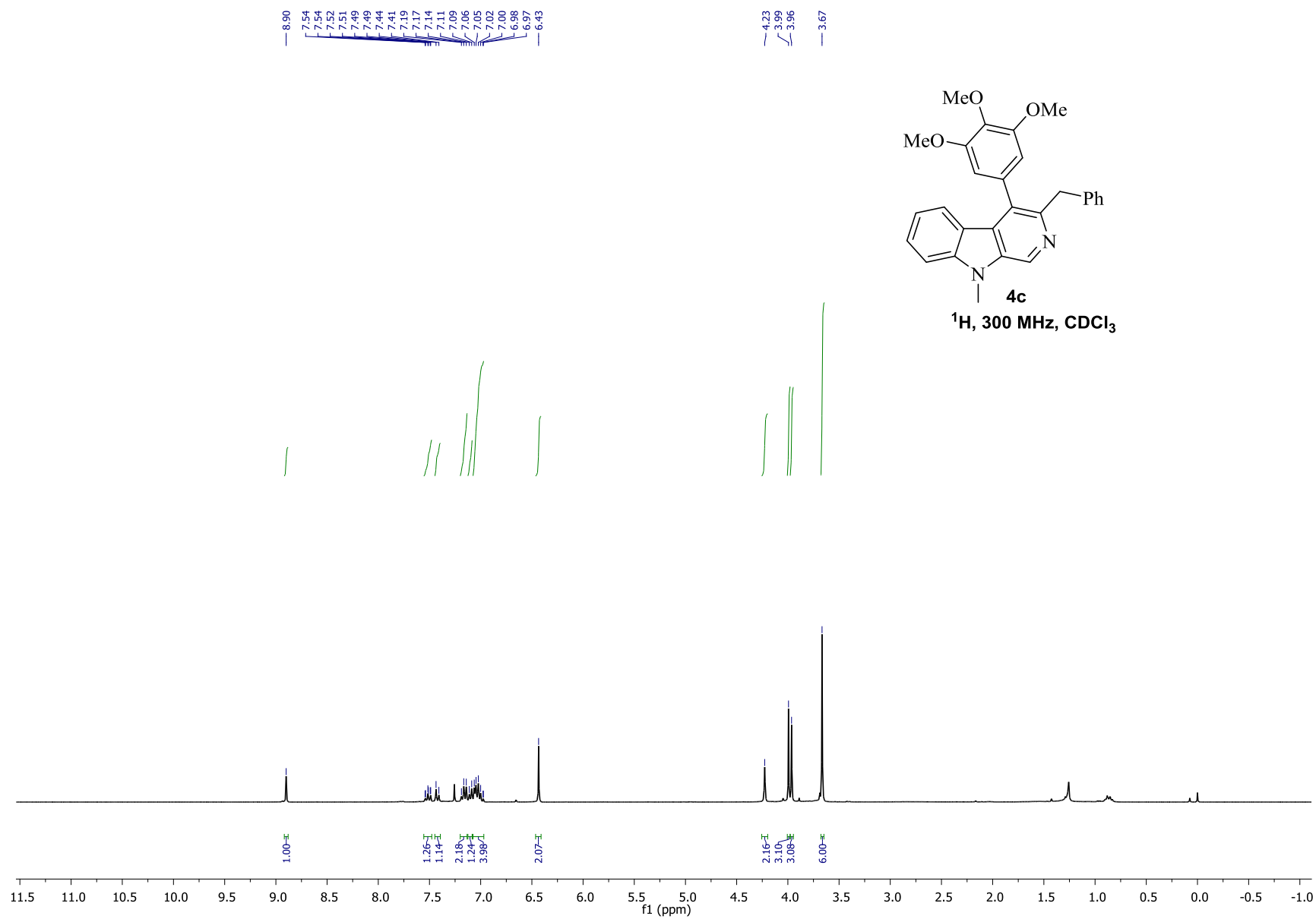


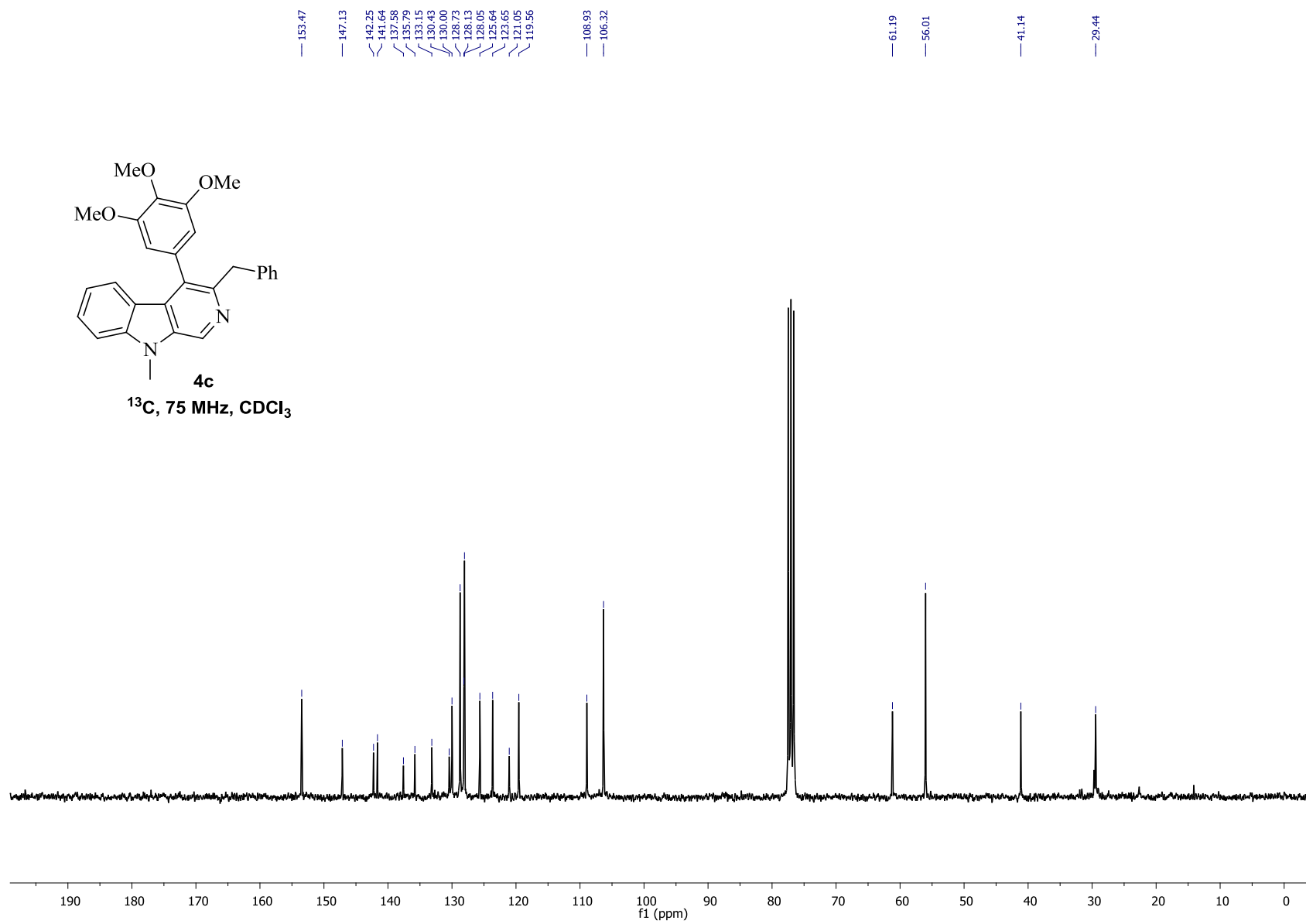


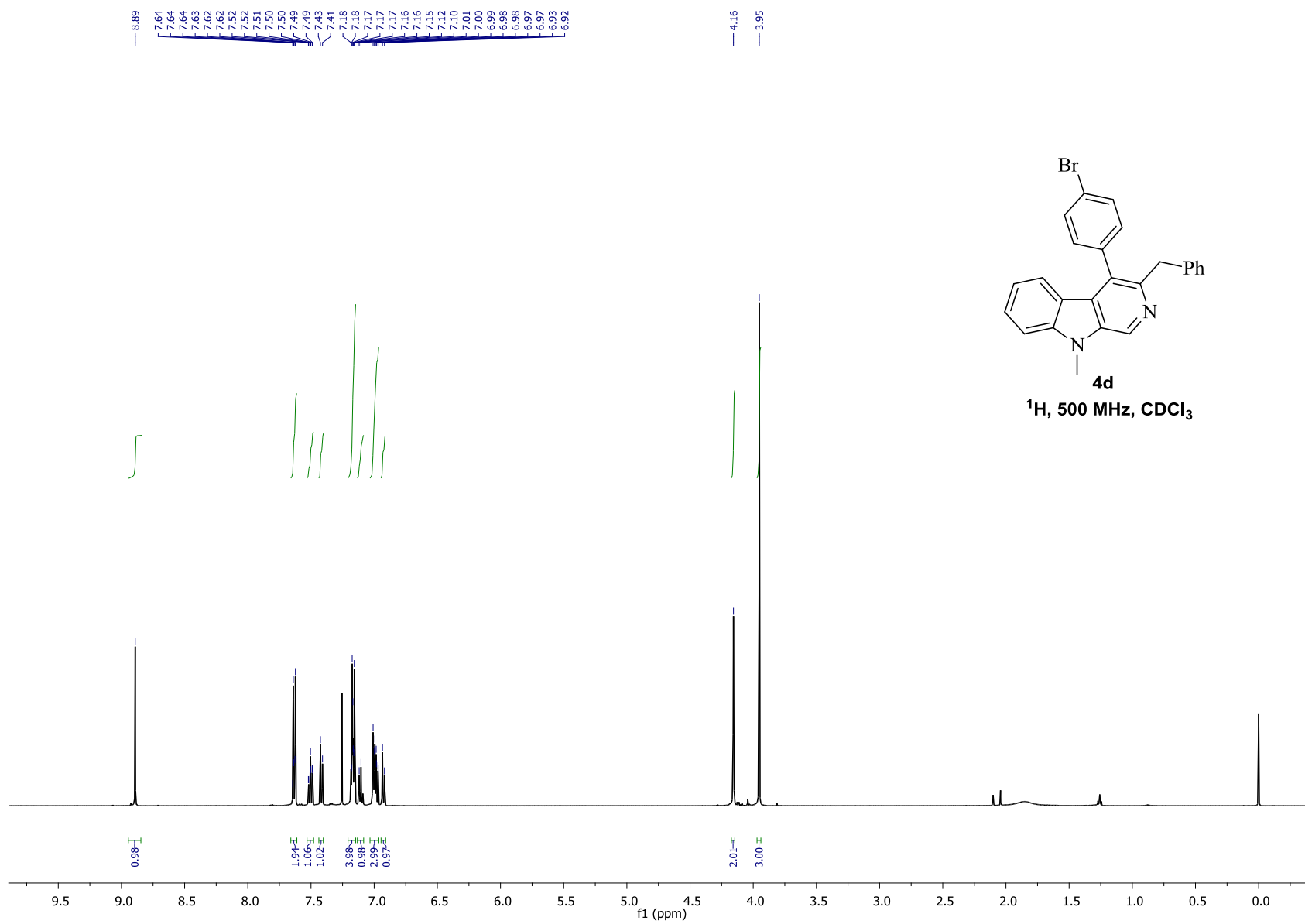


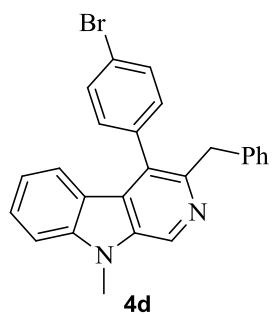
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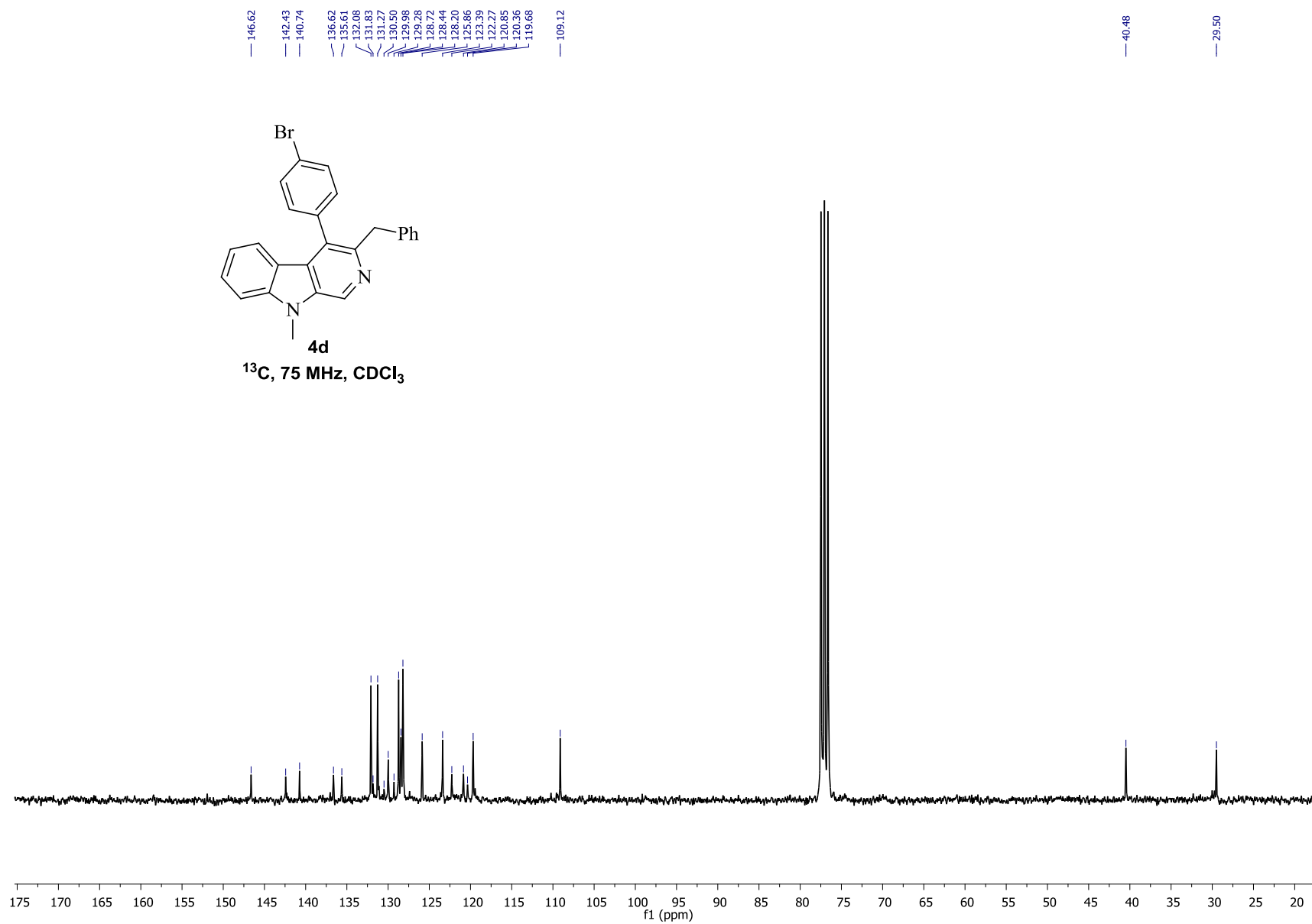


