Supporting Information

Electrochemical Direct C-H Mono and Bis-Chalcogenation of Indolizine Frameworks Under Oxidant-Free Conditions

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General Procedure for Cyclic Voltammetry (CV):

Cyclic voltammetry was performed in a three electrode cell at room temperature. The working electrode was a glassy electrode and the counter electrode was a platinum electrode. The reference was an Ag/AgCl electrode submerged in 3M KCl solution, and separated from the reaction by a salt bridge.

Cyclic Voltammograms graph for KI

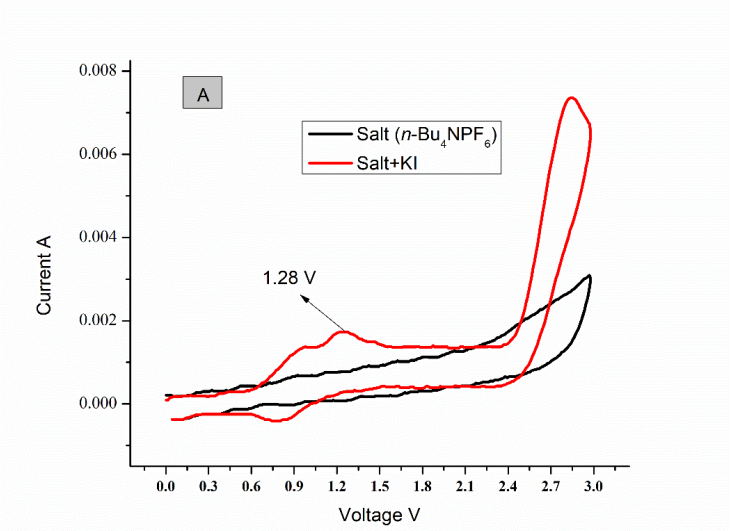
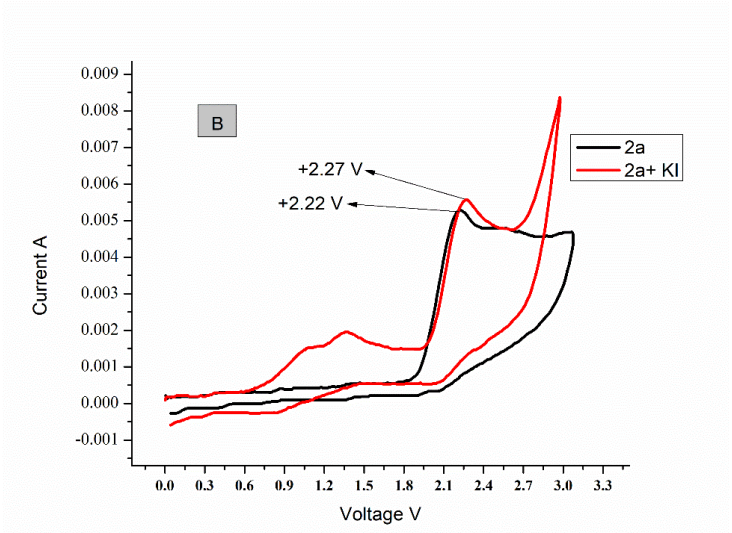


Figure S1. Cyclic voltammograms of reactants and mixture in 0.1 M *n*-Bu_4NPF_6 in CH_3CN using a glassy carbon disk electrode, Pt electrode as counter electrode and Ag/AgCl as reference electrode, at a 200 $mVS^{-}1$. Cyclic voltammograms of salt and salt with KI at a 200 mVS^{-1} (graph A): *n*-Bu_4NPF_6 (0.1 M); (curve salt+KI): *n*-Bu_4NPF_6 (0.1 M), KI (10 mM).

Cyclic Voltammograms graph of 2a



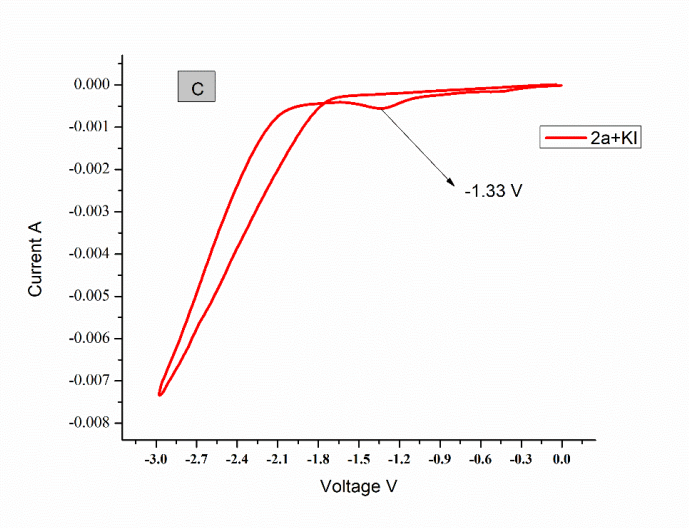


Figure S2. Cyclic voltammograms of **2a** in 0.1 M *n*-Bu_4NPF_6 in CH_3CN using a glassy carbon disk electrode, Pt electrode as counter electrode and Ag/AgCl as reference electrode, at a 200 mVS^{-1}; (graph B and graph C): **2a** (5 mM), *n*-Bu_4NPF_6 (0.1 M) and KI (10 mM) in acetonitrile solvent.

Cyclic Voltammograms graph for 1a

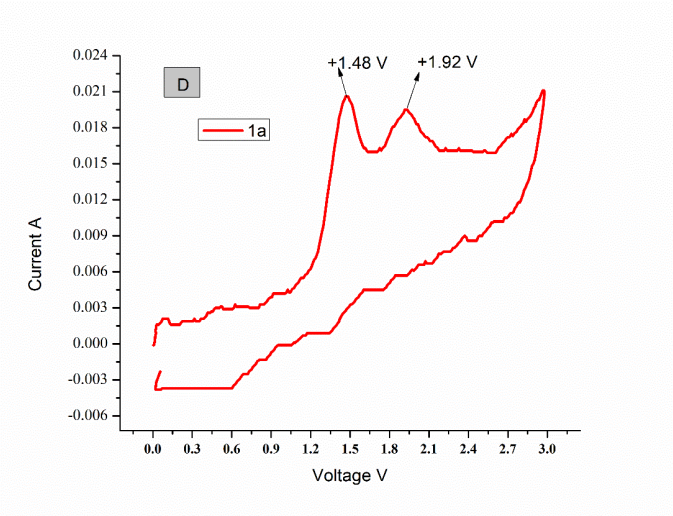


Figure S3. Cyclic voltammograms of **1a** in 0.1 M *n*-Bu_4NPF_6 in CH_3CN using a glassy carbon disk electrode, Pt electrode as counter electrode and Ag/AgCl as reference electrode, at a 200 mVS^{-1}; (graph D): **1a** (5 mM), *n*-Bu_4NPF_6 (0.1 M) in acetonitrile solvent.

