Electronic Supplementary Material (ESI) for RSC Advances
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Supporting Information

Theoretical and experimental investigation of the polyeletrophilic β-enamino diketone: Straightforward and highly regioselective synthesis of 1,4,5-trisubstituted pyrazoles and pyrazolo[3,4-*d*]pyridazinones

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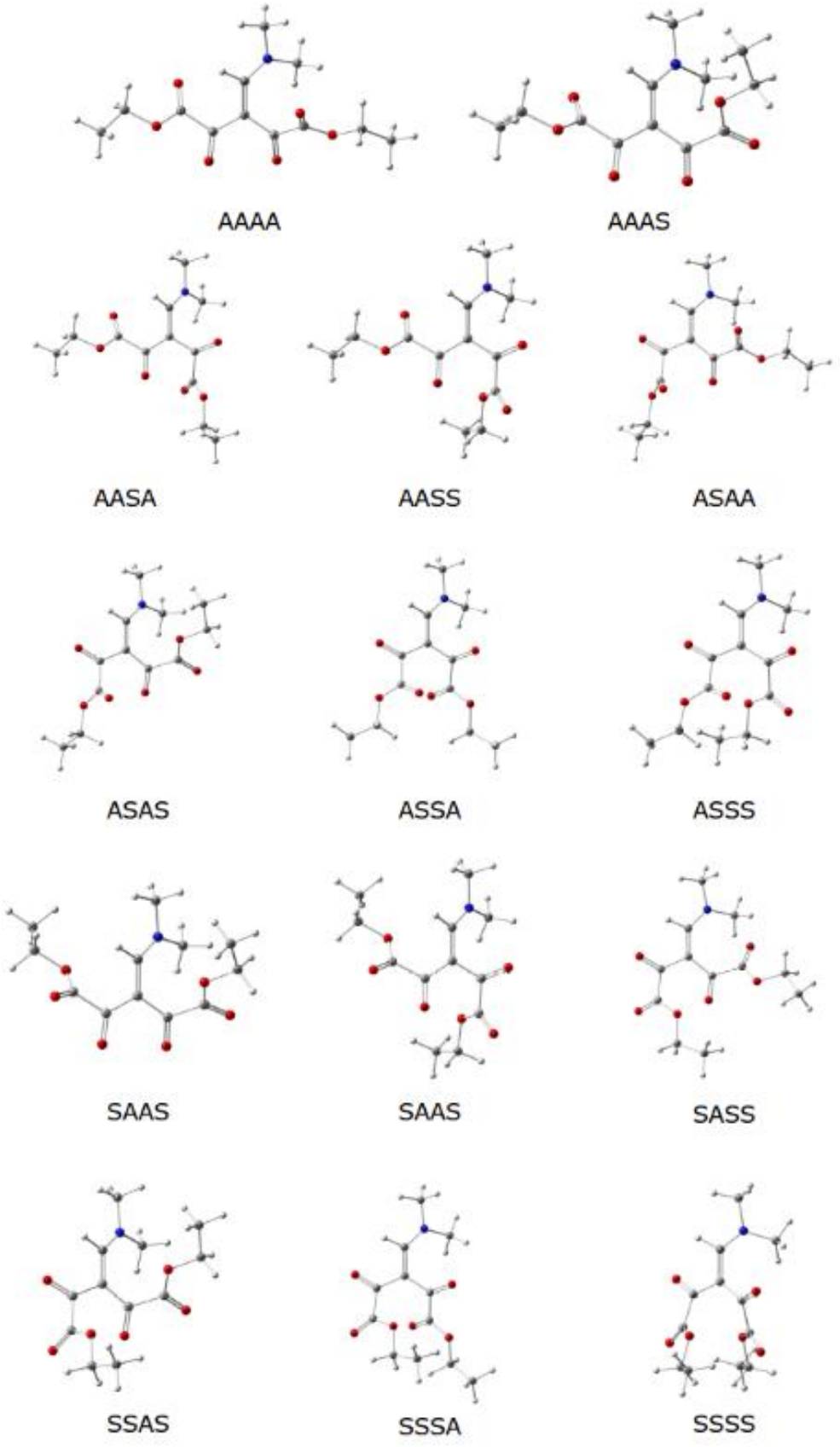


Fig. 1 Conformations of the building block β-enamino diketone (**2**).

Table 1 Dipole moment (Debye) and relative energies (kJ mol^{-1}) for the conformations of building block **2** optimized at M06-2X/6-31+G(d,p) level and IEF-PCM model for solvation effects.

	μ	E_{rel} **gas phase**	E_{rel} **dichloromethane**	E_{rel} **ethanol**
AAAA	7.11	35.26	23.44	21.69
AAAS	9.30	42.97	26.26	23.05
AASA	5.04	9.60	8.42	9.03
AASS	7.31	13.19	8.68	8.65
ASAA	6.92	16.43	9.96	9.95
ASAS	7.26	22.05	11.00	10.00
SAAA	-	→ AAAS	→ SAAS	→ SAAS
SAAS	-	→ AAAS	30.38	25.99
SASA	-	→ AASS	→ SASS	→ SASS
SASS	-	→ AASS	13.73	11.82
SSAA	8.70	17.99	→ SSAS	→ SSAS
SSAS	9.47	24.10	11.11	9.75

Conformer ASSA, gas phase

opt freq=noraman m062x/6-31+g(d,p)geom=connectivity

0 1

C	-1.13452100	-1.29637200	-0.50921800
C	0.29841100	-1.63212500	-0.06538500
C	1.28502500	-0.54736900	-0.06997400
C	0.92352500	0.86340500	-0.21826700
C	-0.40293100	1.31288400	0.42367500
O	-2.03074400	-2.06007200	0.08950100
O	-1.38070600	-0.45763900	-1.34873100
O	1.62506400	1.70047200	-0.75823700
O	-0.86424700	2.42645800	-0.11743400
O	0.57110800	-2.79895000	0.15820000
O	-0.91970600	0.71803100	1.34429800
H	3.75387000	1.76202600	0.02851300
C	2.59793900	-0.99974200	-0.13302900
H	4.73556300	0.99393700	1.32003600
C	3.80082500	0.94852500	0.75669300
H	2.72396100	-2.05570000	-0.37069400
N	3.73199500	-0.35440100	0.11179500
H	2.96040500	1.05158200	1.44630500
C	5.01165100	-0.96988700	-0.21398800
H	5.53814800	-0.36458900	-0.95853500
H	5.63086800	-1.04353200	0.68496100
H	4.84829200	-1.96641400	-0.62420700
C	-3.40135900	-1.80716800	-0.26521500
H	-3.62435100	-0.75998300	-0.03662500
H	-3.51467200	-1.95153500	-1.34371700
C	-2.11979800	2.89559800	0.40285300
H	-2.86433400	2.10622300	0.25770200
H	-2.01065700	3.06575700	1.47811600
C	-4.25469100	-2.76296300	0.53772500
H	-5.31055100	-2.59915900	0.30662900
H	-4.00103700	-3.79845700	0.29926600
H	-4.10215700	-2.60503600	1.60783800
C	-2.47167200	4.15988600	-0.34830700
H	-2.56277800	3.95735800	-1.41781200
H	-3.42410100	4.55338400	0.01656900
H	-1.70100700	4.92051700	-0.20306200

Energy (SCF) = -973.24117121 a.u.
Imaginary Freq. = 0

Conformer ASSS, gas phase

opt freq=noraman m062x/6-31+g(d,p) geom=connectivity

0 1

C	-1.21776800	-0.88703500	-0.69645900
C	0.08708900	-1.30021900	0.00901800
C	1.25086900	-0.45024600	-0.13699200
C	1.20564900	0.89744900	-0.67785100
C	-0.03109500	1.78906900	-0.42435600
O	-2.28266500	-1.35692200	-0.07648000
O	-1.23592000	-0.24400600	-1.72650300
O	2.11495400	1.41901200	-1.31115900
O	-0.72823200	1.39444000	0.63663600
O	0.09783000	-2.38881100	0.57818300
O	-0.28804100	2.75526900	-1.10107900
H	4.12832100	1.36569900	-0.10907800
C	2.47180100	-1.12971500	0.07790500
H	4.69108300	0.77116600	1.48134200
C	3.87196800	0.75816000	0.76149900
H	2.44081500	-2.21657500	0.02548100
N	3.64572800	-0.63048500	0.37708400
H	2.96906500	1.15717900	1.22588800
C	4.83210800	-1.48830900	0.39874300
H	5.56124600	-1.10291000	-0.31764900
H	5.26828900	-1.47454200	1.39996600
H	4.55479900	-2.50458900	0.12363700
C	-3.56573900	-1.05724800	-0.67840100
H	-3.67547100	0.03074900	-0.71791300
H	-3.56224000	-1.44636600	-1.69944000
C	-1.95426400	2.11812200	0.90475400
H	-1.69415900	3.15370800	1.13753000
H	-2.55552000	2.10622200	-0.00934000
C	-4.62616400	-1.70767800	0.17882700
H	-5.60993800	-1.50679600	-0.25248300
H	-4.47858400	-2.78945900	0.22082400
H	-4.60383500	-1.30744800	1.19566600
C	-2.64330600	1.42228600	2.05534300
H	-2.02135000	1.44737900	2.95349300
H	-3.58662500	1.93034900	2.27089400
H	-2.85629100	0.37994900	1.80262500

Energy (SCF) = -973.27287118 a.u.
Imaginary Freq. = 0

Conformer SSSA, gas phase

opt freq=noraman m062x/6-31+g(d,p) geom=connectivity

0 1

C	-0.57519600	2.08349000	-0.28352700
C	0.91575900	1.72860500	-0.44999200
C	1.38809000	0.37756700	-0.11057500
C	0.48882600	-0.74983700	0.13736900
C	-0.79118700	-0.80828400	-0.71783300
O	-1.12178100	1.38494800	0.72810200
O	-1.15241500	2.90672800	-0.93574800
O	0.71155600	-1.65785300	0.91917500
O	-1.73682400	-1.55862200	-0.16625900
O	1.65634100	2.63477900	-0.78322700
O	-0.88585400	-0.25553700	-1.78956300
H	2.74677400	-2.63303500	0.60065600
C	2.75283300	0.32712900	0.14781200
H	4.11675100	-2.55626500	-0.55584500
C	3.20800800	-2.06032900	-0.20785100
H	3.24753200	1.29157500	0.25739300
N	3.56870300	-0.71788400	0.22227700
H	2.49723400	-1.99287400	-1.03434800
C	4.93290100	-0.54958500	0.70582100
H	5.07889000	-1.12744500	1.62389200
H	5.64314500	-0.89900800	-0.04934600
H	5.12128100	0.50260300	0.91923800

C	-2.53364200	1.56865800	0.93101800
H	-2.73074800	2.63478900	1.07333100
H	-3.04817200	1.25222800	0.01597600
C	-2.92931400	-1.73362300	-0.95383200
H	-3.30956600	-0.74872000	-1.24188600
H	-2.65943200	-2.26674300	-1.87060000
C	-2.92279200	0.73532900	2.13239500
H	-4.00226500	0.79986500	2.29501000
H	-2.64819300	-0.31110800	1.97445500
H	-2.41480200	1.09524300	3.03039800
C	-3.91559100	-2.50906700	-0.10973000
H	-4.18224500	-1.94713000	0.78901700
H	-4.82665700	-2.69610300	-0.68398800
H	-3.49081100	-3.46853800	0.19442600

Energy (SCF) = -973.239434
Imaginary Freq. = 0

Conformer SSSS, gas phase

opt freq=noraman m062x/6-31+g(d,p)geom=connectivity

0 1

C	-1.25249700	0.04162700	1.45932700
C	0.22788700	0.47308300	1.49745200
C	1.12600500	0.05299500	0.41143900
C	0.64079700	-0.53204100	-0.84308400
C	-0.70735900	-0.03778000	-1.41565200
O	-1.36928000	-1.17629000	0.91667000
O	-2.16600600	0.69989400	1.88035500
O	1.23596100	-1.37724900	-1.48534900
O	-0.99219100	1.18792200	-0.96205300
O	0.59439400	1.08897700	2.48148300
O	-1.39256200	-0.66995300	-2.17490300
H	3.38577200	-0.80331400	-1.93812400
C	2.46890800	0.08346600	0.76709900
H	4.48635900	0.60190100	-1.75234900
C	3.53609300	0.16022000	-1.44461400
H	2.67249600	0.22618000	1.82798800
N	3.55455700	0.02591000	0.00434500
H	2.72073500	0.82722400	-1.73286300
C	4.87054800	-0.12633700	0.61168500
H	5.33278700	-1.05776800	0.27051600
H	5.51271800	0.71307700	0.32888100
H	4.77426200	-0.15887600	1.69688400
C	-2.26419400	1.74582100	-1.34965200
H	-2.27369400	1.85277000	-2.43836500
H	-3.04889500	1.03615800	-1.06973400
C	-2.40836400	3.06445600	-0.62433300
H	-1.60781300	3.75119900	-0.91024700
H	-3.36724900	3.52250600	-0.88077700
H	-2.37198900	2.90466300	0.45604500
C	-2.70515400	-1.69731500	0.76129100
H	-3.15770500	-1.78185000	1.75343900
H	-3.28709000	-0.97599600	0.17904700
C	-2.57904600	-3.02691100	0.05266800
H	-1.97778800	-3.72160900	0.64428900
H	-3.57134400	-3.46188700	-0.09270000
H	-2.10773800	-2.88986200	-0.92371700

Energy (SCF) = -973.24139261 a.u.
Imaginary Freq. = 0

Conformer ASSA, dichloromethane

opt freq=noraman m062x/6-31+g(d,p)scrf=(iefpcm,solvent=dichloromethane,read)

geom=connectivity

0 1

C	-1.11925400	-1.29753200	-0.53149500
C	0.32404500	-1.61502300	-0.10154700
C	1.29106400	-0.53769500	-0.10515100
C	0.91530000	0.85847600	-0.23663700
C	-0.41617700	1.29350500	0.41161700
O	-2.00048900	-2.04168000	0.10398900
O	-1.38139100	-0.48352500	-1.39485400
O	1.60147300	1.72072400	-0.77130600
O	-0.90012000	2.38980200	-0.13408600
O	0.59746100	-2.79222900	0.11994300
O	-0.91660200	0.69518700	1.34313900
H	3.76916200	1.78199400	0.14998100
C	2.63107700	-0.97377500	-0.19343000
H	4.65005000	0.94883600	1.46397800
C	3.75252200	0.93961300	0.84475600
H	2.78798900	-1.99522600	-0.53572600
N	3.72706000	-0.32836700	0.12323300
H	2.86900000	1.01372600	1.48035200
C	5.03948500	-0.90100800	-0.18289300
H	5.59051100	-0.20599200	-0.82086300
H	5.59173000	-1.05180500	0.74739700
H	4.91480500	-1.84973400	-0.70227500
C	-3.39103600	-1.82515100	-0.24025500
H	-3.62658800	-0.77707500	-0.03431200
H	-3.50944600	-2.00984700	-1.31068200
C	-2.15171400	2.87562700	0.40951800
H	-2.89933800	2.08736700	0.28347600
H	-2.01012800	3.05970300	1.47735600
C	-4.21425700	-2.77279400	0.60013100
H	-5.27331700	-2.62565400	0.37447200
H	-3.95287400	-3.81098500	0.38155600
H	-4.05528900	-2.58278100	1.66430100
C	-2.51252000	4.13315800	-0.34580900
H	-2.63164000	3.92411700	-1.41158700
H	-3.45689900	4.52506900	0.04002700
H	-1.74103600	4.89621600	-0.21751000

radii=bondi

Energy (SCF) = -973.2394674
Imaginary Freq. = 0

Conformer ASSS, dichloromethane

opt freq=noraman m062x/6-31+g(d,p)scrf=(iefpcm,solvent=dichloromethane,read)

geom=connectivity

0 1

C	-1.21776800	-0.88703500	-0.69645900
C	0.08708900	-1.30021900	0.00901800
C	1.25086900	-0.45024600	-0.13699200
C	1.20564900	0.89744900	-0.67785100
C	-0.03109500	1.78906900	-0.42435600
O	-2.28266500	-1.35692200	-0.07648000
O	-1.23592000	-0.24400600	-1.72650300
O	2.11495400	1.41901200	-1.31115900
O	-0.72823200	1.39444000	0.63663600
O	0.09783000	-2.38881100	0.57818300
O	-0.28804100	2.75526900	-1.10107900
H	4.12832100	1.36569900	-0.10907800
C	2.47180100	-1.12971500	0.07790500
H	4.69108300	0.77116600	1.48134200
C	3.87196800	0.75816000	0.76149900
H	2.44081500	-2.21657500	0.02548100
N	3.64572800	-0.63048500	0.37708400
H	2.96906500	1.15717900	1.22588800
C	4.83210800	-1.48830900	0.39874300
H	5.56124600	-1.10291000	-0.31764900
H	5.26828900	-1.47454200	1.39996600
H	4.55479900	-2.50458900	0.12363700
C	-3.56573900	-1.05724800	-0.67840100
H	-3.67547100	0.03074900	-0.71791300
H	-3.56224000	-1.44636600	-1.69944000
C	-1.95426400	2.11812200	0.90475400
H	-1.69415900	3.15370800	1.13753000
H	-2.55552000	2.10622200	-0.00934000
C	-4.62616400	-1.70767800	0.17882700
H	-5.60993800	-1.50679600	-0.25248300
H	-4.47858400	-2.78945900	0.22082400
H	-4.60383500	-1.30744800	1.19566600
C	-2.64330600	1.42228600	2.05534300
H	-2.02135000	1.44737900	2.95349300
H	-3.58662500	1.93034900	2.27089400
H	-2.85629100	0.37994900	1.80262500

radii=bondi

Energy (SCF) = -973.27287118 a.u.
Imaginary Freq. = 0

Conformer SSSS, dichloromethane

opt freq=noraman m062x/6

31+g(d,p)scrf=(iefpcm,solvent=dichloromethane,read)geom=co

nnectivity

0 1

C	-1.23209500	-0.71889100	1.29487100
C	0.26327700	-0.41029300	1.50550000
C	1.13766200	-0.21277200	0.36578900
C	0.65849500	-0.03780000	-0.99506300
C	-0.68053400	0.69417700	-1.24601000
O	-1.43358500	-1.42627200	0.18813800
O	-2.09104000	-0.39284500	2.07877100
O	1.26054300	-0.40405300	-1.99644000
O	-1.01637100	1.47490900	-0.22620300
O	0.64589500	-0.42154800	2.67210600
O	-1.30443000	0.58662500	-2.27465800
H	3.43758400	0.47418100	-2.03886300
C	2.50306800	-0.42676300	0.66211400
H	4.44613000	1.54883600	-1.02571700
C	3.52293500	0.96995700	-1.06953200
H	2.72223400	-0.98441100	1.57066700
N	3.56088500	-0.00717600	0.01271200
H	2.66783900	1.63254300	-0.92772600
C	4.89693700	-0.46267900	0.40181400
H	5.37128800	-0.94407000	-0.45652500
H	5.49493400	0.39809000	0.70862500
H	4.81749500	-1.17584100	1.22059500
C	-2.25650400	2.21694400	-0.34110100
H	-2.19894000	2.83394700	-1.24105000
H	-3.07106600	1.49735000	-0.45839700
C	-2.39972900	3.03952700	0.91777600
H	-1.57060800	3.74463600	1.01540100
H	-3.33375300	3.60500000	0.87401900
H	-2.42344600	2.39286900	1.79827900
C	-2.80364800	-1.77072100	-0.13730800
H	-3.24093700	-2.27797100	0.72567400
H	-3.34644500	-0.83771300	-0.31414000
C	-2.76148200	-2.64663100	-1.36740800
H	-2.20809200	-3.56726600	-1.16686200
H	-3.78184300	-2.90963300	-1.65678700
H	-2.28696400	-2.11915500	-2.19854500

radii=bondi

Energy (SCF) = -973.27243715 a.u.
Imaginary Freq. = 0

Conformer ASSA, ethanol

opt freq=noraman m062x/6-

31+g(d,p)scrf=(iefpcm,solvent=ethanol,read)

geom=connectivity

0 1

C	-1.11338900	-1.29964300	-0.53550200
C	0.32941000	-1.61405900	-0.10064100
C	1.29362800	-0.53765400	-0.10980800
C	0.91184200	0.85506000	-0.24532500
C	-0.41766900	1.28730700	0.40978700
O	-1.99589600	-2.03880800	0.10302000
O	-1.37364300	-0.49006700	-1.40415000
O	1.58959000	1.71939000	-0.78916700
O	-0.90792900	2.38066600	-0.13502000
O	0.60118700	-2.79121000	0.13034800
O	-0.91210000	0.68786700	1.34415600
H	3.76670600	1.78908600	0.14582200
C	2.63798700	-0.97001300	-0.19641800

H	4.63732000	0.96249400	1.46952300
C	3.74432000	0.94988600	0.84425300
H	2.80075600	-1.98892800	-0.54321200
N	3.72751300	-0.32029600	0.12538800
H	2.85584900	1.02432100	1.47266600
C	5.04517400	-0.88810800	-0.17082300
H	5.59831700	-0.18774700	-0.80066500
H	5.58793300	-1.03835800	0.76481300
H	4.92795400	-1.83539900	-0.69418700
C	-3.38804600	-1.82444600	-0.24344200
H	-3.62247400	-0.77472900	-0.04541300
H	-3.50567600	-2.01909700	-1.31200400
C	-2.15732100	2.86764800	0.41706000
H	-2.90499800	2.07868100	0.29707100
H	-2.00666100	3.05428800	1.48297900
C	-4.21123700	-2.76484100	0.60465500
H	-5.26987100	-2.61767000	0.37745200
H	-3.95176800	-3.80510000	0.39351900
H	-4.05288700	-2.56626500	1.66742700
C	-2.52363700	4.12355200	-0.33781500
H	-2.65115600	3.91327200	-1.40246000
H	-3.46559500	4.51454100	0.05459000
H	-1.75238500	4.88783800	-0.21501900

radii=bondi

Energy (SCF) = -973.27665182 a.u.
Imaginary Freq. = 0

Conformer ASSS, ethanol

opt freq=noraman m062x/6-31+g(d,p)scrf=(iefpcm,solvent=ethanol,read)

geom=connectivity

0 1

C	-1.21856000	-0.88797100	-0.69796700
C	0.08815400	-1.30086900	0.00501800
C	1.25047100	-0.45337900	-0.14276600
C	1.20417400	0.89189100	-0.68369700
C	-0.03150600	1.78468500	-0.42885100
O	-2.28088500	-1.35807000	-0.07624000
O	-1.23872200	-0.24422700	-1.72841400
O	2.11201100	1.41467500	-1.32061200
O	-0.72599000	1.39650100	0.63306200
O	0.09822800	-2.39045000	0.57516600
O	-0.28826500	2.74825900	-1.11192100
H	4.12882500	1.36724500	-0.09335100
C	2.47544300	-1.13278000	0.07137300
H	4.66911600	0.77132800	1.50324500
C	3.85974100	0.75897800	0.77282700
H	2.45076700	-2.21897400	0.00572400
N	3.64265800	-0.62949400	0.38056900
H	2.94972600	1.15506300	1.22533000
C	4.83453300	-1.48089700	0.40698300
H	5.56669500	-1.08391900	-0.29958200
H	5.26015300	-1.46993900	1.41245300
H	4.56561300	-2.49652700	0.12198300
C	-3.56840500	-1.05555700	-0.67063800
H	-3.67826500	0.03247000	-0.70050100
H	-3.56891500	-1.43930600	-1.69358800
C	-1.95053000	2.12424600	0.90561200
H	-1.68560400	3.15914700	1.13530300
H	-2.55631700	2.10939300	-0.00516000
C	-4.62363100	-1.71242000	0.18771800
H	-5.60914100	-1.50832600	-0.23791900
H	-4.47637600	-2.79466200	0.22065200
H	-4.59662400	-1.31835200	1.20682100
C	-2.63504400	1.43292200	2.06107500
H	-2.00775100	1.45708300	2.95556100
H	-3.57448800	1.94621600	2.28063000
H	-2.85606700	0.39192400	1.80996200

radii=bondi

Energy (SCF) = -973.27781476 a.u.
Imaginary Freq. = 0

Conformer SSSS, ethanol

opt freq=noraman m062x/6-31+g(d,p)scrf=(iefpcm,solvent=ethanol,read)

geom=connectivity

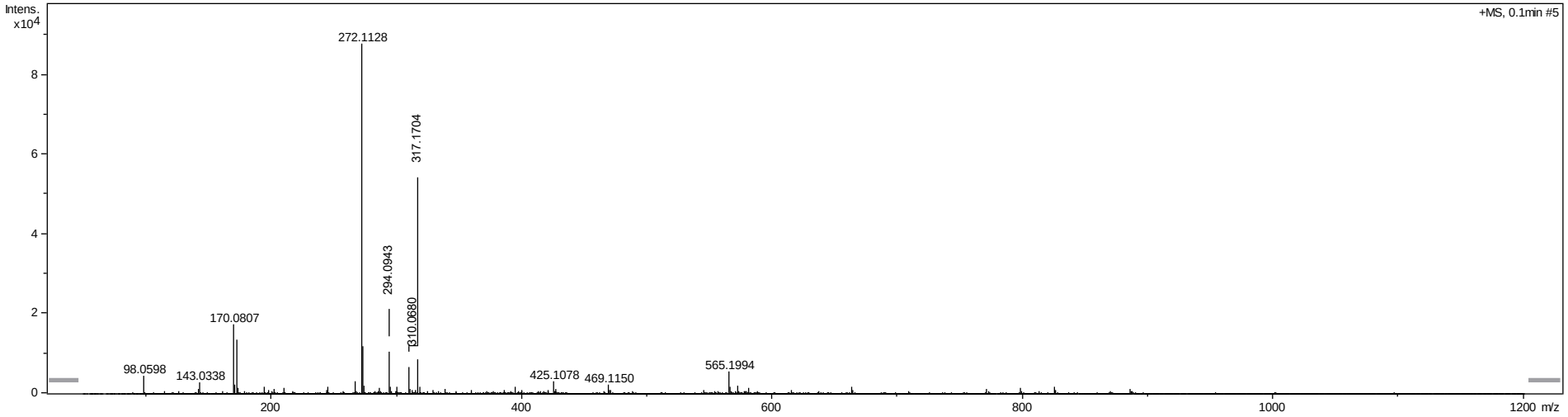
0 1

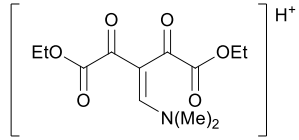
C	-1.23371900	-0.76164900	1.27596000
C	0.26261400	-0.45701000	1.49158400
C	1.13597100	-0.23375100	0.35926000
C	0.65580900	-0.02046600	-0.99390600
C	-0.67655500	0.73054600	-1.22316400
O	-1.44434600	-1.42707400	0.14721700
O	-2.08678000	-0.46610900	2.07970500
O	1.25194300	-0.36640500	-2.00718400
O	-1.00704800	1.48547600	-0.18445500
O	0.64416700	-0.49441200	2.65951400
O	-1.30015100	0.65500600	-2.25605000
H	3.43249200	0.51996200	-2.02678800
C	2.50456600	-0.45742900	0.64763600
H	4.43661900	1.57170800	-0.98675700
C	3.51526500	0.99164700	-1.04524800
H	2.72635800	-1.04573300	1.53578700
N	3.55811900	-0.01504200	0.01015300
H	2.65762900	1.64673400	-0.88551500
C	4.89751700	-0.47653900	0.38350400
H	5.37193600	-0.92624600	-0.49160800
H	5.49017700	0.37794000	0.71648900
H	4.82230500	-1.21616200	1.17860800
C	-2.24063600	2.24309700	-0.28235000
H	-2.18194300	2.86920300	-1.17564700
H	-3.06273700	1.53230500	-0.40031200
C	-2.36441800	3.05559400	0.98495200
H	-1.52695900	3.75096400	1.08141800
H	-3.29244200	3.63144500	0.95294300
H	-2.38904800	2.40277600	1.86100200
C	-2.81819800	-1.76398800	-0.17713900
H	-3.24623100	-2.29768800	0.67428500