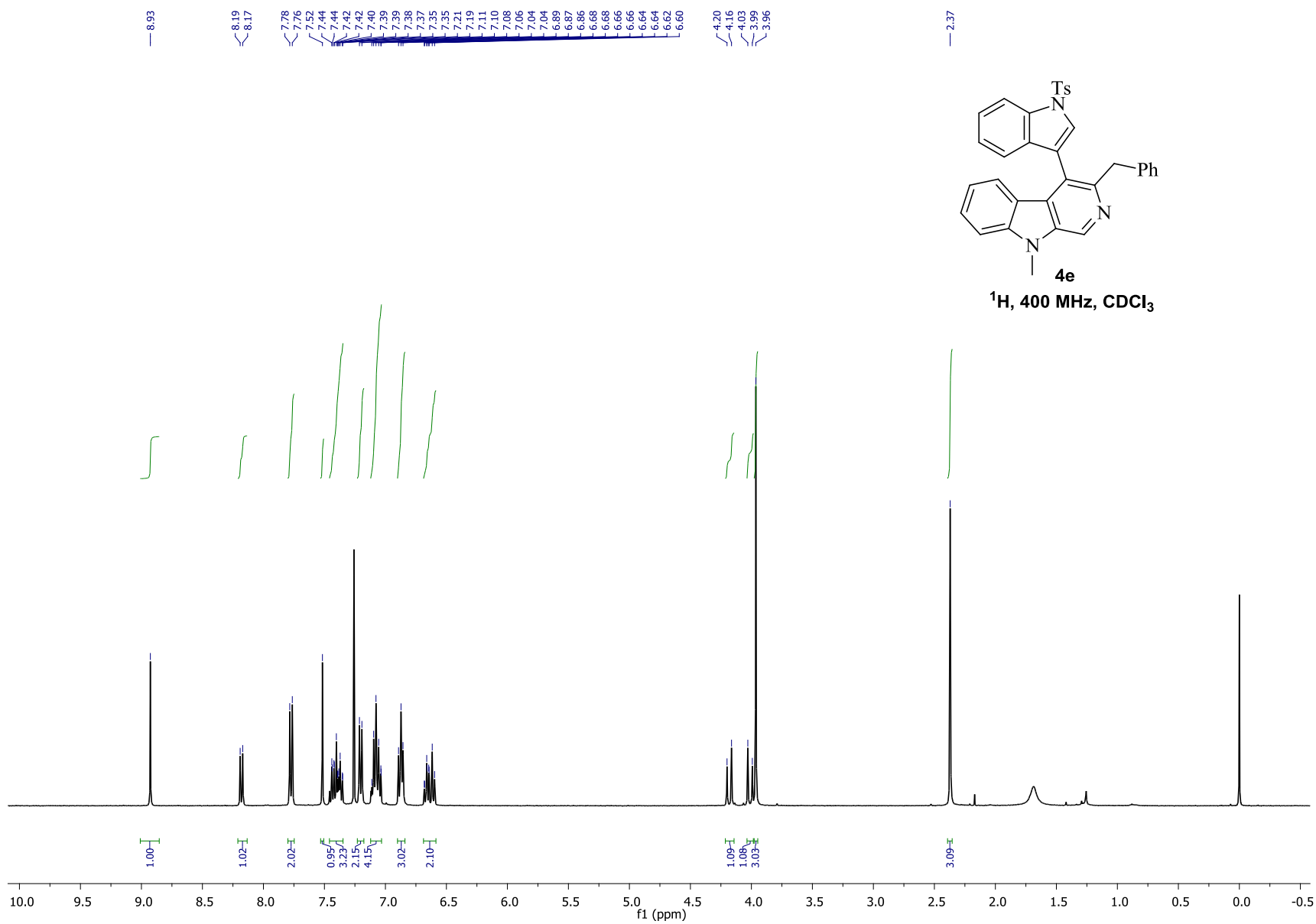


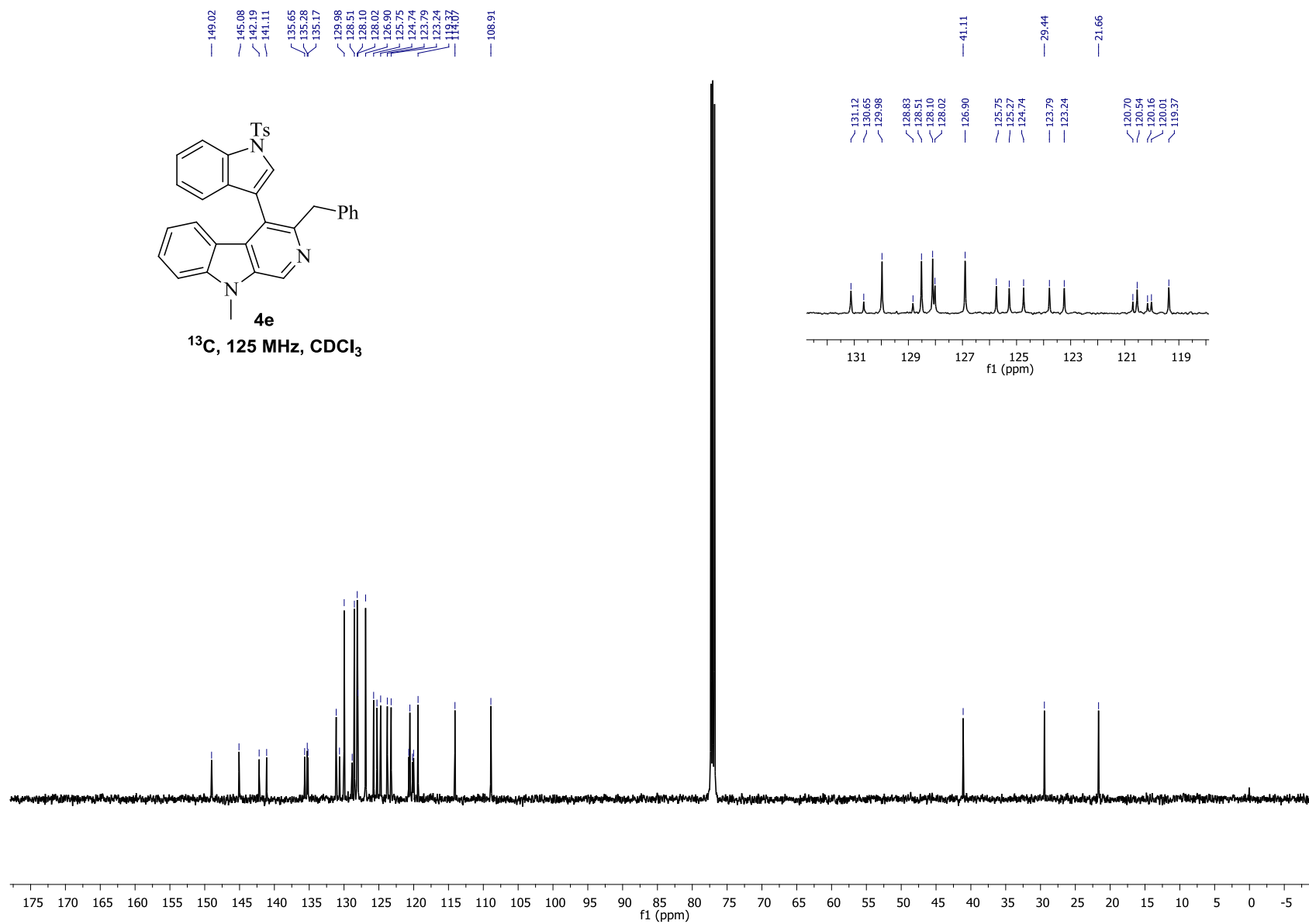


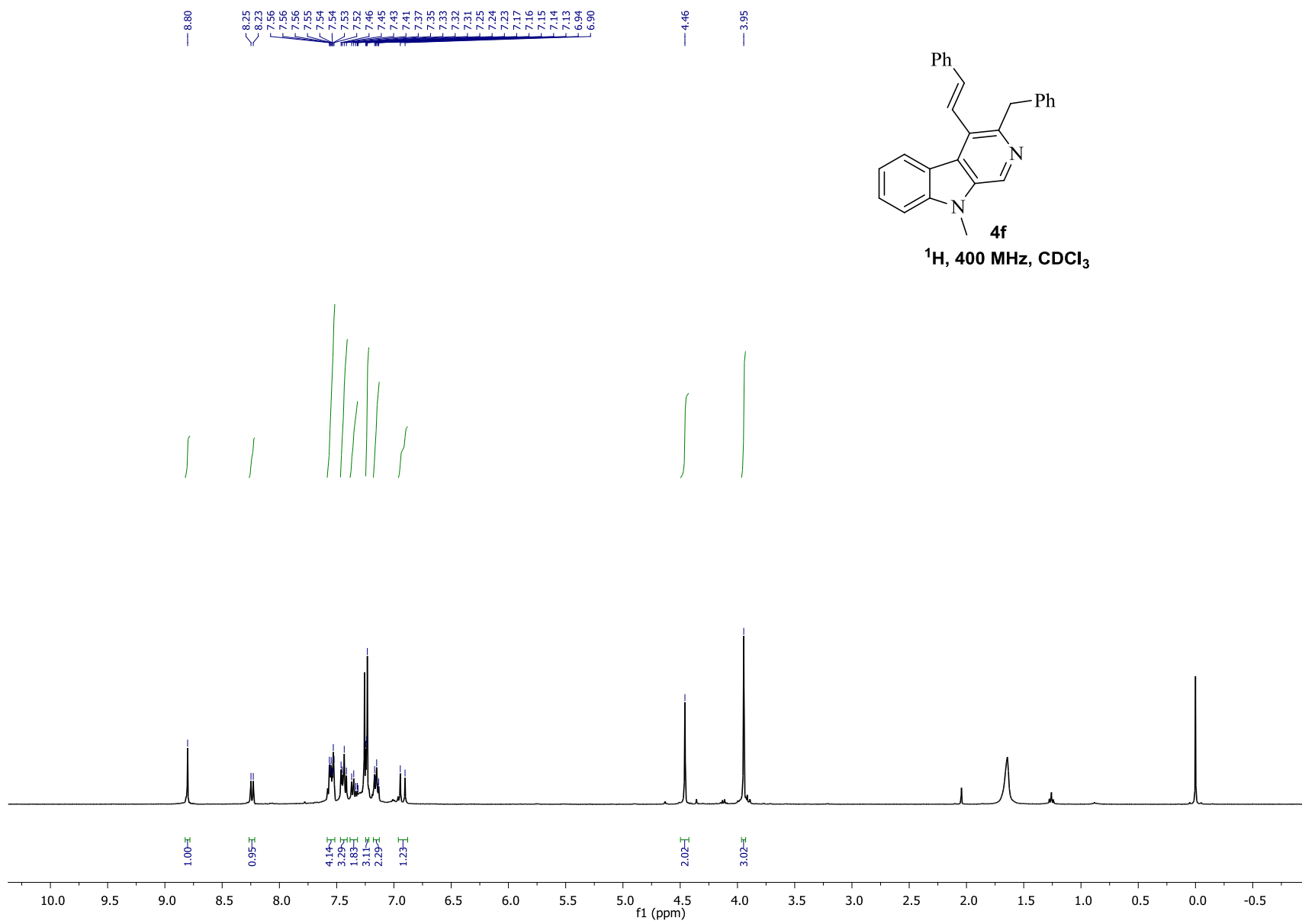


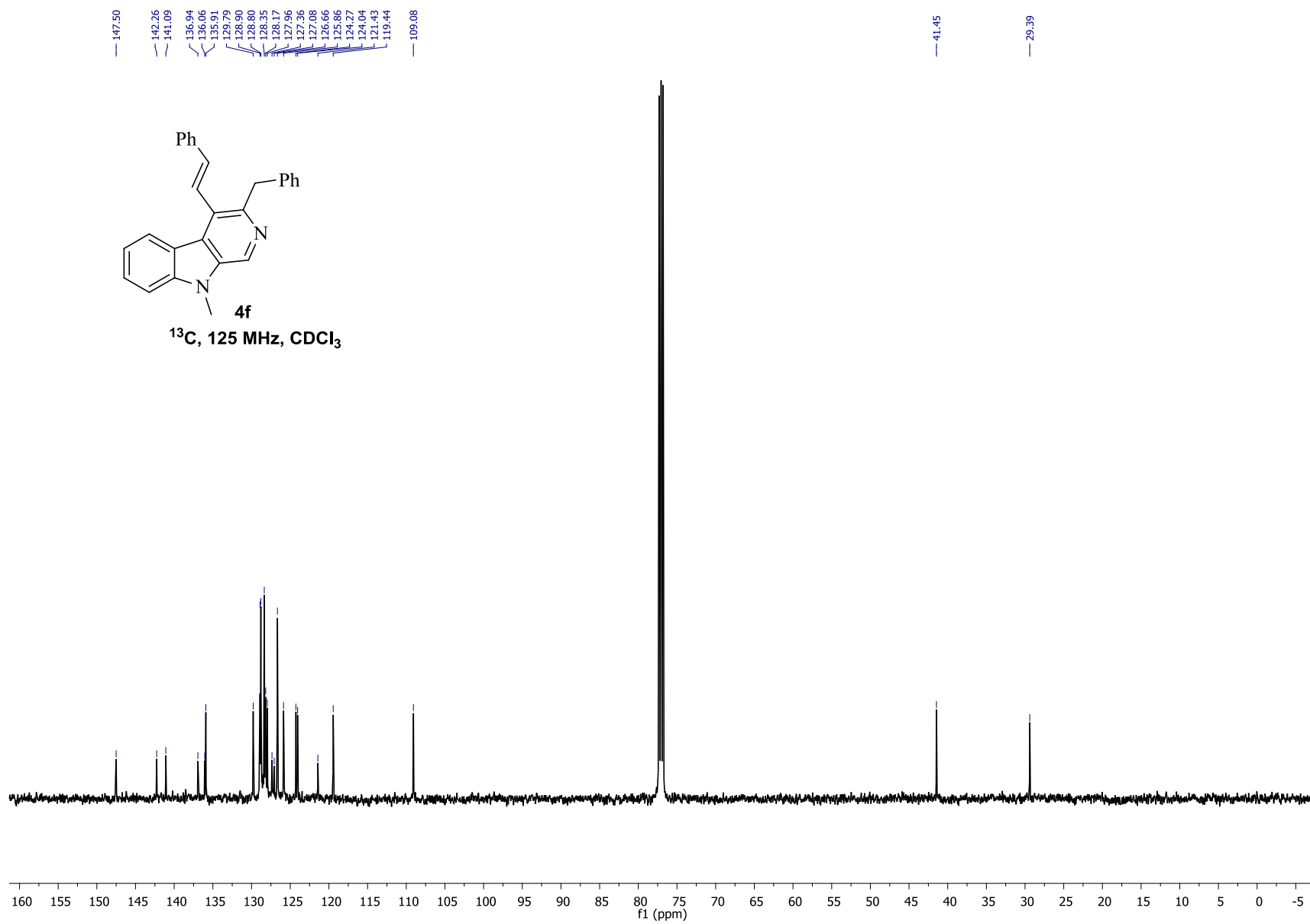
^{13}C , 75 MHz, CDCl_3

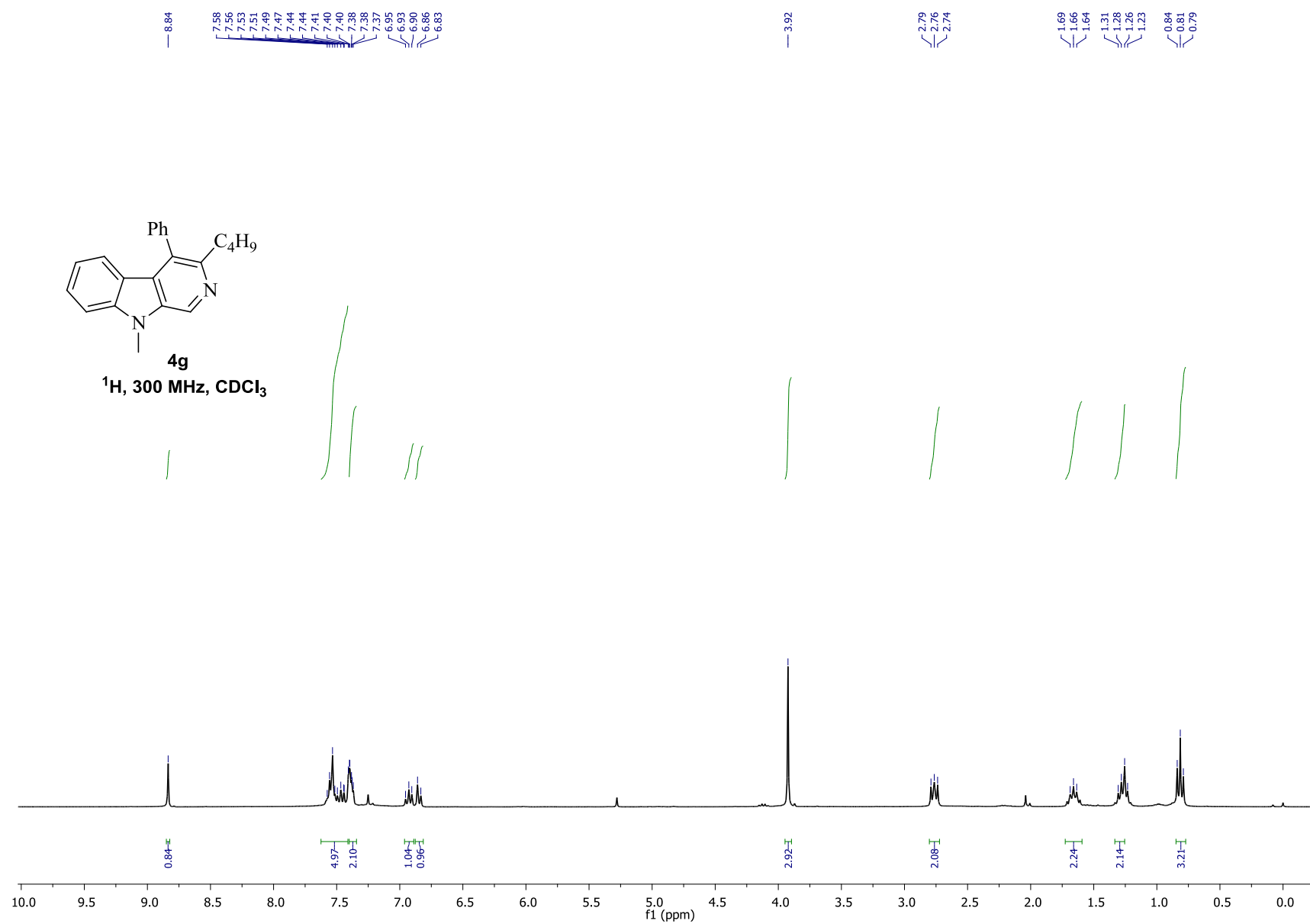


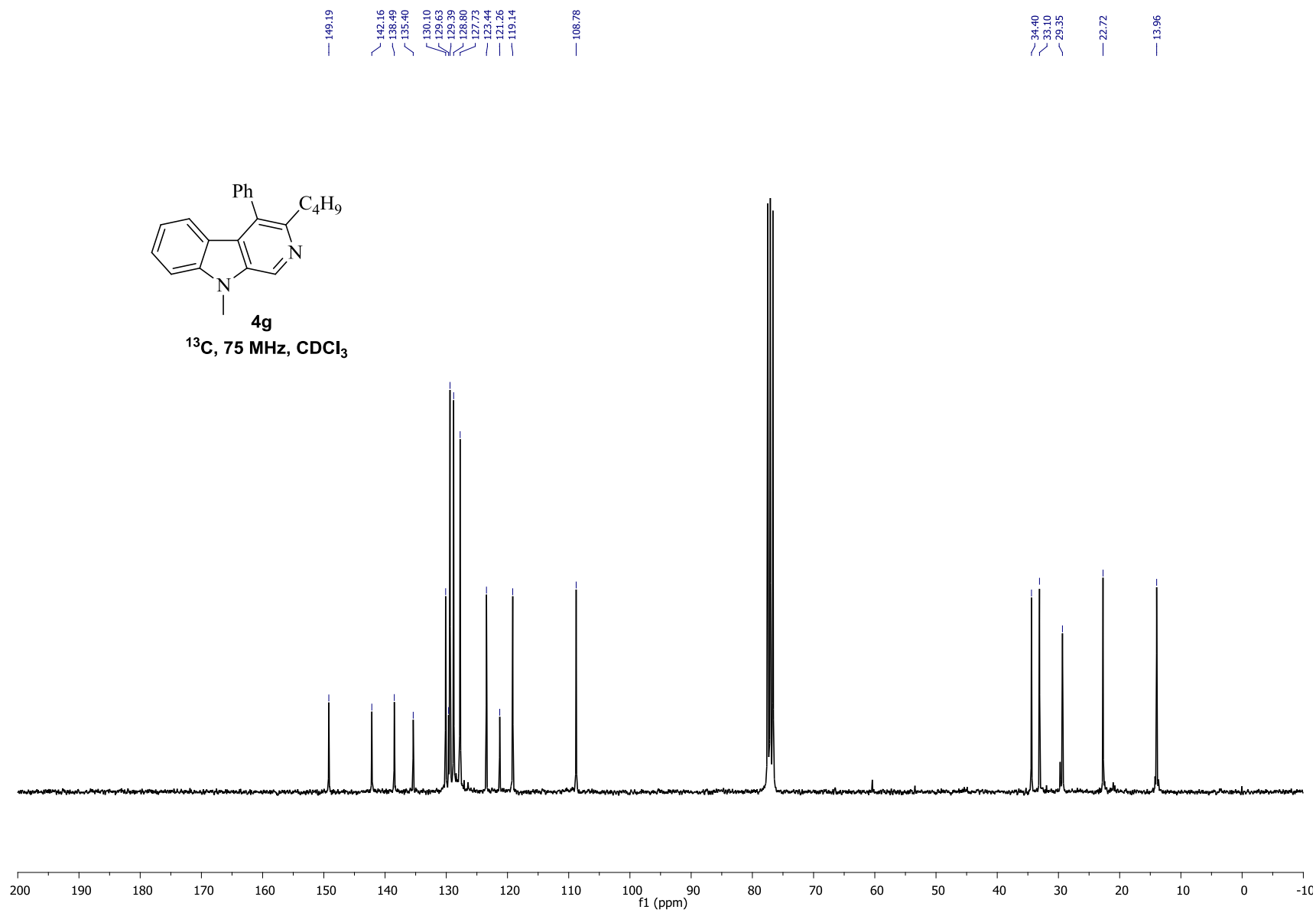


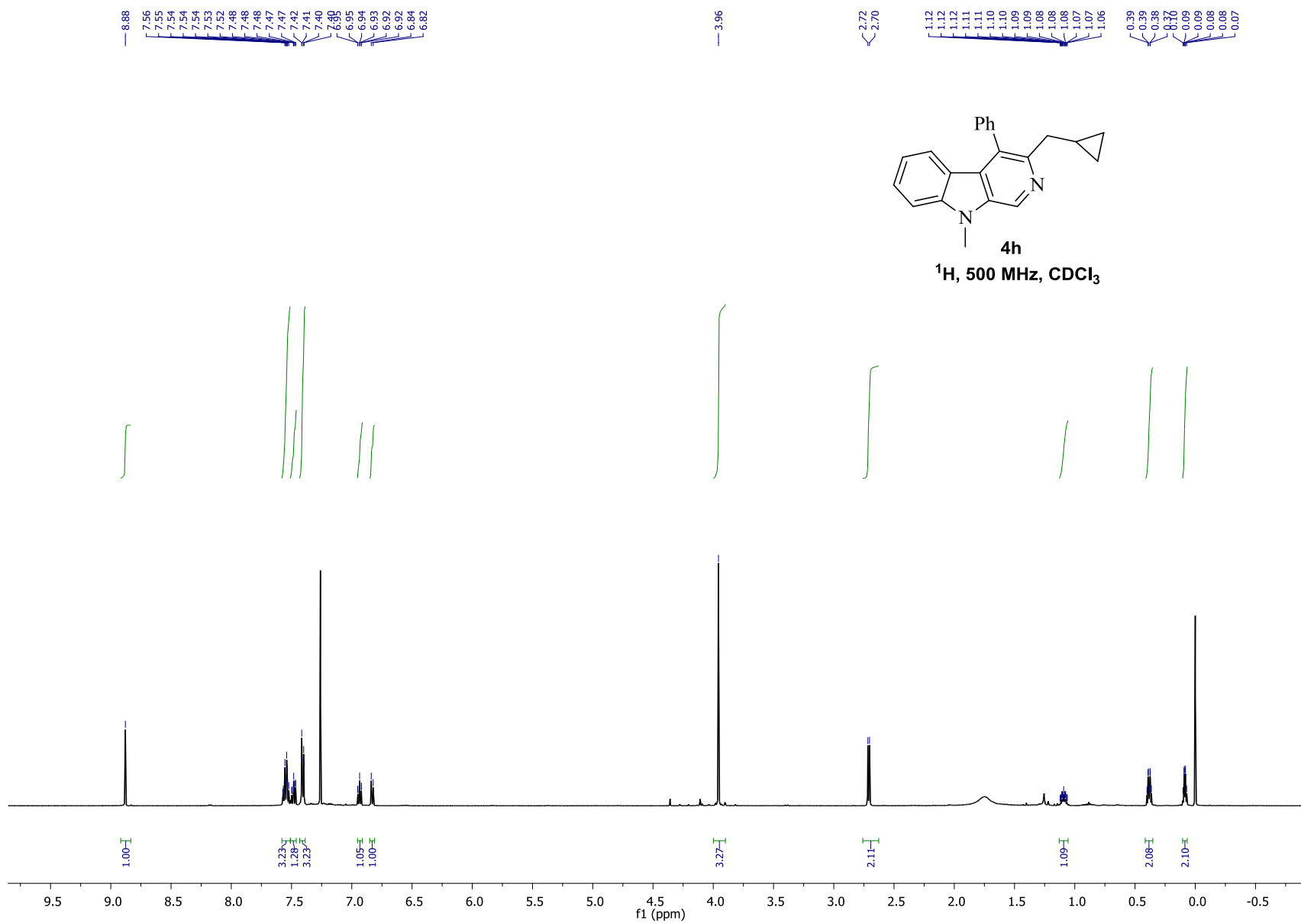




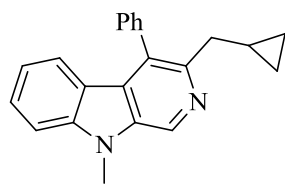




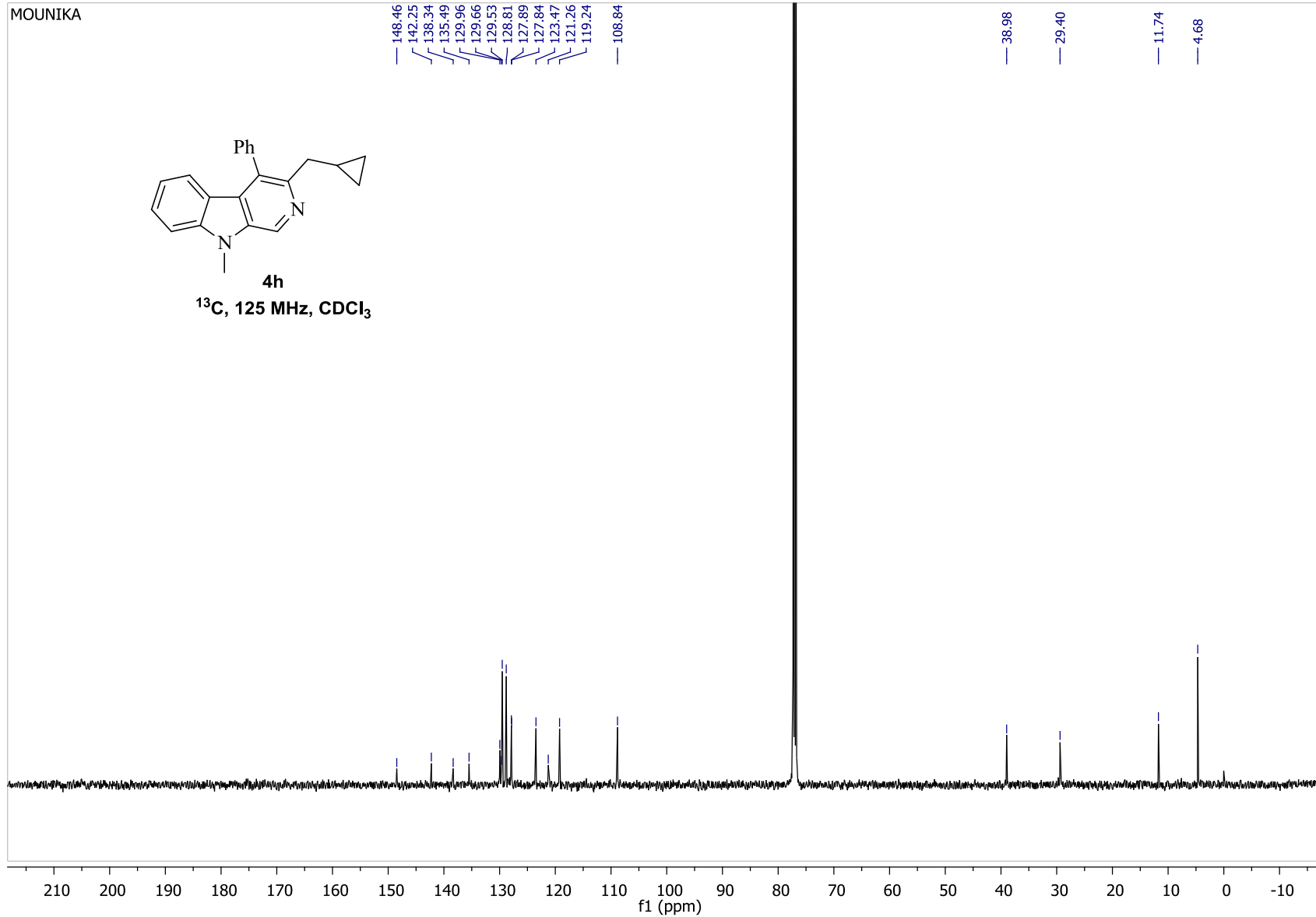