Cyclic Voltammograms graph for 6a

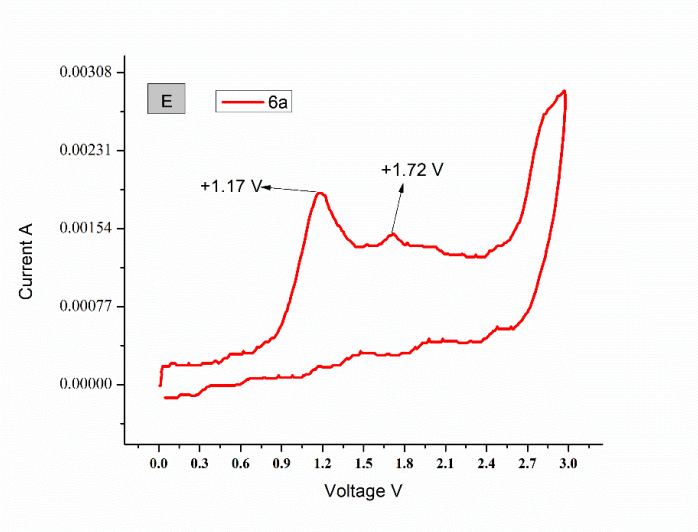


Figure S4. Cyclic voltammograms of **6a** in 0.1 M *n*-Bu_4NPF_6 in CH_3CN using a glassy carbon disk electrode, Pt electrode as counter electrode and Ag/AgCl as reference electrode, at a 200 mVS^{-1}; (graph E): **6a** (5 mM), *n*-Bu_4NPF_6 (0.1 M) in acetonitrile solvent.

Cyclic Voltammograms graph for 1a+2a

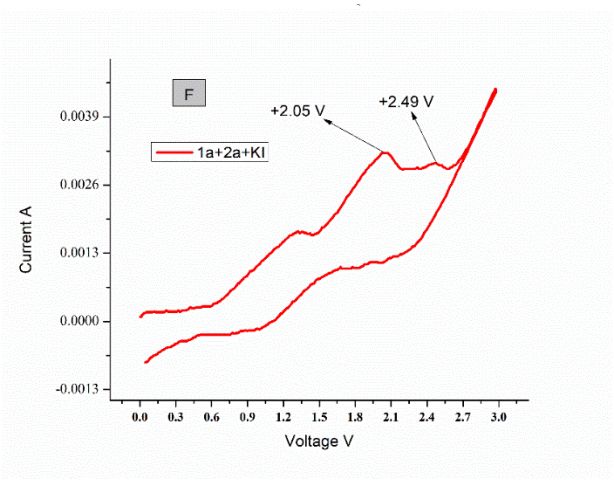


Figure S5. Cyclic voltammograms of reactants and mixture in 0.1 M *n*-Bu_4NPF_6 in CH_3CN using a glassy carbon disk electrode, Pt electrode as counter electrode and Ag/AgCl as reference electrode, at a 200 mVS^{-1}; (graph F): **1a** (5 mM) + **2a** (5 mM)+ *n*-Bu_4NPF_6 (0.1 M), KI (10 mM) in acetonitrile solvent.

Cyclic Voltammograms graph for 6a+2a

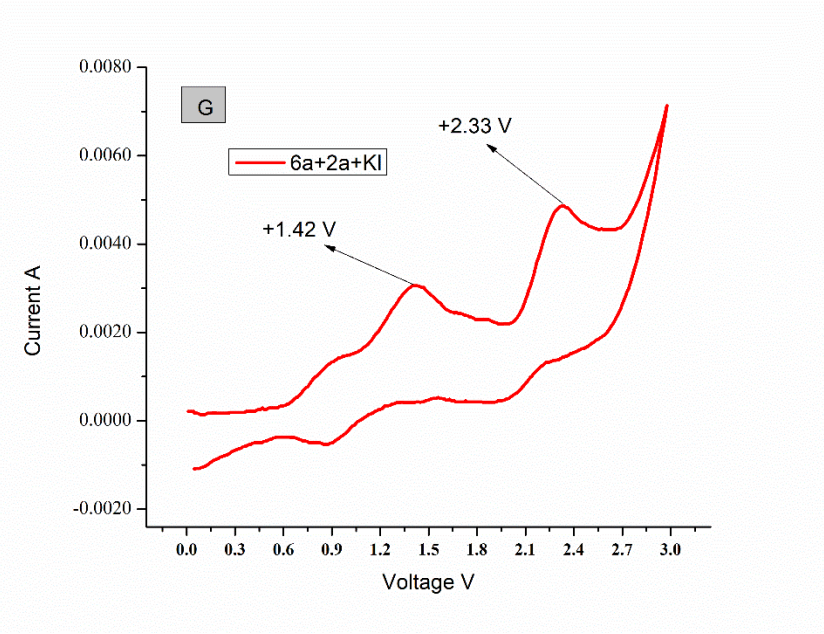
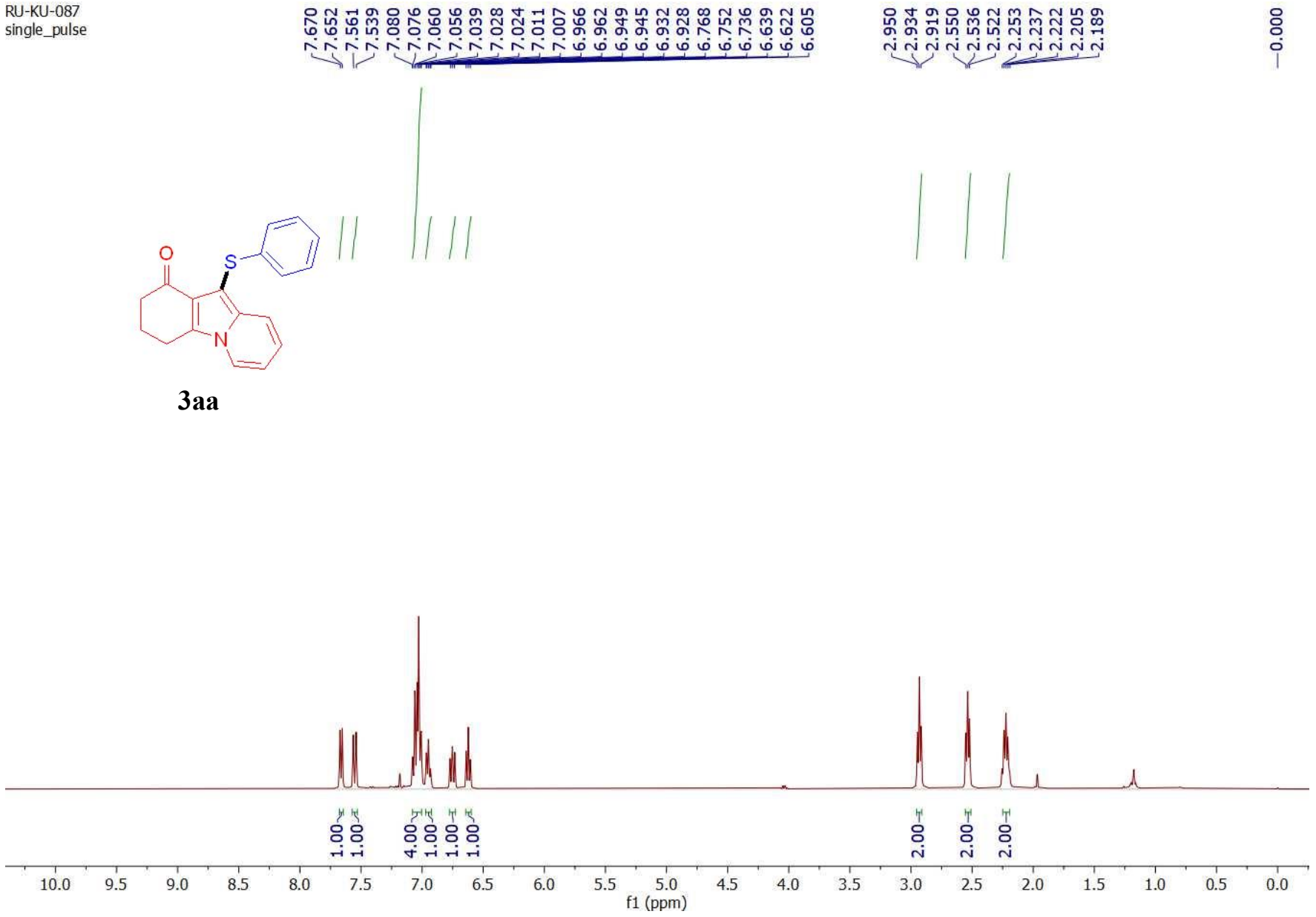