H	-3.36268800	-0.82663800	-0.32212000
C	-2.78574200	-2.60515500	-1.43129100
H	-2.22995500	-3.53050200	-1.26125600
H	-3.80874200	-2.86122300	-1.71733500
H	-2.32071900	-2.05478200	-2.25302700

radii=bondi

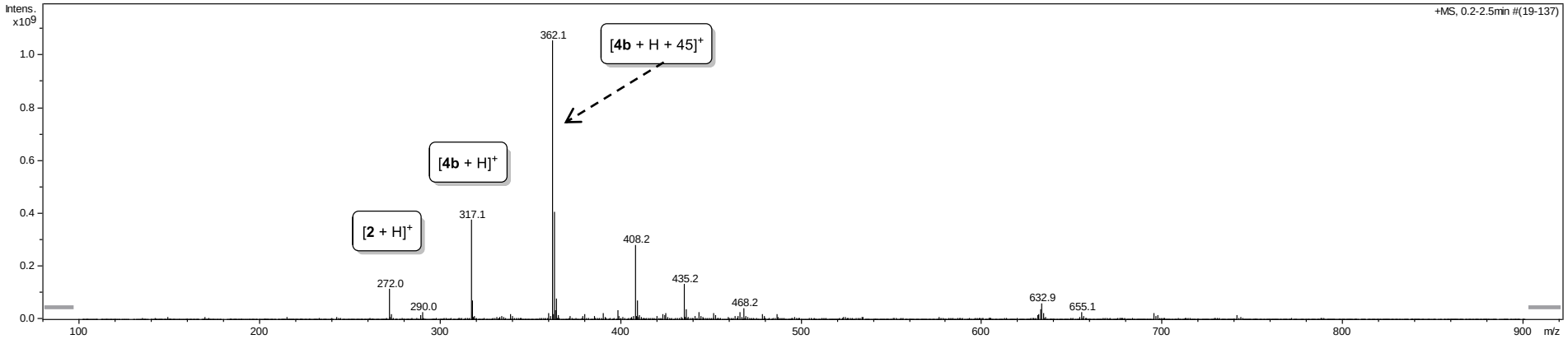
Energy (SCF) = -973.27712525 a.u.
Imaginary Freq. = 0

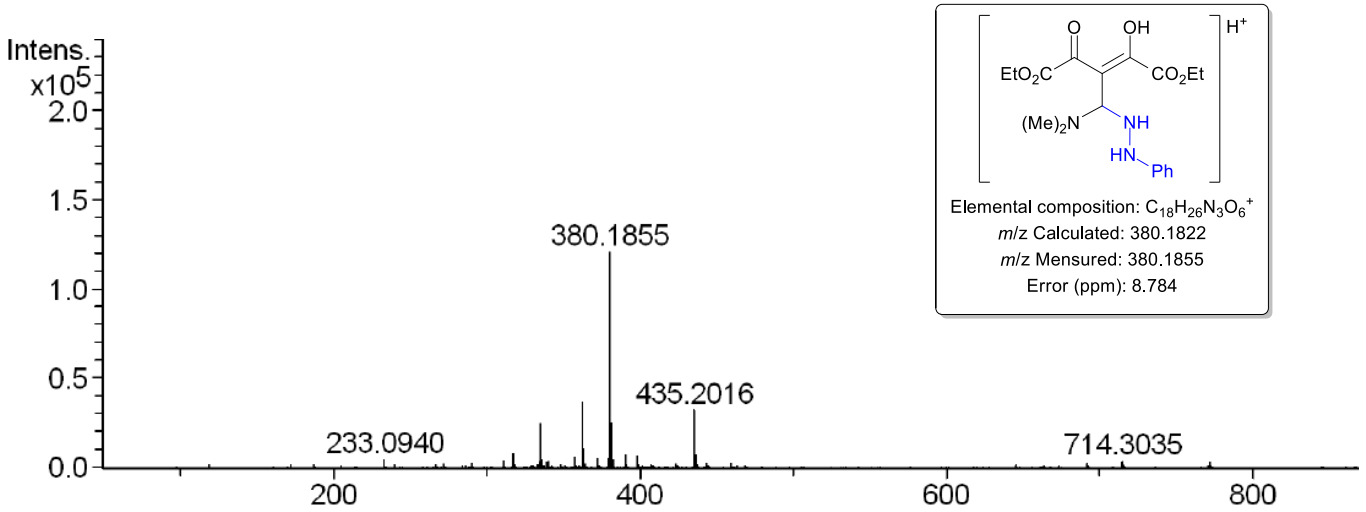




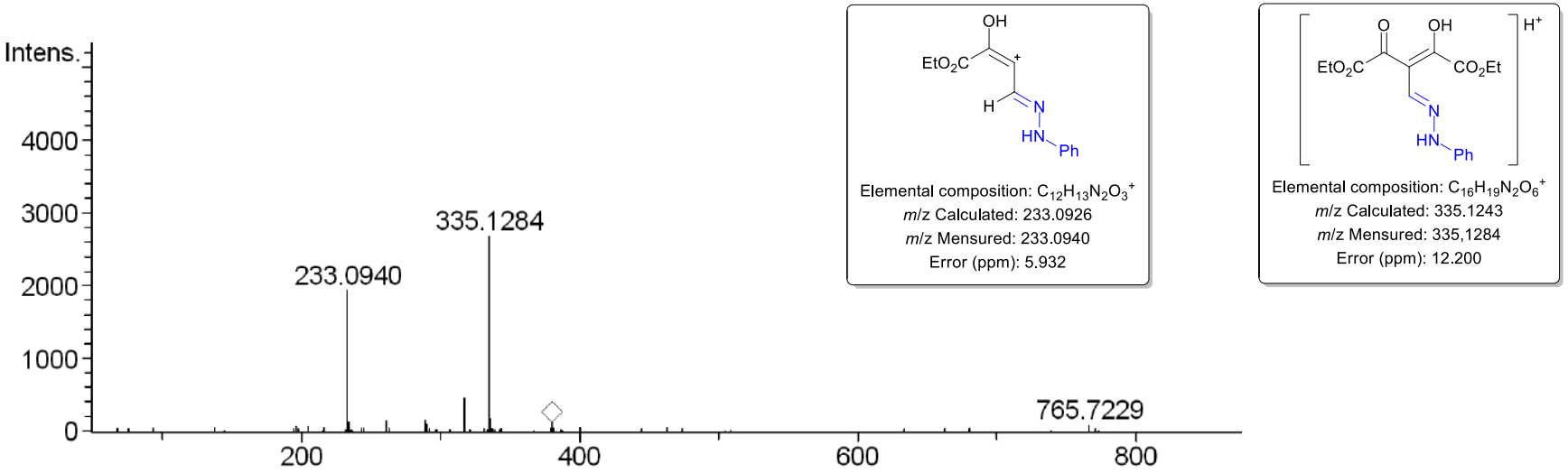
[2 + H]$^+$

Elemental composition: $C_{12}H_{18}NO_6^+$
m/z Calculated: 272,1134
m/z Mensured: 272.1128
Error (ppm): 2.250

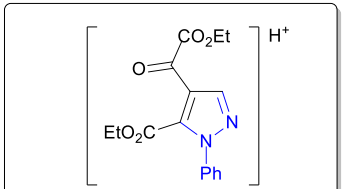




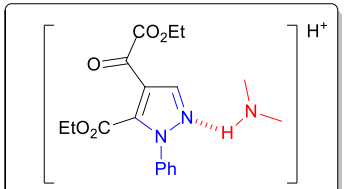
ESI(+)-MS for the reaction of **2** with phenylhydrazine in ethanol at 0°C after 3 min of reaction.



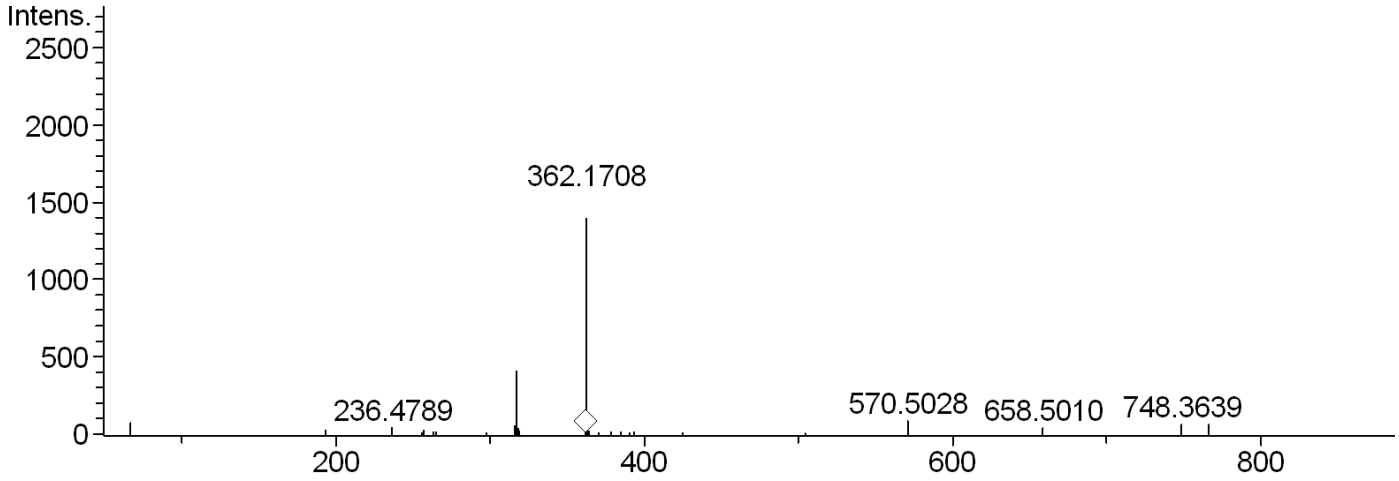
ESI(+)-MS/MS of the ion of m/z 380.1855.



Elemental composition: $C_{16}H_{17}N_2O_5^+$
m/z Calculated: 317.1137
m/z Mensured: 317.1104
Error (ppm): 10.554

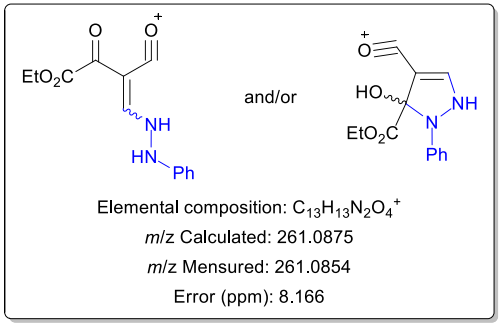


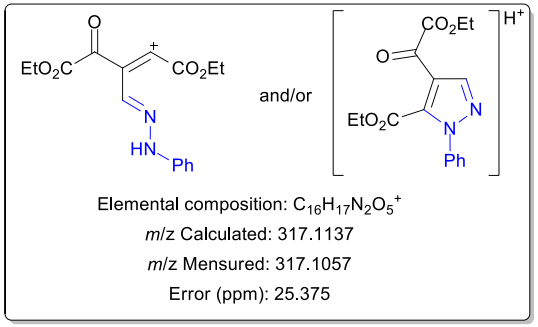
Elemental composition: $C_{18}H_{24}N_3O_5^+$
m/z Calculated: 362.1716
m/z Mensured: 362.1708
Error (ppm): 1.645

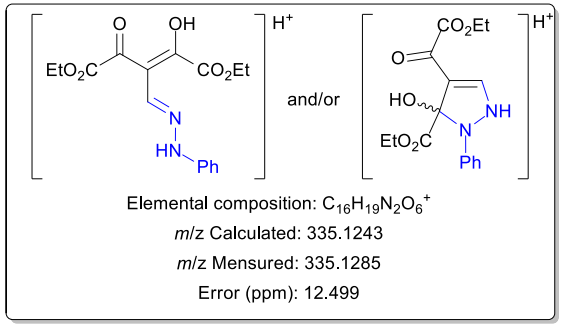


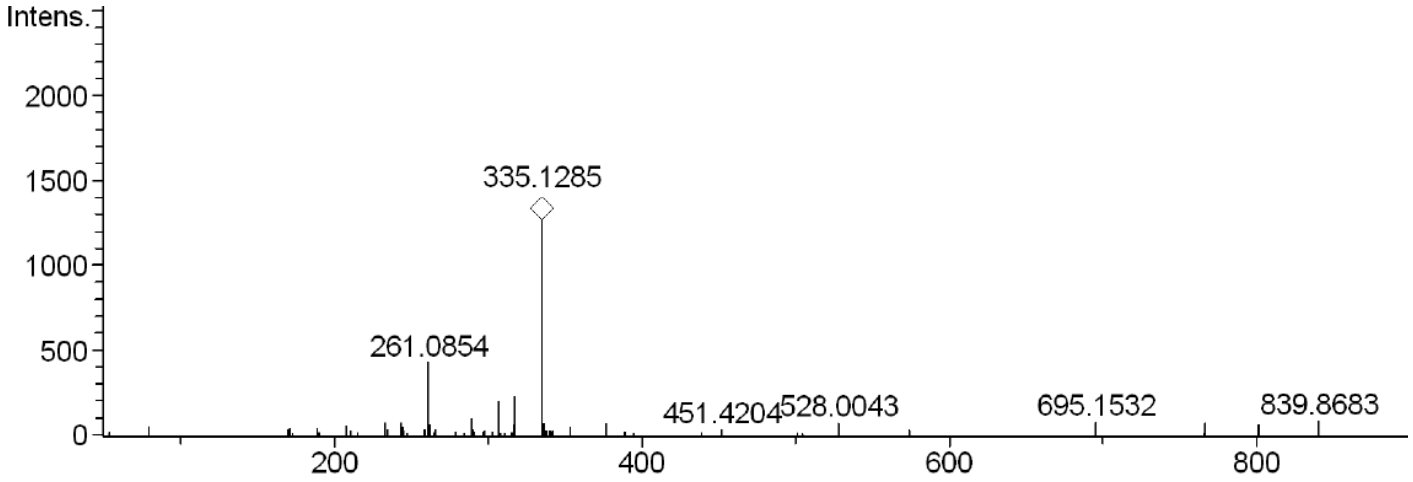
#	m/z	I
1	67.0484	77
2	193.3849	31
3	236.4789	46
4	257.1181	26
5	316.1349	56
6	317.1104	410
7	318.0931	38
8	319.0747	20
9	362.1708	1391
10	363.0638	56
11	363.1684	107
12	363.4798	21
13	364.3064	24
14	378.1956	19
15	384.4528	19
16	570.5028	93
17	658.5010	48
18	748.3639	70
19	765.6334	32
20	765.7351	68

ESI(+)-MS/MS of the ion of m/z 362.1708.



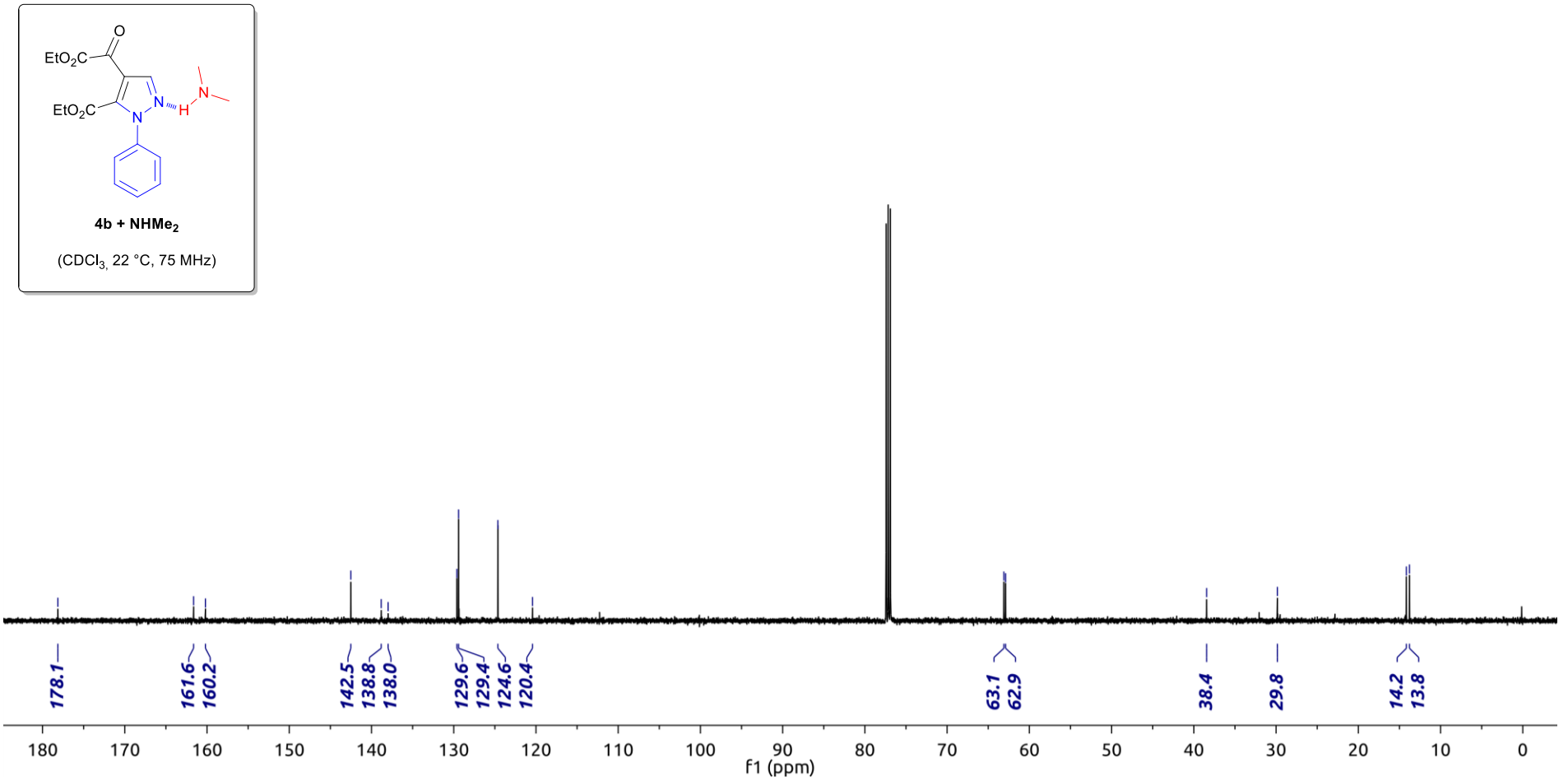


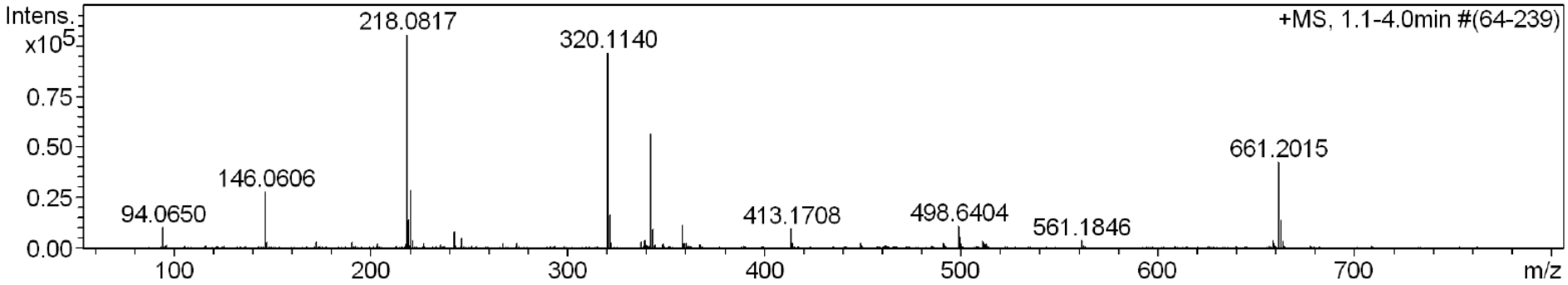


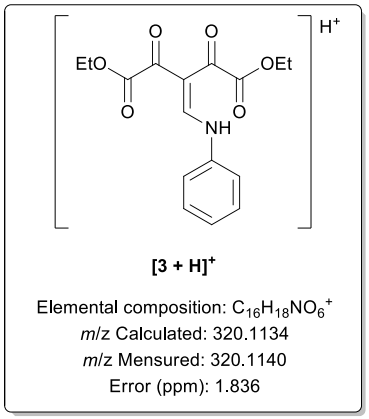


#	m/z	I
1	79.9090	52
2	208.0666	56
3	233.0689	71
4	243.0760	72
5	244.5418	47
6	261.0854	428
7	262.1013	62
8	289.1048	98
9	307.1028	196
10	316.7394	64
11	317.1057	227
12	335.1285	1266
13	336.1152	67
14	376.6198	65
15	528.0043	70
16	695.1532	77
17	765.6097	64
18	765.7341	72
19	800.7716	63
20	839.8683	80

ESI(+)-MS/MS of the ion of m/z 335.1285.