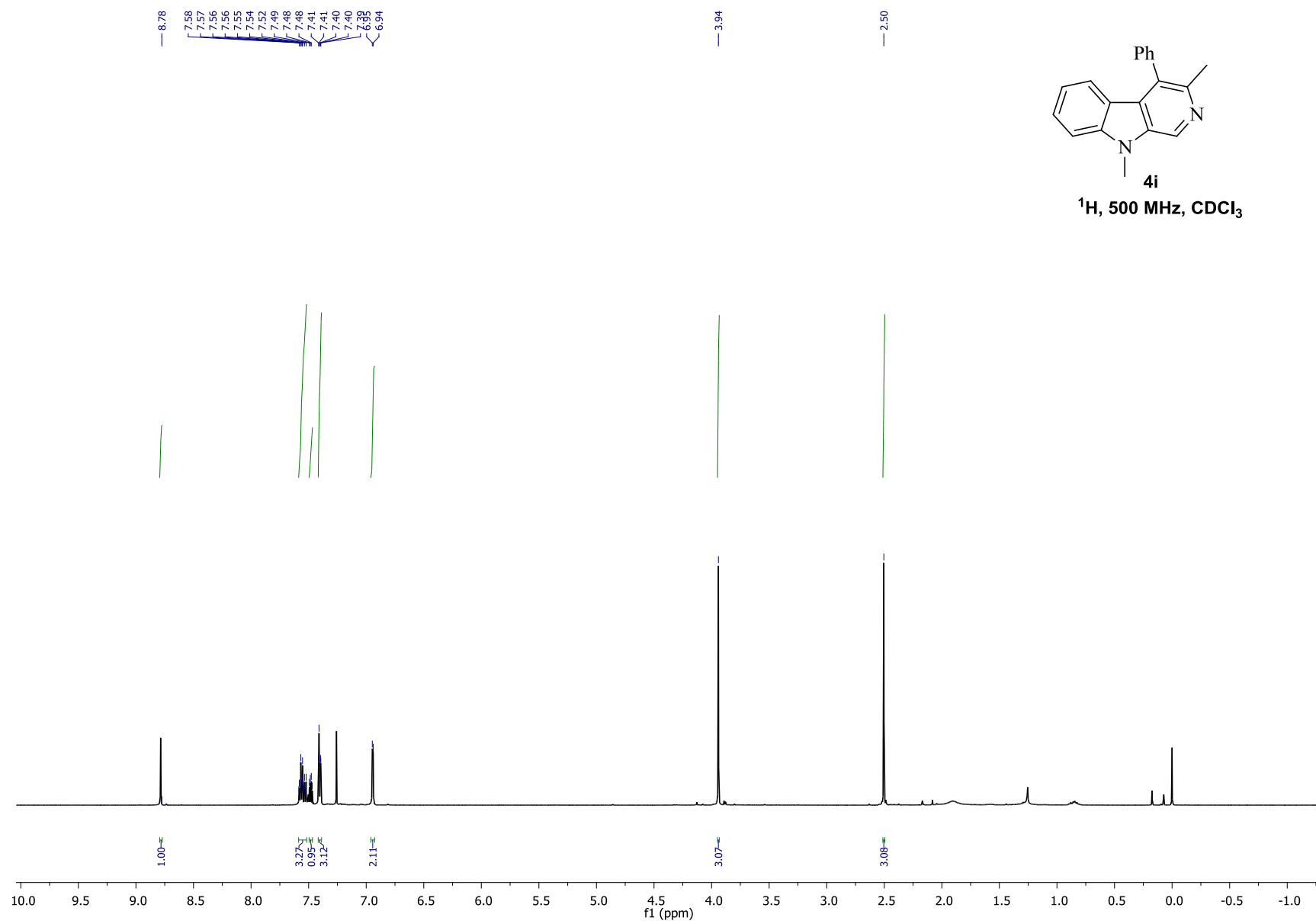


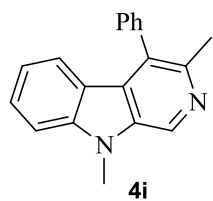
MOUNIKA



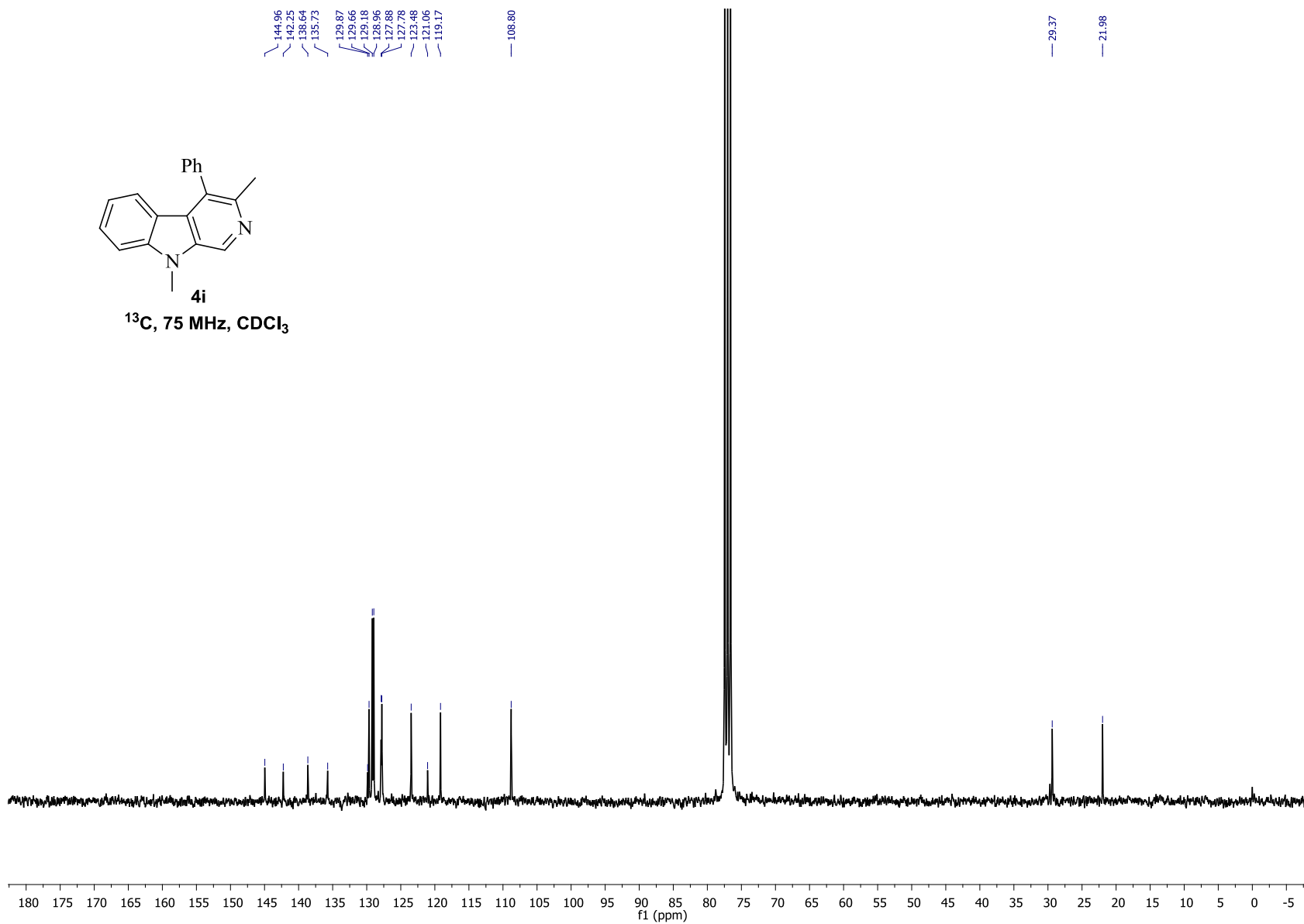
4h
 ^{13}C , 125 MHz, CDCl_3

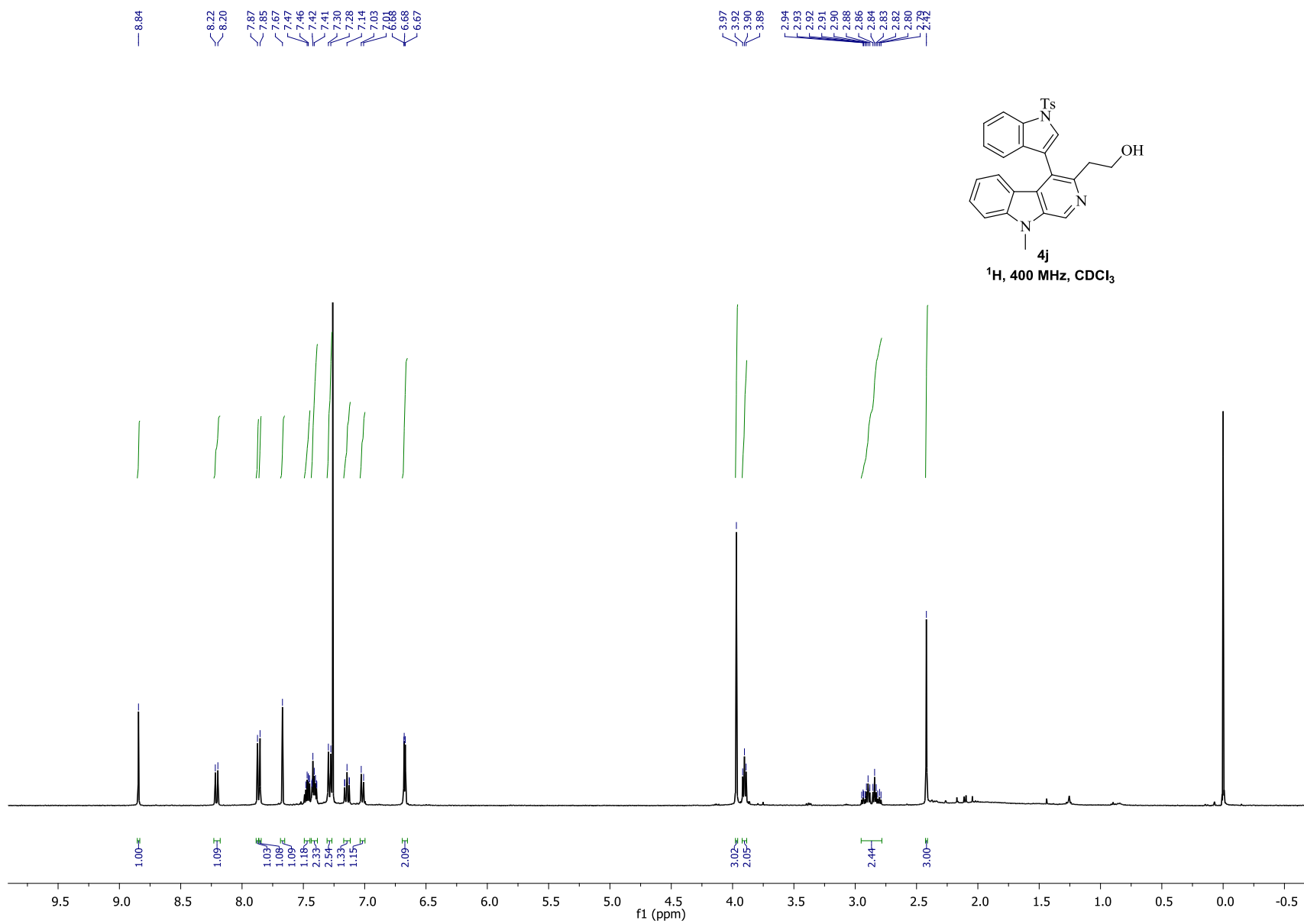


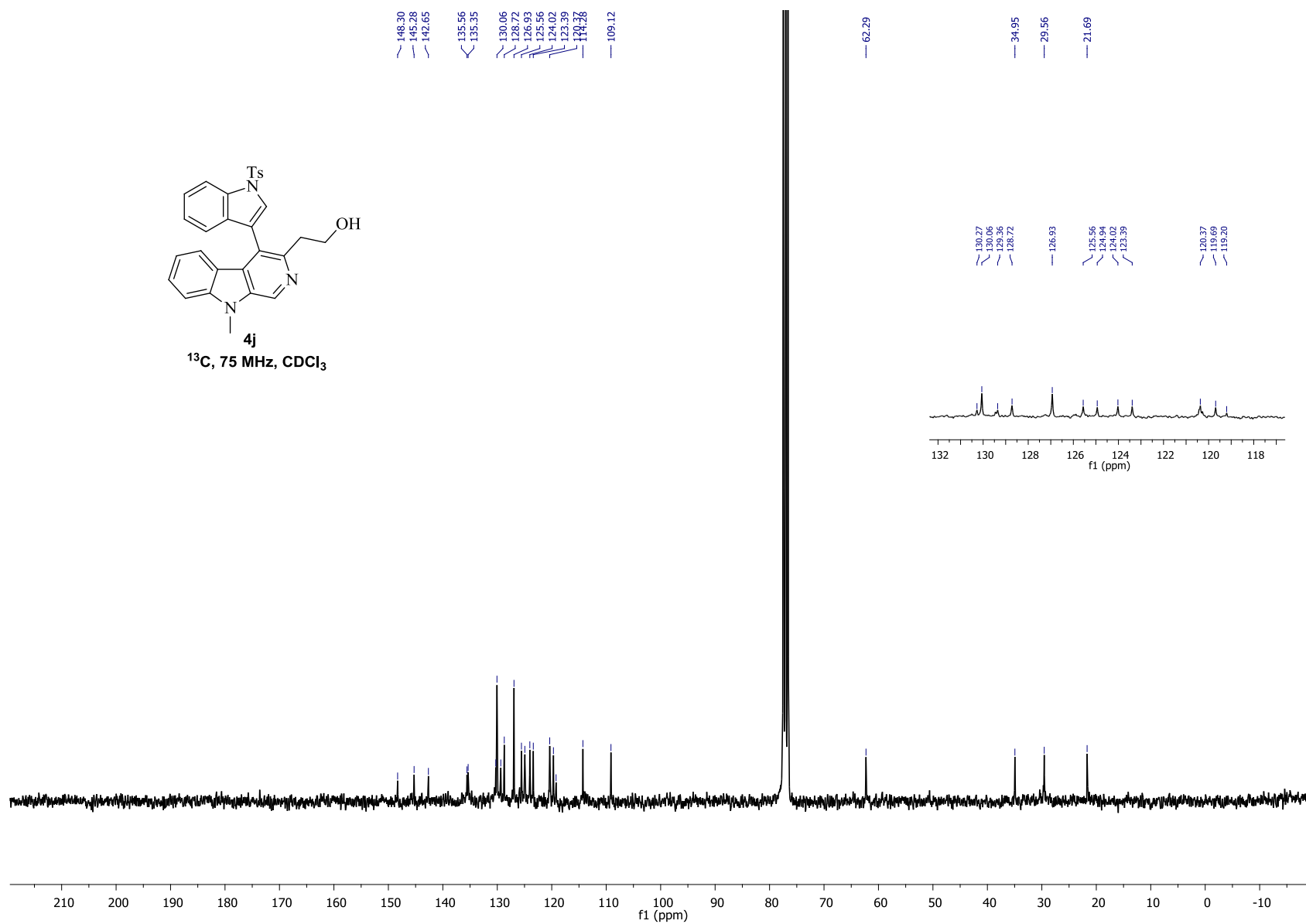




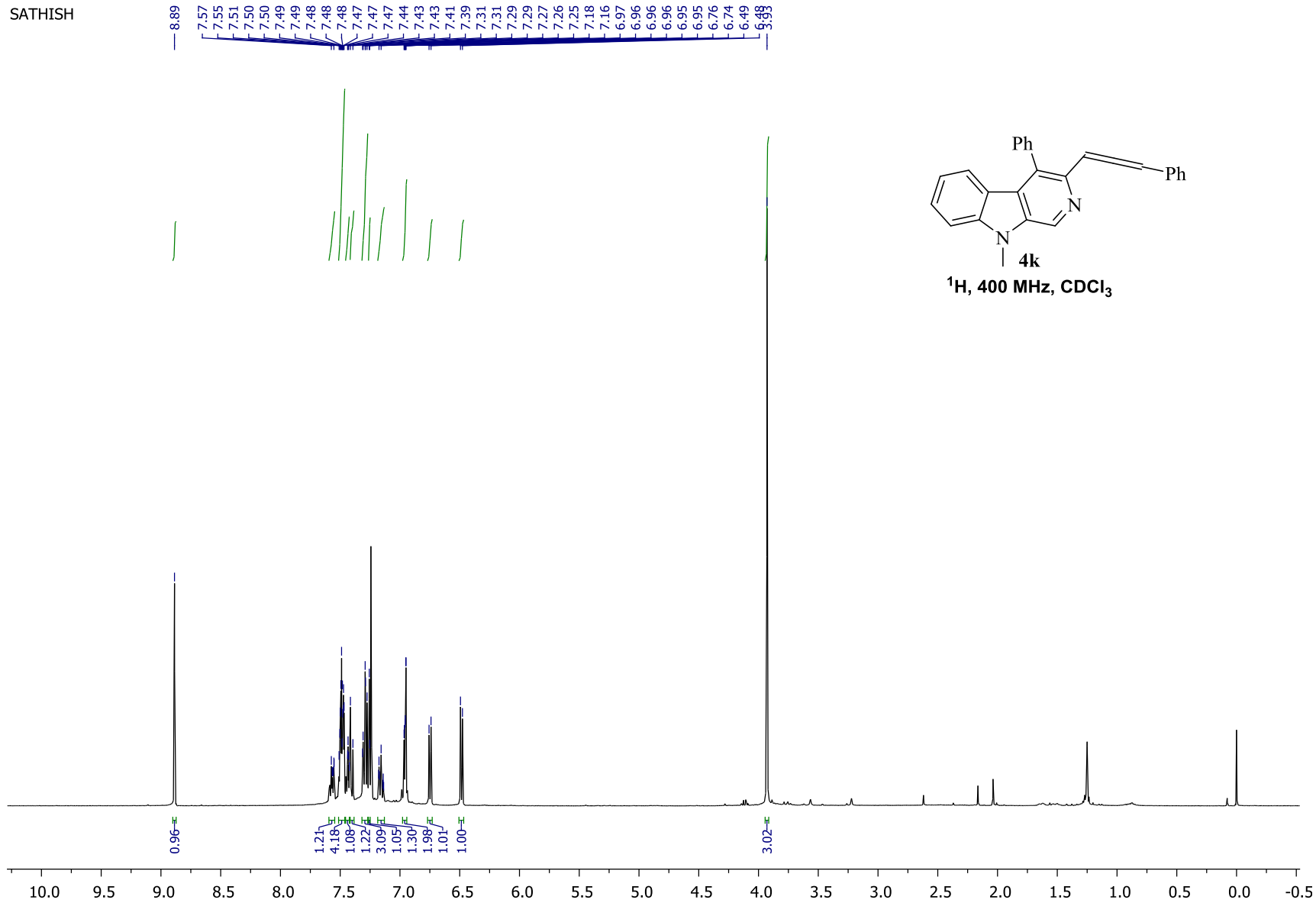
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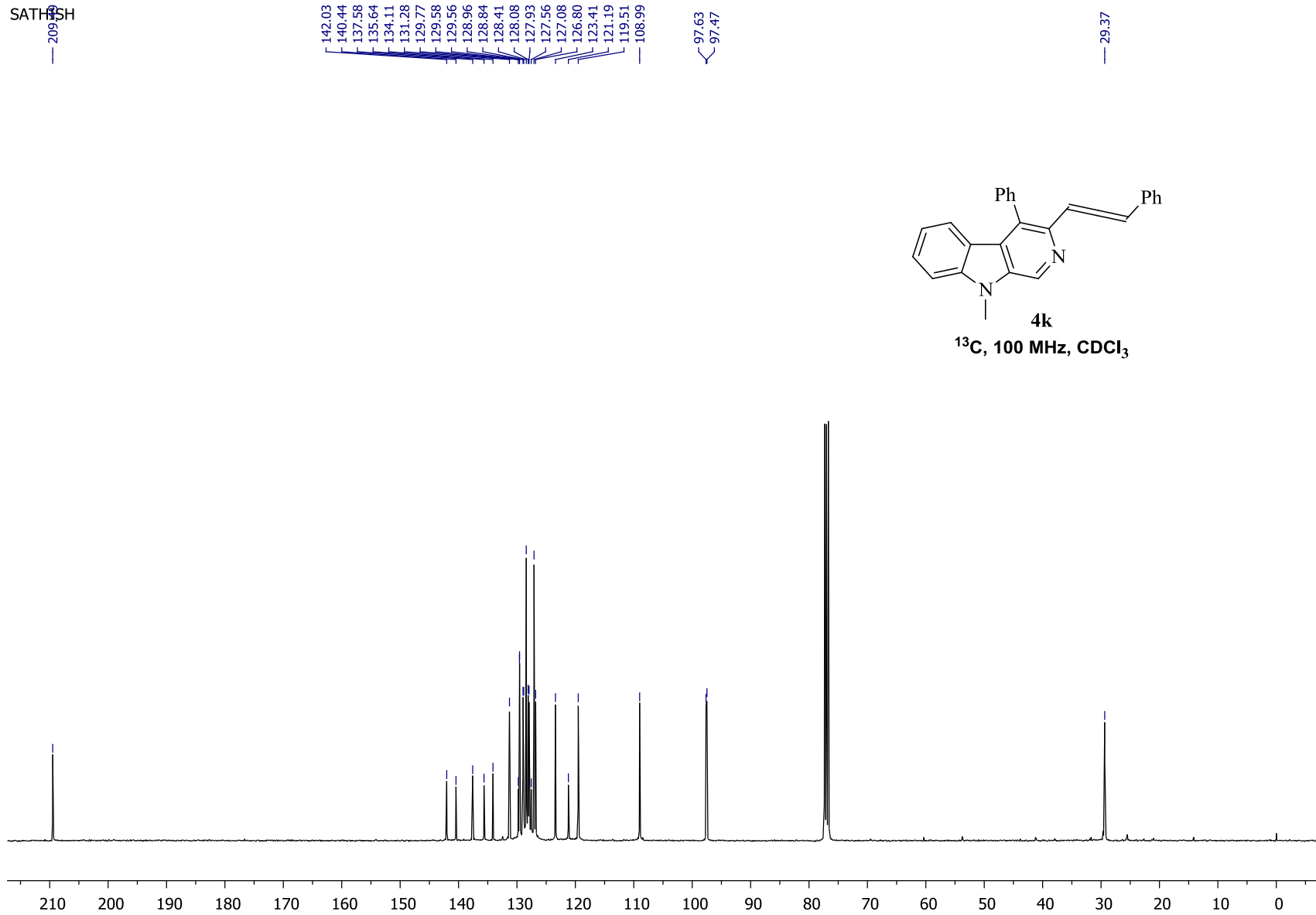