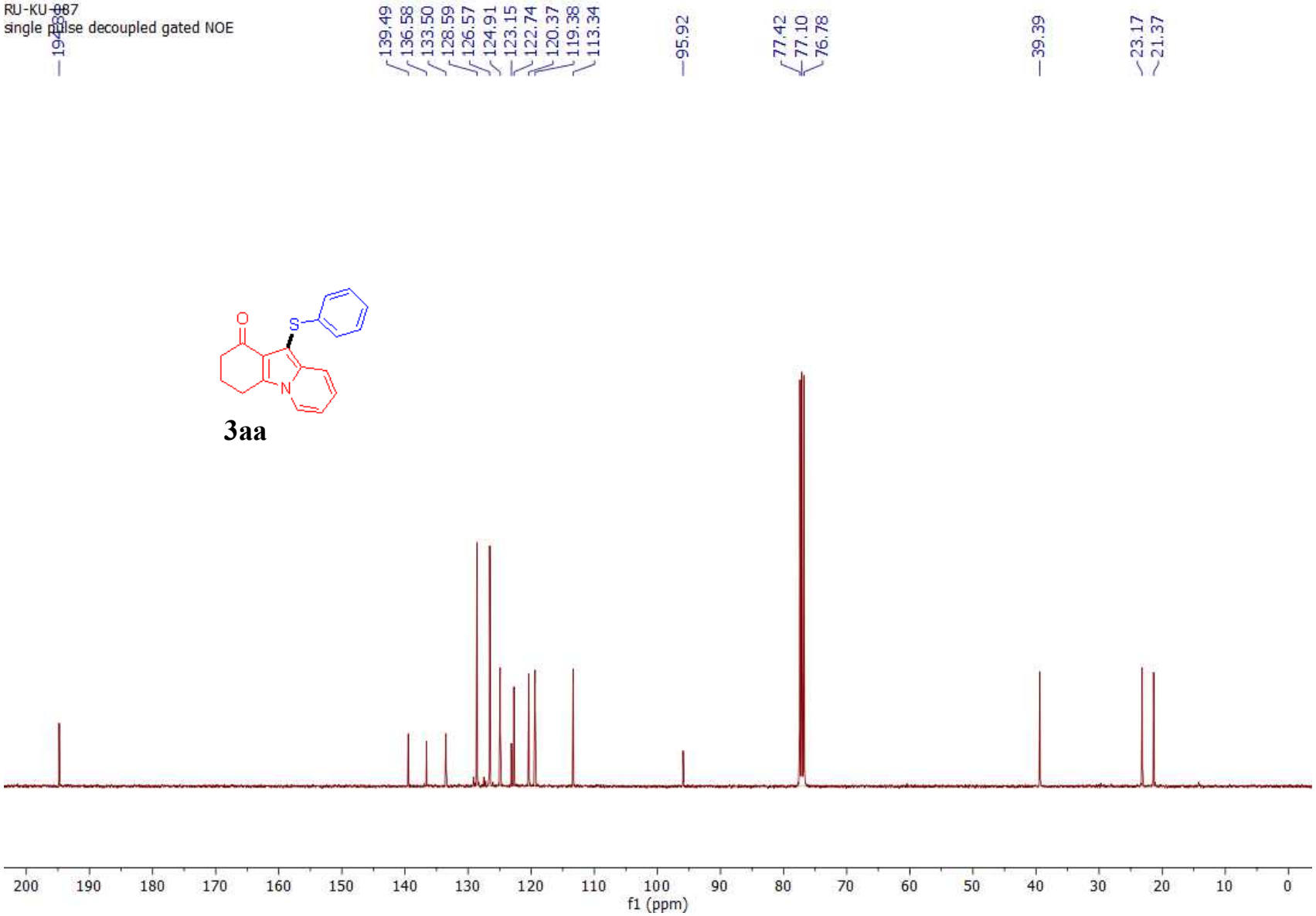
Figure S6. Cyclic voltammograms of reactants and mixture in 0.1 M *n*-Bu_4NPF_6 in CH_3CN using a glassy carbon disk electrode, Pt electrode as counter electrode and Ag/AgCl as reference electrode, at a 200 mVS^{-1}; (graph F): **6a** (5 mM) + **2a** (5 mM)+ *n*-Bu_4NPF_6 (0.1 M), KI (10 mM) in acetonitrile solvent.

^{1}H NMR spectrum of 3aa (400 MHz, $CDCl_3$)