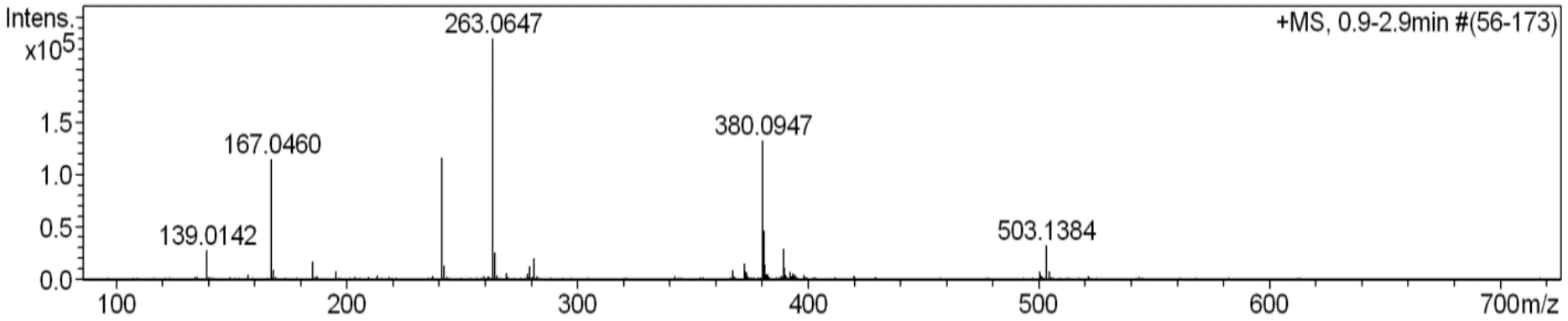




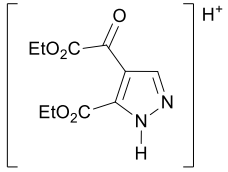


$[3 + H]^+$

Elemental composition: $C_{16}H_{18}NO_6^+$
m/z Calculated: 320.1134
m/z Mensured: 320.1140
Error (ppm): 1.836



#	m/z	I
1	139.0142	26659
2	167.0460	112781
3	168.0481	8853
4	185.0560	16039
5	241.0826	114344
6	242.0847	12561
7	263.0647	228587
8	264.0665	24598
9	279.0382	11560
10	281.0737	18919
11	367.0860	7683
12	372.1054	14013
13	380.0947	132355
14	380.5953	46207
15	381.0962	12975
16	389.0990	27659
17	389.6000	9782
18	500.1309	7094
19	503.1384	32051
20	504.1409	7130



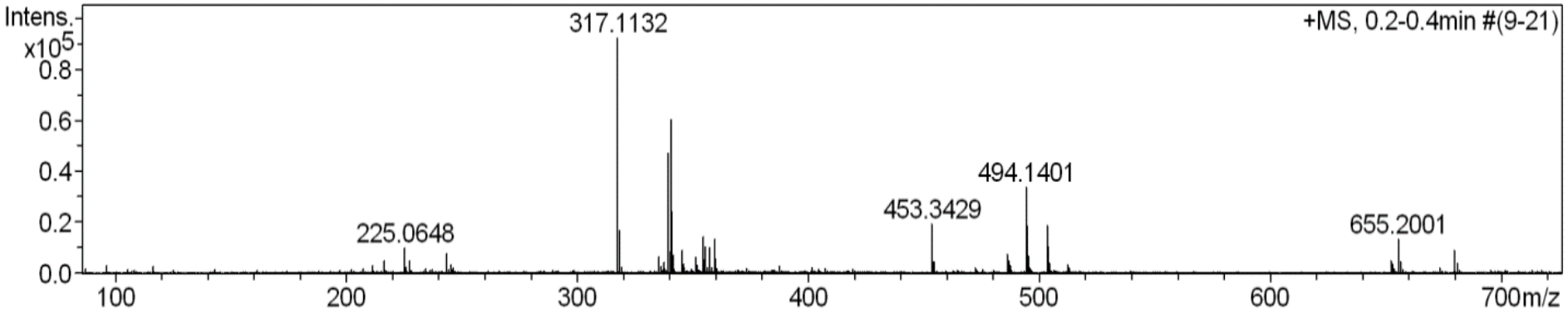
[4a + H]$^+$

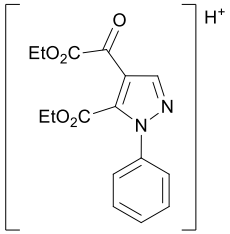
Elemental composition: $C_{10}H_{13}N_2O_5^+$

m/z Calculated: 241.0824

m/z Mensured: 241.0826

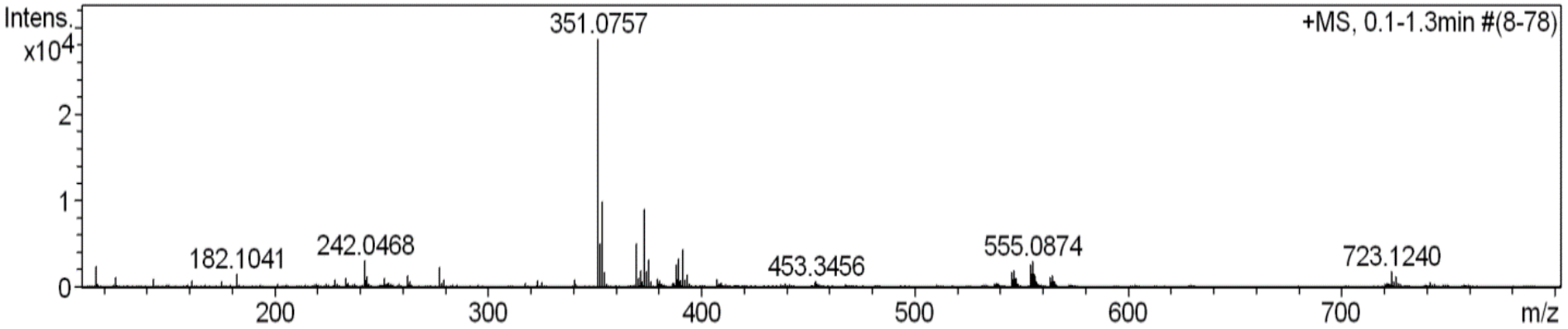
Error (ppm): 0.637

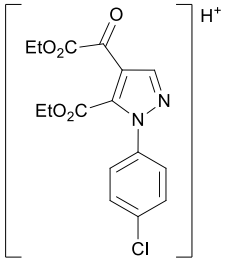




[4b + H]$^+$

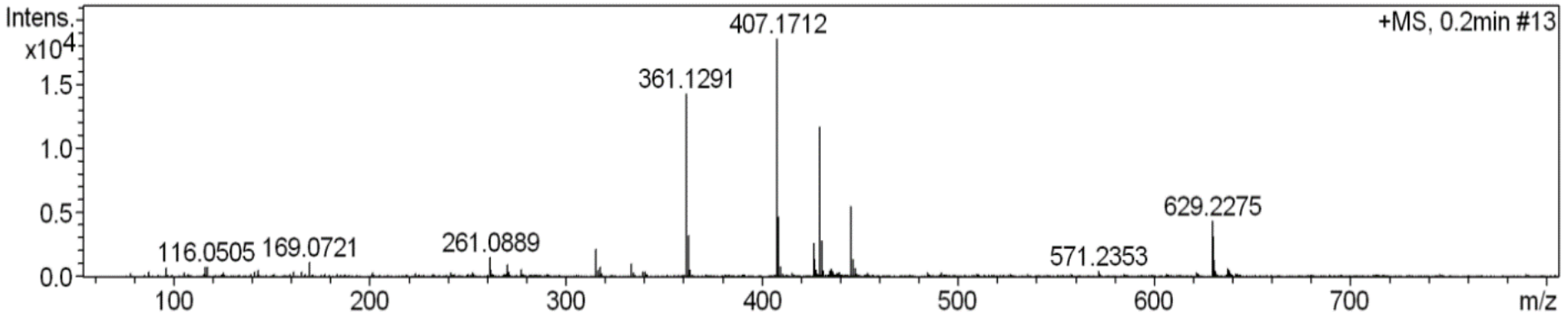
Elemental composition: $C_{16}H_{17}N_2O_5^+$
m/z Calculated: 317.1137
m/z Mensured: 317.1132
Error (ppm): 1.724

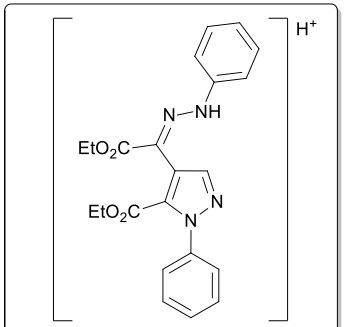




[4c + H]$^+$

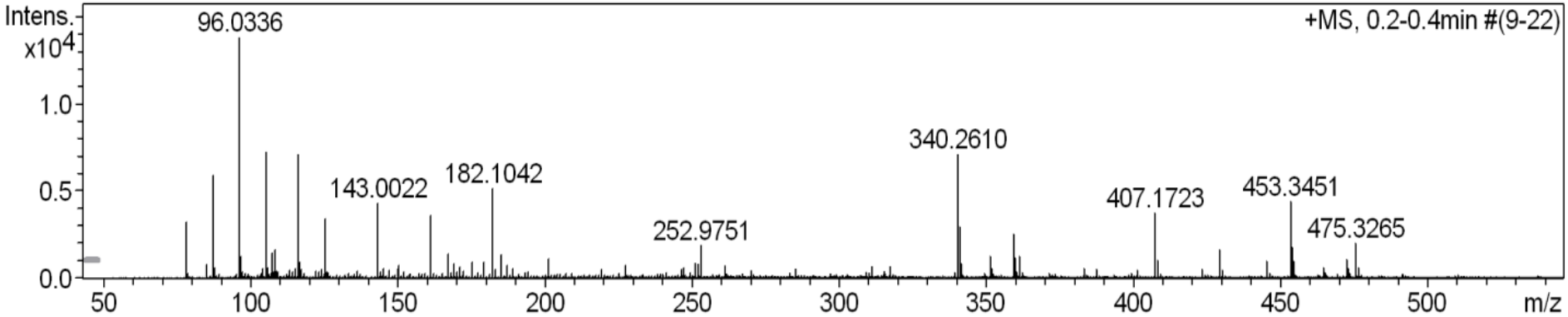
Elemental composition: $C_{16}H_{16}ClN_2O_5^+$
m/z Calculated: 351.0747
m/z Mensured: 351.0757
Error (ppm): 2.637

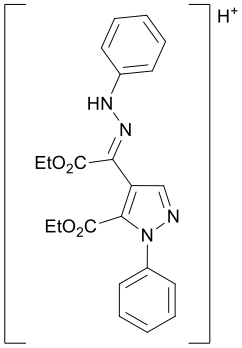




[5b(*E*) + H]$^+$

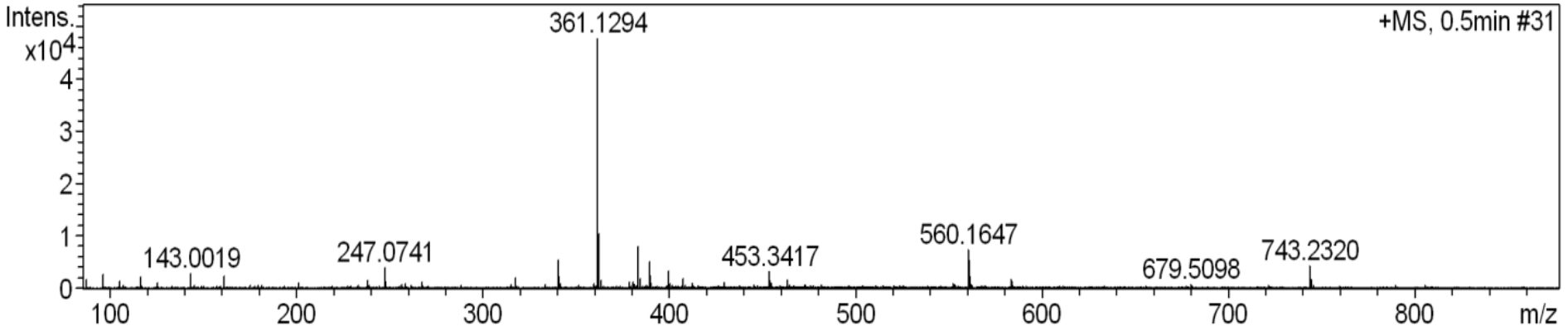
Elemental composition: $C_{22}H_{23}N_4O_4^+$
m/z Calculated: 407.1719
m/z Mensured: 407.1712
Error (ppm): 1.793

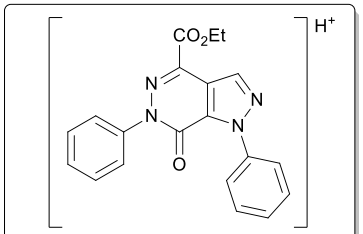




[5b(*Z*) + H]$^+$

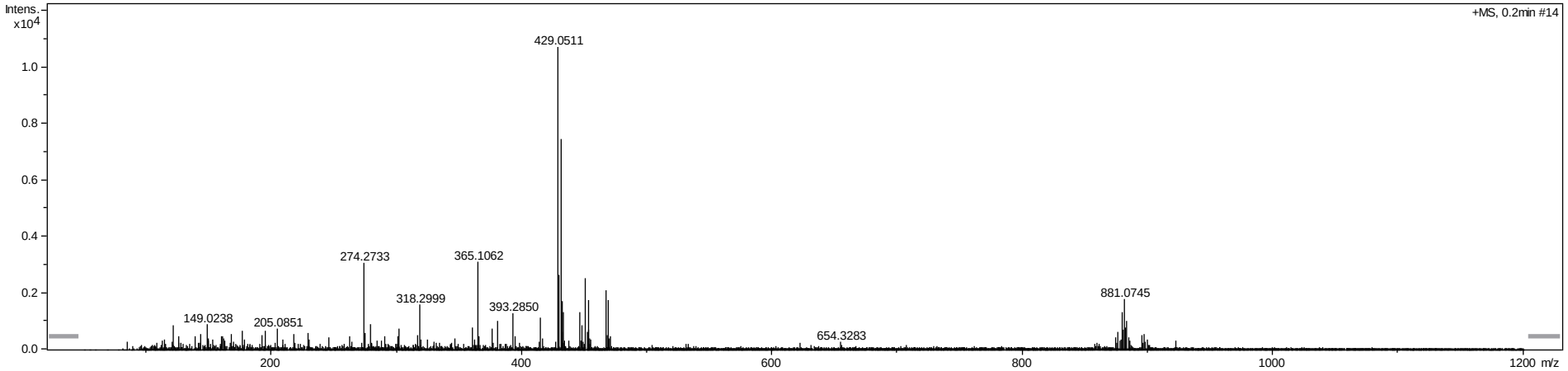
Elemental composition: $C_{22}H_{23}N_4O_4^+$
m/z Calculated: 407.1719
m/z Mensured: 407.1723
Error (ppm): 0.908

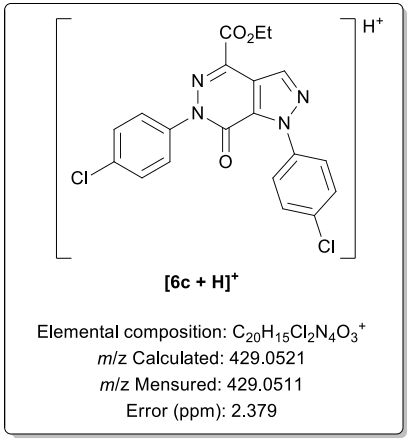




[6b + H]$^+$

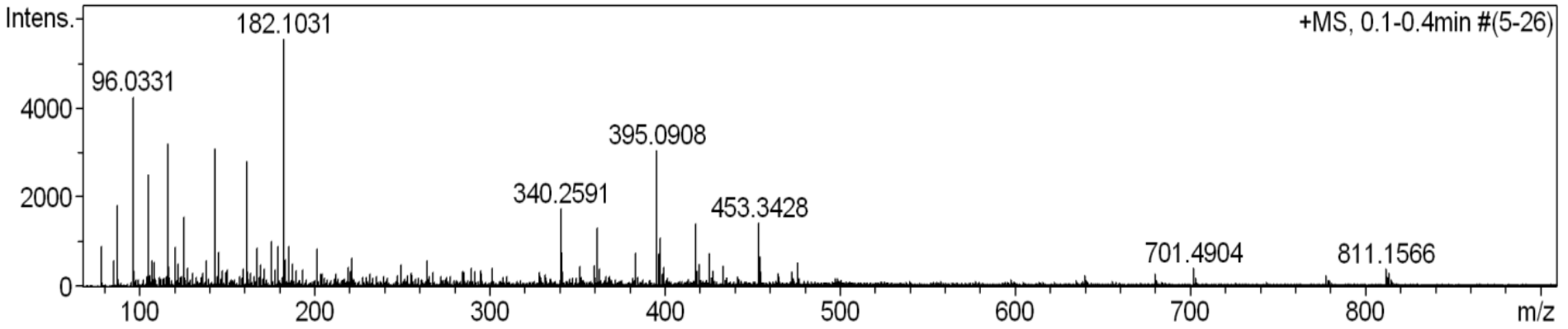
Elemental composition: $C_{20}H_{17}N_4O_3^+$
m/z Calculated: 361.1301
m/z Mensured: 361.1294
Error (ppm): 1.843

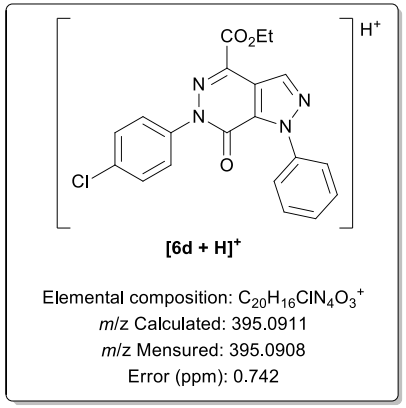




[6c + H]$^+$

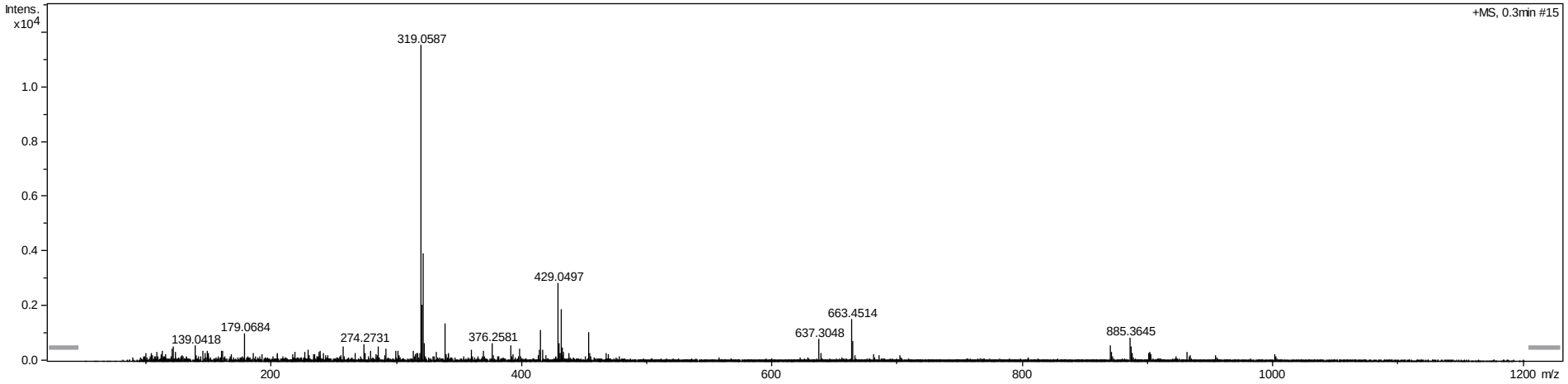
Elemental composition: $C_{20}H_{15}Cl_2N_4O_3^+$
m/z Calculated: 429.0521
m/z Mensured: 429.0511
Error (ppm): 2.379

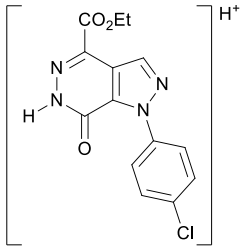




[6d + H]$^+$

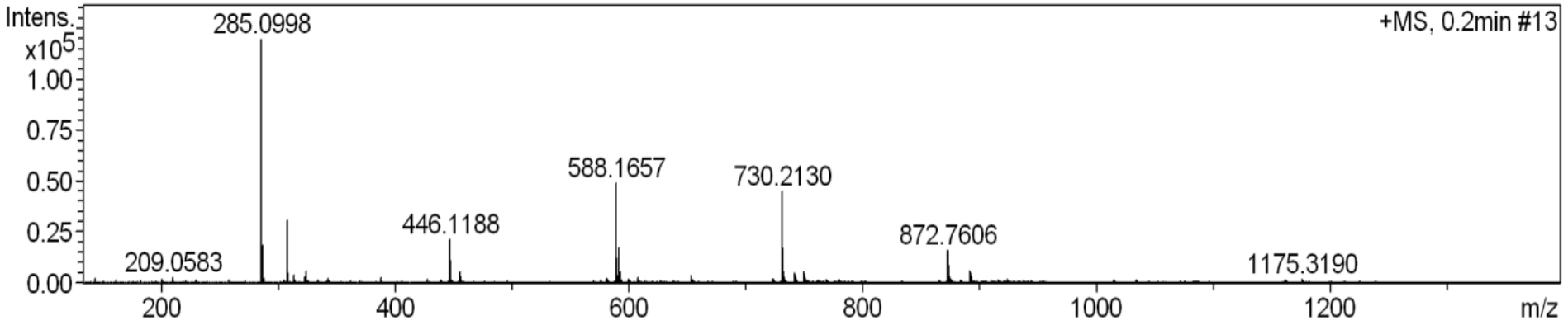
Elemental composition: $C_{20}H_{16}ClN_4O_3^+$
m/z Calculated: 395.0911
m/z Mensured: 395.0908
Error (ppm): 0.742

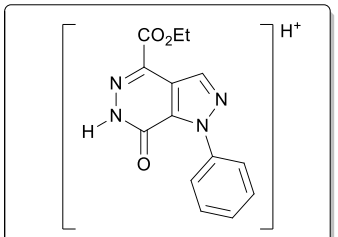




[6e + H]$^+$

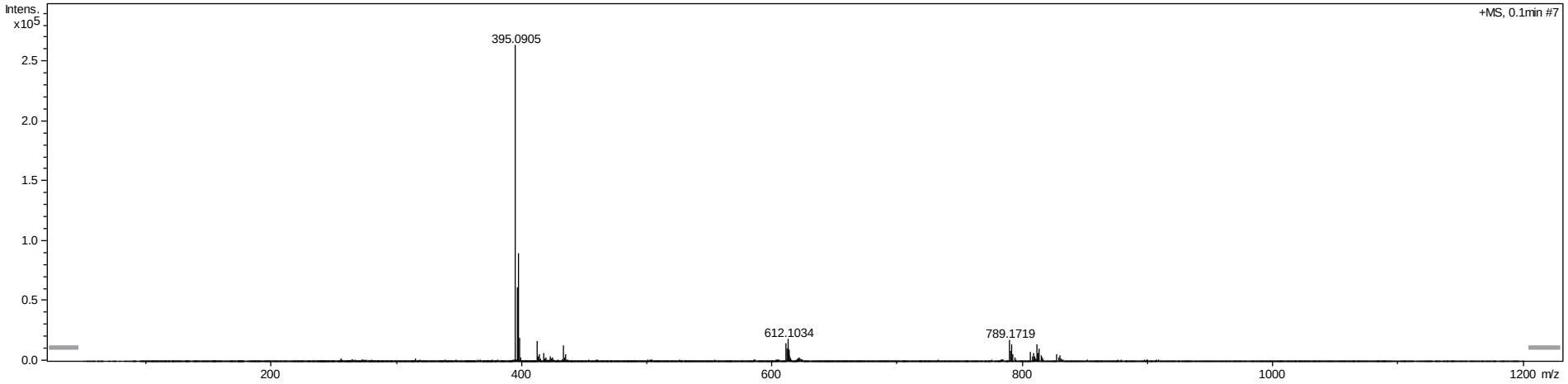
Elemental composition: $C_{14}H_{12}ClN_4O_3^+$
m/z Calculated: 319.0598
m/z Mensured: 319.0587
Error (ppm): 3.426

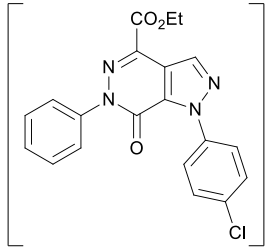




[6f + H]$^+$

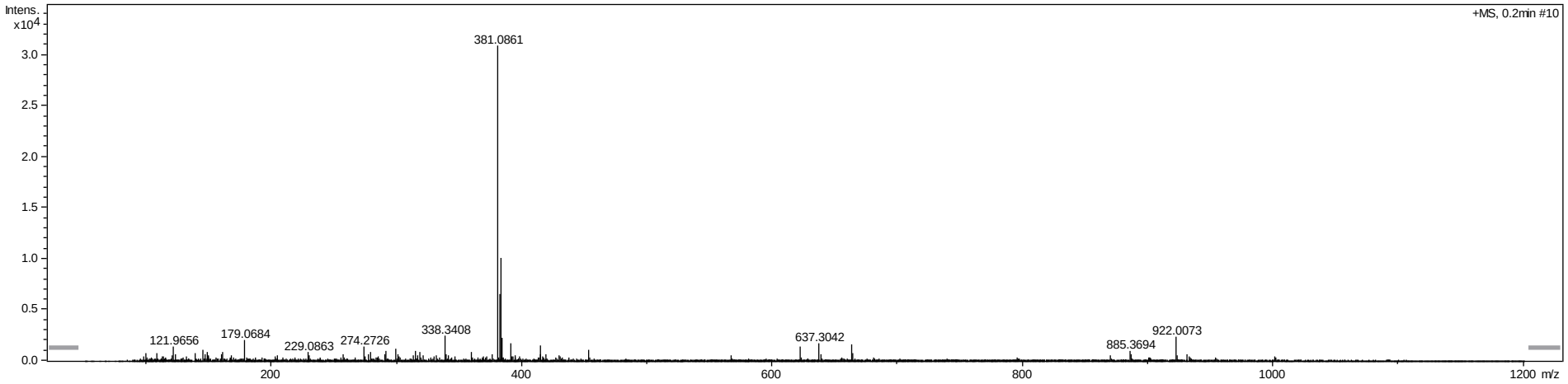
Elemental composition: $C_{14}H_{13}N_4O_3^+$
m/z Calculated: 285.0988
m/z Mensured: 285.0998
Error (ppm): 3.629

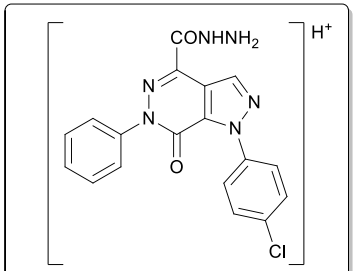




[6g + H]

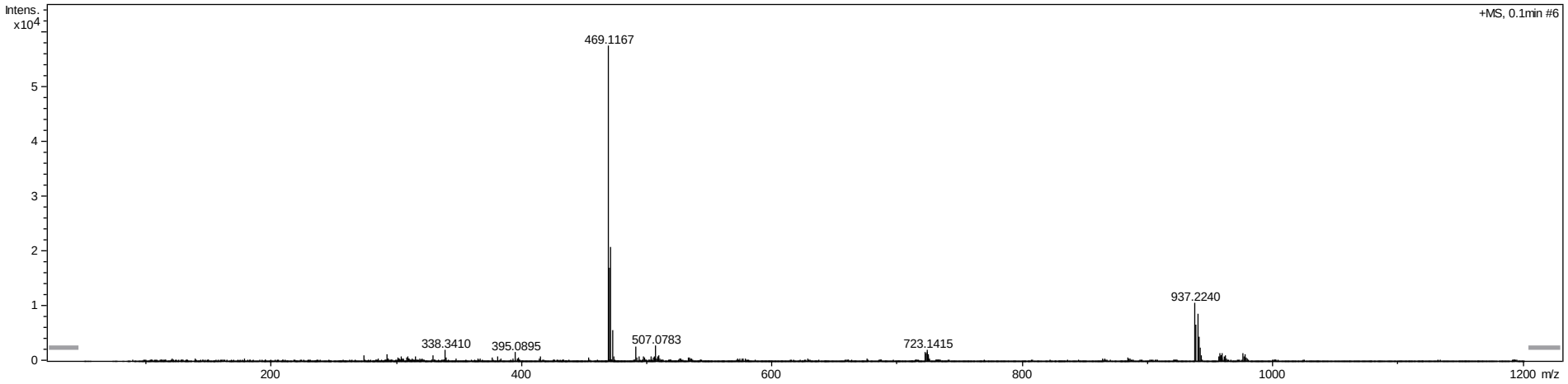
Elemental composition: $C_{20}H_{16}ClN_4O_3^+$
m/z Calculated: 395.0911
m/z Mensured: 395.0905
Error (ppm): 1.501

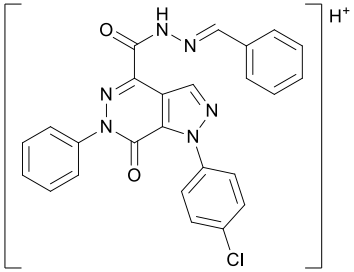




[7 + H]