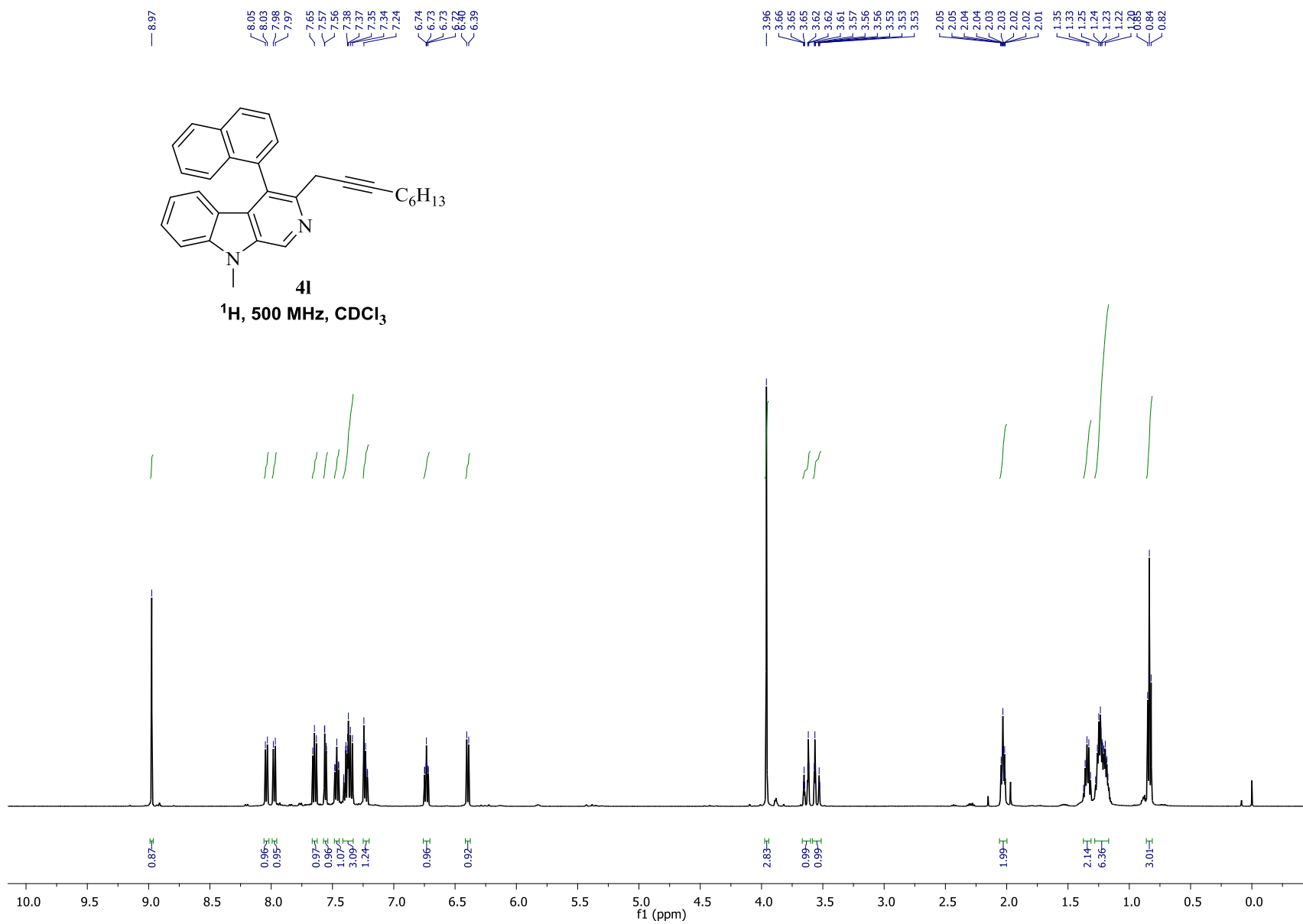


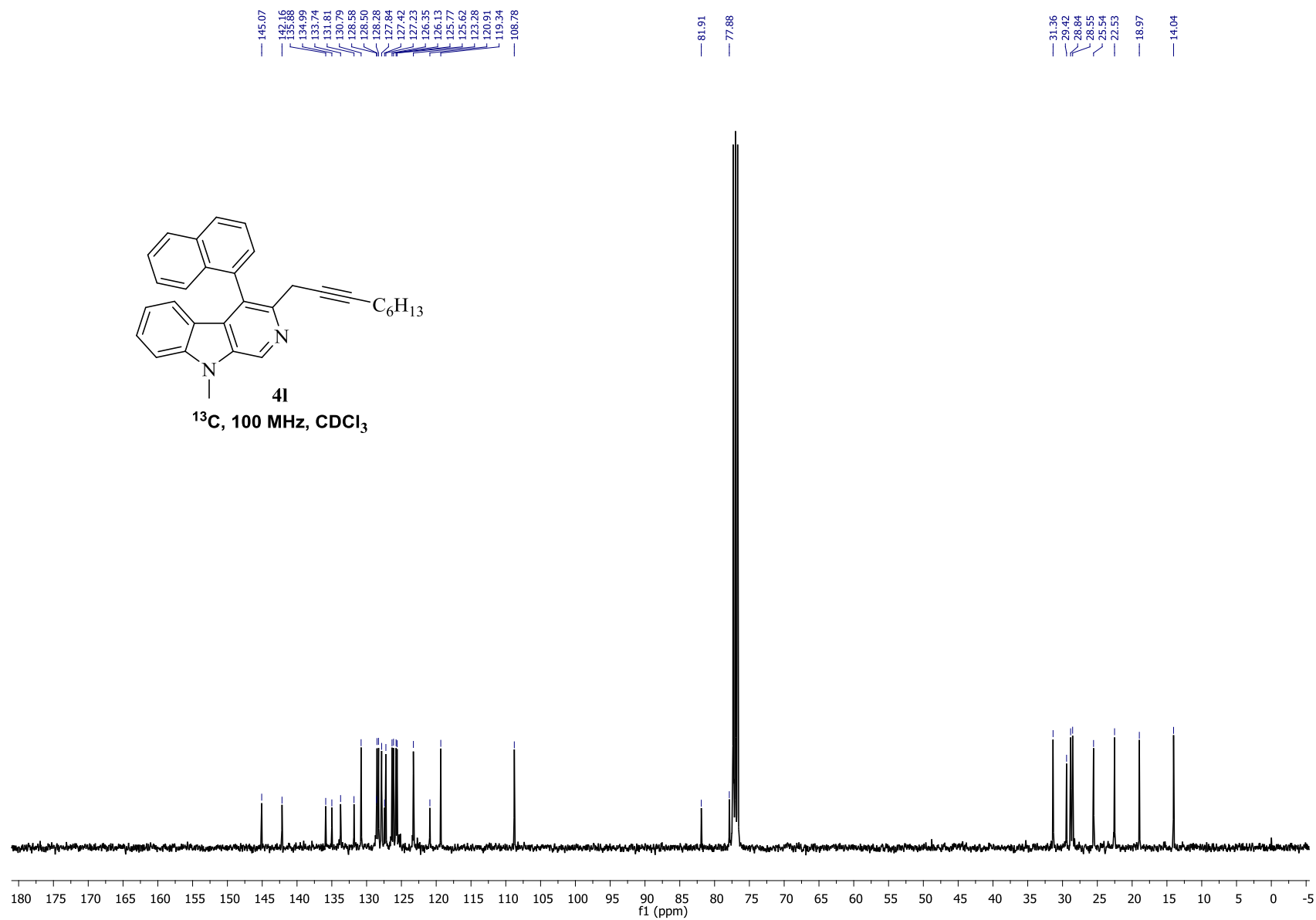
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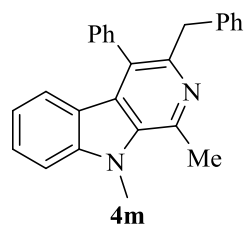
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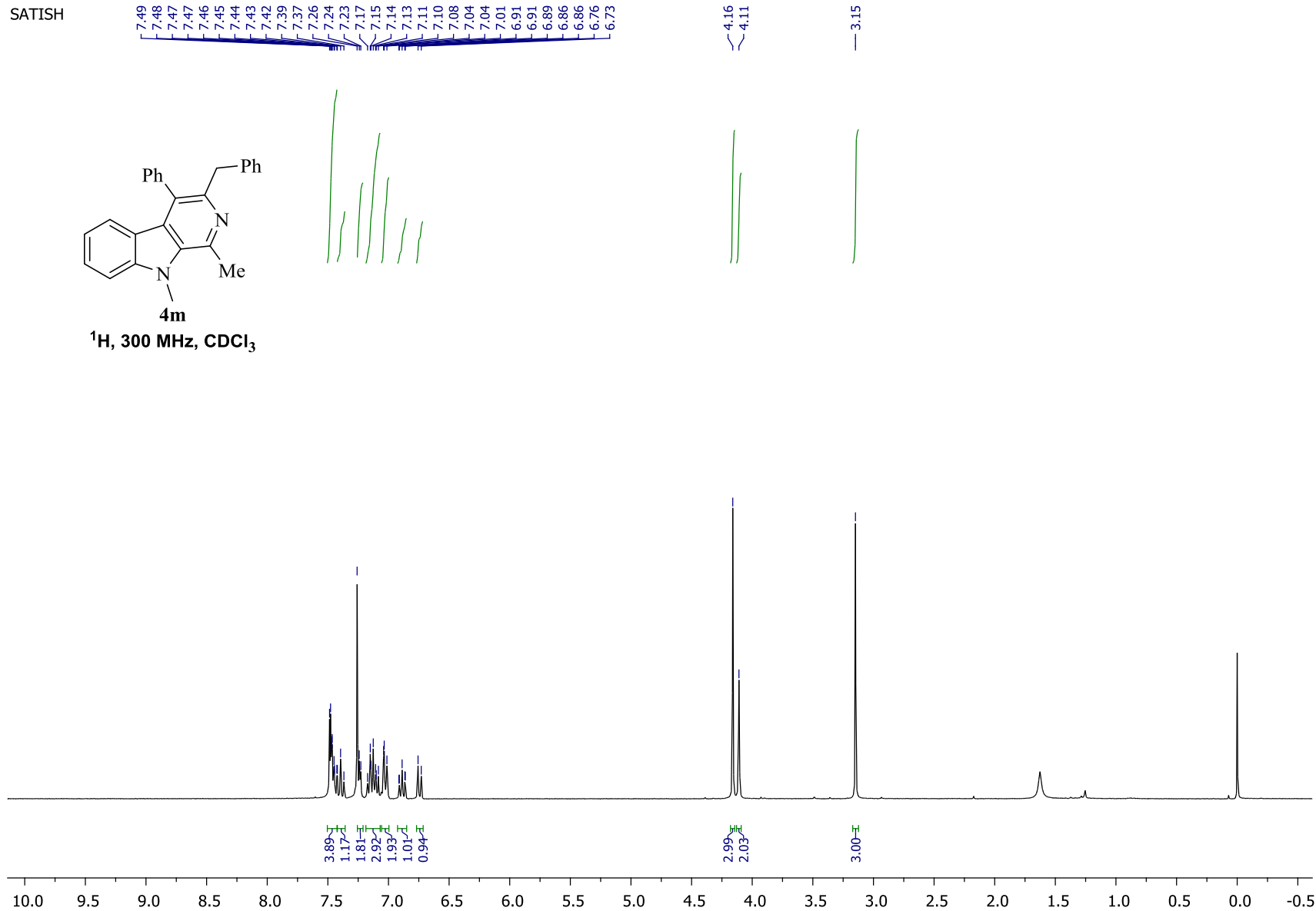




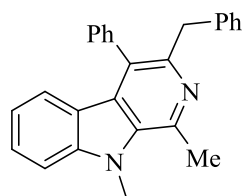
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¹H, 300 MHz, CDCl₃

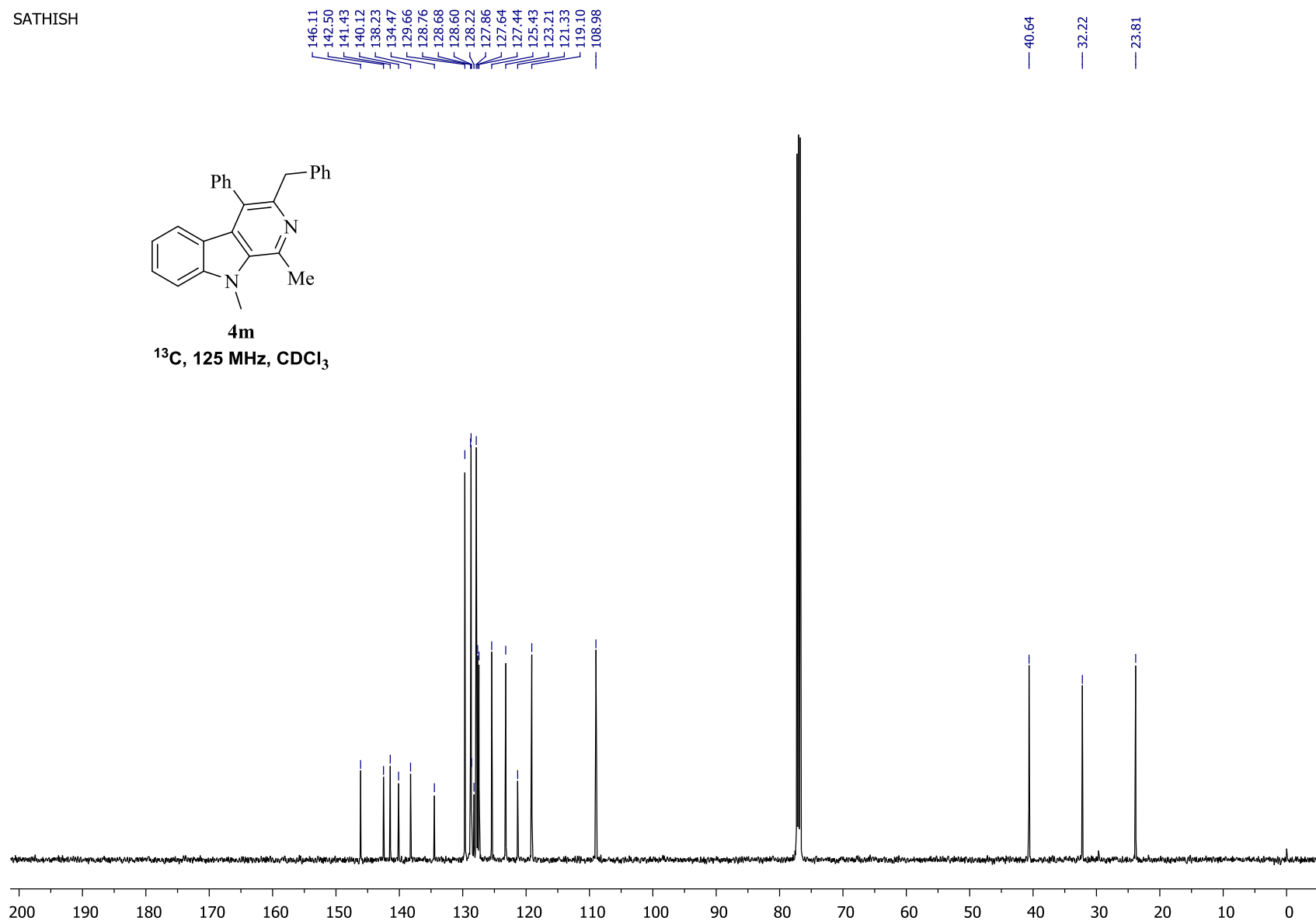


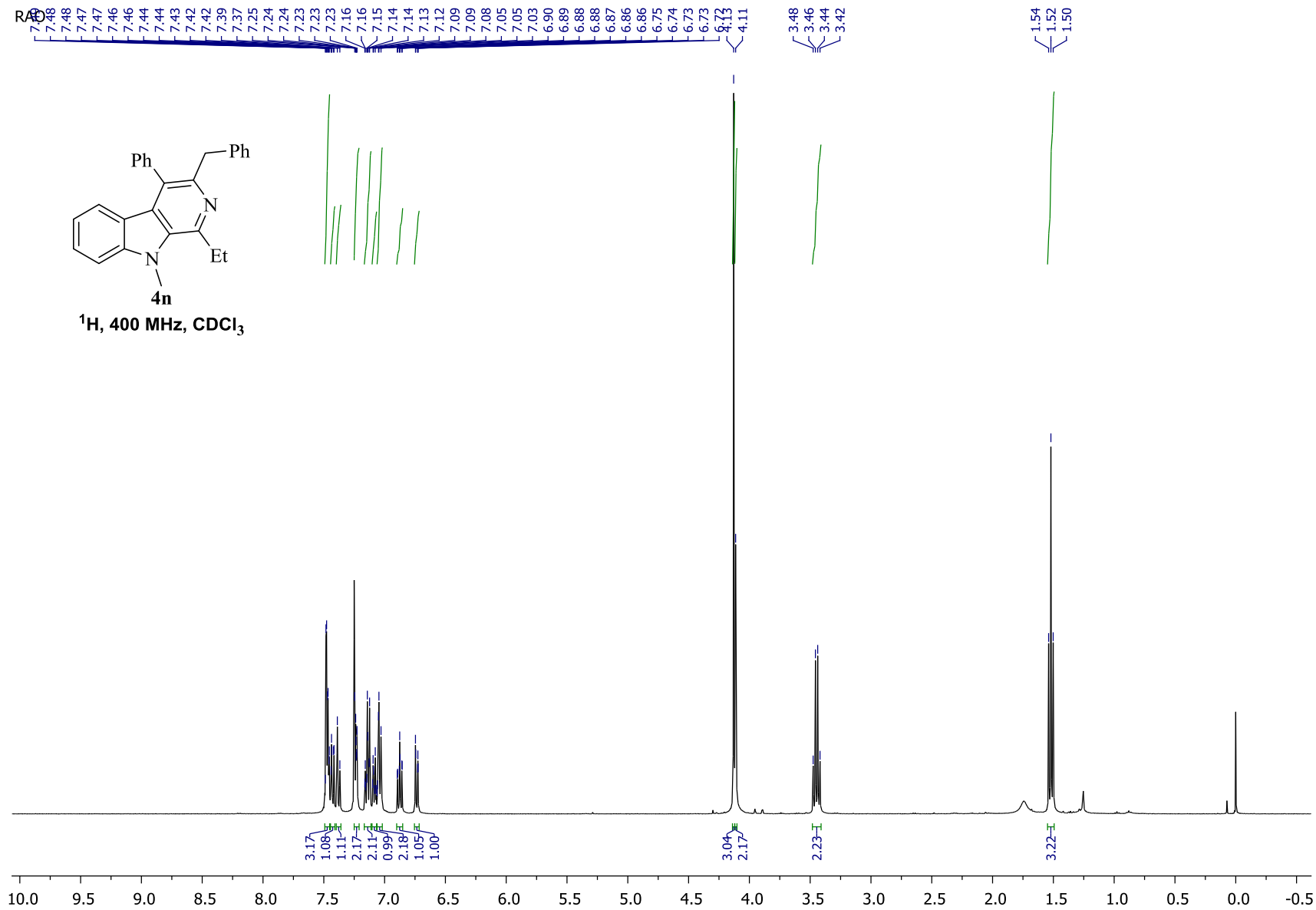
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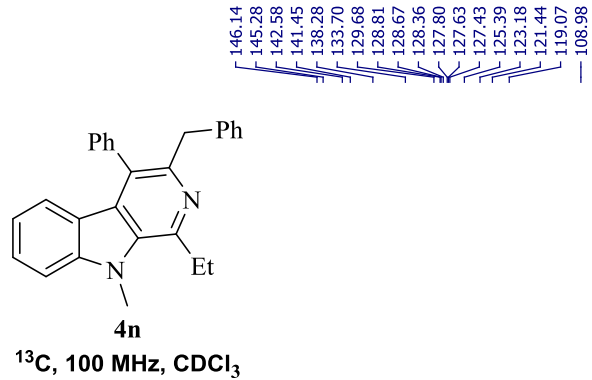
4m