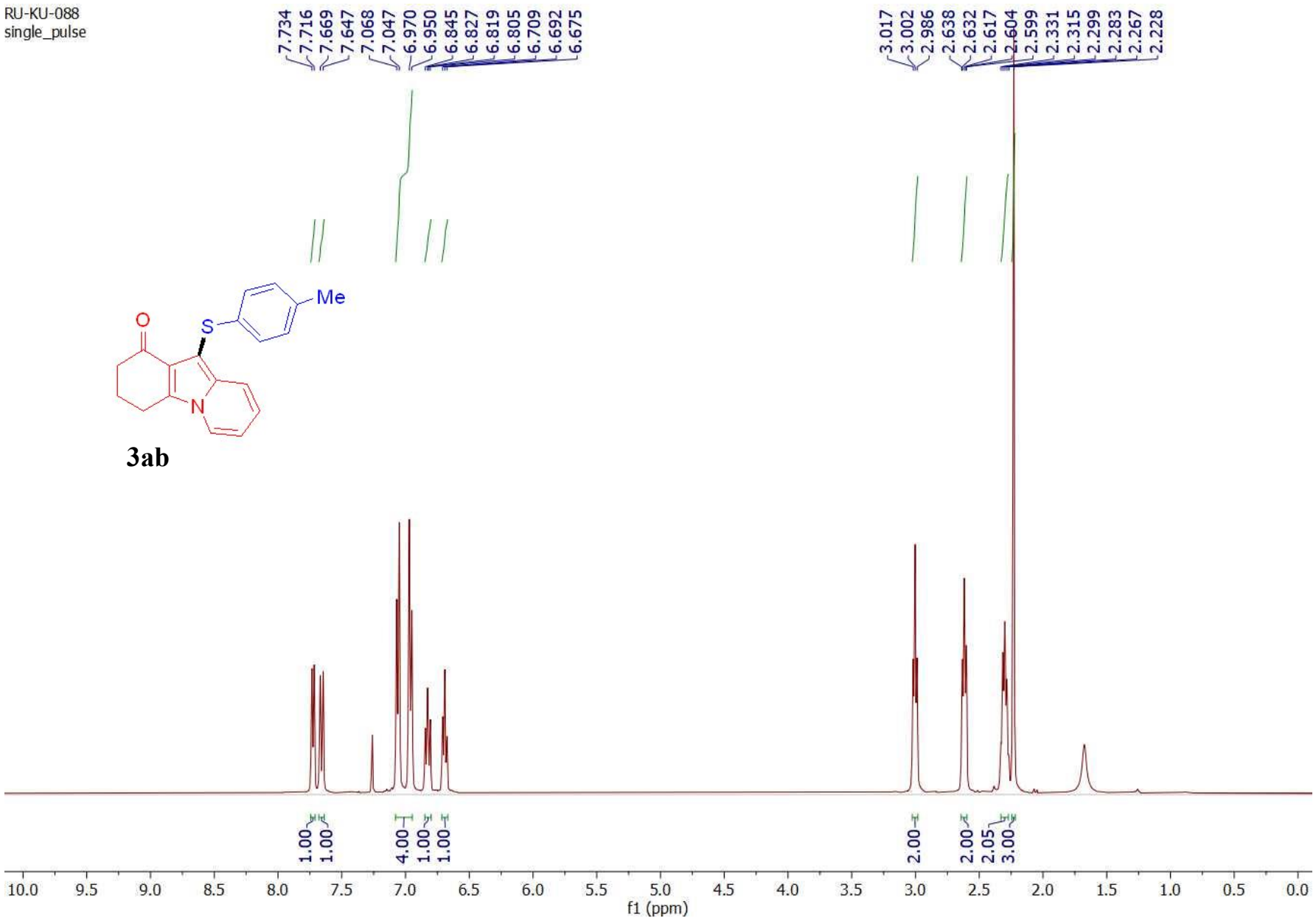


3aa

$^{13}C\{H\}$ NMR spectrum of 3aa (100 MHz, $CDCl_3$)

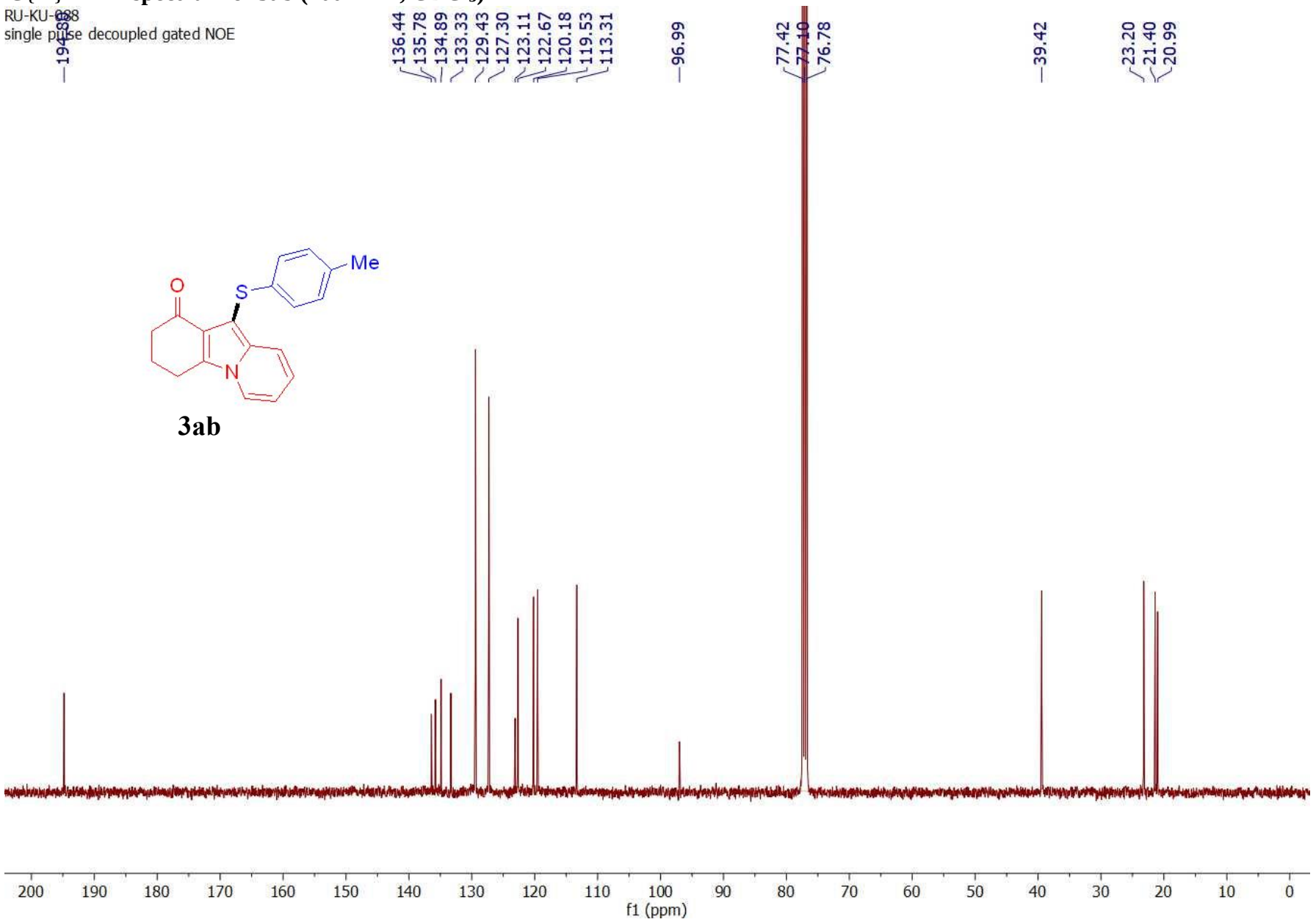


^{1}H NMR spectrum of 3ab (400 MHz, $CDCl_3$)