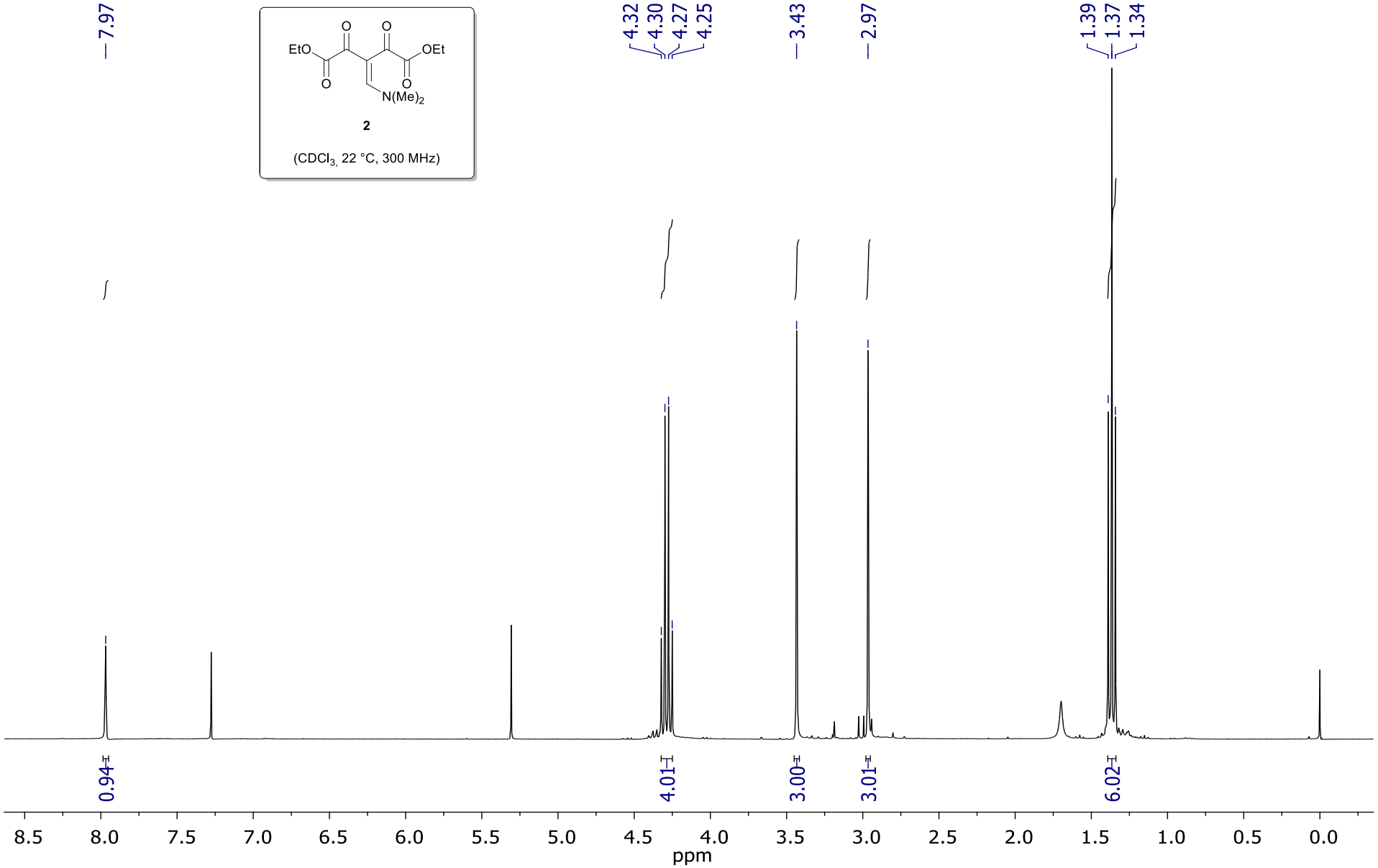
Elemental composition: $C_{18}H_{14}ClN_6O_2^+$
m/z Calculated: 381.0867
m/z Mensured: 381.0861
Error (ppm): 1.513

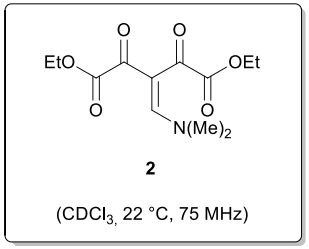




[8 + H]$^+$

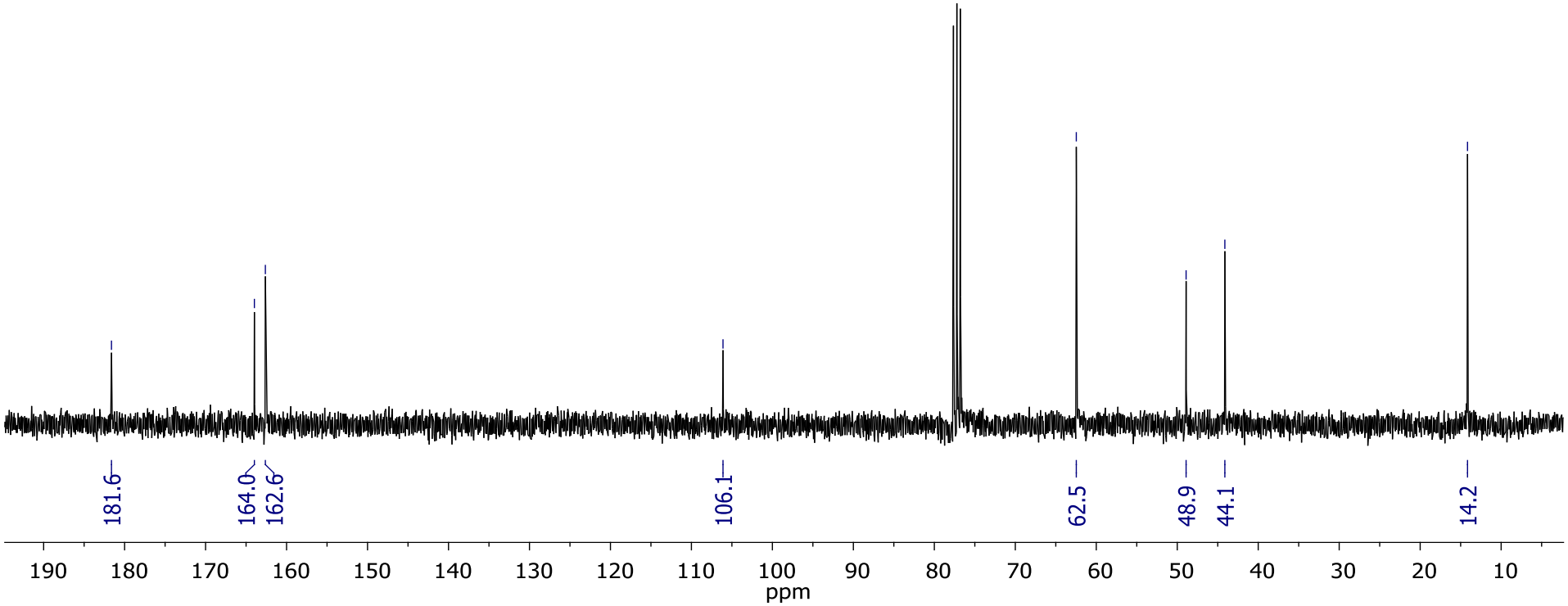
Elemental composition: $C_{25}H_{18}ClN_6O_2^+$
m/z Calculated: 469.1180
m/z Mensured: 469.1167
Error (ppm): 2.721

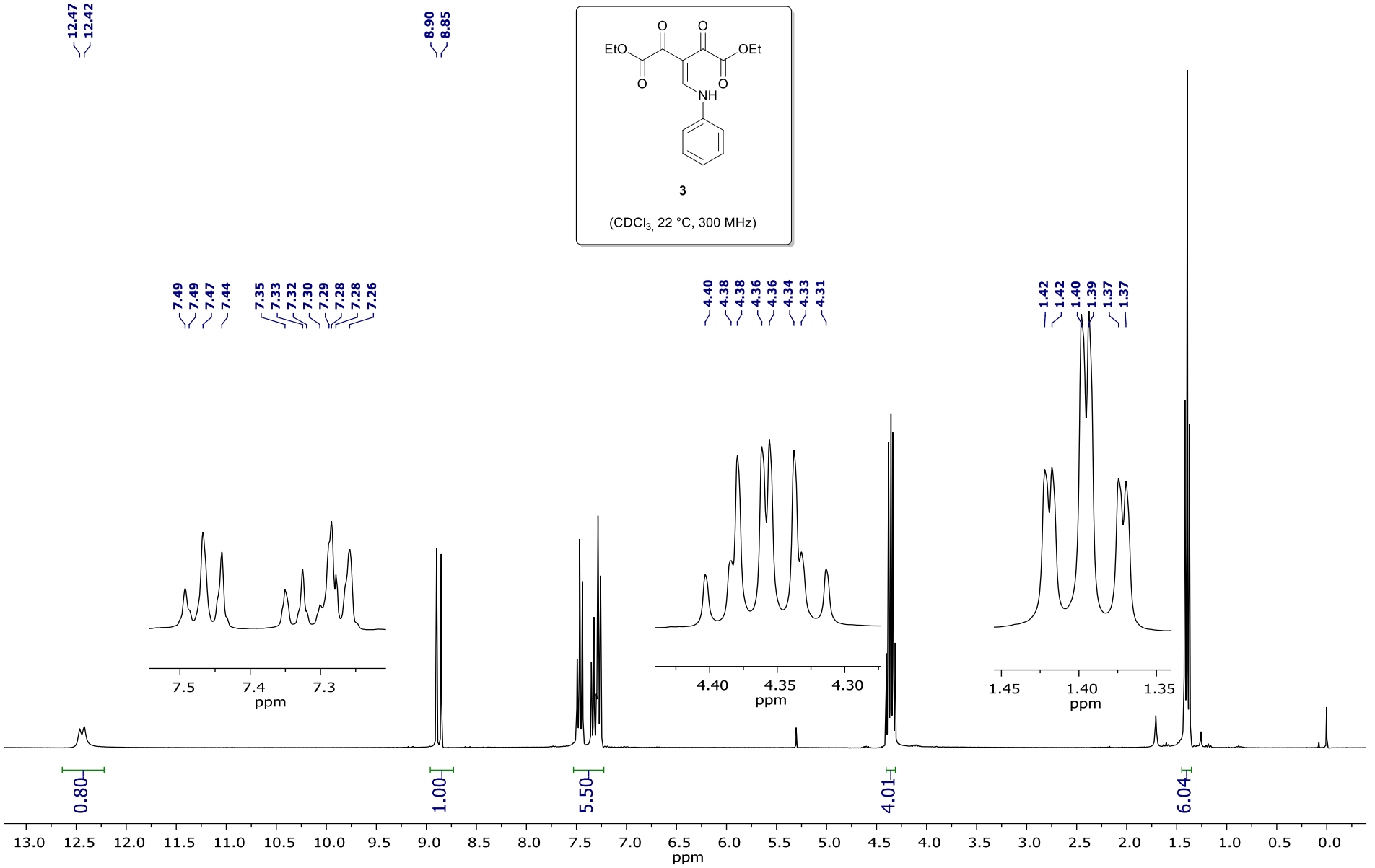


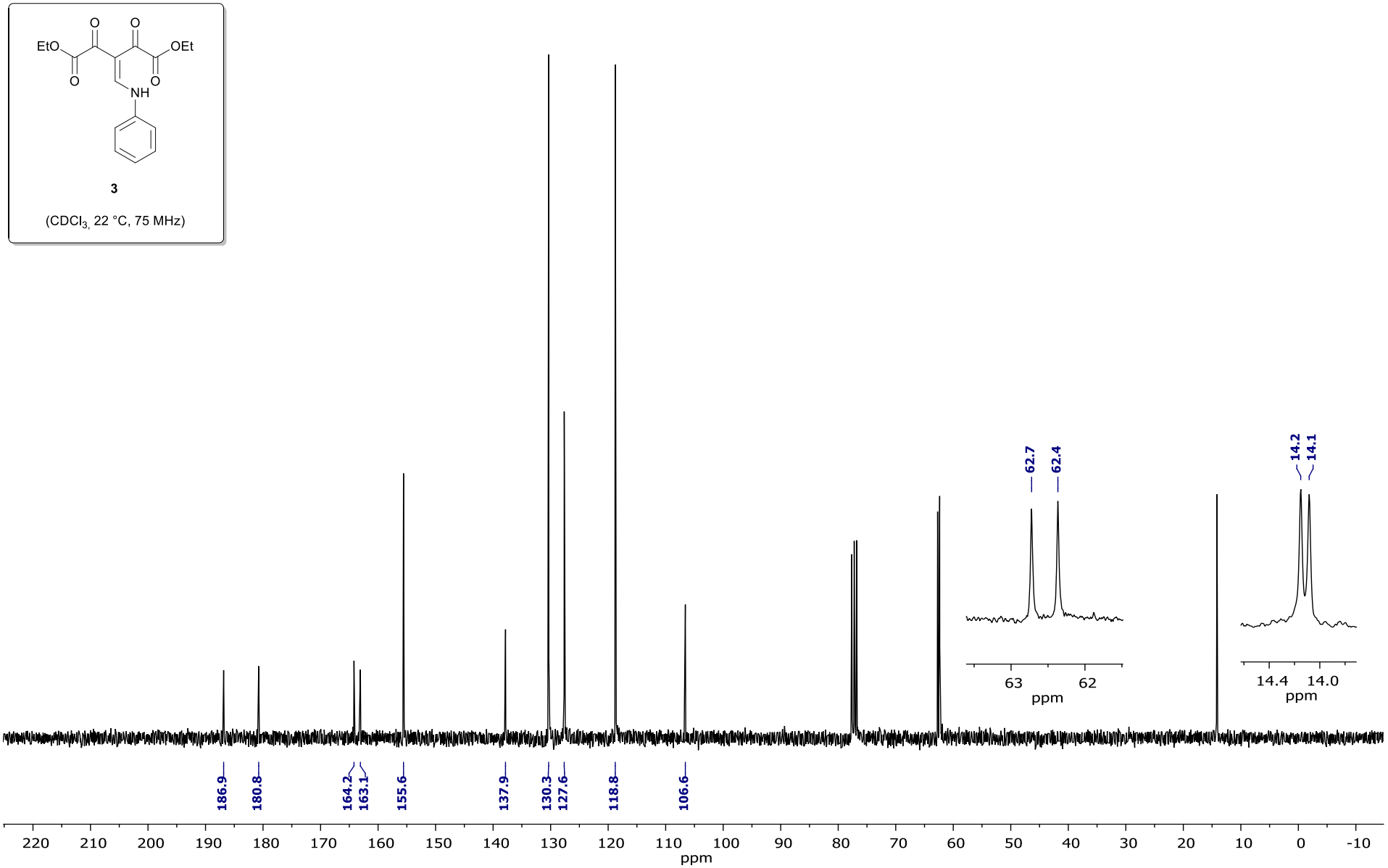


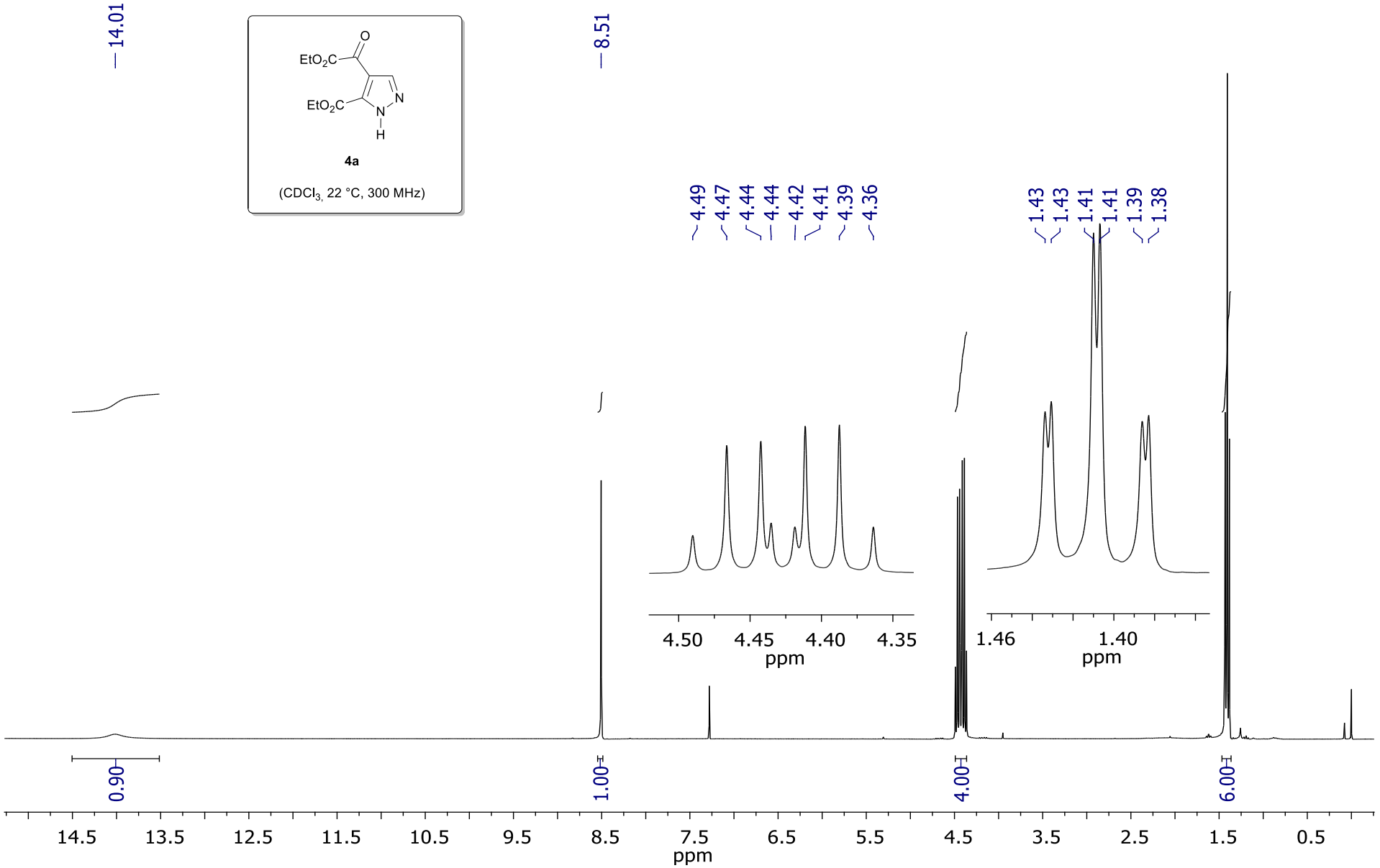
2

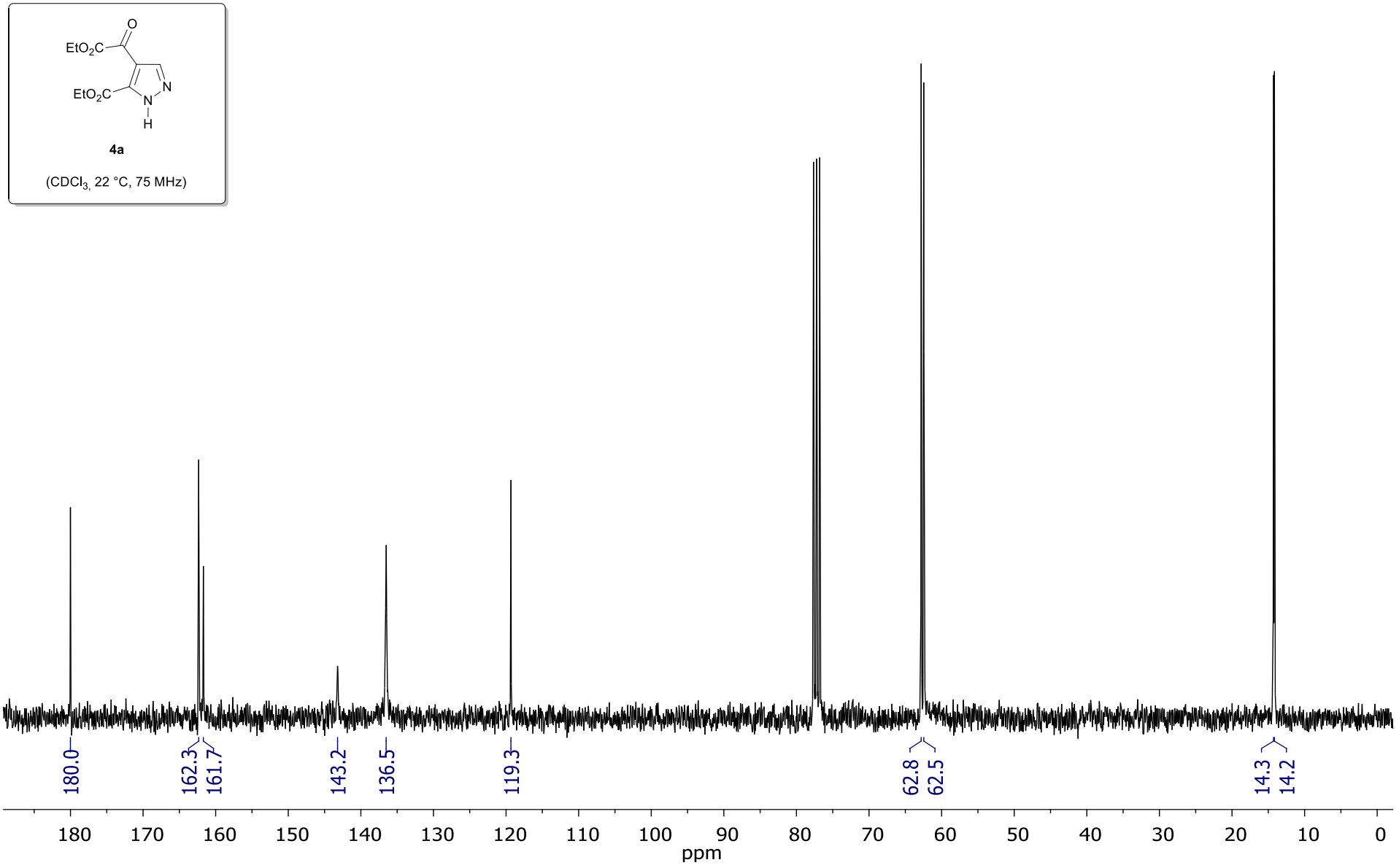
($CDCl_3$, 22 °C, 75 MHz)