^{13}C , 125 MHz, CDCl_3

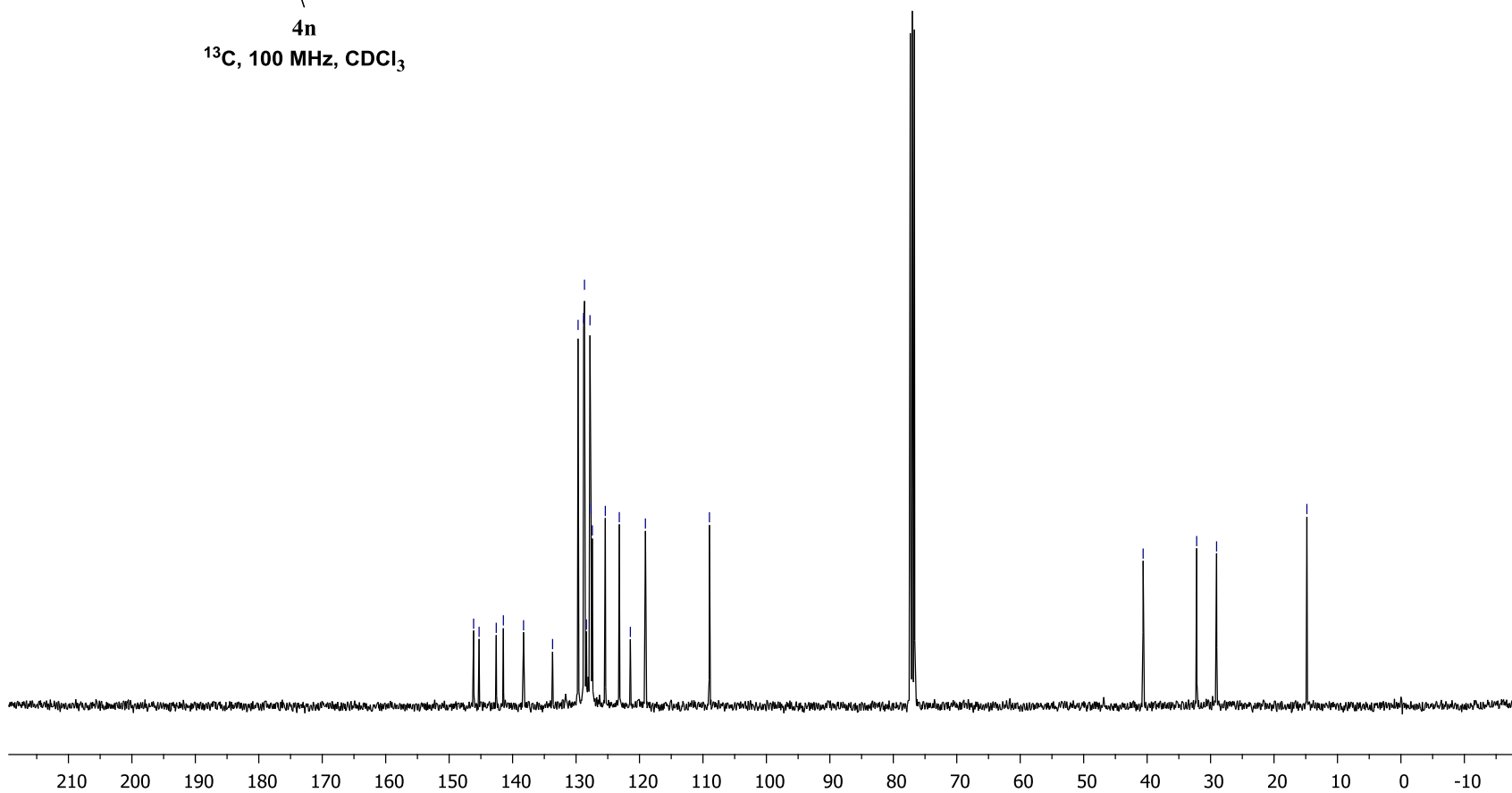


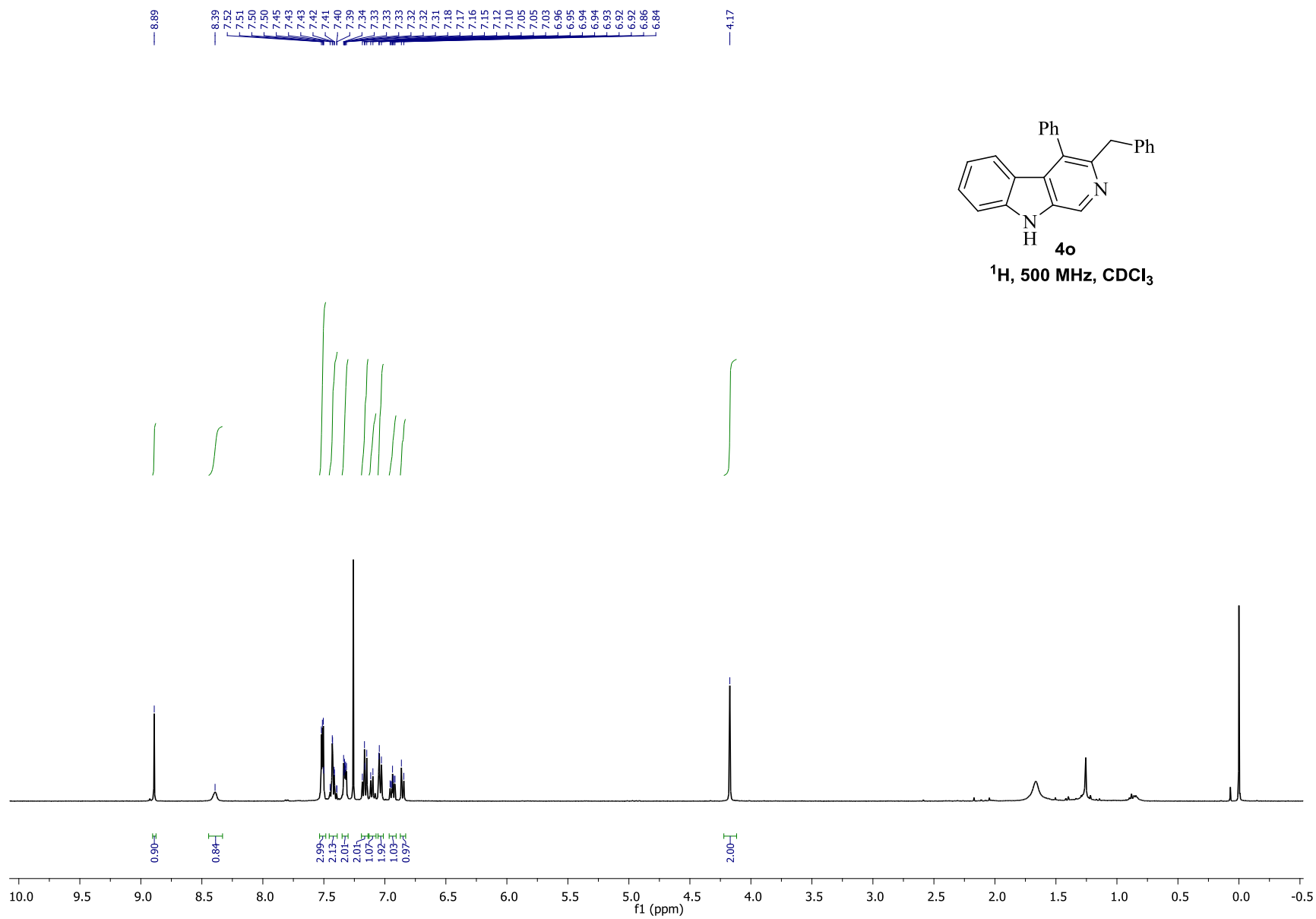


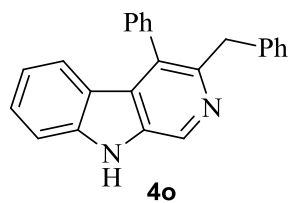
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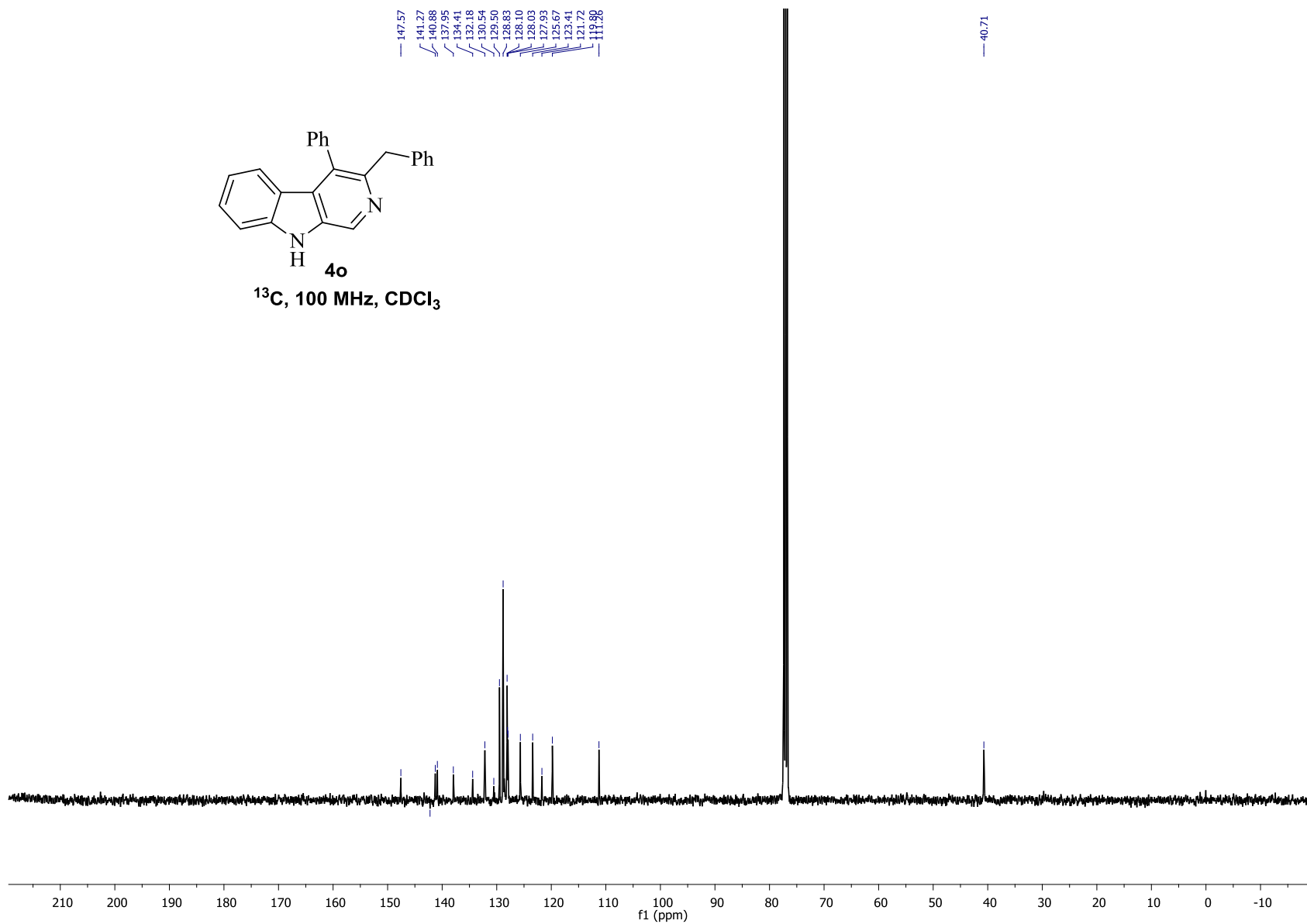
40.63
32.19
29.05
14.82