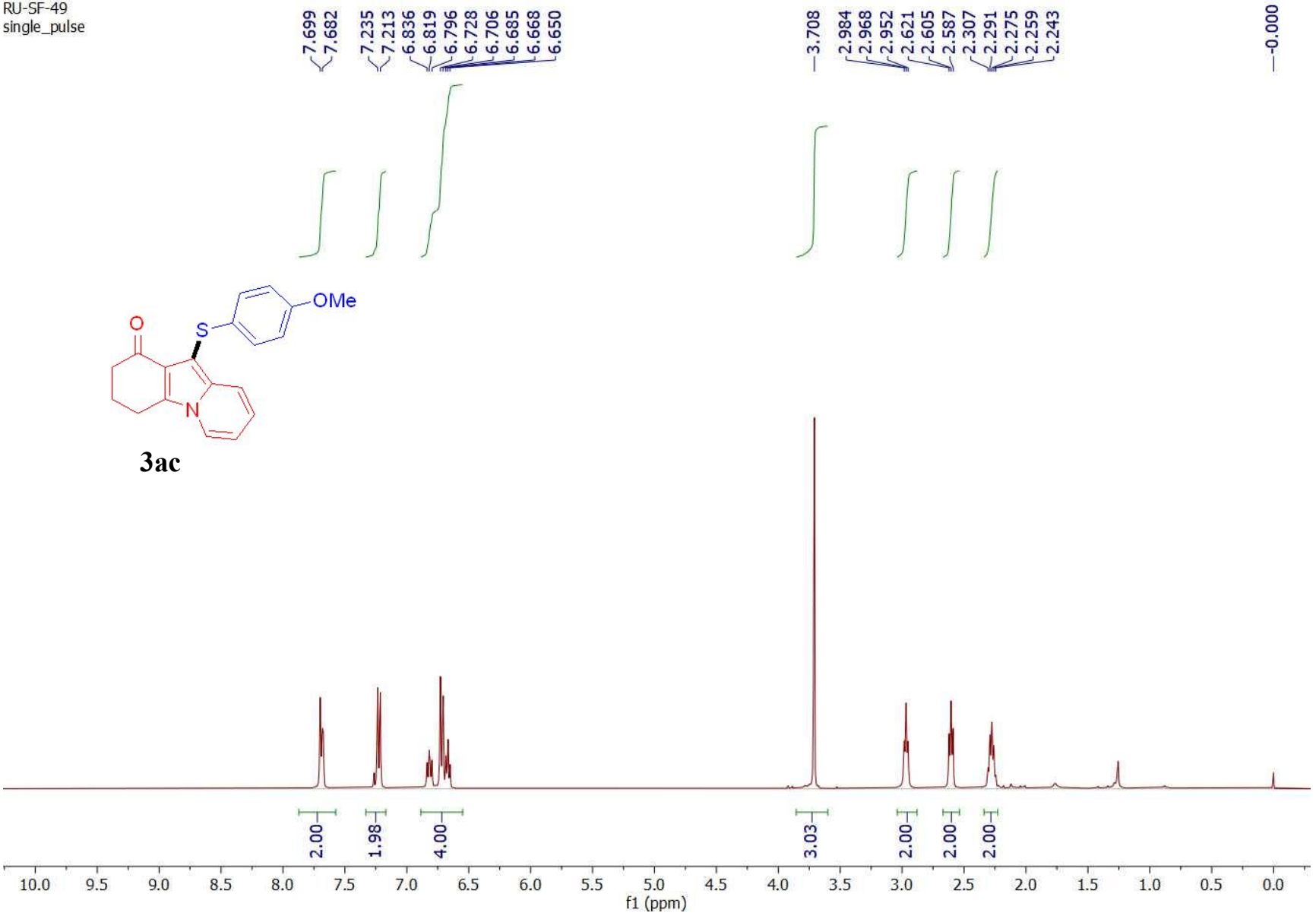
3ab

$^{13}C\{H\}$ NMR spectrum of 3ab (100 MHz, $CDCl_3$)



3ab

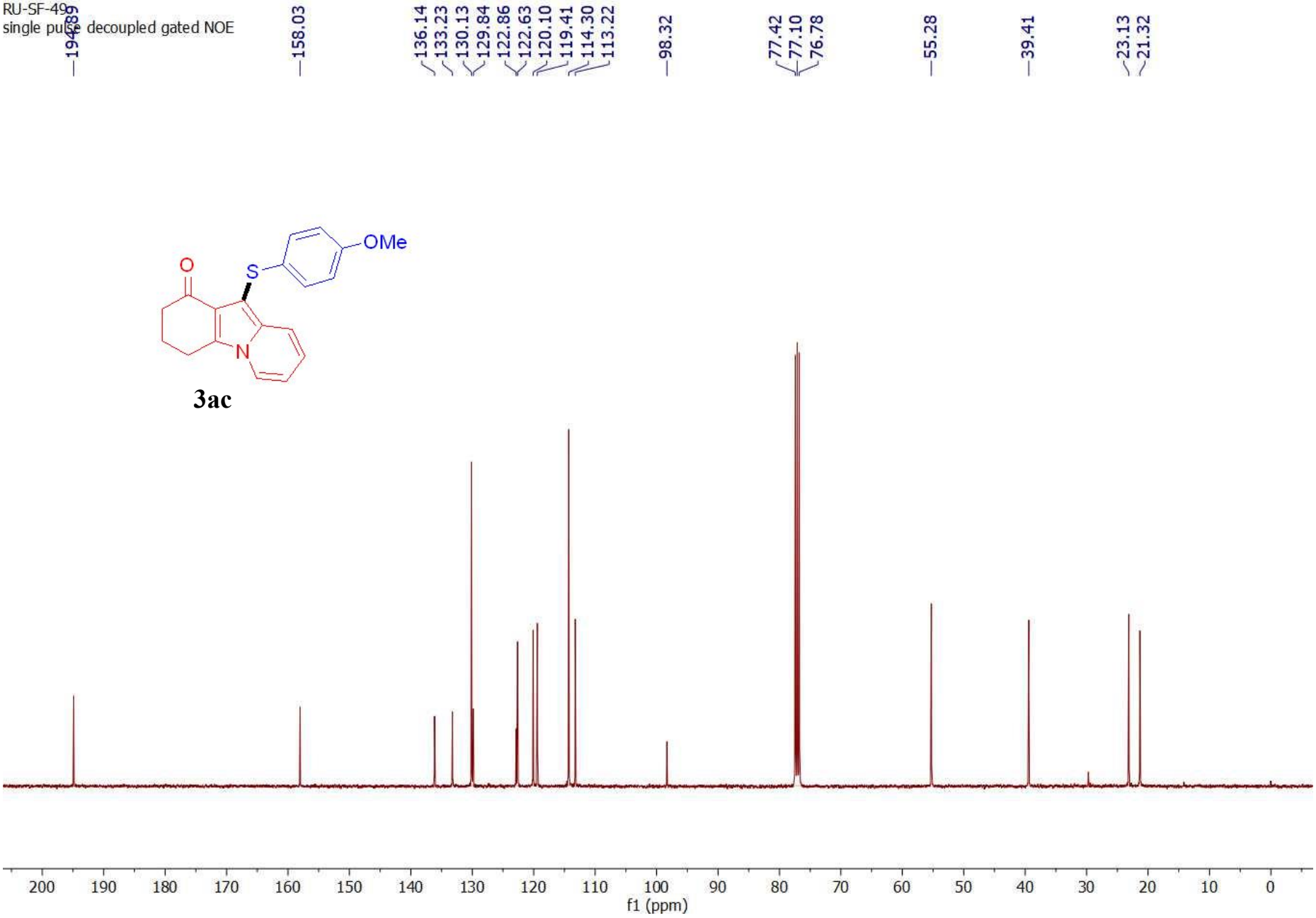
^{1}H NMR spectrum of 3ac (400 MHz, $CDCl_3$)