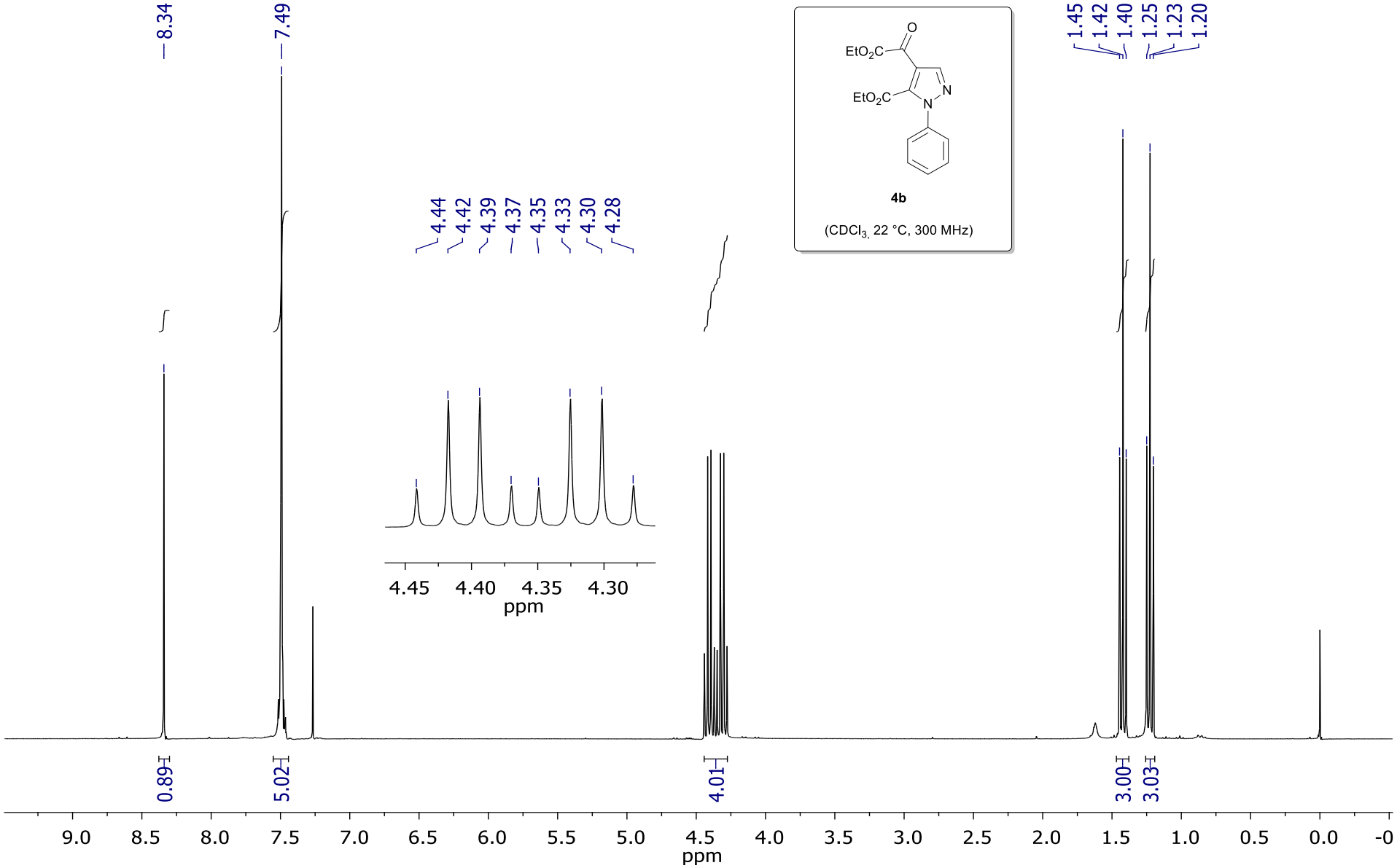


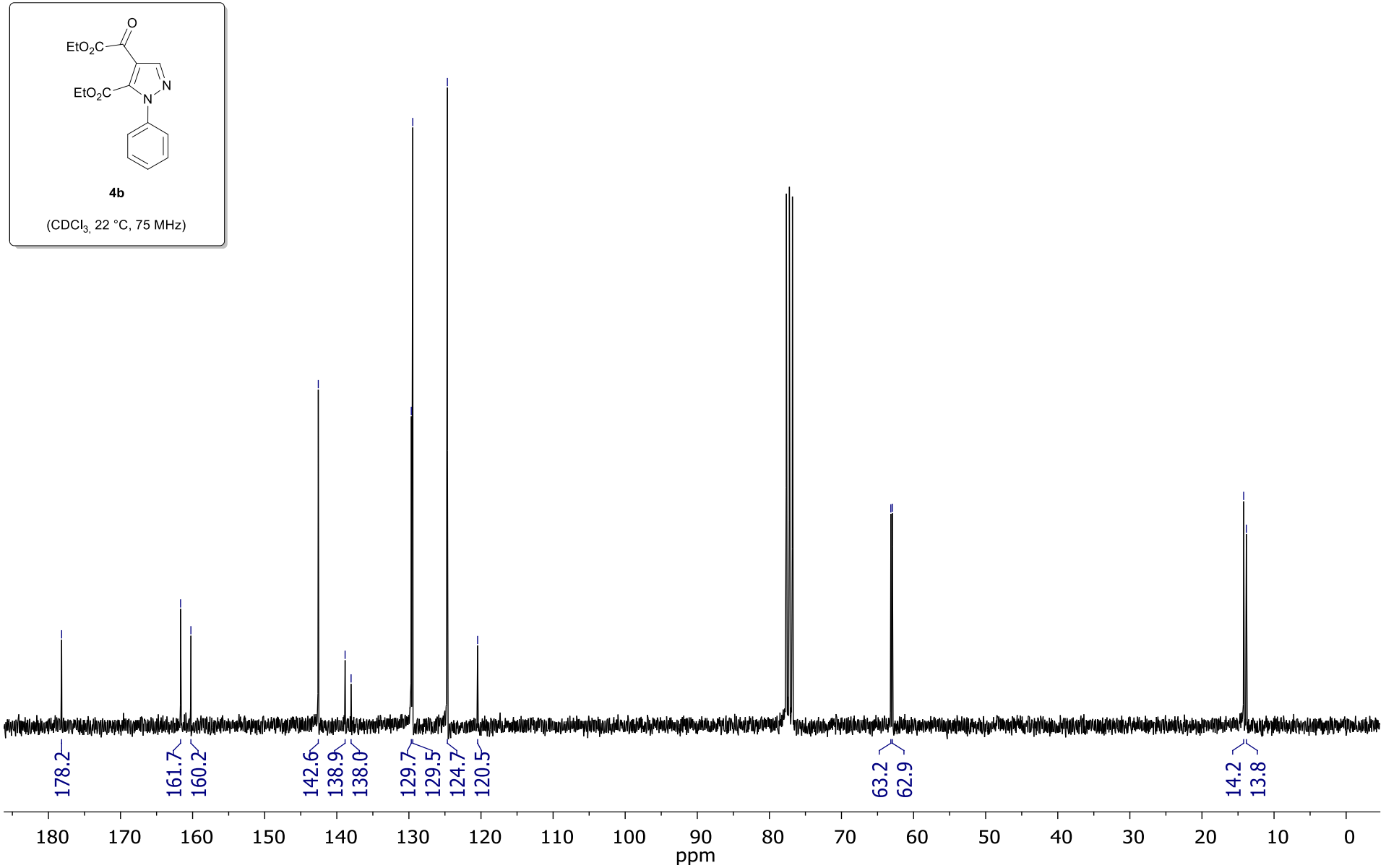


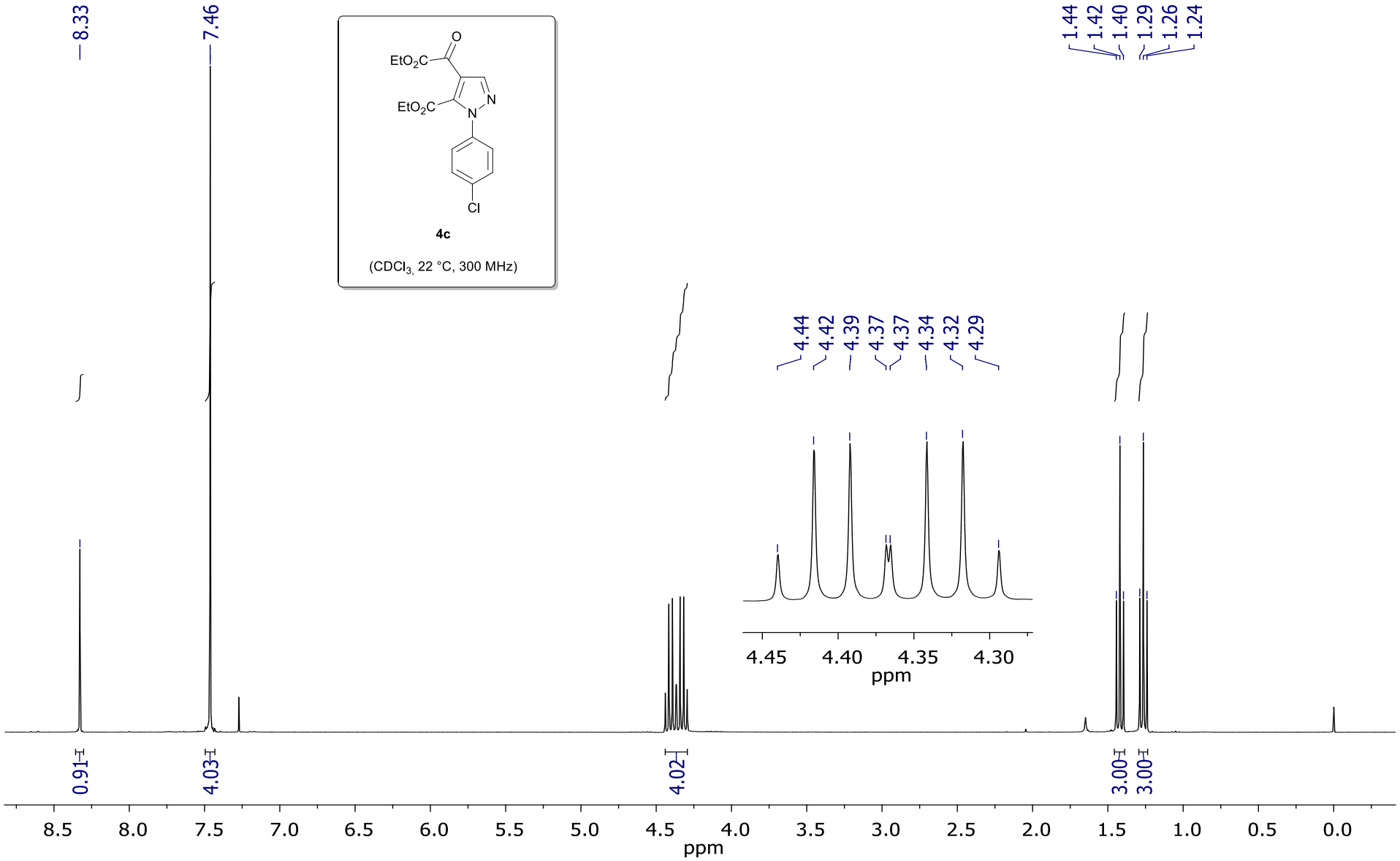


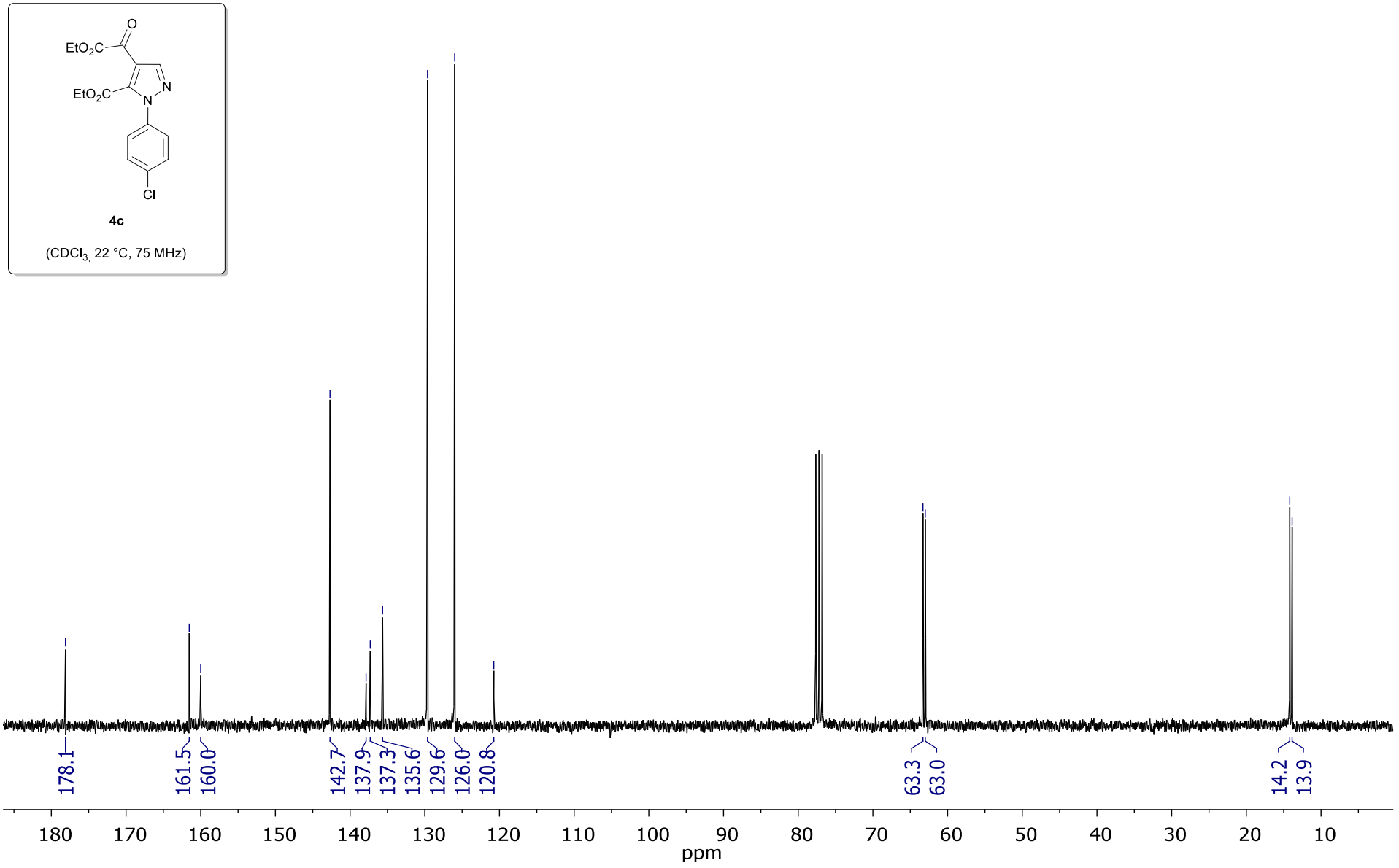


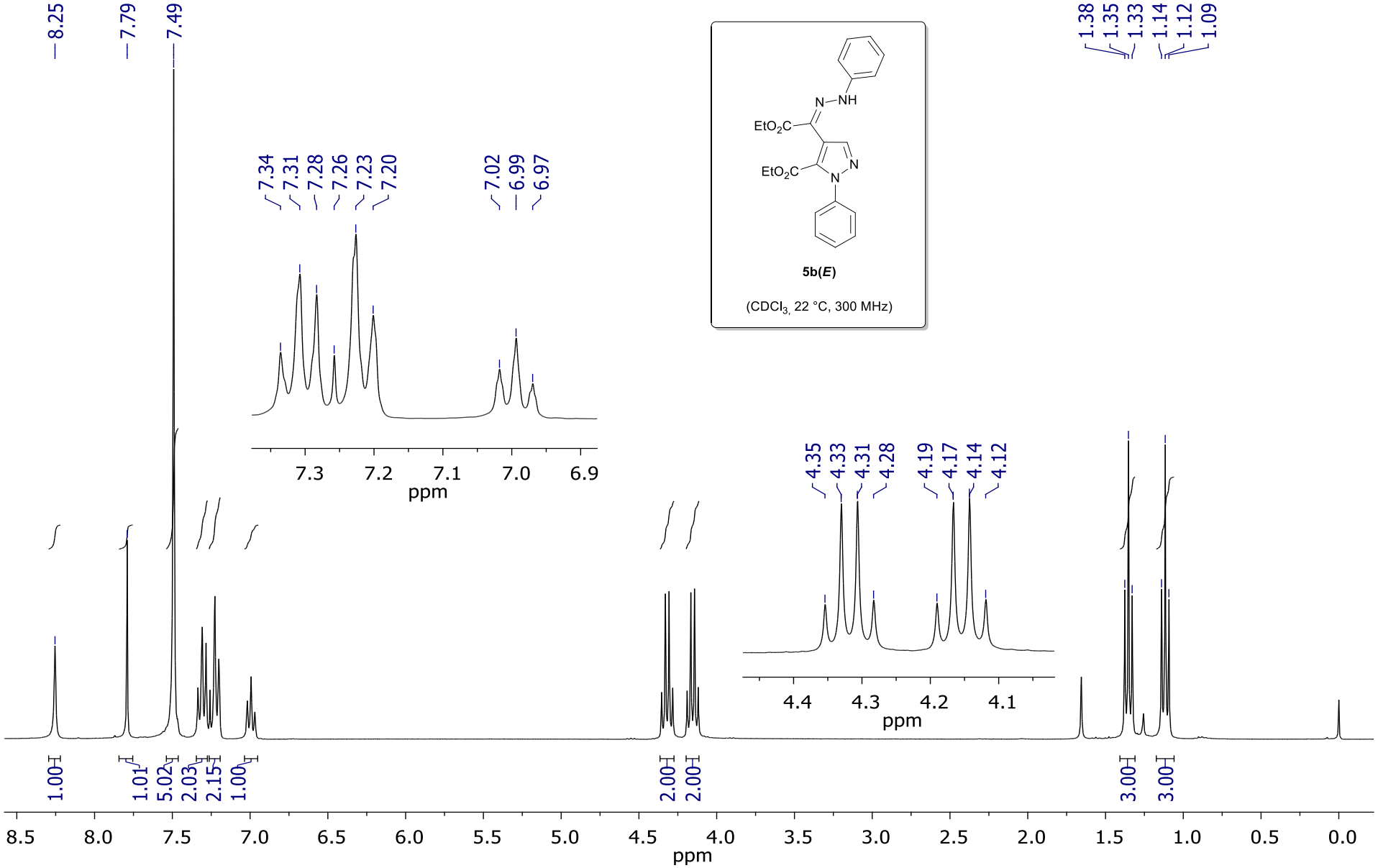


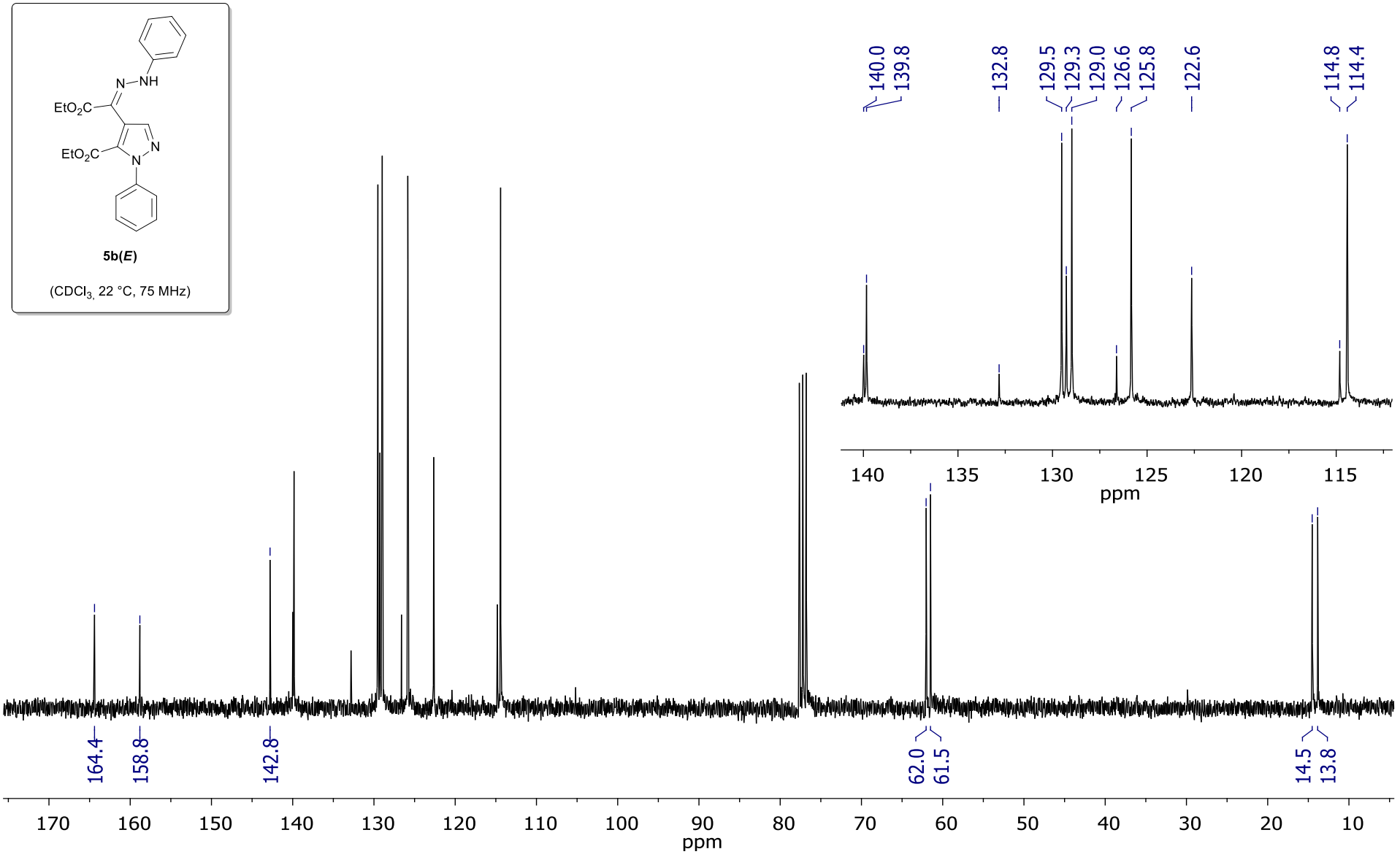


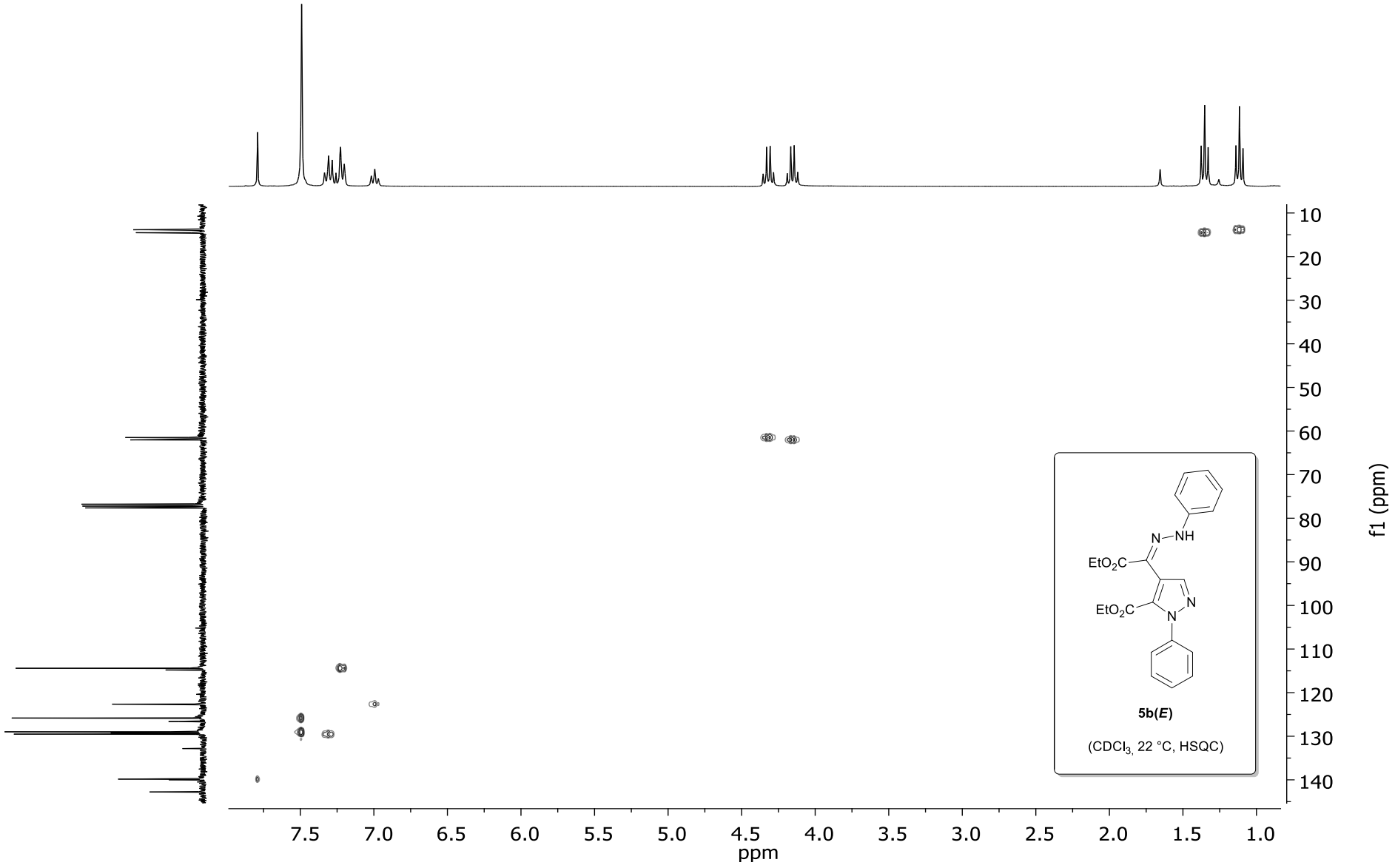


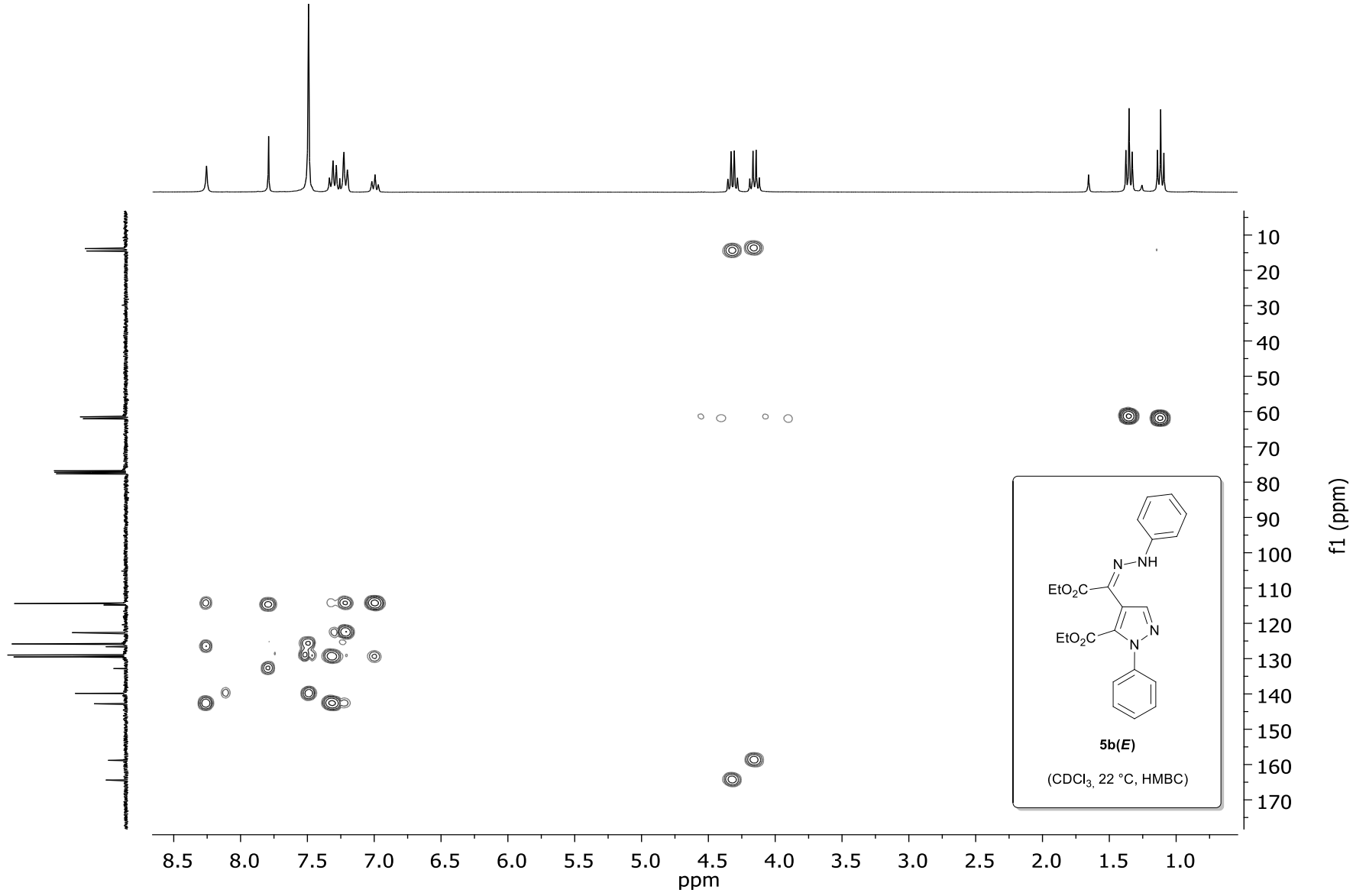