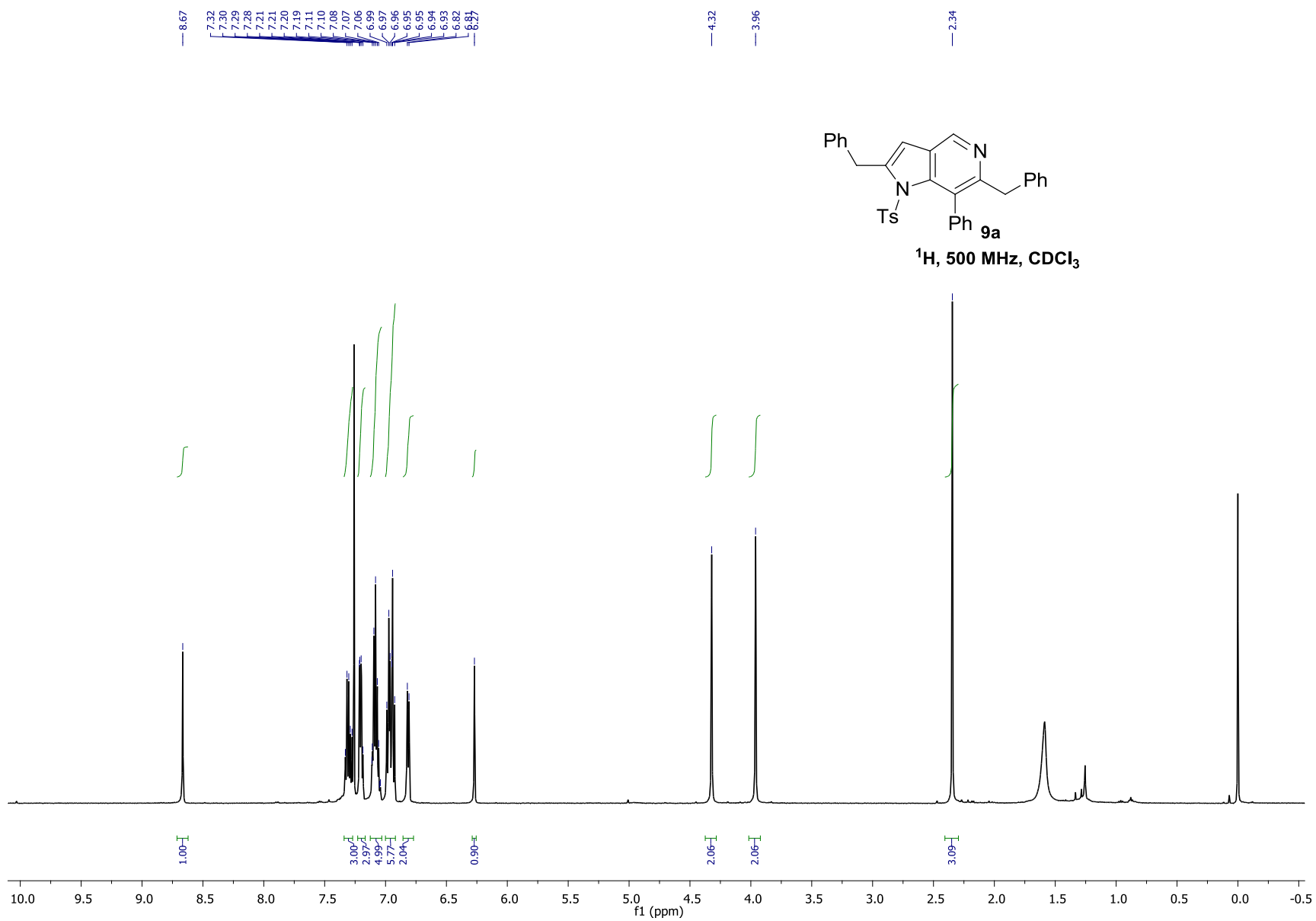


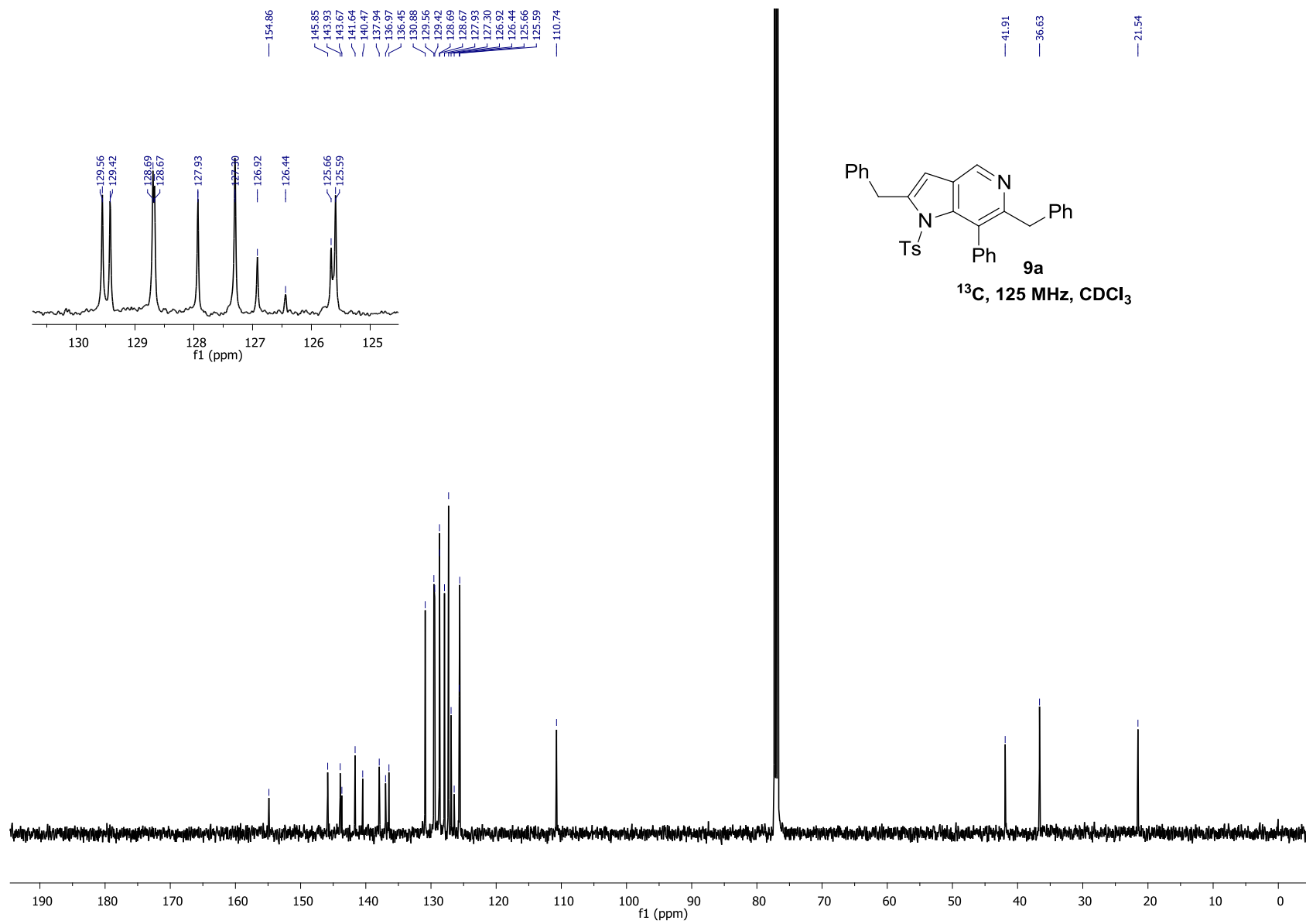


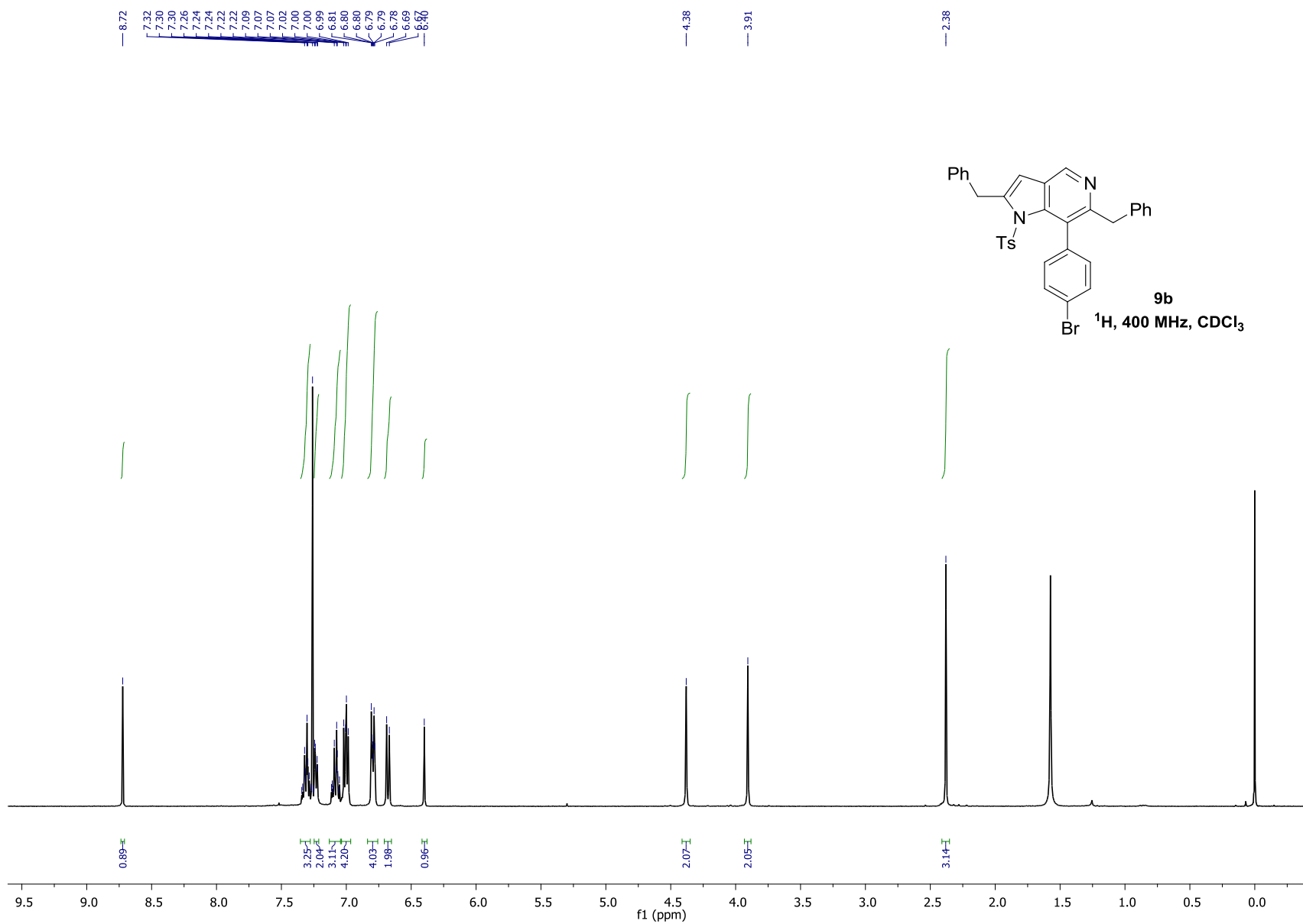


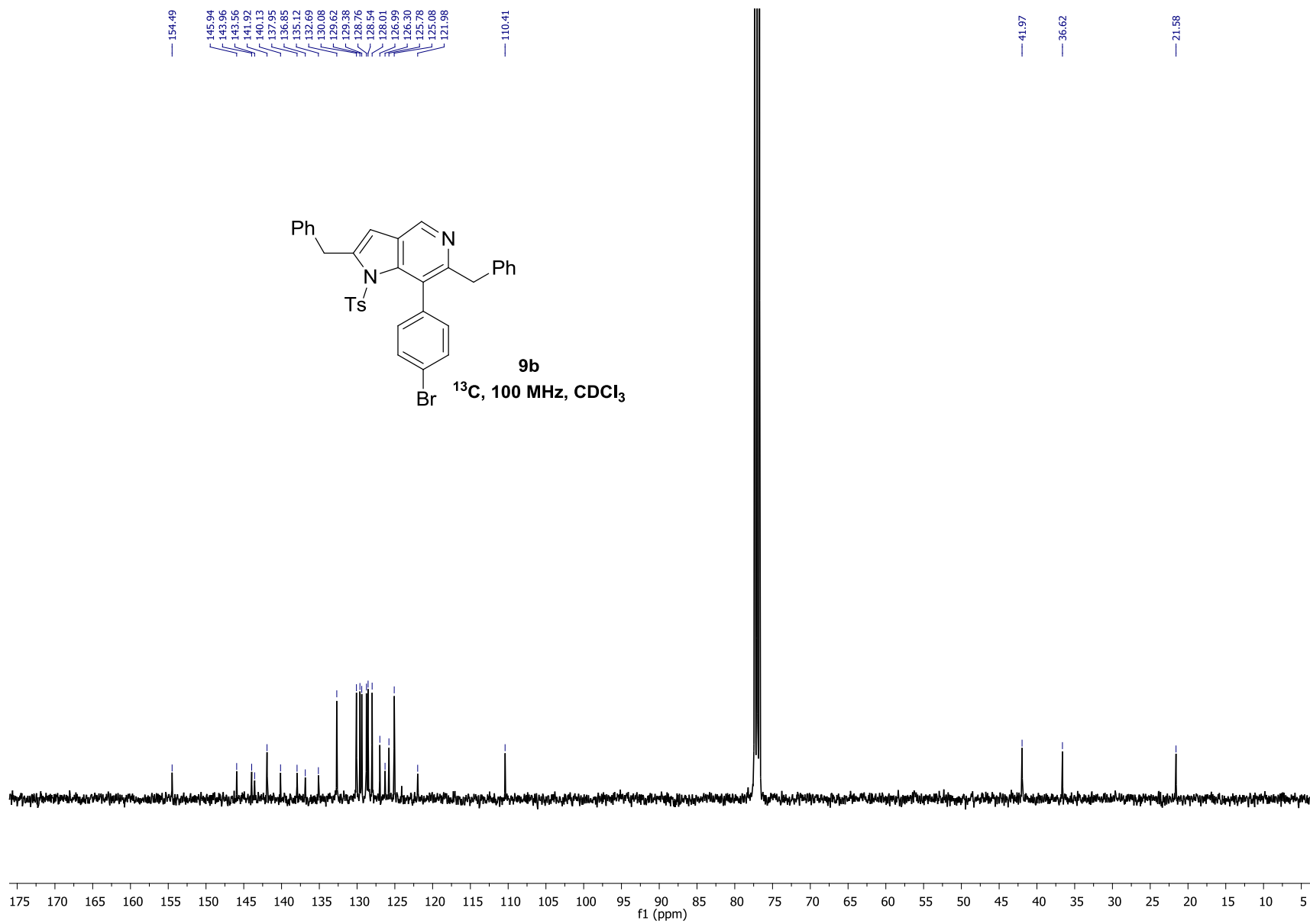
^{13}C , 100 MHz, CDCl_3

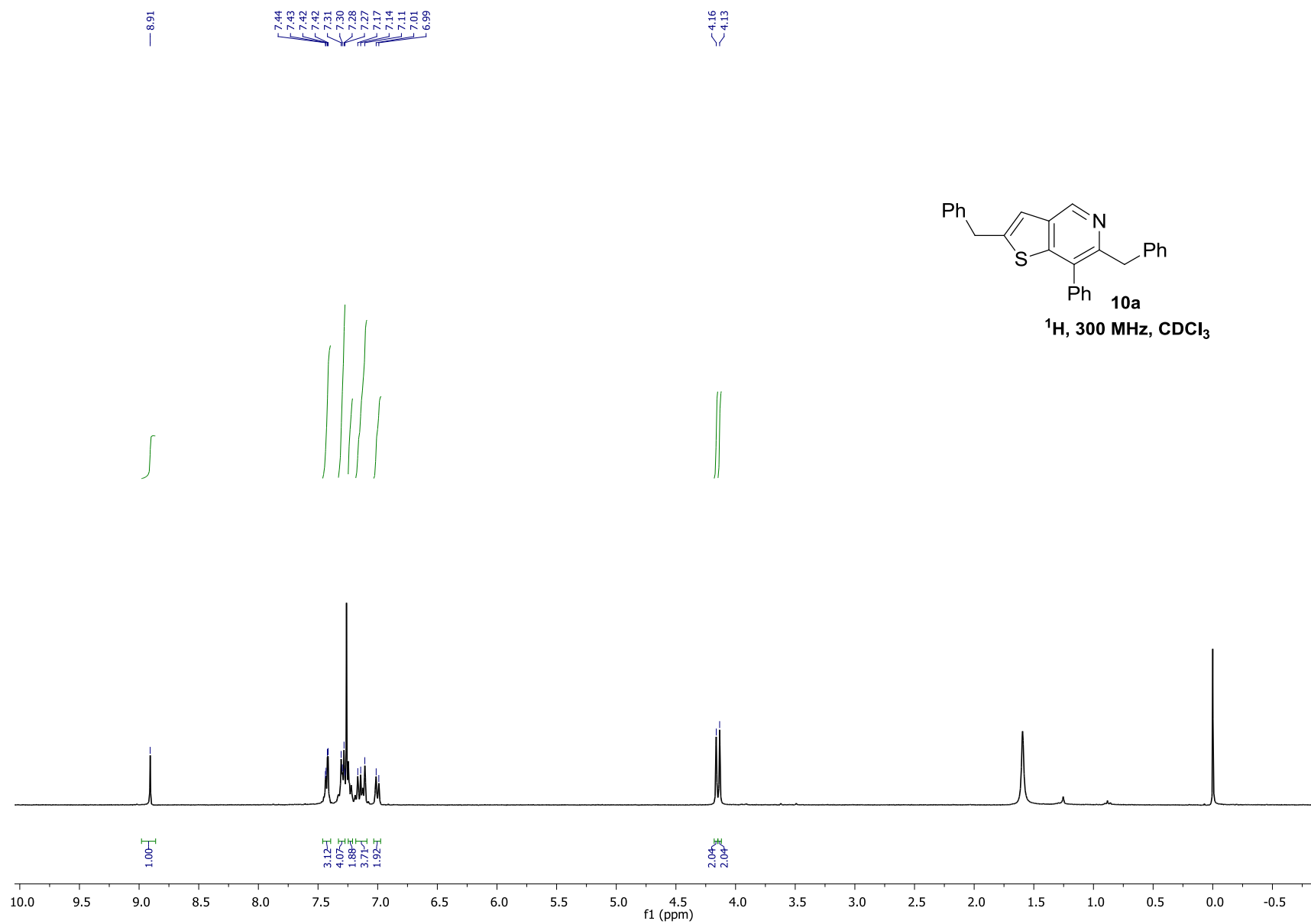


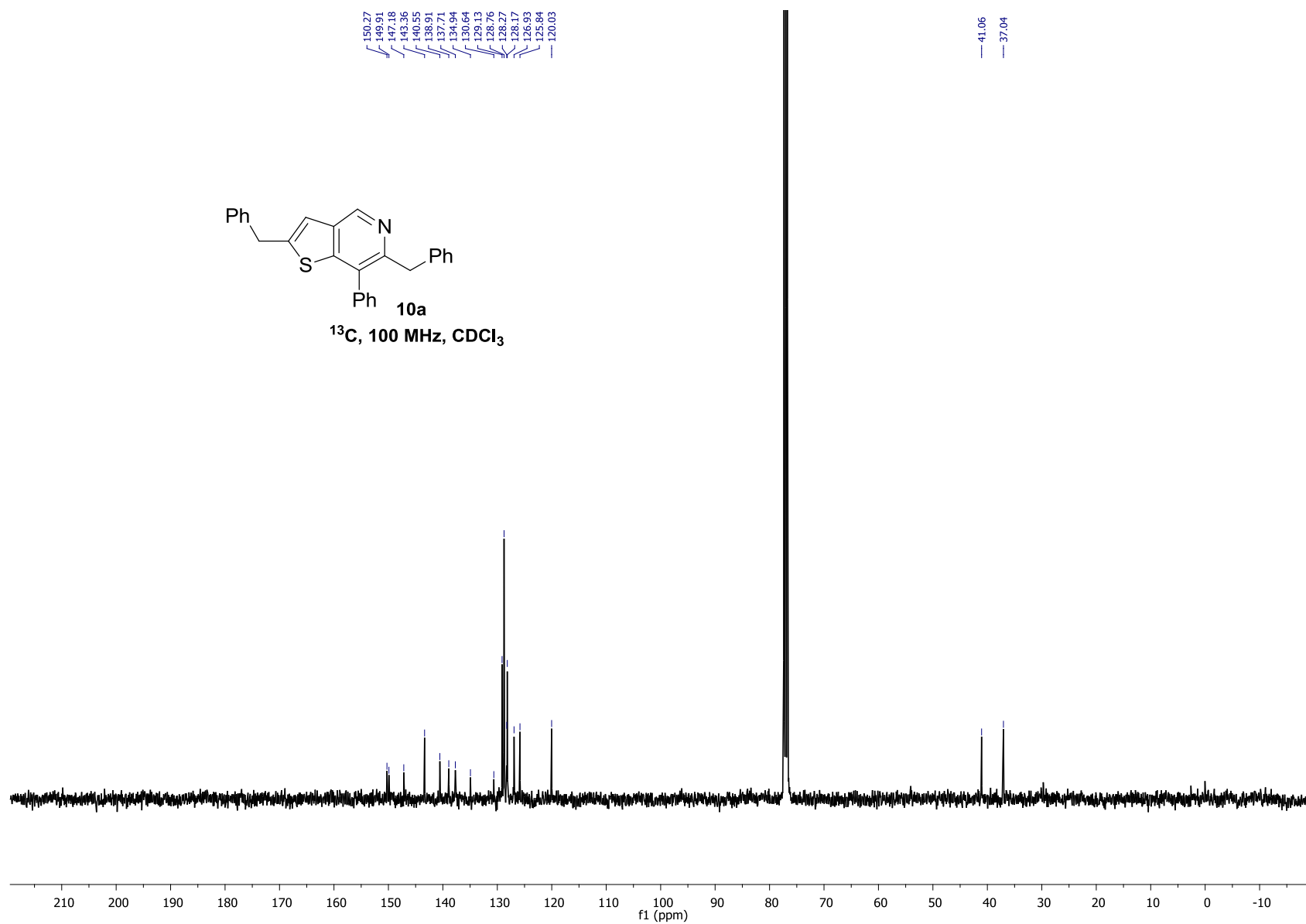


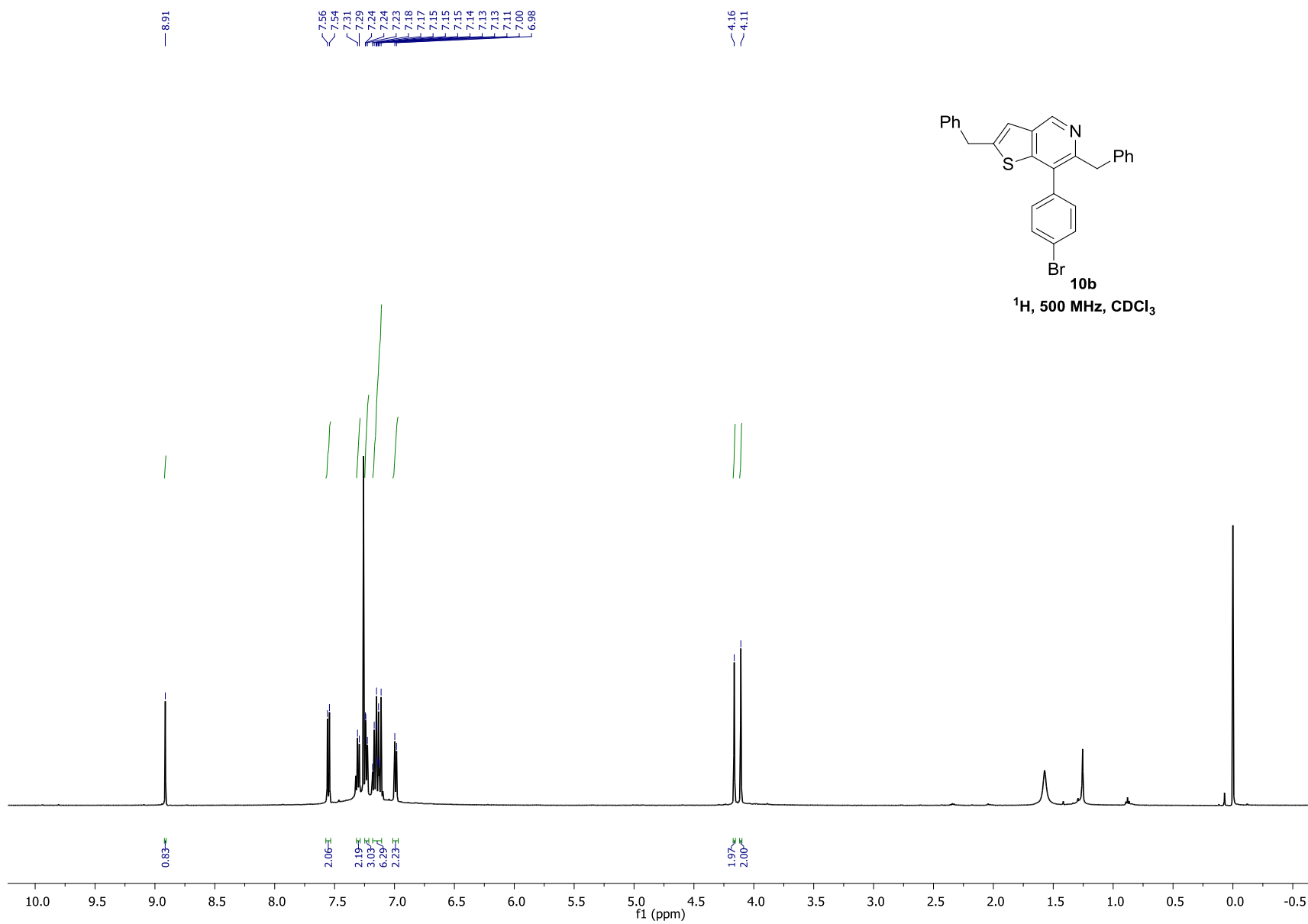


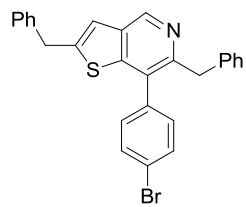






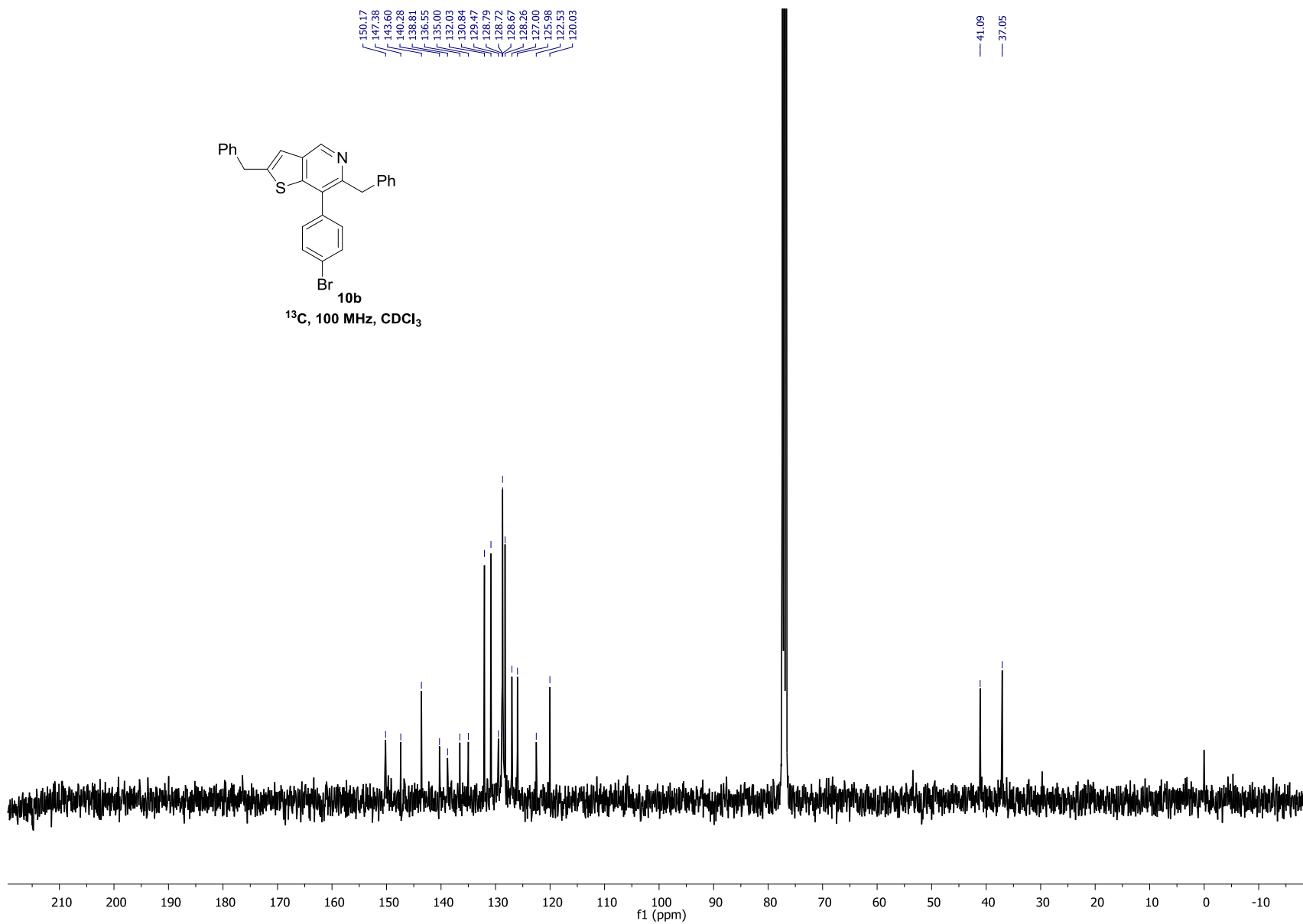


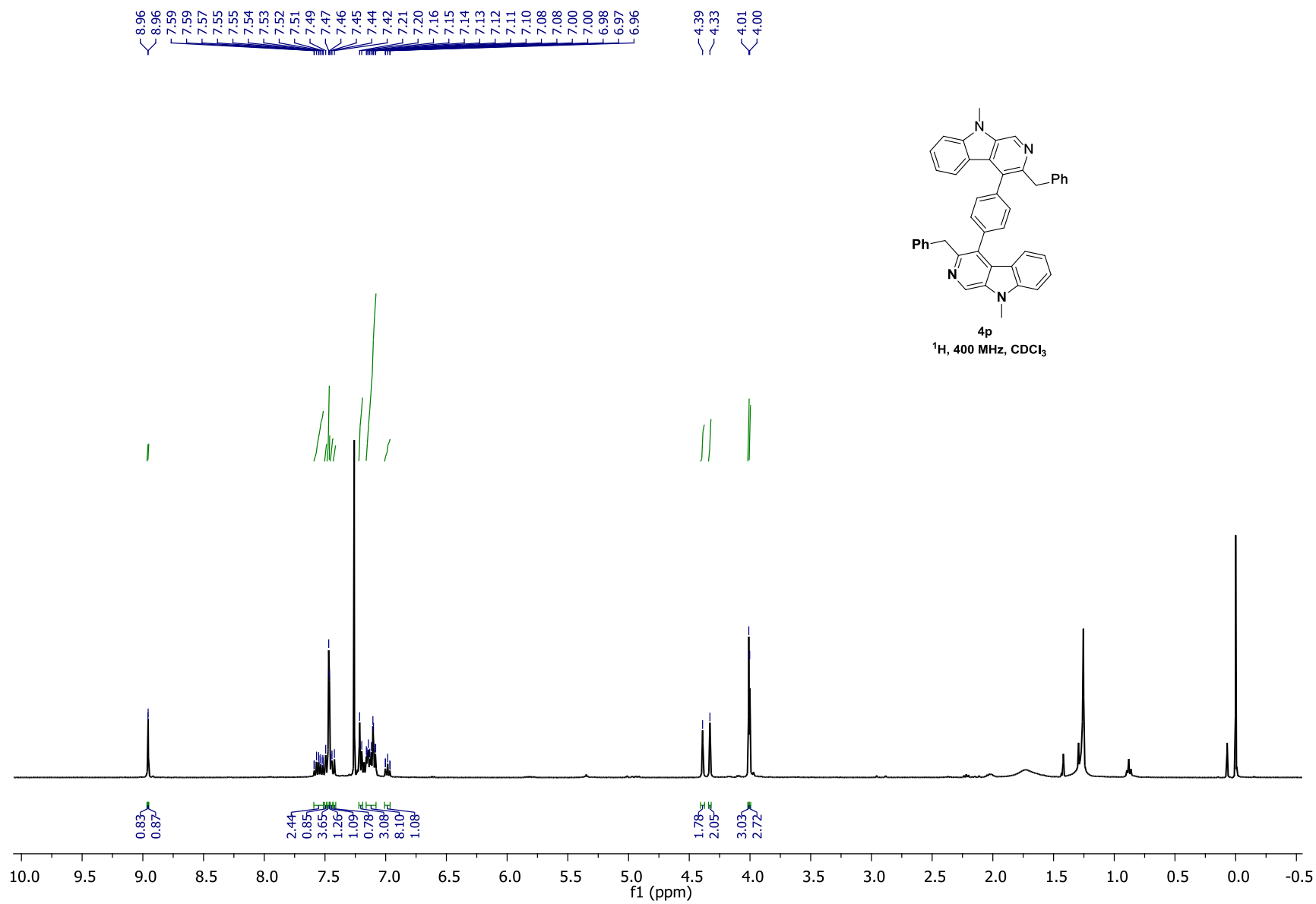


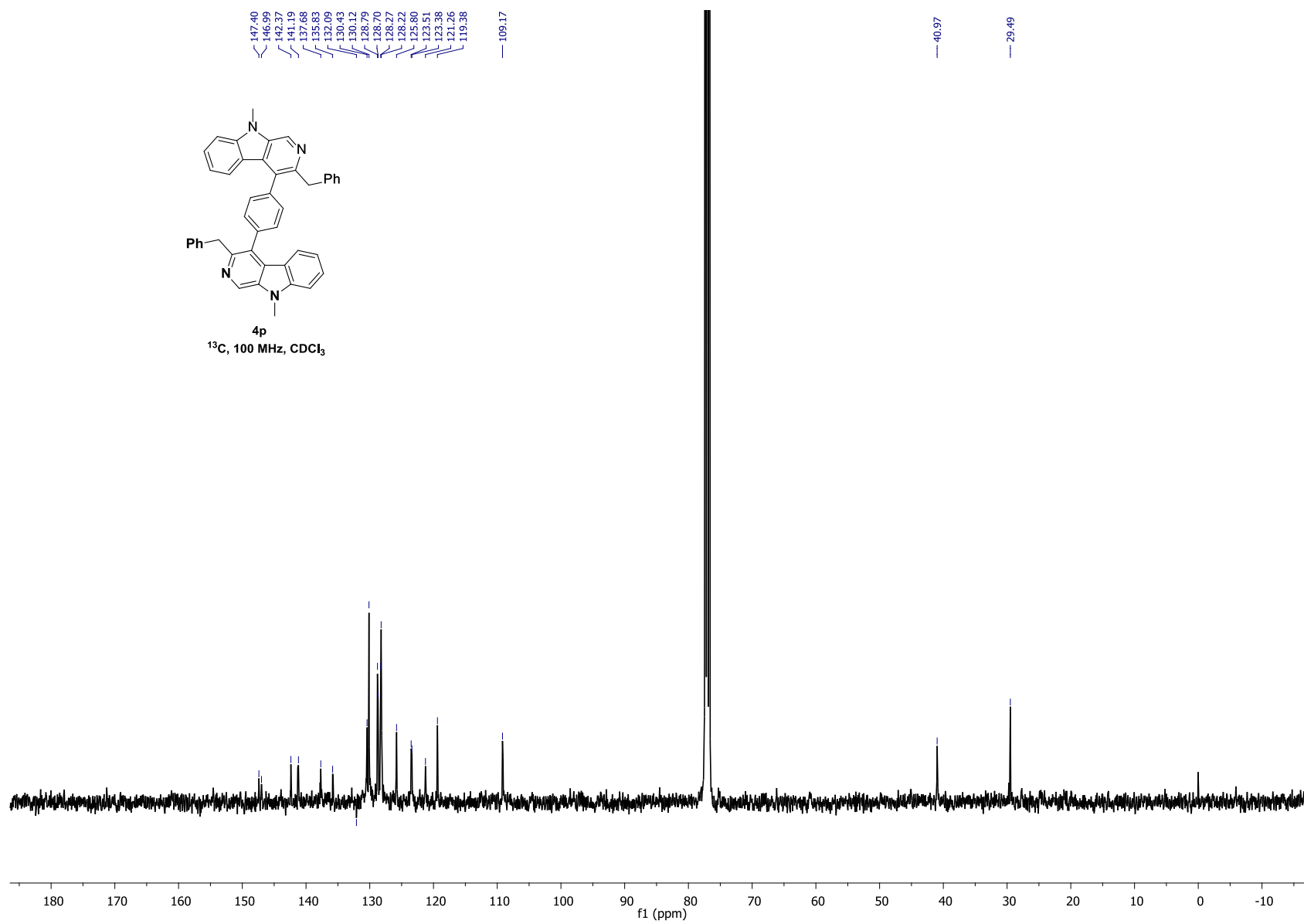


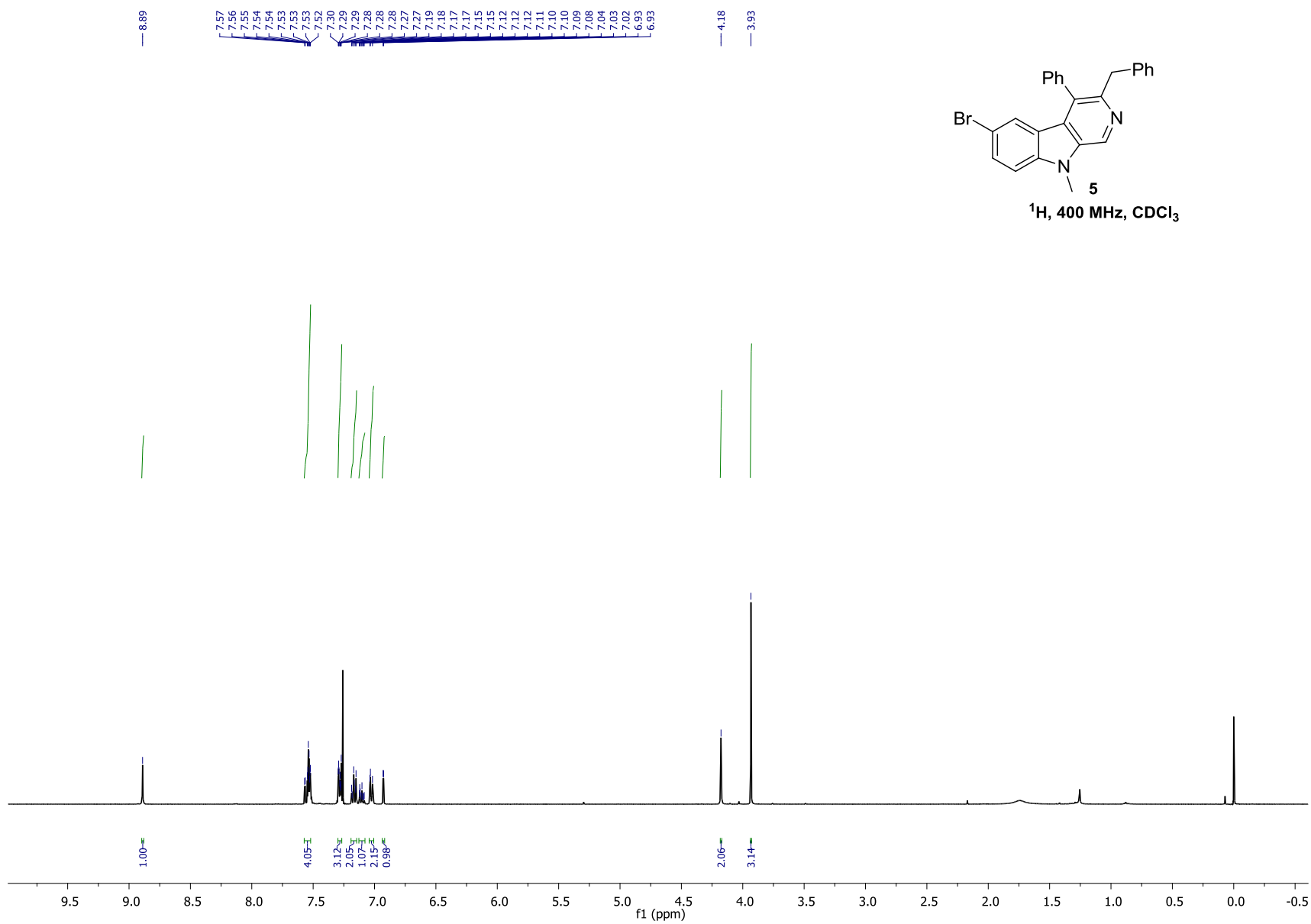
10b

^{13}C , 100 MHz, CDCl_3

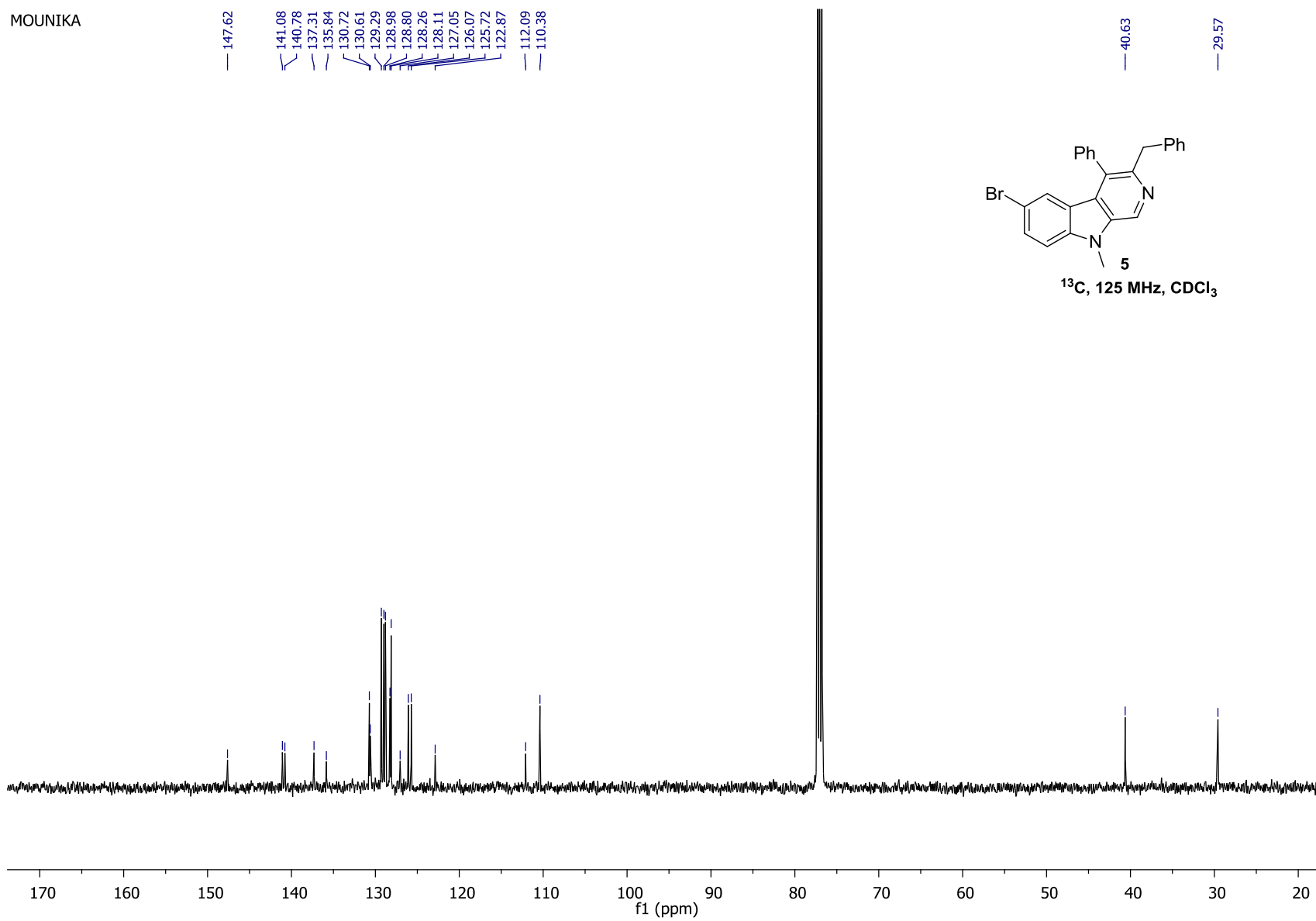


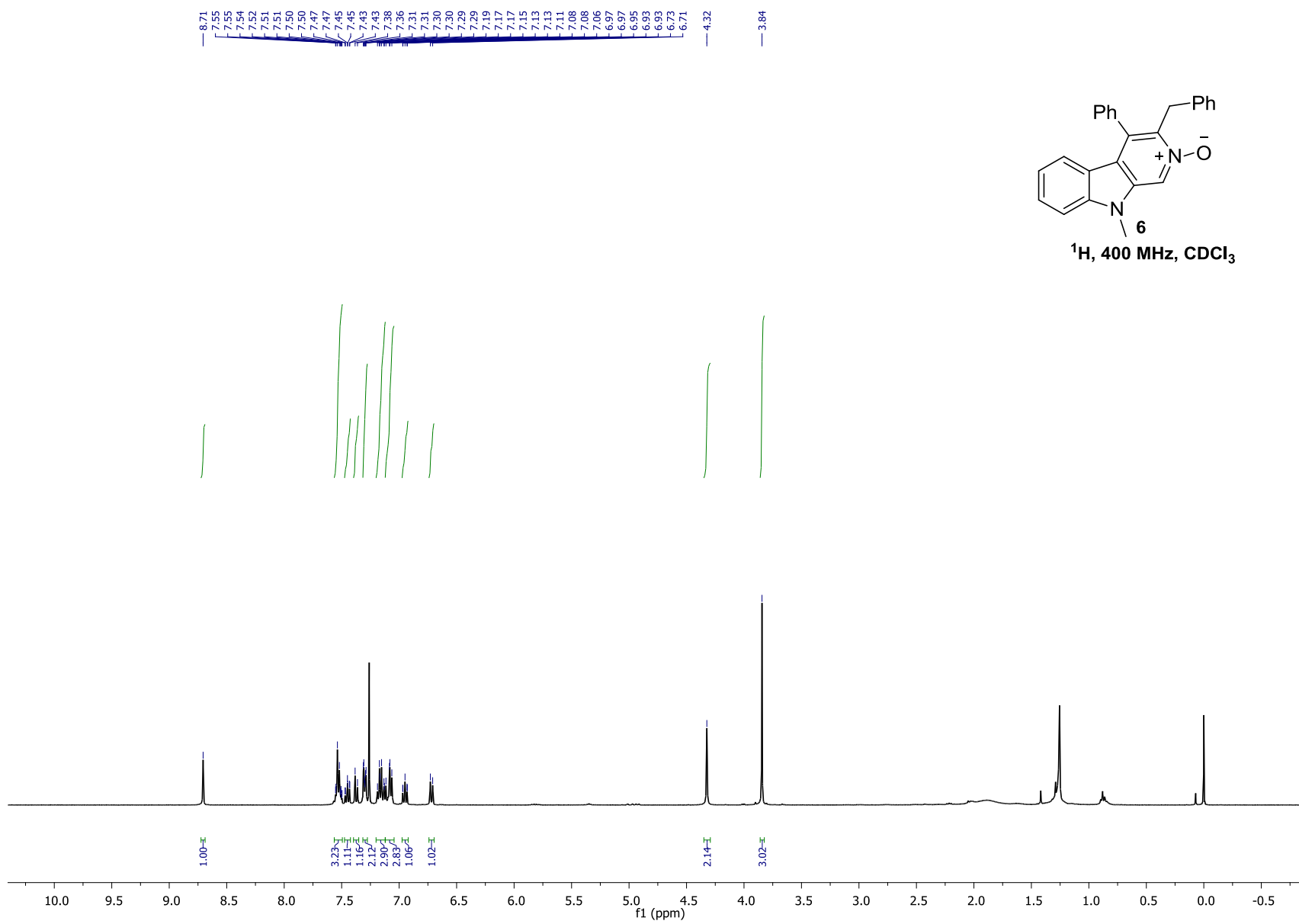


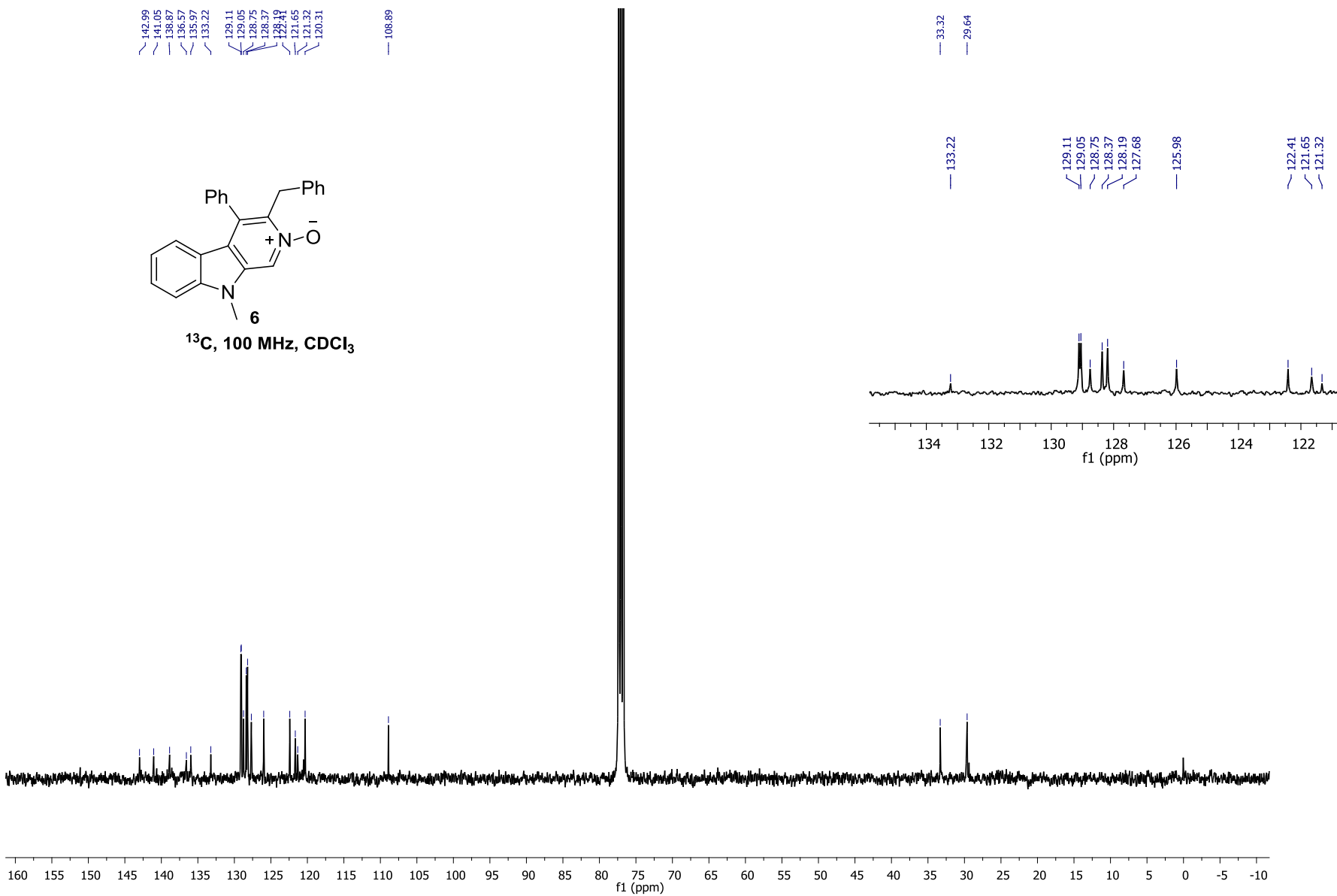




MOUNIKA







1. Theoretical Calculations of β -carboline derivatives

Computational data of β -carboline derivatives such as Z-matrices or cartesian coordinates, the number of imaginary frequencies, and computed total energies of target or optimized structures were measured using density functional theory (DFT) and Time-dependent density functional theory (TDDFT) calculations by Gaussian 09 package with a functional basis set of the B3LYP/6-31G (d, p) in vacuum. The resultant total energy of optimized structures and other absolute energy values as shown in Table S1, S2 and Figure S1. The calculated HOMO-LUMO energy level values represented in Figure 1 and Table 4 in manuscript.

Compound: 4a

Z-matrices

0 1	X	Y	Z
C	-5.11380700	0.76318600	-1.15585000
C	-4.79718900	-0.54793800	-0.81293300
C	-3.49955400	-0.80539600	-0.35803600
C	-2.53249200	0.23047800	-0.23099000
C	-2.88102500	1.54122900	-0.58649800
C	-4.16837700	1.79779900	-1.04693900
C	-1.32612300	-0.39727800	0.27516400
C	-1.62563500	-1.77501100	0.42369000
C	-0.65404300	-2.64701600	0.91242600
H	-0.85012200	-3.70702300	1.06181600
C	0.87713900	-0.90506900	1.08655300
C	-0.03785800	0.05457600	0.61140400
H	-6.11452400	0.98970300	-1.51214100
H	-5.53769900	-1.33699500	-0.89297100
H	-2.15692800	2.34306300	-0.50034500
H	-4.44880000	2.80932900	-1.32342100
N	-2.93320900	-2.01335700	0.02500600
N	0.56321300	-2.21081400	1.23239900
C	2.30194200	-0.54198200	1.47360900
H	2.34971400	0.50154800	1.79431200

H	2.56555600	-1.16319800	2.33657800
C	3.32633300	-0.77047200	0.36851300
C	3.50155300	-2.04298400	-0.19480700
C	4.12848400	0.28045000	-0.09165800
C	4.45346900	-2.25457600	-1.19121500
H	2.88066100	-2.86210500	0.15531900
C	5.08402900	0.07011600	-1.08859400
H	4.00263300	1.27282900	0.33334200
C	5.24934400	-1.19878800	-1.64267400
H	4.57704300	-3.24749800	-1.61520200
H	5.69777200	0.89912700	-1.43046000
H	5.99205300	-1.36554900	-2.41771400
C	0.32167900	1.49982400	0.47665600
C	0.95664900	1.97791900	-0.67893700
C	0.01385800	2.40748400	1.50175900
C	1.27408300	3.33119000	-0.80643100
H	1.20310200	1.28365700	-1.47603100
C	0.33430600	3.75970900	1.37520500
H	-0.48020800	2.04721100	2.39954900
C	0.96426000	4.22537900	0.21960900
H	1.76458600	3.68569700	-1.70842800
H	0.09065300	4.44883800	2.17875900
H	1.21259400	5.27802200	0.11996400
C	-3.61534900	-3.28914200	0.07338900
H	-4.32420400	-3.35959500	-0.75534500
H	-4.15904200	-3.43351800	1.01547200
H	-2.88892500	-4.09646500	-0.03939200

Imaginary frequencies: 0

Compound: 4c

Z-matrices

0 2

C	4.42355300	-2.91754500	-1.41600100
C	4.95897700	-1.70525700	-0.99108900
C	4.07911400	-0.75827600	-0.45631600
C	2.68618700	-1.01866600	-0.33134600
C	2.17642800	-2.24879900	-0.77013500
C	3.04829200	-3.18860200	-1.30988200
C	2.10172500	0.16613900	0.26810200
C	3.16808900	1.07876900	0.47002500
C	2.91667000	2.32193100	1.04816900
H	3.70927100	3.04318700	1.23733400
C	0.65005500	1.82890500	1.21642400
C	0.80351700	0.55013700	0.64629800
H	5.08524900	-3.67010200	-1.83489700
H	6.02352400	-1.51045700	-1.06937700
H	1.11773100	-2.46423400	-0.68563300
H	2.66430800	-4.14502900	-1.65046500
N	4.35331300	0.51778300	0.01656000
N	1.68404300	2.67672900	1.40865000
C	-0.70312100	2.35734800	1.66368700
H	-1.34323900	1.52967000	1.98006700
H	-0.52198600	2.98578900	2.54268000
C	-1.43804500	3.18041000	0.61245900
C	-0.81872700	4.27639800	-0.00550800
C	-2.75878700	2.87510200	0.26134000
C	-1.50182800	5.04046100	-0.95125200
H	0.20426300	4.52207000	0.26325600
C	-3.44666700	3.64114500	-0.68349300
H	-3.25432000	2.03052000	0.73318500
C	-2.81836800	4.72596000	-1.29571000
H	-1.00546200	5.88619600	-1.41935600
H	-4.47313400	3.39003400	-0.93691500