3ac

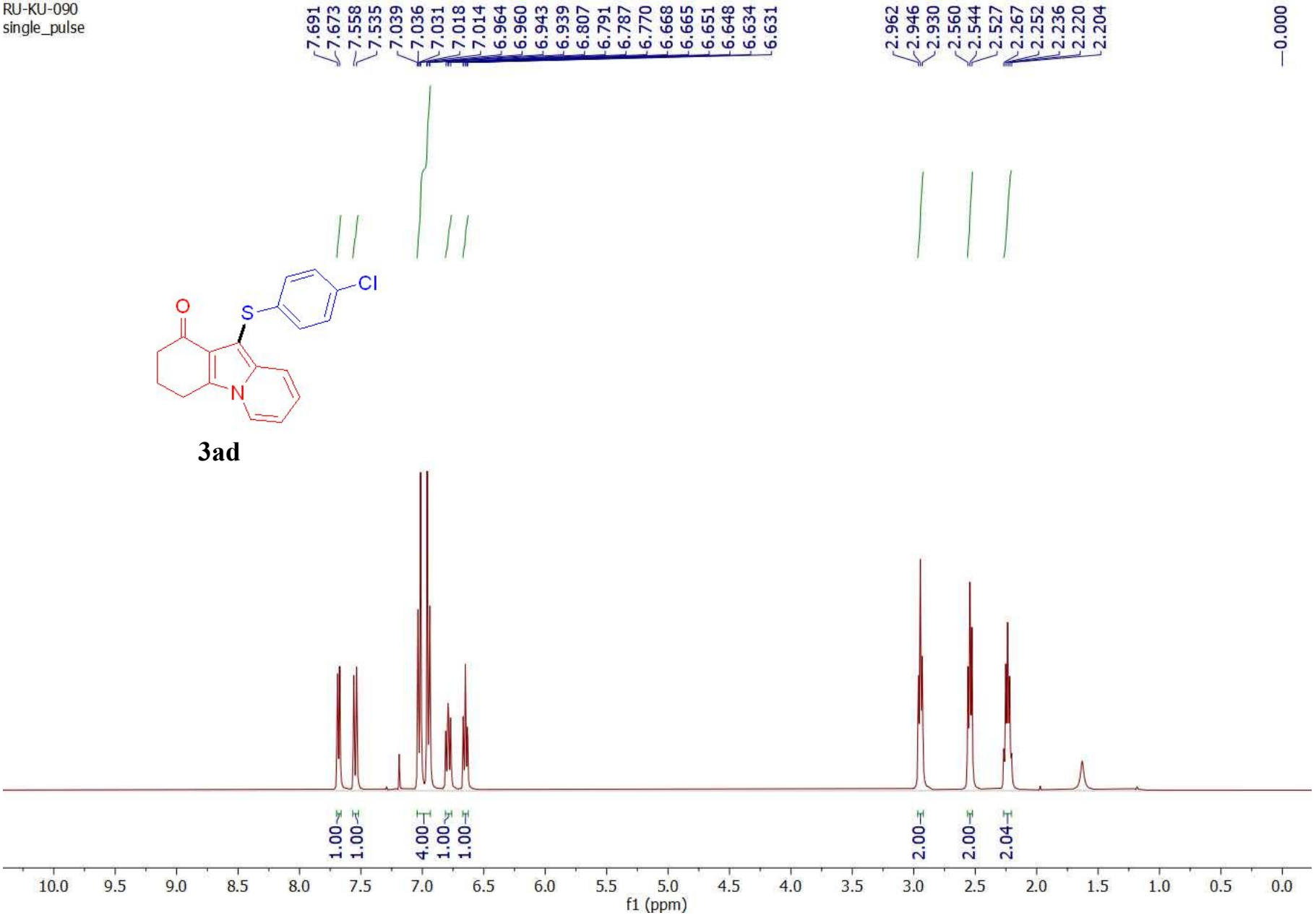
$^{13}C\{H\}$ NMR spectrum of 3ac (100 MHz, $CDCl_3$)

RU-SF-49
single pulse decoupled gated NOE



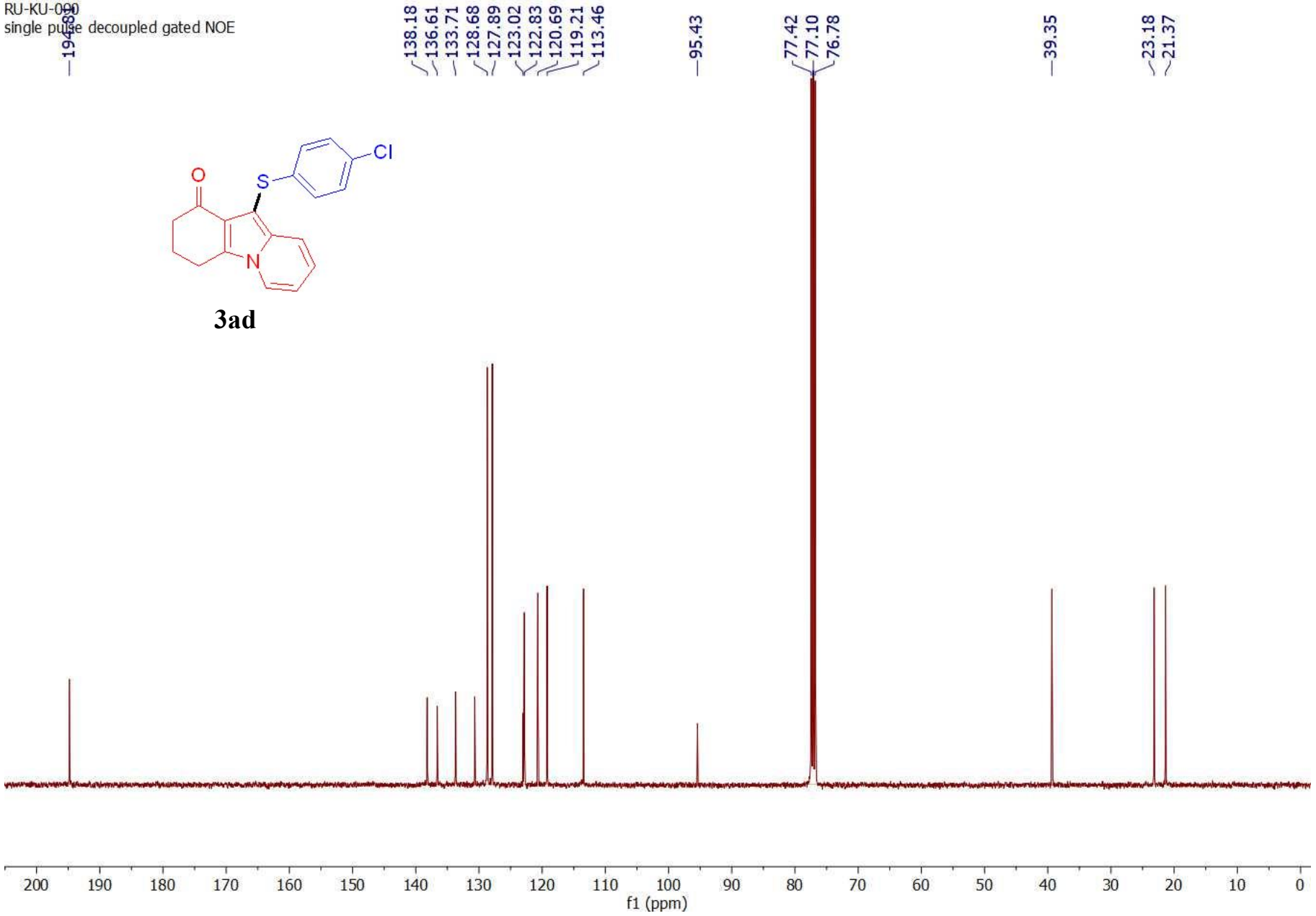
3ac

^{1}H NMR spectrum of 3ad (400 MHz, $CDCl_3$)