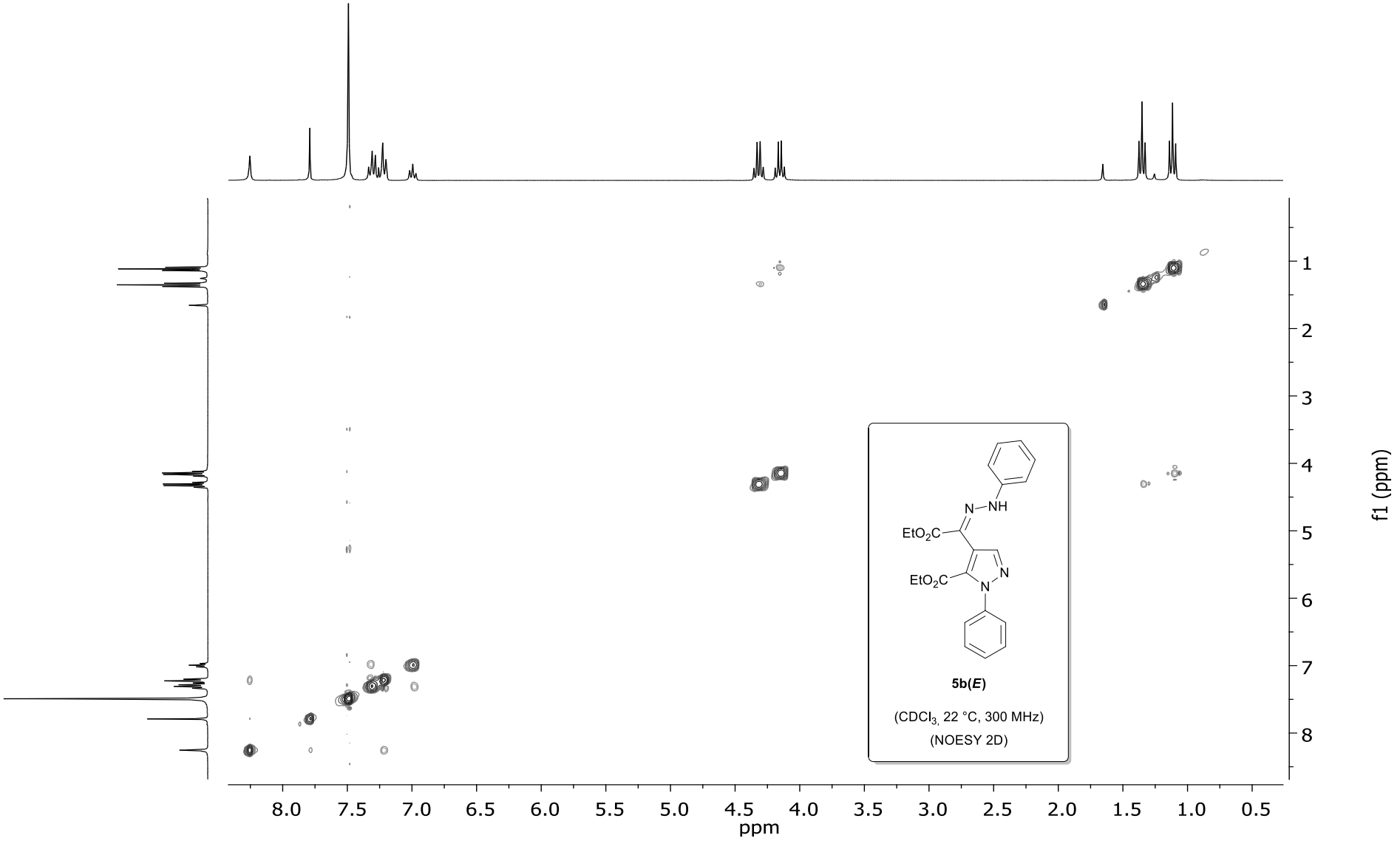


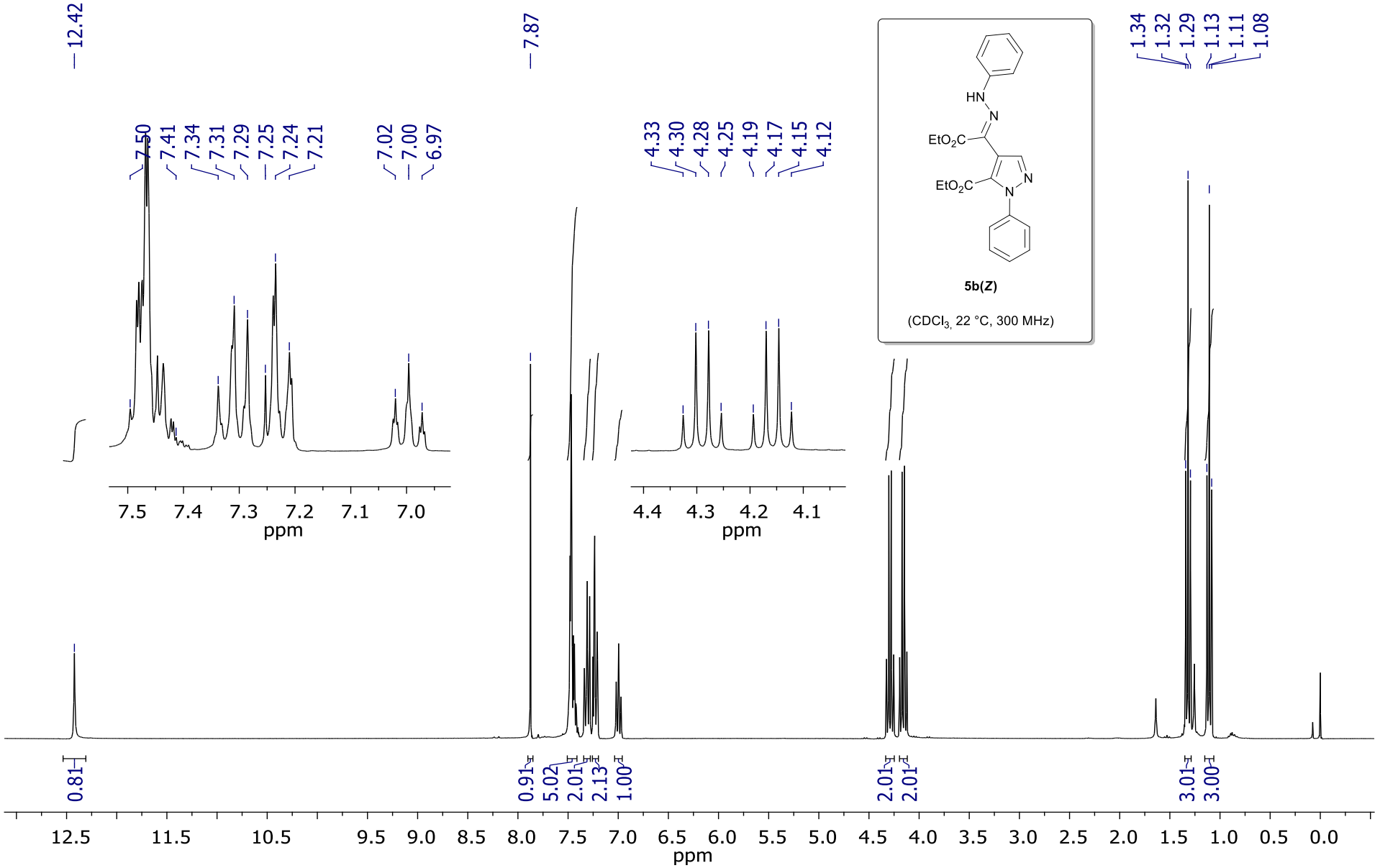


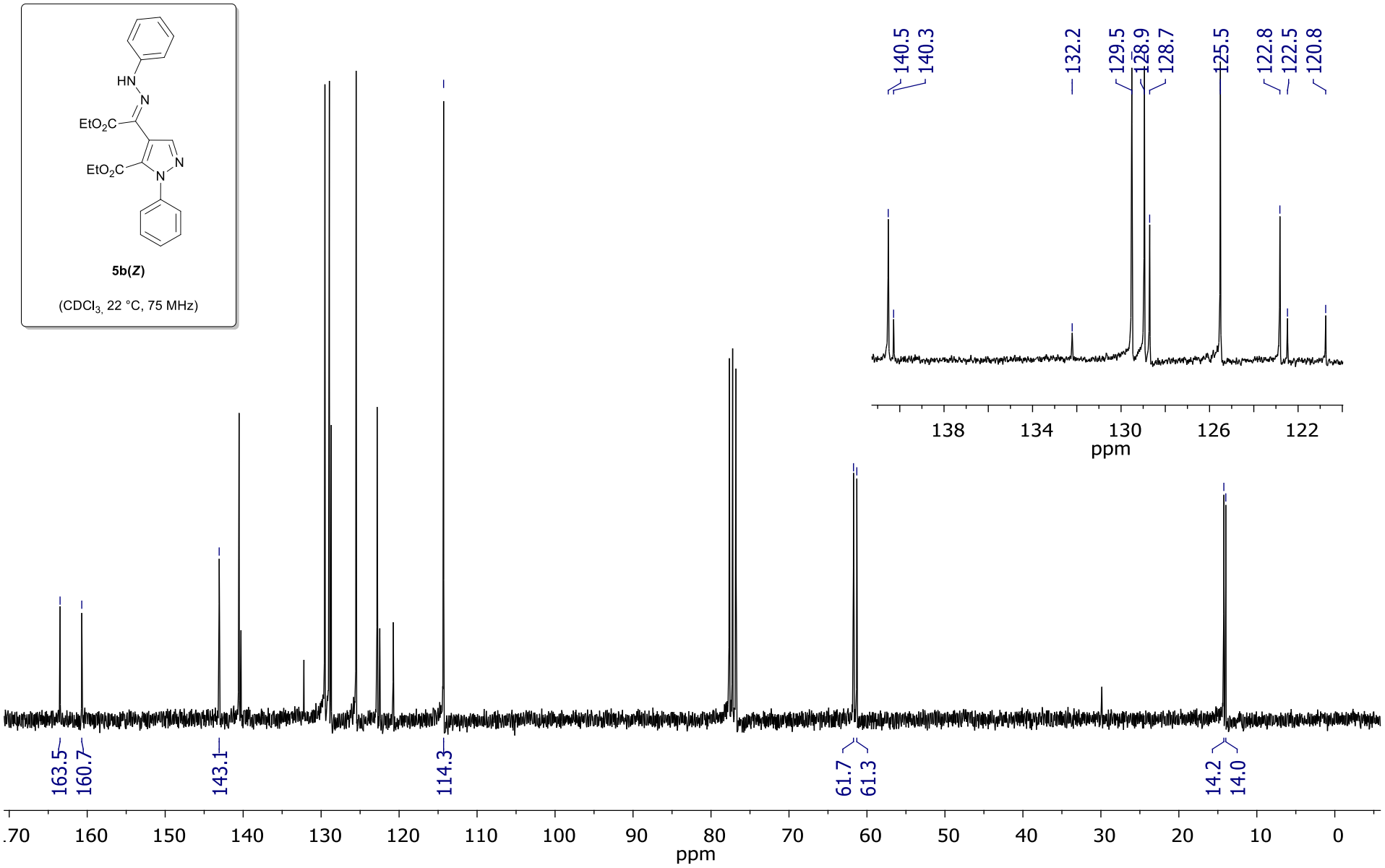


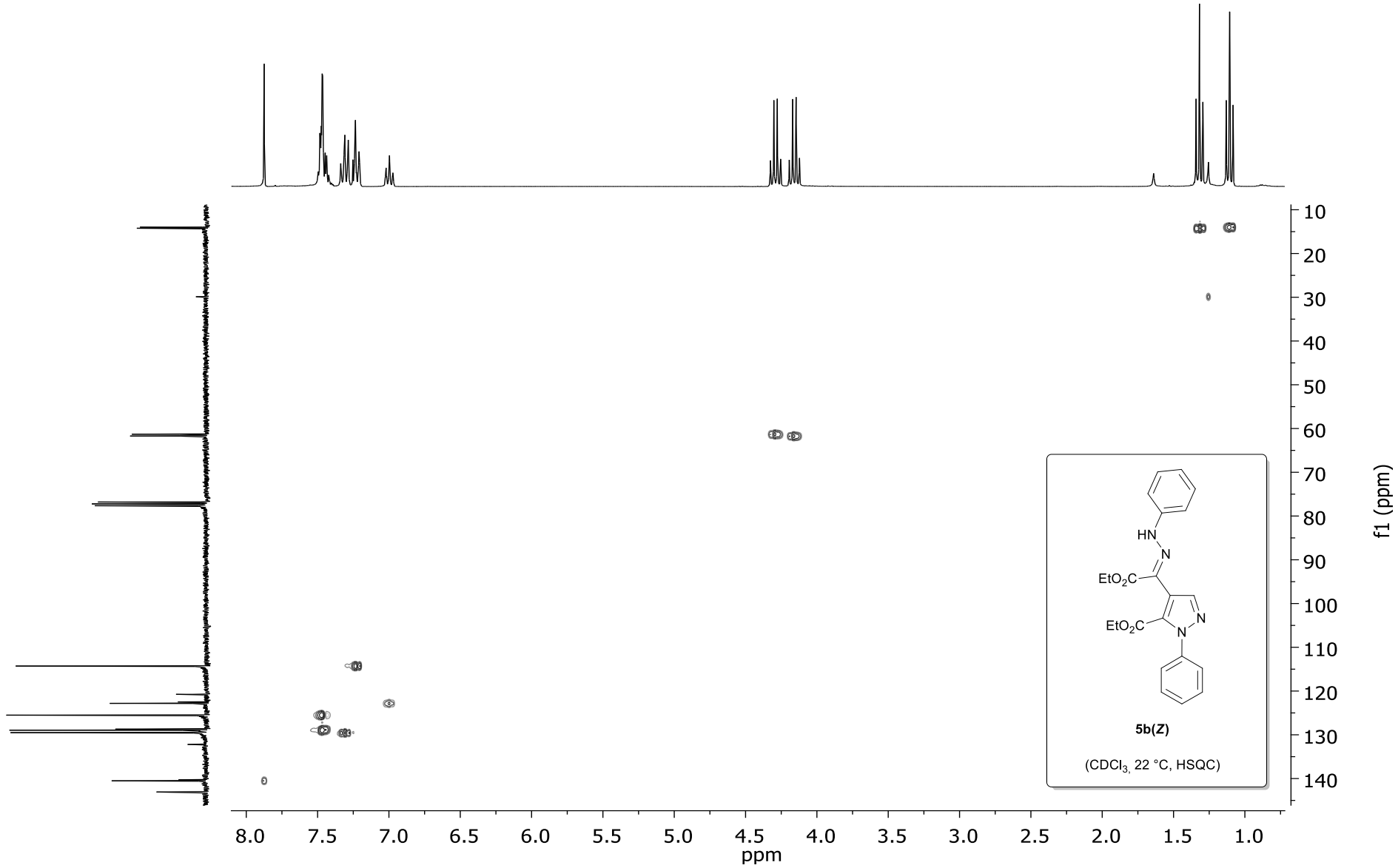


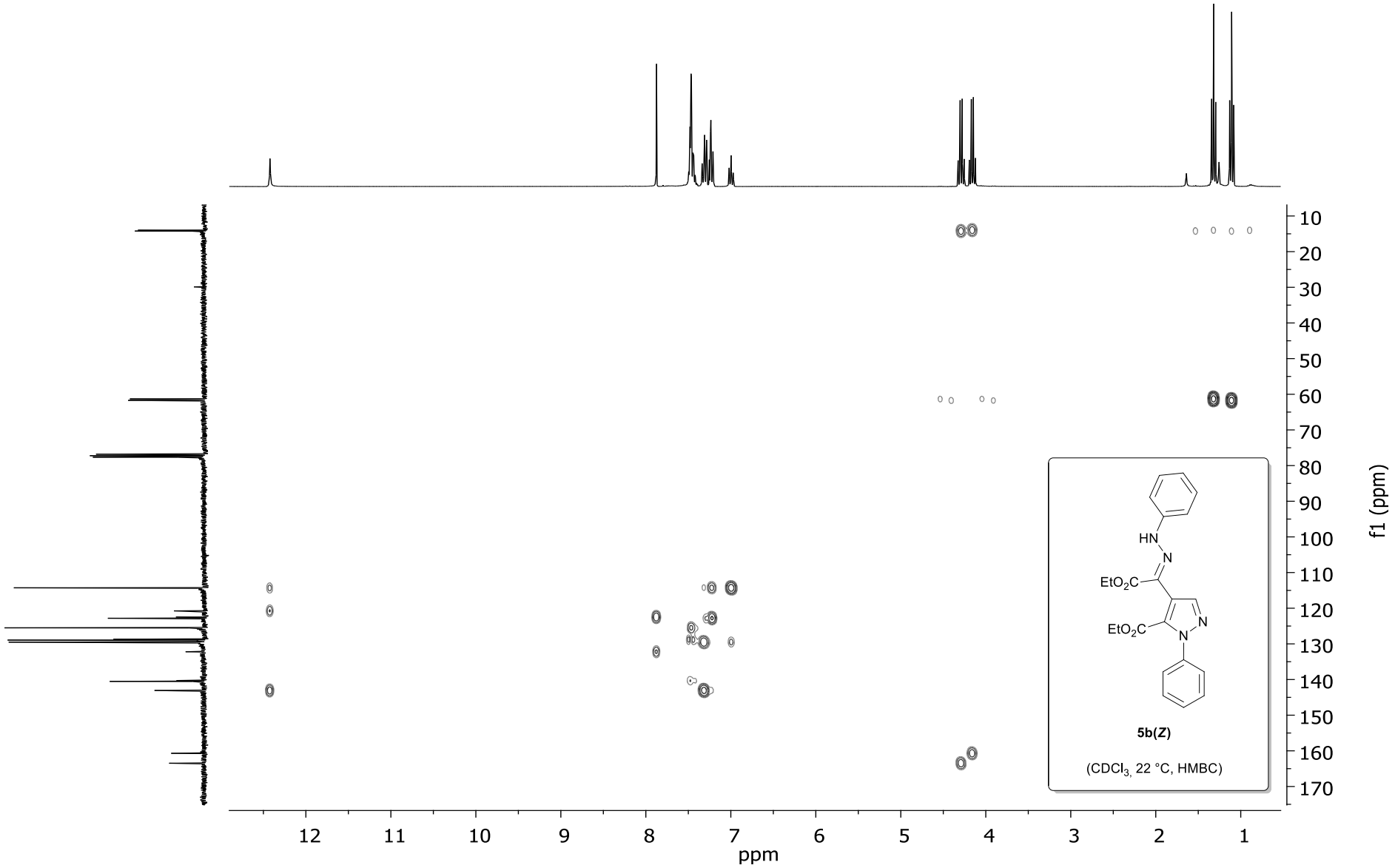


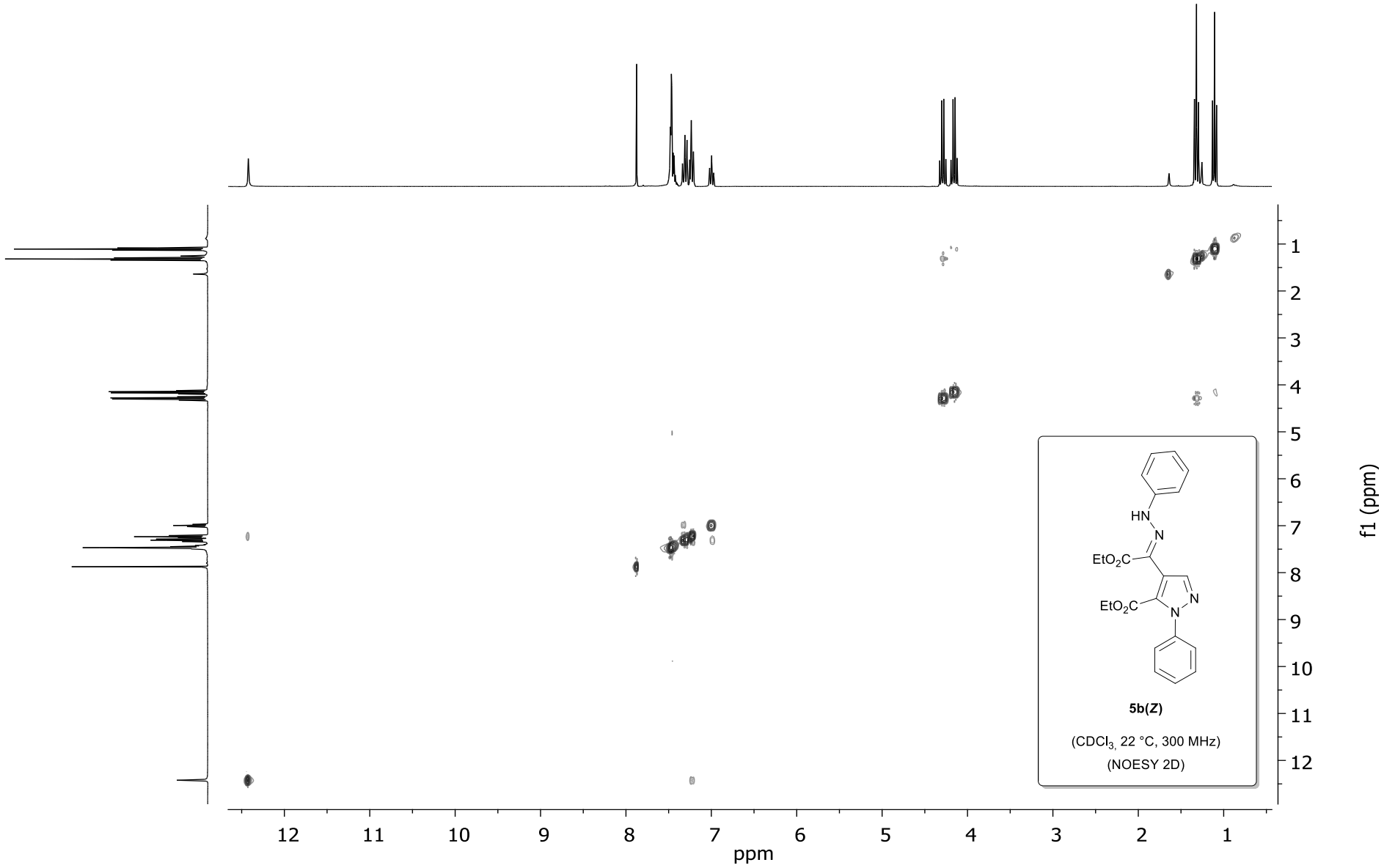


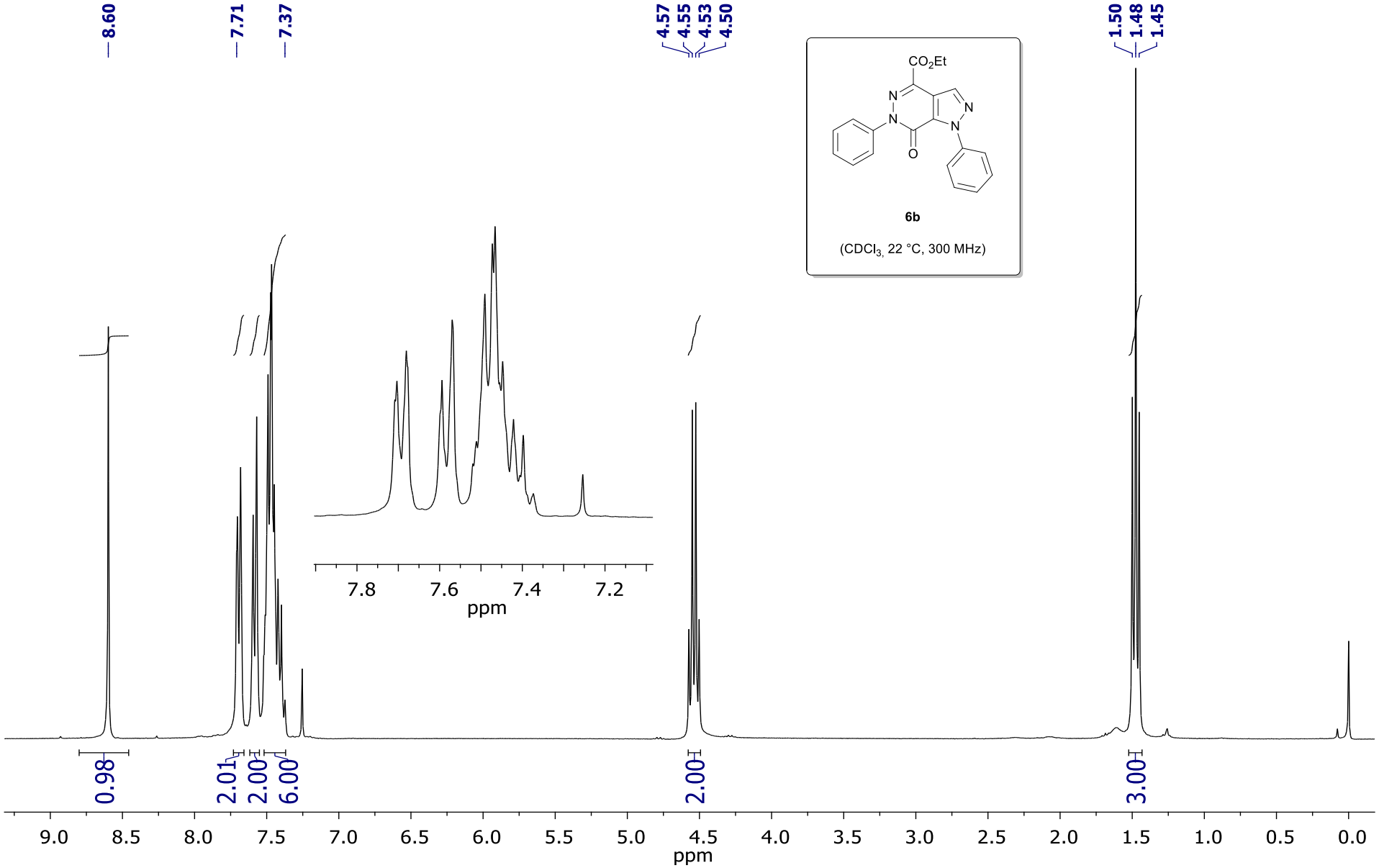


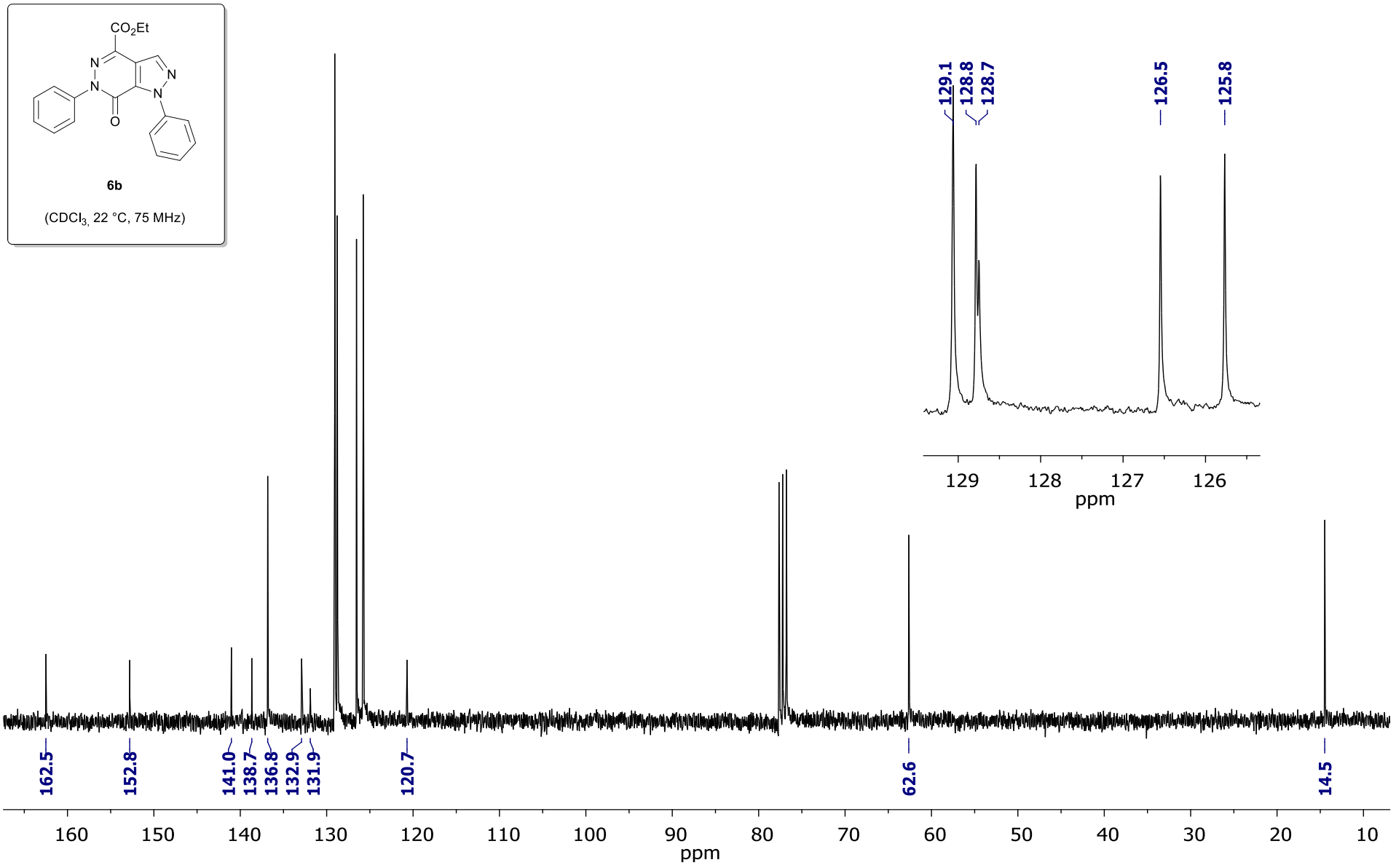


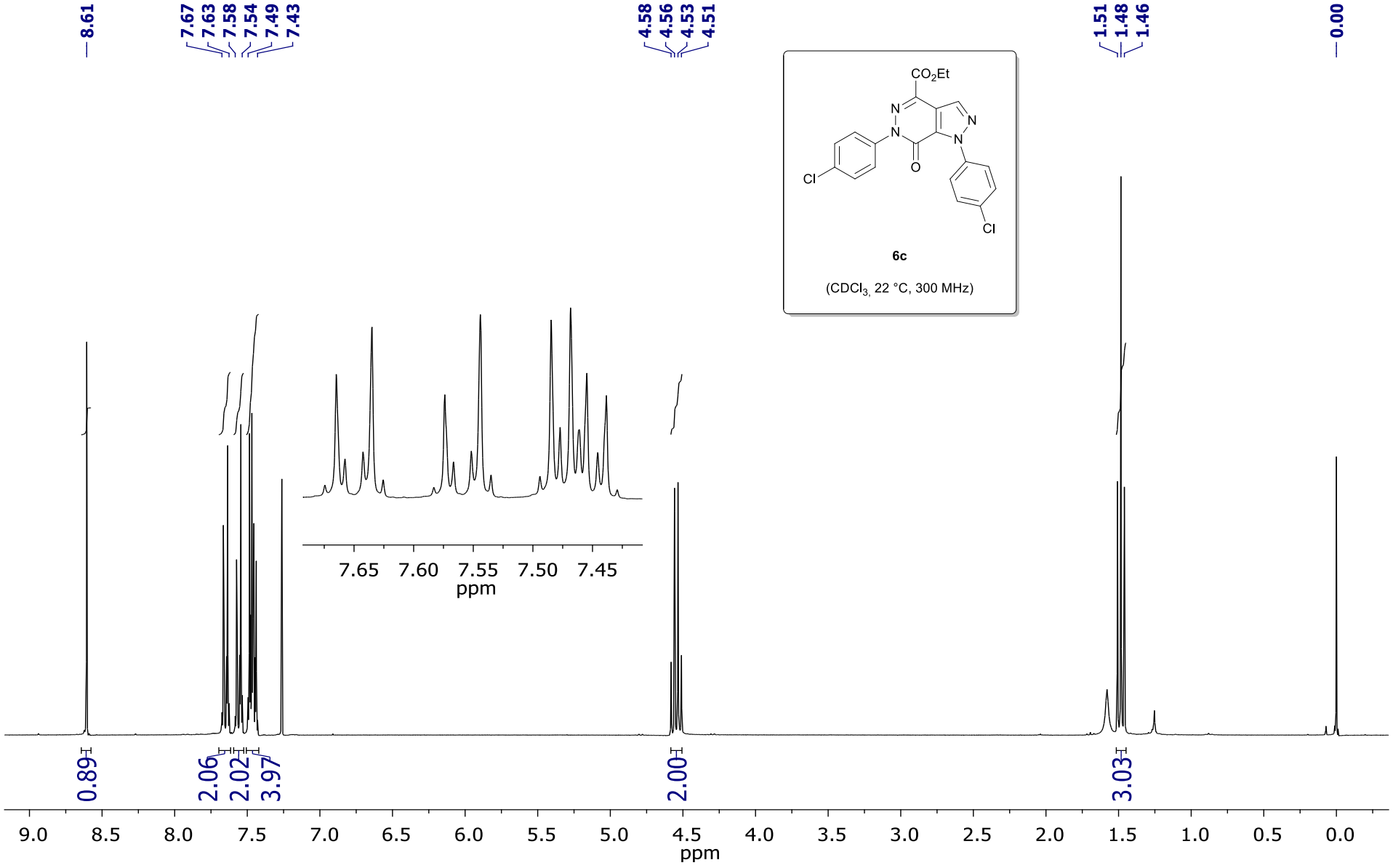