H	-3.35001800	5.32332700	-2.03085000

C	-0.35360800	-0.37699600	0.45063000
C	-1.15441600	-0.26950900	-0.69421100
C	-0.63381200	-1.36953800	1.39638900
C	-2.22201000	-1.14943100	-0.88337900
H	-0.93269700	0.47902500	-1.44477500
C	-1.69358700	-2.26059800	1.19990700
H	-0.02562000	-1.48031700	2.28754700
C	-2.49819700	-2.16167600	0.05432900
C	5.66513300	1.12475100	0.09538200
H	6.26241400	0.82557700	-0.76963900
H	6.20037300	0.83799700	1.00927400
H	5.56687200	2.21185500	0.07299200
O	-3.56336800	-3.01154100	-0.11867900
O	-3.03851100	-1.12217200	-1.98706200
O	-1.88635100	-3.26239700	2.11841600
C	-3.11224800	0.01199600	-2.74536400
H	-3.75596700	-0.11508600	-3.60566000
H	-3.01350100	0.96962800	-2.24338900
C	-3.32536000	-4.08449900	-1.03736300
H	-2.49045600	-4.70949200	-0.69929800
H	-3.11989600	-3.70306900	-2.04287300
H	-4.24041700	-4.67969600	-1.05537000
C	-3.10614500	-3.19752500	2.86656900
H	-3.08420400	-4.04654200	3.55262900
H	-3.97900900	-3.27144900	2.21286400
H	-3.15662000	-2.26733500	3.44682600

Imaginary frequencies: 0

Compound: 4f

Z-matrices

0	1		
C	-4.08745100	3.62317500	-0.21702500
C	-2.84952100	4.20408800	0.03628100
C	-1.72749700	3.36847200	0.05668100
C	-1.82615600	1.96558000	-0.16825400
C	-3.09063800	1.41516300	-0.43006700
C	-4.20767800	2.24343300	-0.45371700
C	-0.46779700	1.44303700	-0.10192700
C	0.37071500	2.56605000	0.13045800
C	1.75524800	2.41949700	0.15679700
H	2.42347900	3.26514600	0.30675500
C	1.56064600	0.14357000	-0.21769400
C	0.14374200	0.17989900	-0.25337800
H	-4.97386400	4.25035000	-0.23939100
H	-2.76113800	5.27335700	0.19793100
H	-3.19814000	0.35532300	-0.62320900
H	-5.18510200	1.81828900	-0.65922700
N	-0.40050800	3.71104700	0.26346900
N	2.32515800	1.22787700	-0.02071700
C	2.28910400	-1.18944400	-0.39165800
H	1.83465400	-1.92611800	0.28163400
H	2.09775100	-1.56534700	-1.40716800
C	3.78305300	-1.15043500	-0.15644400
C	4.67134500	-0.90706700	-1.21015600
C	4.31020100	-1.37754500	1.12025000
C	6.04943500	-0.88768400	-0.99600000
H	4.27817400	-0.72924400	-2.20801300
C	5.68739900	-1.35897100	1.34090300
H	3.63388100	-1.57084100	1.94935800
C	6.56284300	-1.11407100	0.28192900
H	6.72247400	-0.69879900	-1.82780400
H	6.07675000	-1.54023500	2.33895800

H	7.63594500	-1.10354200	0.45032500
C	-0.60670700	-1.07533800	-0.43651500
C	-1.64884500	-1.46943200	0.31998300
H	-0.22825600	-1.74938900	-1.20303800
H	-1.96428700	-0.81745200	1.13295800
C	-2.41094100	-2.71817200	0.19596100
C	-3.31924300	-3.06090400	1.21408000
C	-2.28462100	-3.59636700	-0.89788200
C	-4.06014900	-4.23948300	1.15466700
H	-3.43642100	-2.39292100	2.06358100
C	-3.02348800	-4.77353700	-0.95716300
H	-1.61308900	-3.34928500	-1.71436200
C	-3.91393000	-5.10330300	0.06906800
H	-4.75216800	-4.48223100	1.95587900
H	-2.91062700	-5.43524900	-1.81118800
H	-4.49109200	-6.02167200	0.01761500
C	0.10899800	5.05399200	0.44220600
H	-0.60901700	5.64619900	1.01422500
H	0.29877600	5.55712300	-0.51447100
H	1.04036700	5.01885400	1.01108600

Imaginary frequencies: 0

Compound: 4i

Z-matrices

0 1			
C	-2.90442500	-2.99342900	-0.04289700
C	-3.42743500	-1.70361600	-0.02503000
C	-2.52403800	-0.63581300	0.00041600
C	-1.11723200	-0.84831600	-0.00384400
C	-0.62053900	-2.15899800	-0.02288000
C	-1.51755200	-3.22238200	-0.04127700
C	-0.50563400	0.46753100	0.00904300

C	-1.57097100	1.40365000	0.01744800
C	-1.29393100	2.76926500	0.00853600
H	-2.08303100	3.51885100	-0.00277000
C	0.99142000	2.34849300	0.01048000
C	0.81277600	0.95024600	0.00867200
H	-3.58511800	-3.83961900	-0.06296900
H	-4.49998800	-1.53974100	-0.03794500
H	0.44843400	-2.33885500	-0.02540900
H	-1.14385000	-4.24139500	-0.05784500
N	-2.78384300	0.72730700	0.03242100
N	-0.03893200	3.22009400	0.00834400
C	2.37141400	2.96571300	0.01429100
H	2.97988000	2.59428700	0.84557400
H	2.92152100	2.73621400	-0.90536800
C	1.98027800	0.01680700	0.00752700
C	2.47159700	-0.51409100	1.20968400
C	2.60436400	-0.34937000	-1.19414500
C	3.55812100	-1.38977300	1.20987900
H	1.99441700	-0.23841600	2.14571800
C	3.69035300	-1.22566400	-1.19447000
H	2.22941700	0.05254500	-2.13110400
C	4.17023400	-1.74828400	0.00760800
H	3.92584400	-1.79200300	2.14958000
H	4.16046000	-1.50076500	-2.13432300
C	-4.09455700	1.33970300	-0.00681400
H	-4.80643500	0.72177400	0.54599900
H	-4.46249700	1.46863900	-1.03260100
H	-4.05540000	2.31788500	0.47708000
H	5.01564400	-2.43010500	0.00759800
H	2.27466000	4.04886700	0.10005900