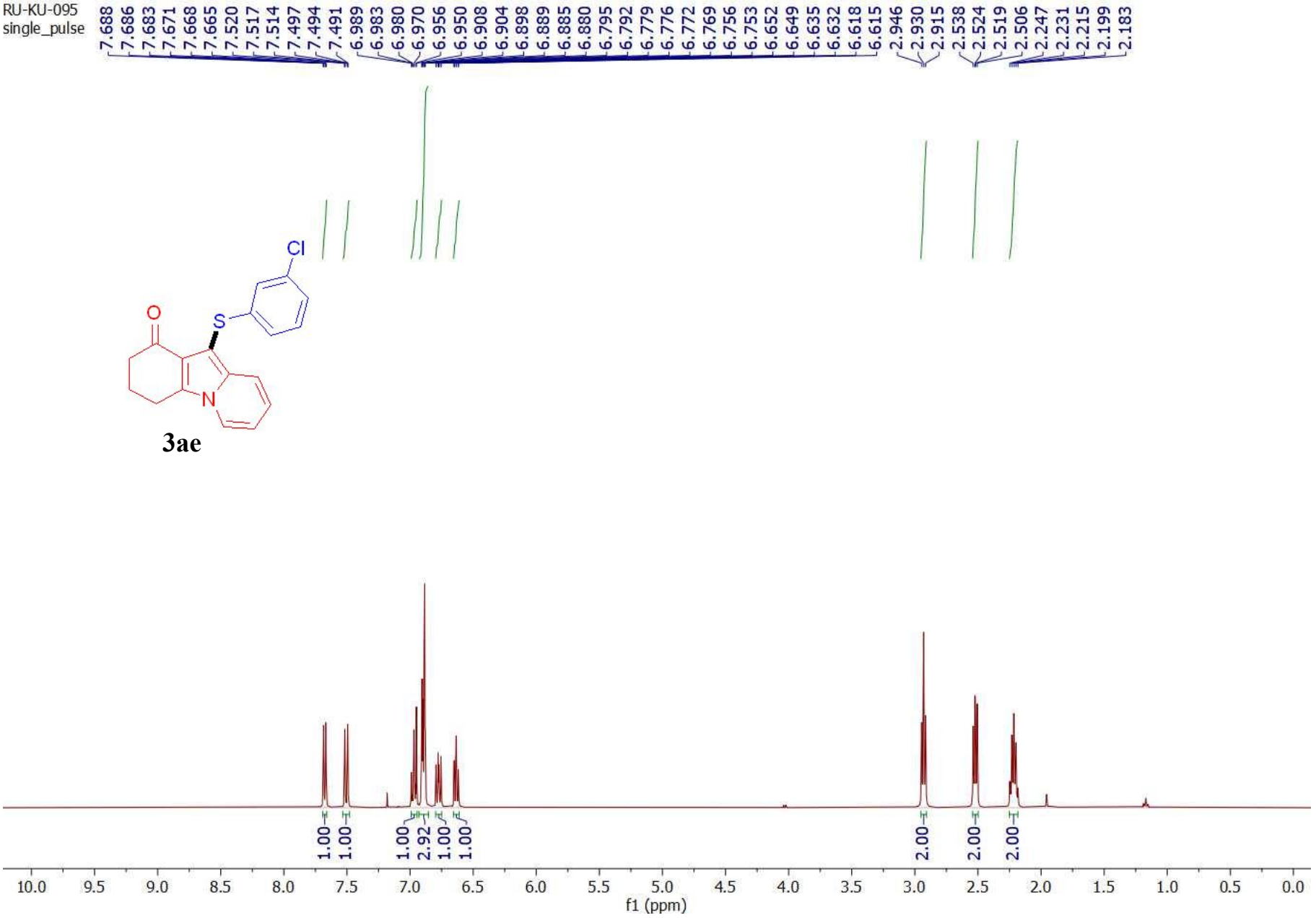
3ad

$^{13}C\{H\}$ NMR spectrum of 3ad (100 MHz, $CDCl_3$)



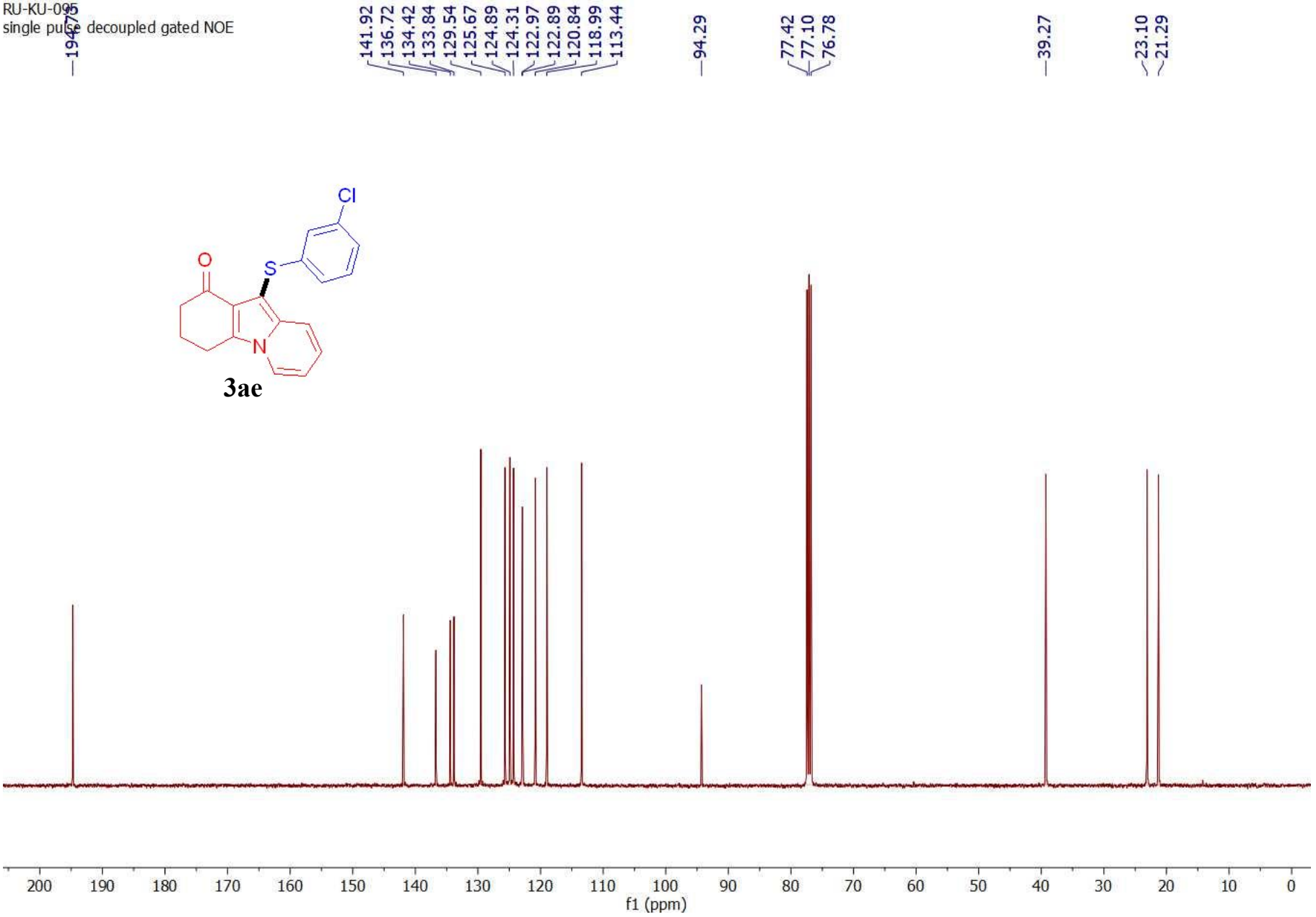
3ad

^{1}H NMR spectrum of 3ae (400 MHz, $CDCl_3$)