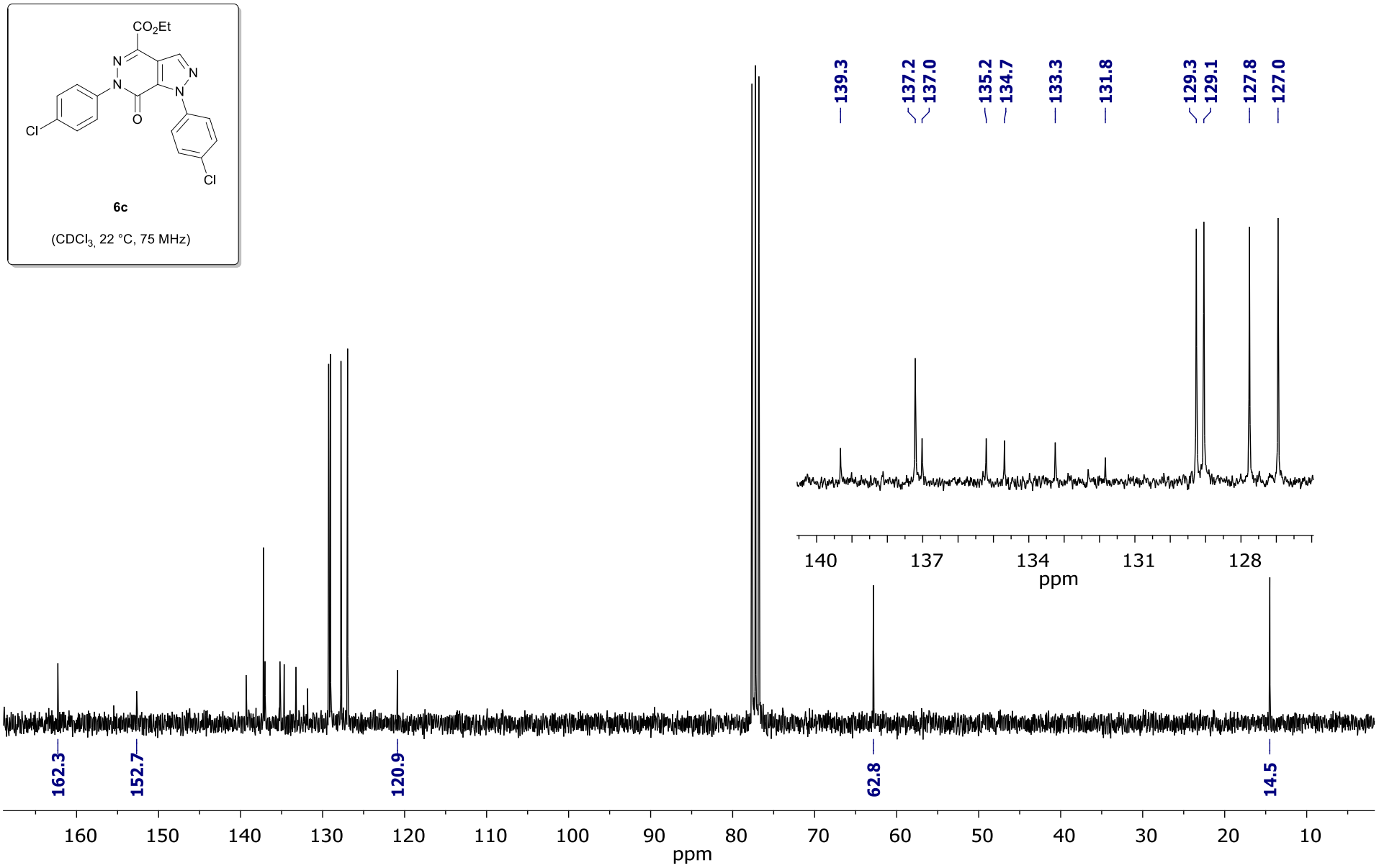


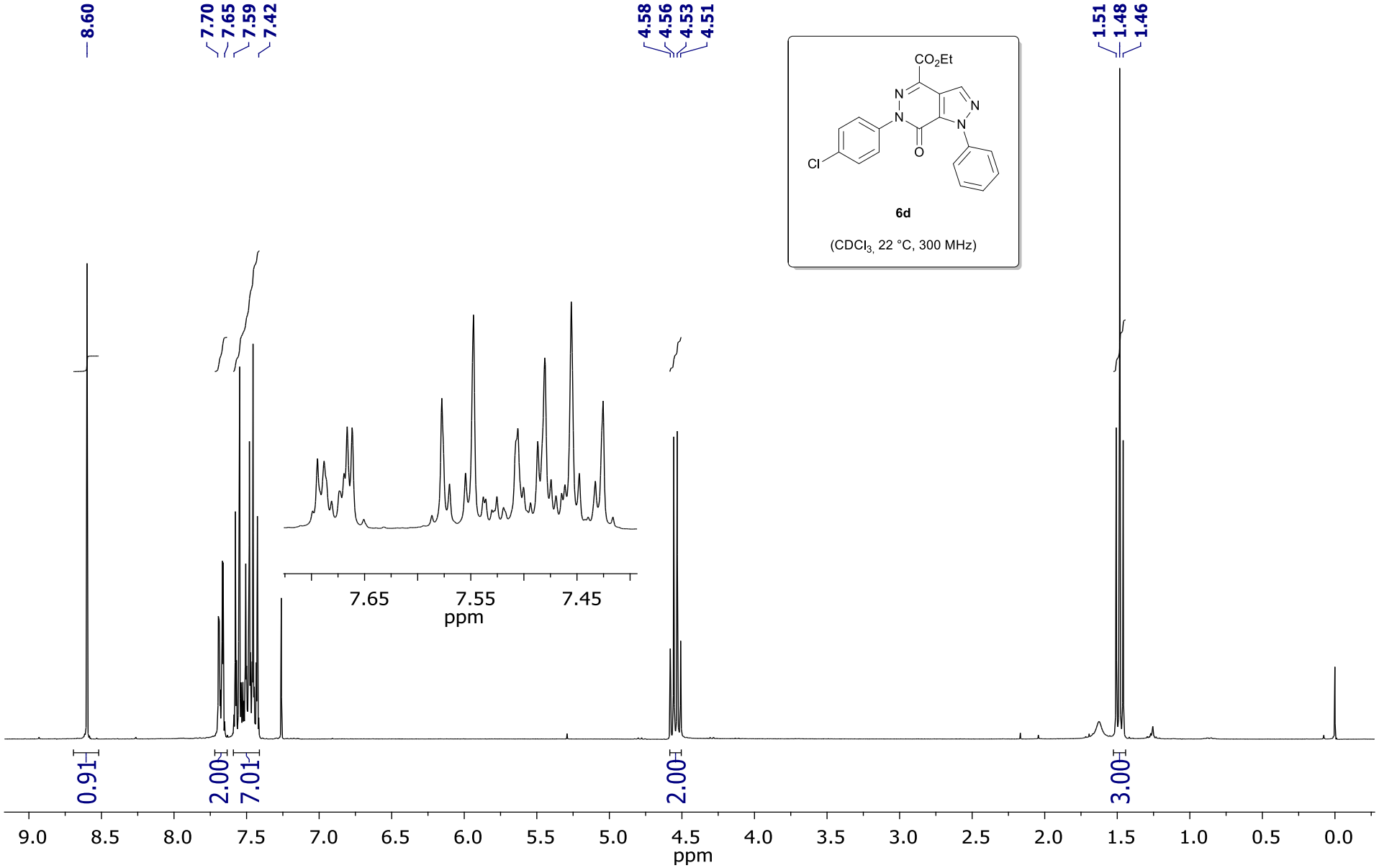


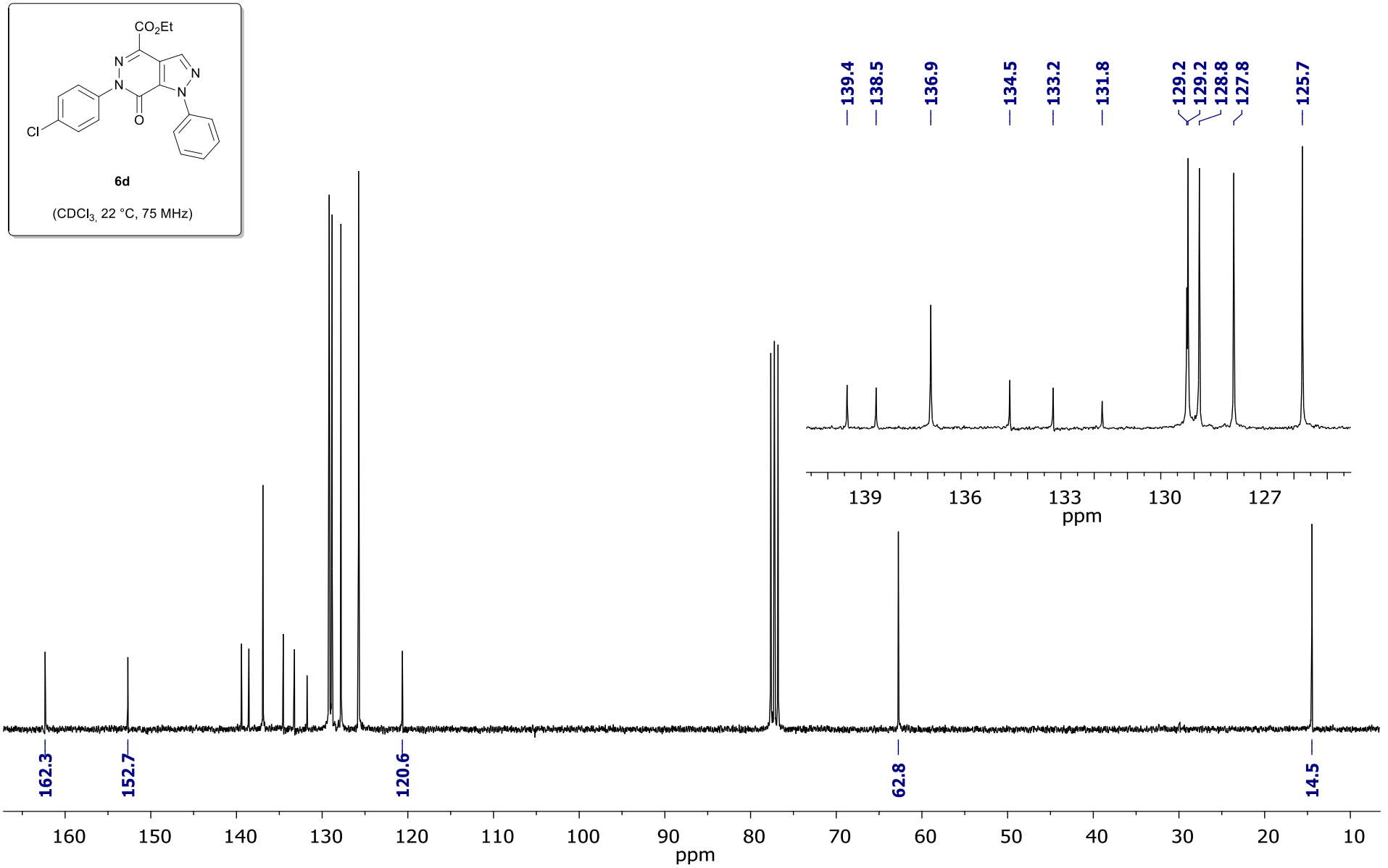


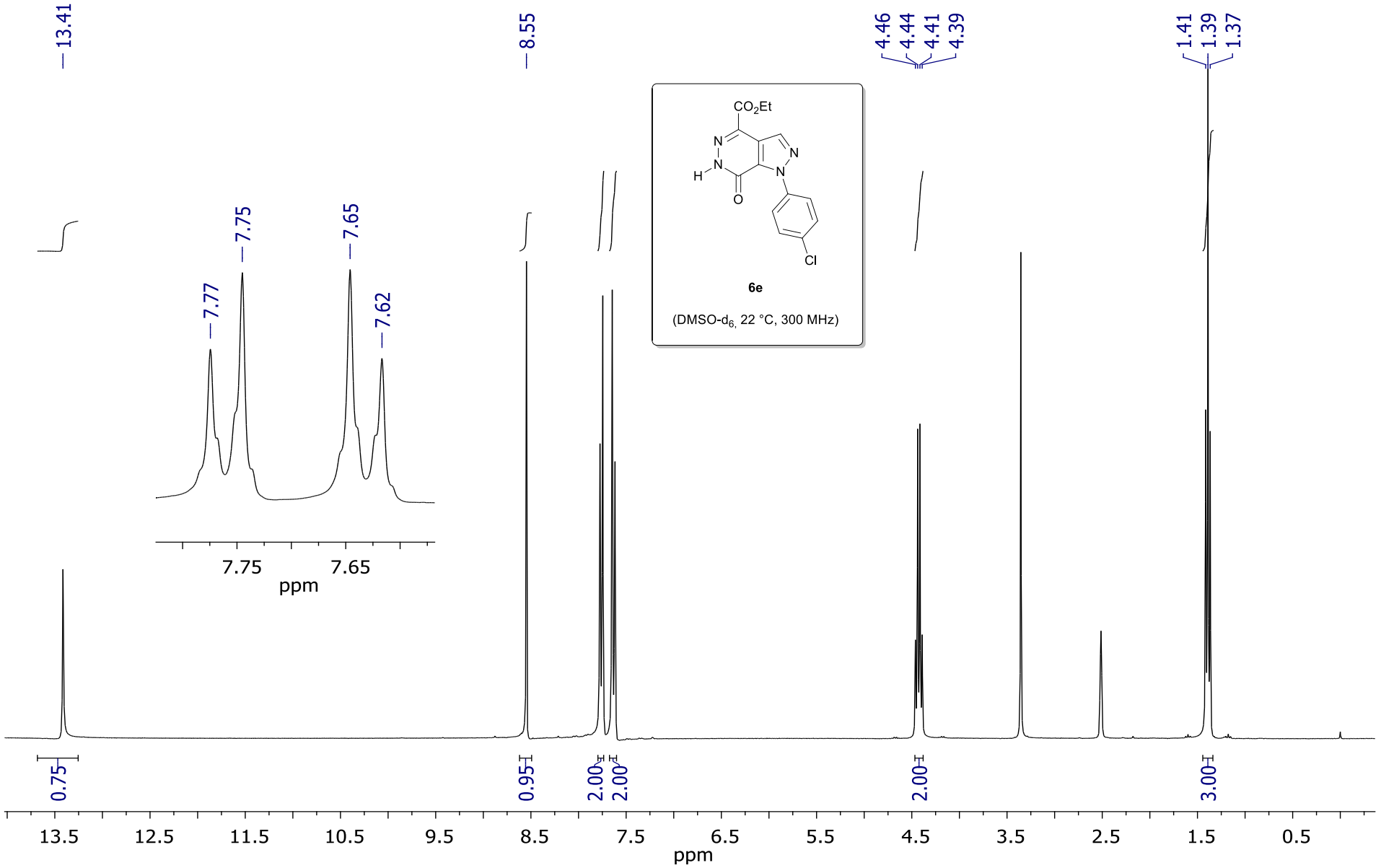


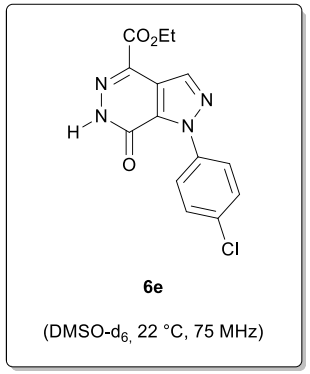






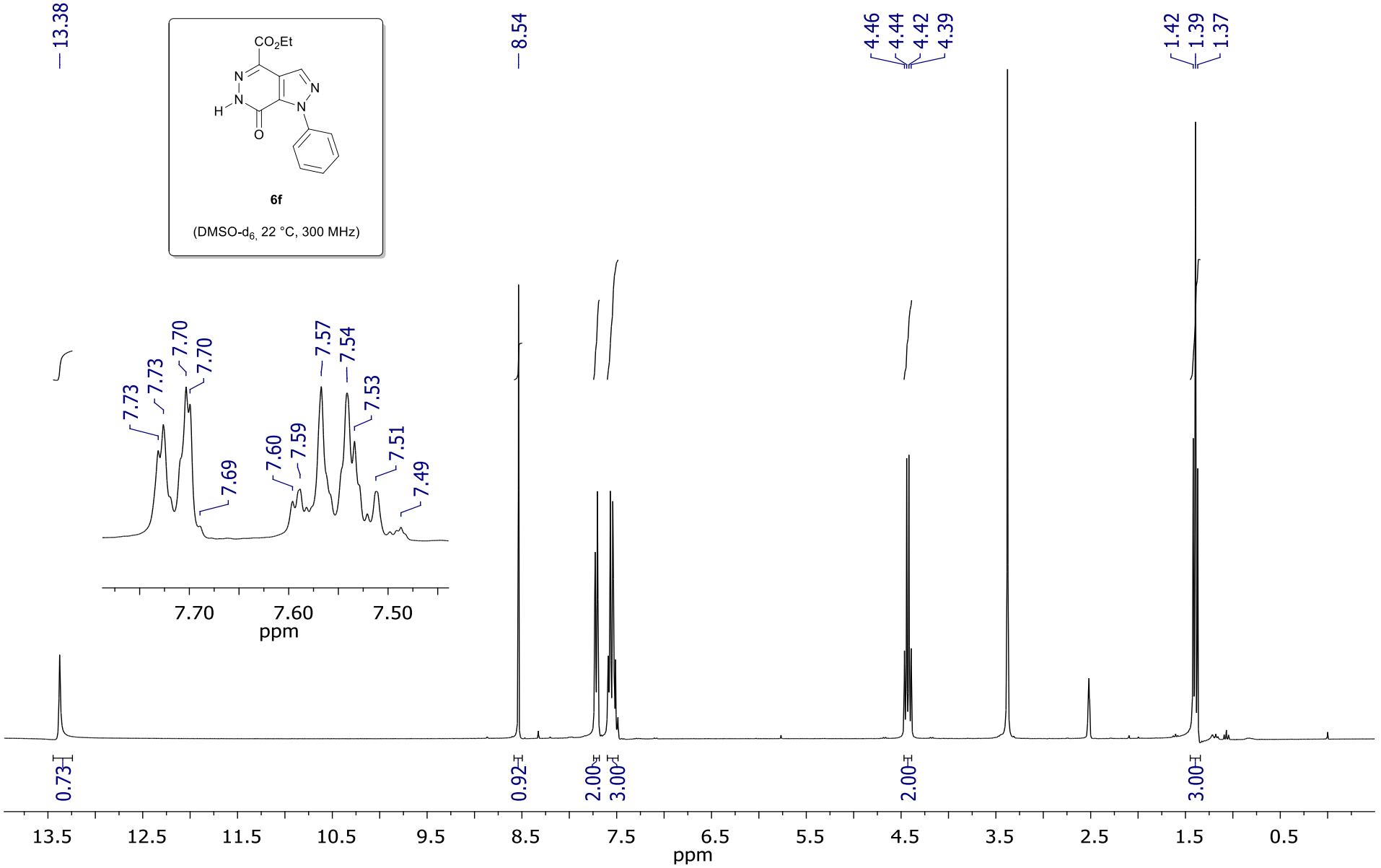






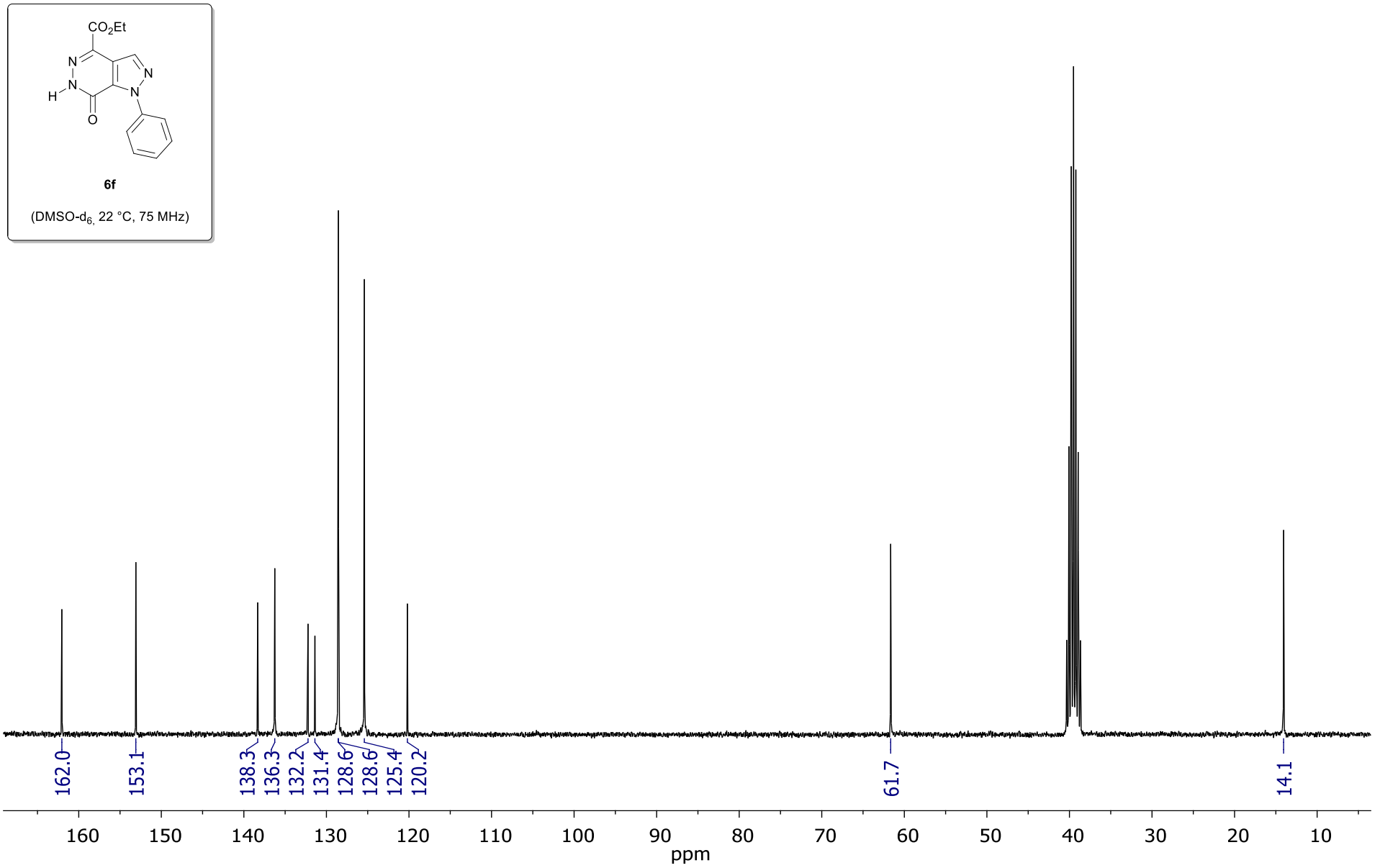
6e

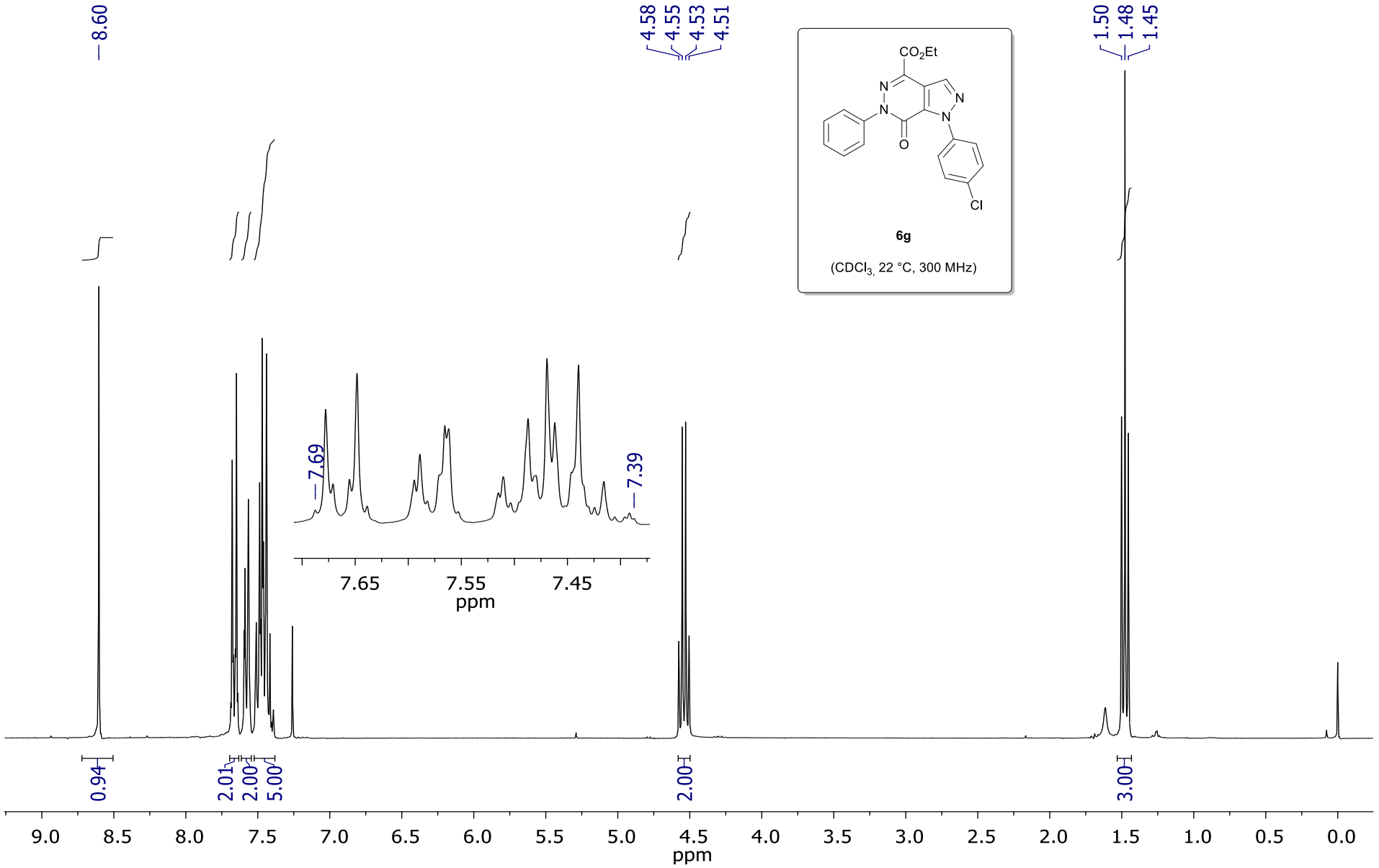