Imaginary frequencies: 0

Compound : 4p

Z-matrices

0 1			
C	5.01709200	-4.64448000	3.03792300
C	3.74912000	-4.21512800	2.63984000
C	3.67745300	-3.20457700	1.67219500
C	4.85164800	-2.63233000	1.11019900
C	6.11325300	-3.08038200	1.52497700
C	6.18975800	-4.08556600	2.48981300
C	4.40897800	-1.64927500	0.14348700
C	2.98058100	-1.62825400	0.18277400
C	2.28282500	-0.71642200	-0.63887500
C	4.32781200	-0.03871100	-1.62977700
C	5.08632100	-0.83543100	-0.76650700
H	5.09996400	-5.42226700	3.79044400
H	2.85711200	-4.64556200	3.08083900
H	7.01707800	-2.65105000	1.10419600
H	7.15835900	-4.44072500	2.82507200
N	2.54902100	-2.60992700	1.09435100
N	2.97456300	0.01625100	-1.54634200
C	4.97269300	0.85349700	-2.67452600
H	5.91992800	0.40944600	-3.00136200
H	4.30545100	0.87920500	-3.54391800
C	5.22867000	2.27809800	-2.19141800
C	4.15673500	3.10449900	-1.80895400
C	6.53343600	2.79030500	-2.12357000
C	4.38894500	4.41144700	-1.37092500
H	3.14747600	2.70717000	-1.84880700
C	6.76766300	4.09981500	-1.68529600
H	7.37053100	2.16281100	-2.41877100
C	5.69546700	4.91442400	-1.30763000
H	3.55151100	5.03845500	-1.07965900
H	7.78381600	4.48019200	-1.63984800
H	5.87401600	5.93013300	-0.96836400
C	1.20005400	-3.14317100	1.26531800

H	0.68290300	-2.70224300	2.12447100
H	1.26327500	-4.22553100	1.40989600
H	0.60801400	-2.94968300	0.37176200
H	6.16985100	-0.82816500	-0.81829800
C	0.82647600	-0.42530400	-0.57459200
C	0.16538200	-0.23066600	0.65238500
C	0.09651300	-0.23439200	-1.76286200
C	-1.18905000	0.11204100	0.69229300
H	0.72115100	-0.31939300	1.58023700
C	-1.25760500	0.09998800	-1.72316600
H	0.60923600	-0.34136700	-2.71175800
C	-1.92438800	0.27485000	-0.49484900
H	-1.67698400	0.27131900	1.64780500
H	-1.80809100	0.23151900	-2.64949200
C	-5.01533900	-4.43301400	-1.59157600
C	-6.04972700	-3.50868100	-1.43650200
C	-5.70247900	-2.18541400	-1.13826500
C	-4.34073400	-1.77546300	-1.00703200
C	-3.32216700	-2.72838300	-1.16818400
C	-3.66593300	-4.04959100	-1.45822700
C	-4.36375500	-0.35038800	-0.70833700
C	-5.73563100	0.03099200	-0.66907300
C	-6.08779800	1.35396900	-0.40362400
C	-3.81864600	1.94135700	-0.19279500
C	-3.37710700	0.62594600	-0.45976800
H	-5.25674200	-5.46551400	-1.82360700
H	-7.08470700	-3.81187000	-1.54994600
H	-2.28207900	-2.44056800	-1.07742000
H	-2.88527400	-4.79174600	-1.58845200
N	-6.53473800	-1.08467700	-0.92140400
N	-5.13979300	2.27756800	-0.17293300
C	-2.86411900	3.09015500	0.08473300
H	-1.89245100	2.89047600	-0.37534100
H	-3.28463800	3.97604100	-0.40640200
C	-2.66003100	3.40120700	1.56673000
C	-3.75714100	3.68925400	2.39851000
C	-1.36905400	3.43385900	2.11881300

C	-3.56428700	3.99833100	3.74847700
H	-4.75561100	3.66501300	1.97439400
C	-1.17473000	3.74567100	3.47049300
H	-0.51301400	3.21361900	1.48716000
C	-2.27244500	4.02772200	4.29027300
H	-4.42149600	4.21985000	4.37760200
H	-0.16880800	3.76804800	3.87928200
H	-2.12422900	4.27028000	5.33818000
C	-7.98798400	-1.09447500	-0.98759500
H	-8.36939700	-2.04183700	-0.59676600
H	-8.35385500	-0.96289300	-2.01368200
H	-8.38832600	-0.29007000	-0.36649500
H	-7.11768900	1.69482600	-0.38050200

Imaginary frequencies: 0

Compound: 4d

Z-matrices

0 1			
C	3.61205500	-3.93898500	-1.17328300
C	4.40672900	-2.84735600	-0.81912300
C	3.76124800	-1.69494100	-0.35487800
C	2.34042600	-1.62779300	-0.22940100
C	1.56704600	-2.74141700	-0.59507200
C	2.20790800	-3.88858100	-1.06487800
C	2.03282600	-0.30126400	0.28411300
C	3.27897100	0.37123200	0.44058100
C	3.31315300	1.67748700	0.92797100
H	4.23823000	2.22364900	1.08052600
C	0.96614200	1.70397000	1.09489300
C	0.84531800	0.38098900	0.61593300
H	4.08694000	-4.84473200	-1.53684100

H	5.48685000	-2.89970900	-0.89951600
H	0.48747400	-2.71374200	-0.51323100
H	1.61900500	-4.75414400	-1.34903300
N	4.31432500	-0.47505100	0.04415900
N	2.17441000	2.31761300	1.24325400
C	-0.23405700	2.55381500	1.47526700
H	-1.06638800	1.91488600	1.78363400
H	0.06267400	3.15143100	2.34520000
C	-0.71060900	3.49394000	0.36919400
C	0.16218100	4.44708300	-0.18600700
C	-2.03413600	3.43973200	-0.09665200
C	-0.28101600	5.32076400	-1.18358600
H	1.18612900	4.49016100	0.17073300
C	-2.47959700	4.31565400	-1.09488000
H	-2.71899100	2.70936900	0.32515000
C	-1.60354900	5.25858600	-1.64240100
H	0.40412000	6.05257000	-1.60141700
H	-3.50743200	4.26064100	-1.44118500
H	-1.94654700	5.93924000	-2.41560000
C	-0.48538600	-0.28680500	0.47284600
C	-1.27599900	-0.08040700	-0.67190300
C	-0.96620900	-1.14588900	1.47842200
C	-2.51473300	-0.71587400	-0.81324900
H	-0.92227600	0.58366200	-1.45277300
C	-2.20442100	-1.78396600	1.34817700
H	-0.36674600	-1.31575700	2.36693100
C	-2.96070200	-1.55988600	0.20040800
H	-3.11995400	-0.55473600	-1.69713500
H	-2.57169500	-2.44258200	2.12593800
C	5.73363900	-0.15597000	0.07478000
H	6.24052200	-0.64748200	-0.76001100
H	6.20703800	-0.47439800	1.01202600
H	5.86918900	0.92204900	-0.03861600
Br	-4.68436100	-2.44751500	0.00970600

Imaginary frequencies: 0

Compound: 4j

Z-matrices

0 1			
C	5.20841500	1.97627200	-1.14492800
C	5.34885600	0.59399900	-1.06587100
C	4.25579800	-0.14395900	-0.59985600
C	3.04295200	0.48572100	-0.20568000
C	2.93148400	1.88001700	-0.29734500
C	4.01471400	2.61522800	-0.76602300
C	2.16055500	-0.57296000	0.23700400
C	2.87895400	-1.78325500	0.08838200
C	2.28125200	-2.99187200	0.44564200
H	2.79530300	-3.94481100	0.33256600
C	0.34795700	-1.89314900	1.12136900
C	0.85031400	-0.62933600	0.74619400
H	6.04164500	2.57271000	-1.50509400
H	6.27822500	0.11286300	-1.35250500
H	2.01505700	2.37999200	-0.00525500
H	3.93903600	3.69531300	-0.84176700
N	4.13517300	-1.51720300	-0.43660200
N	1.05015700	-3.03396100	0.94816600
C	-1.02052200	-2.07517600	1.74814100
H	-1.39956000	-3.05500500	1.44412100
C	-1.04065300	-2.01595800	3.27945700
C	0.06088800	0.61294300	0.92686900
C	-0.11198900	1.32315100	2.07963200
H	0.32851700	1.05737900	3.03015000
C	-0.90628700	2.48458100	1.80038400
C	-1.37240100	3.53584200	2.60506300
C	-1.21060100	2.46676100	0.41609700
C	-2.13854000	4.53721700	2.02501300
H	-1.13388700	3.55797700	3.66448000
C	-1.97244600	3.48289500	-0.17463800
C	-2.43249400	4.50566800	0.65039600
H	-2.50914400	5.35652900	2.63366800

H	-2.17914700	3.48529700	-1.23553100
H	-3.02375100	5.30432000	0.21252100
N	-0.59159800	1.31674000	-0.12912000
S	-0.90387500	0.69592500	-1.71533200
O	-1.32638000	1.85209400	-2.50136700
C	-2.30543500	-0.39794400	-1.51397300
C	-3.57739100	0.13903200	-1.28927600
C	-2.11079900	-1.77377900	-1.62568600
C	-4.65851500	-0.72535400	-1.16077600
H	-3.71827000	1.21220200	-1.22471800
C	-3.21110500	-2.62221600	-1.50121500
H	-1.11701700	-2.16613900	-1.80750400
C	-4.49476700	-2.11691100	-1.26393800
H	-5.64917600	-0.31445500	-0.98576800
H	-3.06523800	-3.69485800	-1.59016500
C	-5.68120300	-3.03761800	-1.11611000
H	-6.08068500	-3.00280600	-0.09591500
H	-5.41378000	-4.07434700	-1.33439400
H	-6.49441000	-2.74754600	-1.78991200
C	5.17453100	-2.49213000	-0.68904800
H	5.76036800	-2.18799000	-1.56006300
H	4.72187600	-3.46004000	-0.91340200
H	5.85071100	-2.60964900	0.16723000
H	-1.71858000	-1.31532000	1.38394100
O	0.25296800	-0.10208700	-2.09772800
H	-2.09089800	-2.07278100	3.61212700
H	-0.64605700	-1.04567900	3.61589700
O	-0.27769100	-3.09374400	3.80166400
H	-0.24558500	-2.99333500	4.76126000

Imaginary frequencies: 0

Compound: 6

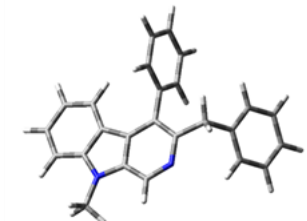
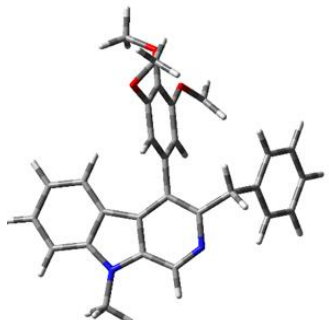
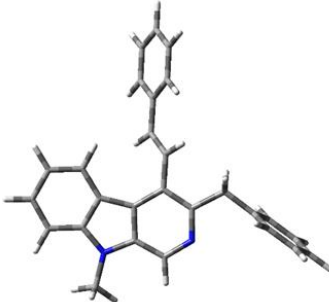
Z-matrices

0 1			
C	-5.19849600	0.96307600	-1.10376500
C	-4.88878800	-0.37672400	-0.85523500
C	-3.58963200	-0.67639600	-0.43520500
C	-2.60361200	0.33922200	-0.24768100
C	-2.94261700	1.67716900	-0.50635500
C	-4.23747600	1.97814500	-0.93325000
C	-1.39598600	-0.33529700	0.19682200
C	-1.70391500	-1.72525700	0.25477900
C	-0.76140700	-2.65630400	0.65258800
H	-0.90860000	-3.72094100	0.74156500
C	0.85270600	-0.87730400	0.93226900
C	-0.09543900	0.07953200	0.54497100
H	-6.19969200	1.22396200	-1.43141400
H	-5.63805500	-1.15033900	-0.98156700
H	-2.21224900	2.46591800	-0.37570600
H	-4.50884600	3.00902700	-1.13462700
N	-3.02332800	-1.92403500	-0.13780500
N	0.49618000	-2.22718300	0.97712700
C	2.27002500	-0.56390800	1.35365900
H	2.28291300	0.42776300	1.81346600
H	2.54536200	-1.30262100	2.11397300
C	3.30308300	-0.59853800	0.22725200
C	3.55766600	-1.78440300	-0.48731600
C	4.03307500	0.55659700	-0.09721900
C	4.51548200	-1.80318800	-1.50621500
H	3.00993100	-2.68194500	-0.21970500
C	4.99522600	0.53473600	-1.11458700
H	3.84631100	1.47748300	0.44782300
C	5.23734100	-0.64556600	-1.82499400
H	4.70367100	-2.72571100	-2.04762700
H	5.55227600	1.43707300	-1.34928500

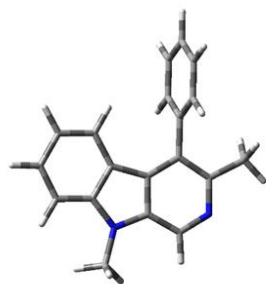
H	5.98266900	-0.66528300	-2.61439200
C	0.26298100	1.53364800	0.51619700
C	0.86497100	2.10295400	-0.61941400
C	-0.02744300	2.35697100	1.61950900
C	1.16728300	3.46912300	-0.65122600
H	1.09816400	1.47353000	-1.47121700
C	0.27921500	3.72171700	1.58753400
H	-0.49563500	1.92492000	2.49849900
C	0.87549100	4.28131900	0.45099200
H	1.63140800	3.89616400	-1.53450900
H	0.05179800	4.34517700	2.44646200
C	-3.70989800	-3.20586800	-0.19110000
H	-4.45561100	-3.18911600	-0.98974300
H	-4.21042800	-3.44422200	0.75559000
H	-2.99282700	-3.99832600	-0.41985800
H	1.11170700	5.34037200	0.42534900
O	1.39209300	-3.14463900	1.35920200

Imaginary frequencies: 0

Table S1. Optimized structures and total energy values of β -carboline derivatives using B3LYP/6-31G (d, p) method.

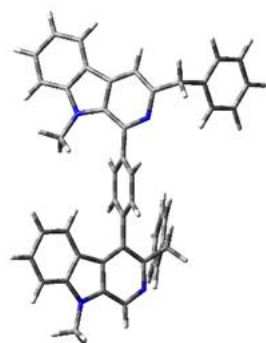
β -carboline derivatives	Optimized structures	Total energy (a.u.)
4a		-1074.2693982
4c		-1417.16588698
4f		-1151.67110260

4i



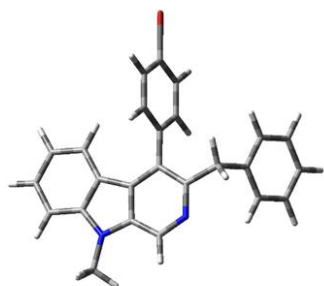
-843.21341257

4p



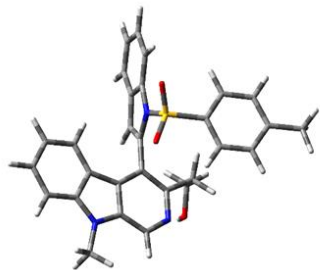
-1916.28172870

4d



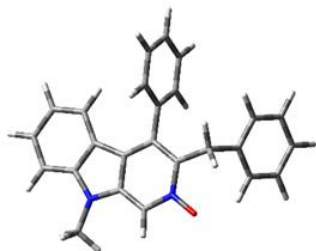
-3645.37258288

4j



-1908.23934122

6



-1149.43301198

Table S2. Absolute energy values (electronic and thermal energies) of β -carboline derivatives using B3LYP/6-31G (d, p) method.

β -carboline derivatives	Sum of electronic and thermal energies (values in Hartrees)			
	Enthalpy (ΔH)	Zero-point energy (ΔE_{ZPE})	Free energy (ΔG)	Total energy (ΔE_{tot})
4a	-1073.863879	-1073.886194	-1073.939114	-1073.864823
4c	-1416.669240	-1416.699862	-1416.763578	-1416.670184
4f	-1151.230203	-1151.254830	-1151.312122	-1151.231147
4i	-842.894149	-842.912314	-842.958948	-842.895093
4p	-1915.576784	-1915.616146	-1915.693250	-1915.577729
4d	-3644.975652	-3644.999444	-3645.055532	-3644.976596
4j	-1907.724976	-1907.757414	-1907.824097	-1907.725920414
6	-1149.022338	-1149.045498	-1149.098754	-1149.023282

2. Oscillator strength calculations of β -carboline derivatives:

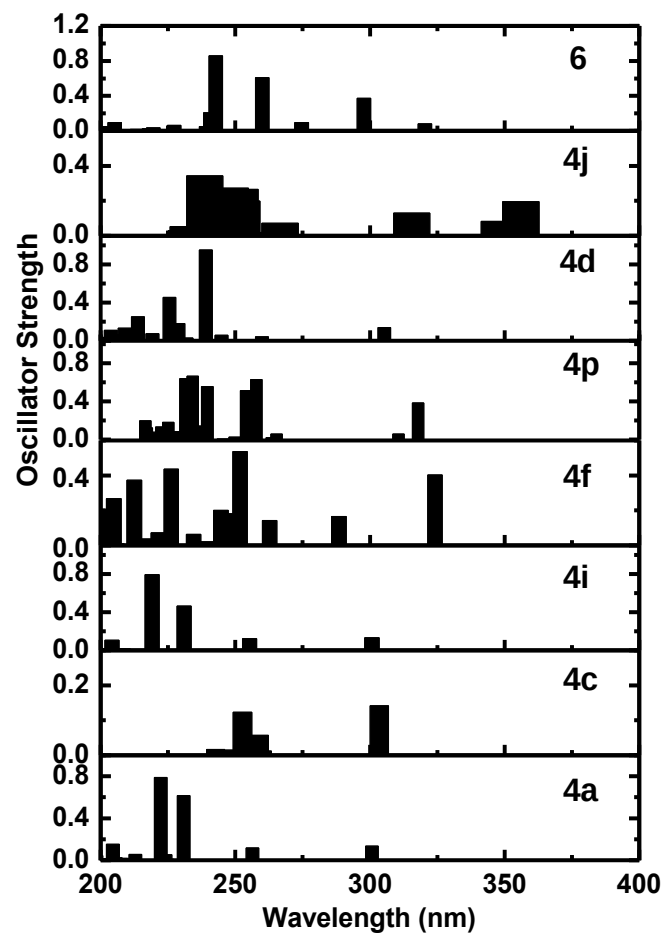


Figure S1. Oscillator strength values of **4a-6** based β -carboline derivatives using TDDFT calculations.

3. Emission studies of 4a-6 β -carboline in CHCl_3 at excitation wavelength of 290 nm:

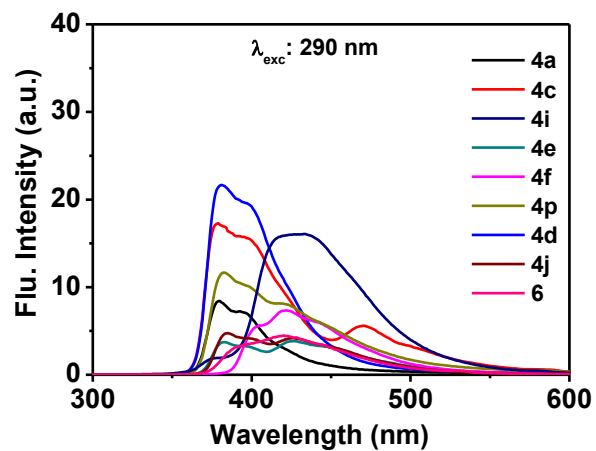


Figure S2. Emission spectra of 4a-6 based β -carboline in CHCl_3 at excitation wavelength of 290 nm.

4. Cyclic Voltammetry of electron donor appended β -carboline in CHCl_3 :

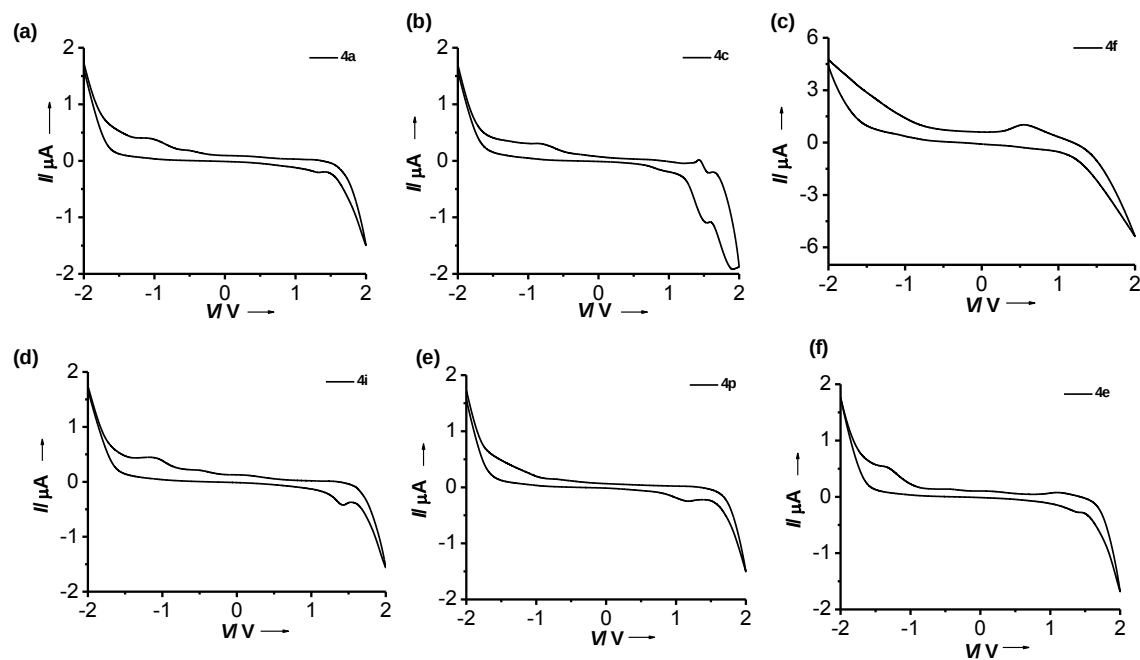


Figure S3. Cyclic voltammograms of electron donor linked β -carboline in chloroform at scan rate of 200 mV/s using 0.1 M tetrabutyl ammonium hexafluorophosphate (NBu_4PF_6) as supporting electrolyte at 25 °C.

5. Cyclic Voltammetry of electron acceptor linked β -carboline in CHCl_3 :

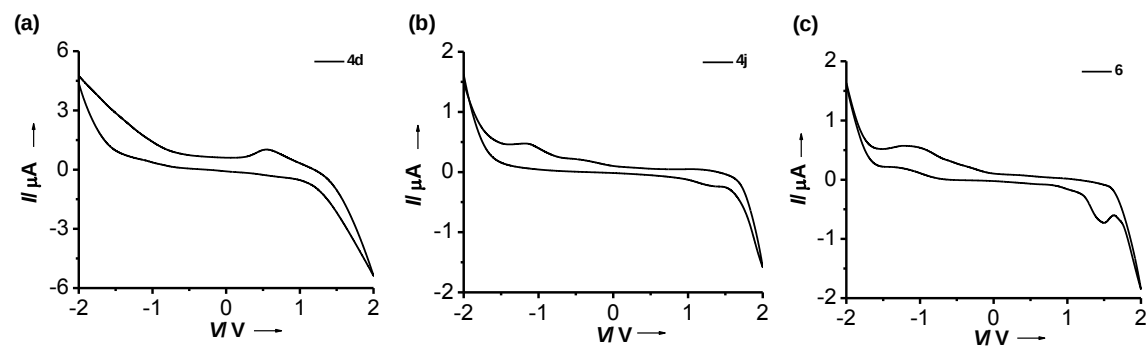


Figure S4. Cyclic voltammograms of electron acceptor linked β -carboline in chloroform at scan rate of 200 mV/s recorded at 25 °C.