(DMSO-d_6, 22 °C, 75 MHz)

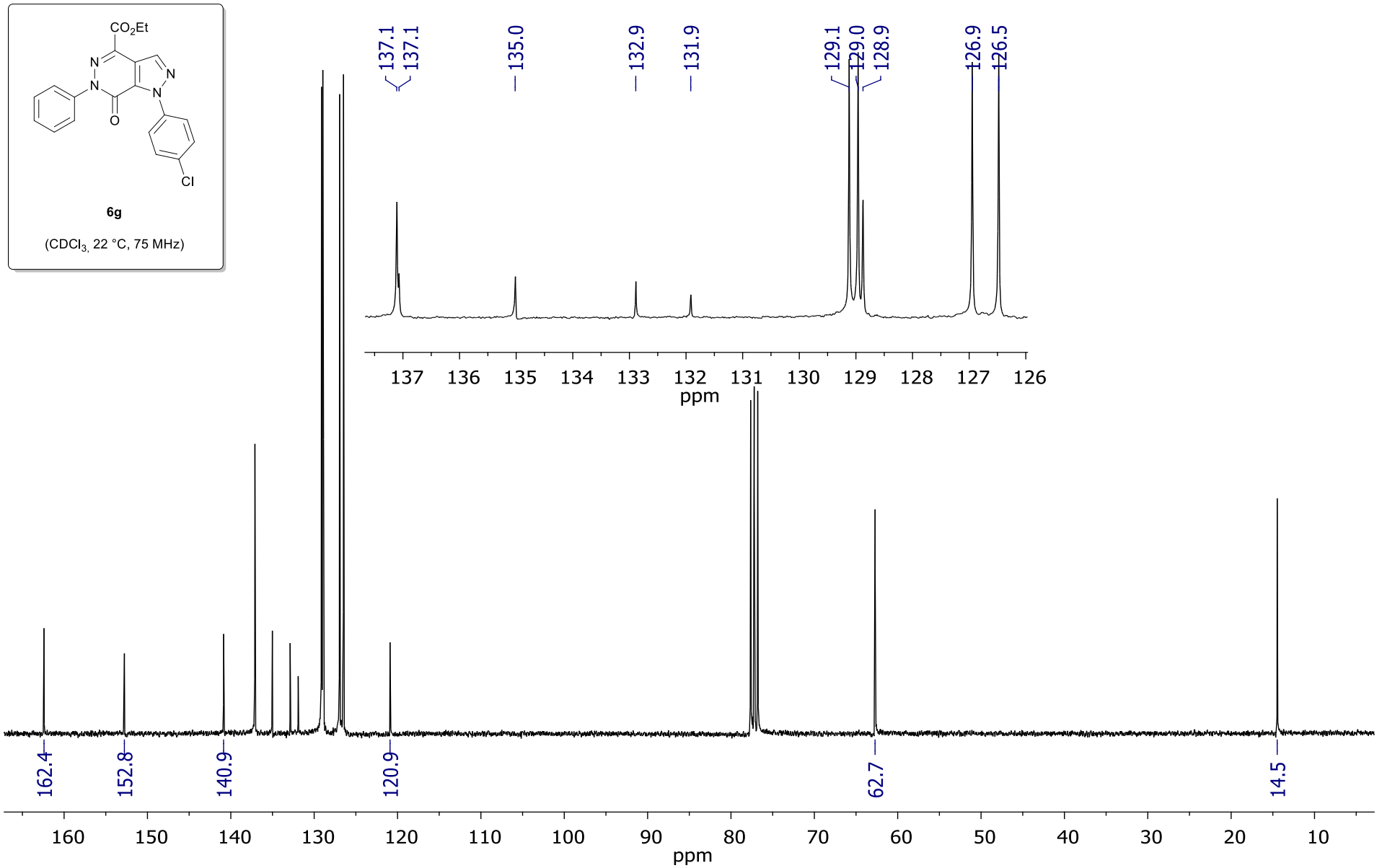


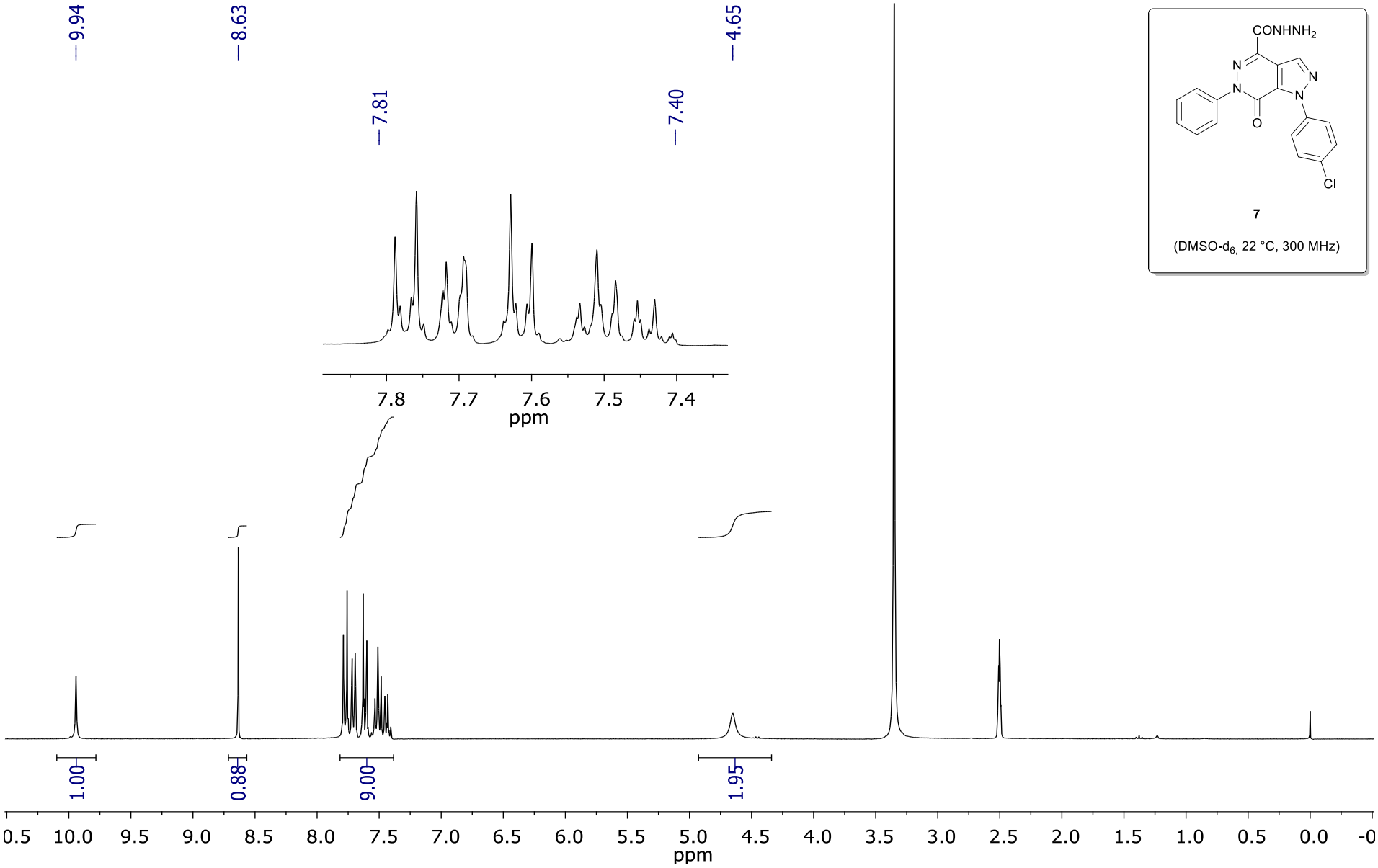
6f

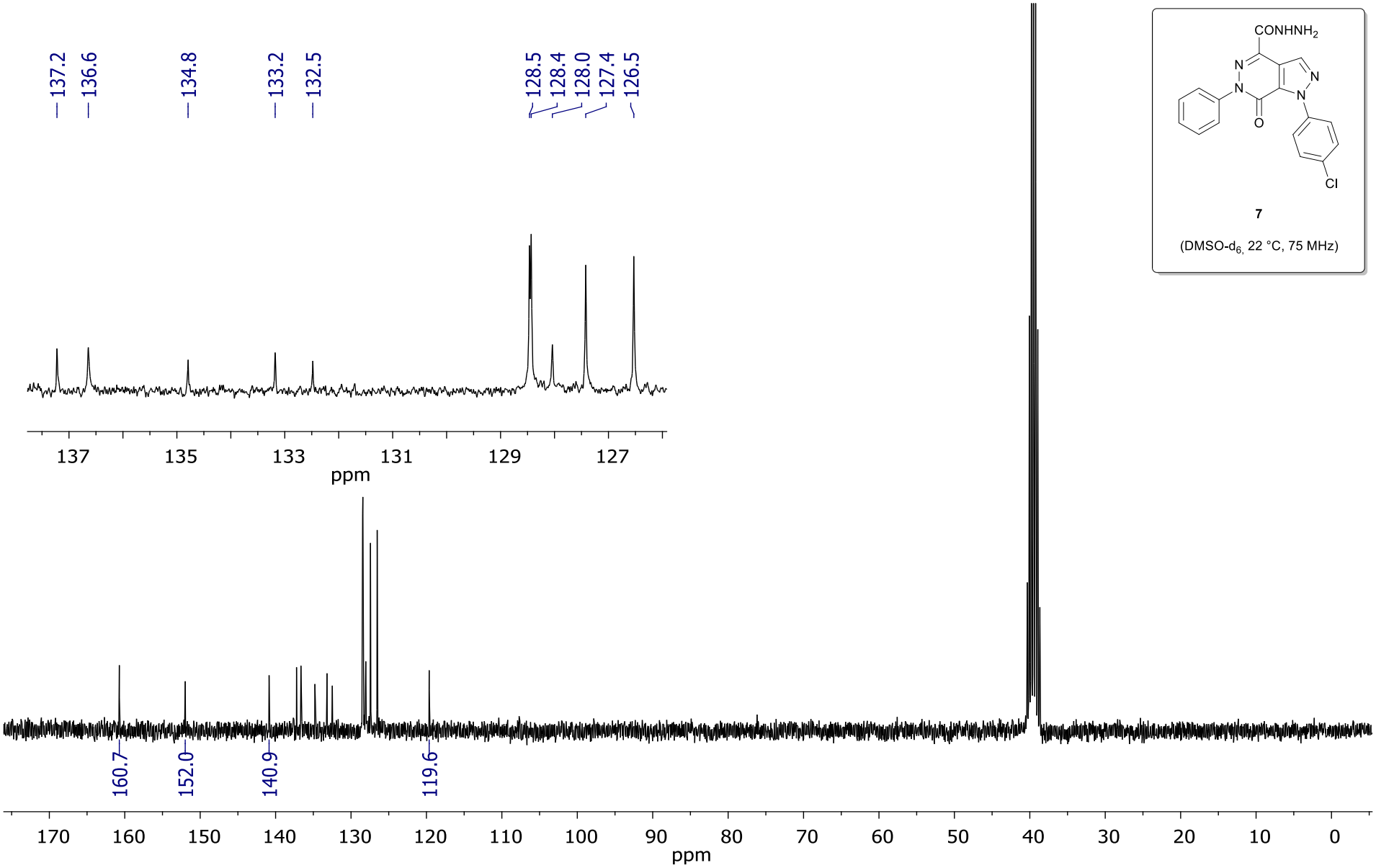
(DMSO-d_6, 22 °C, 300 MHz)

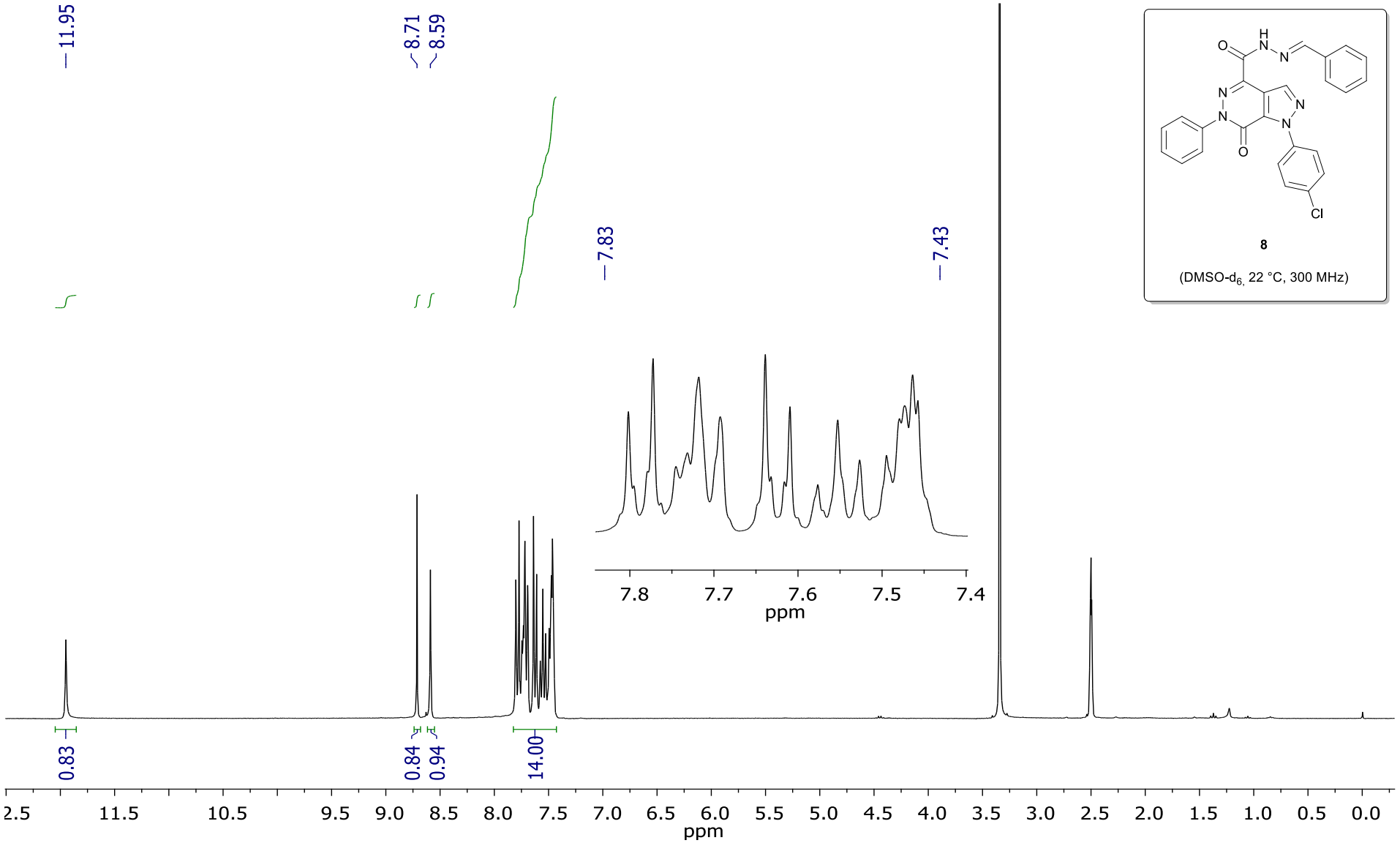


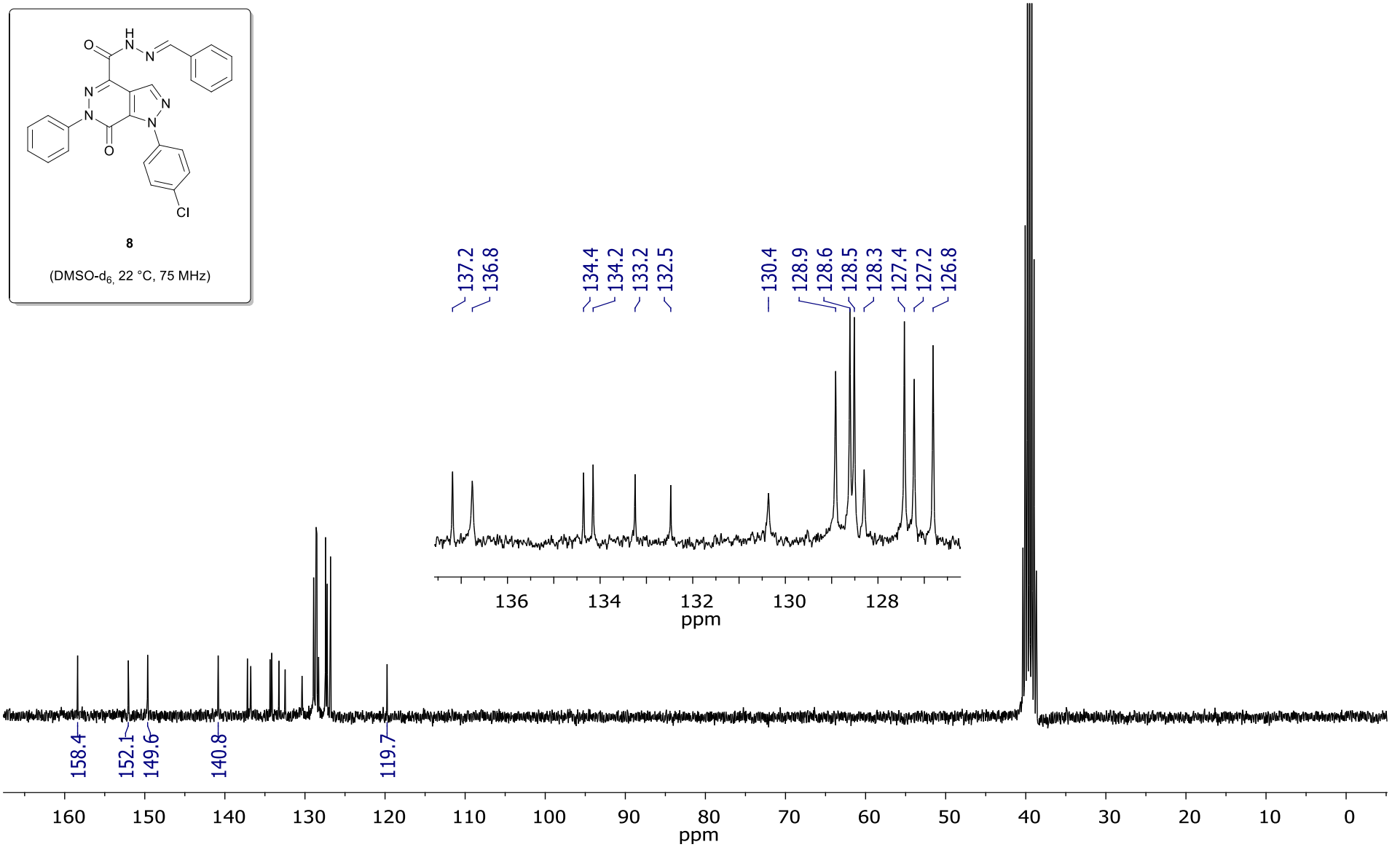


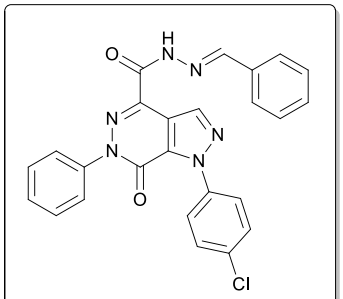












8

(DMSO-d_6, 22 °C, 300 MHz)

(NOESY 2D)