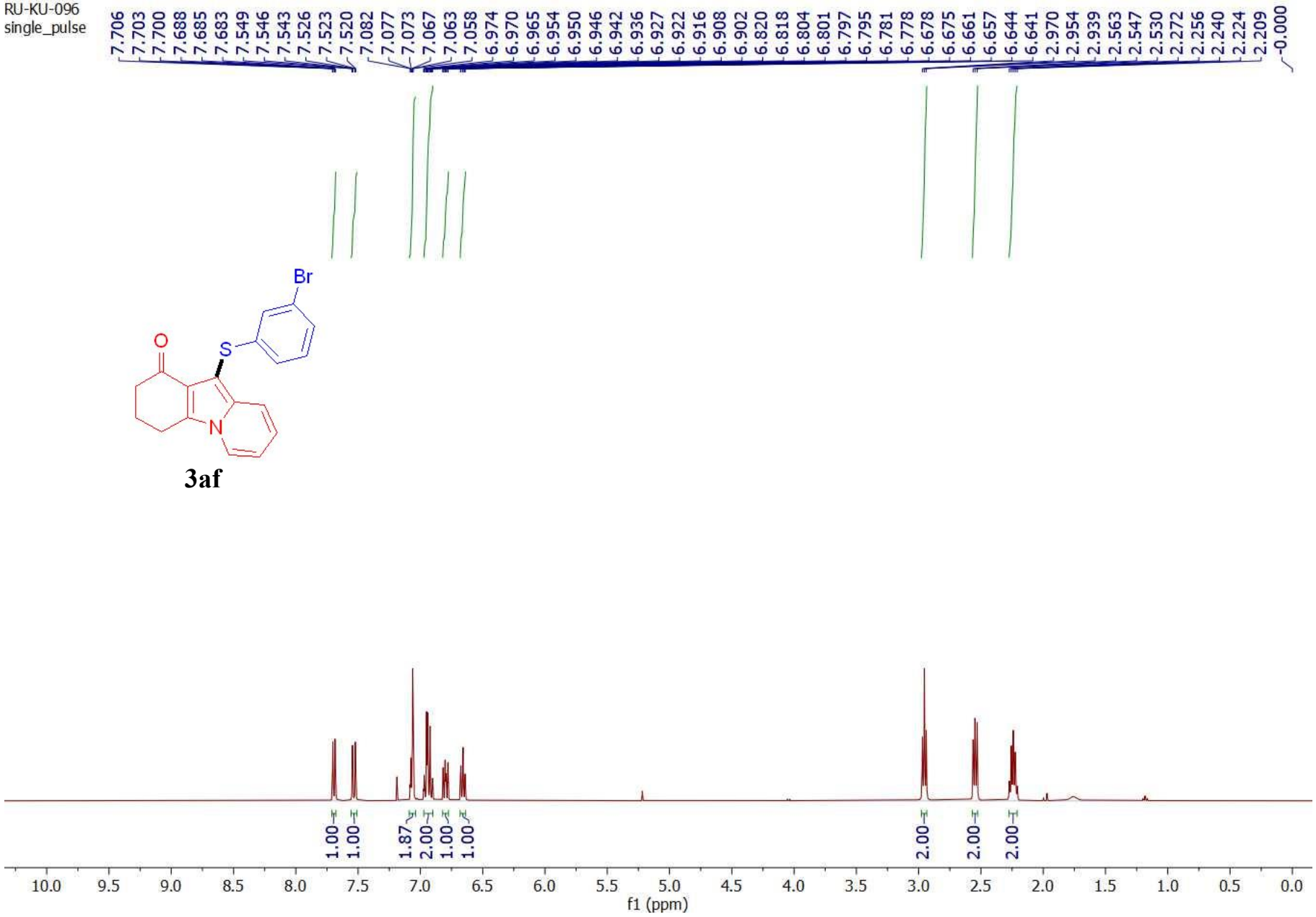


3ae

$^{13}C\{H\}$ NMR spectrum of 3ae (100 MHz, $CDCl_3$)

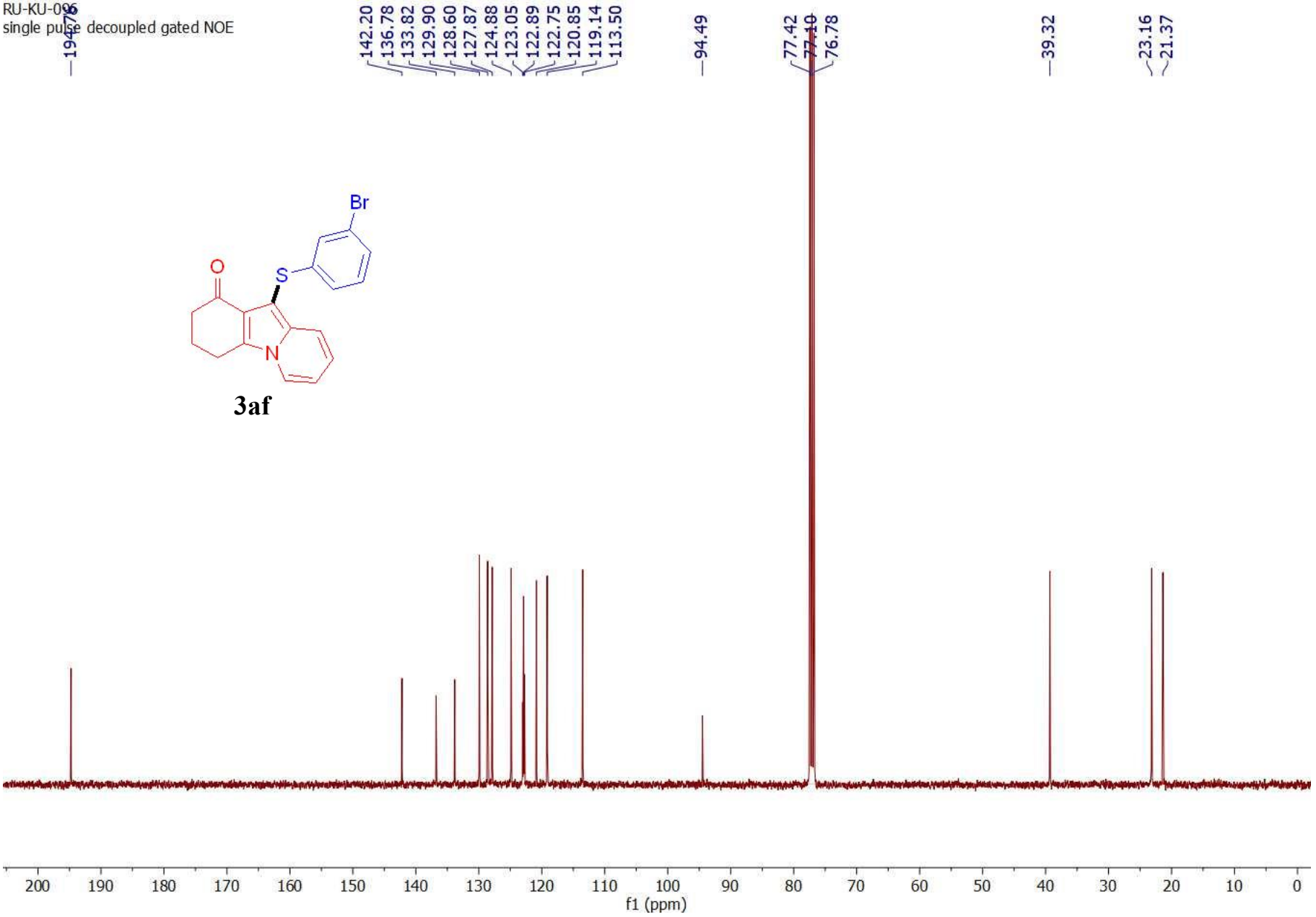


^{1}H NMR spectrum of 3af (400 MHz, $CDCl_3$)



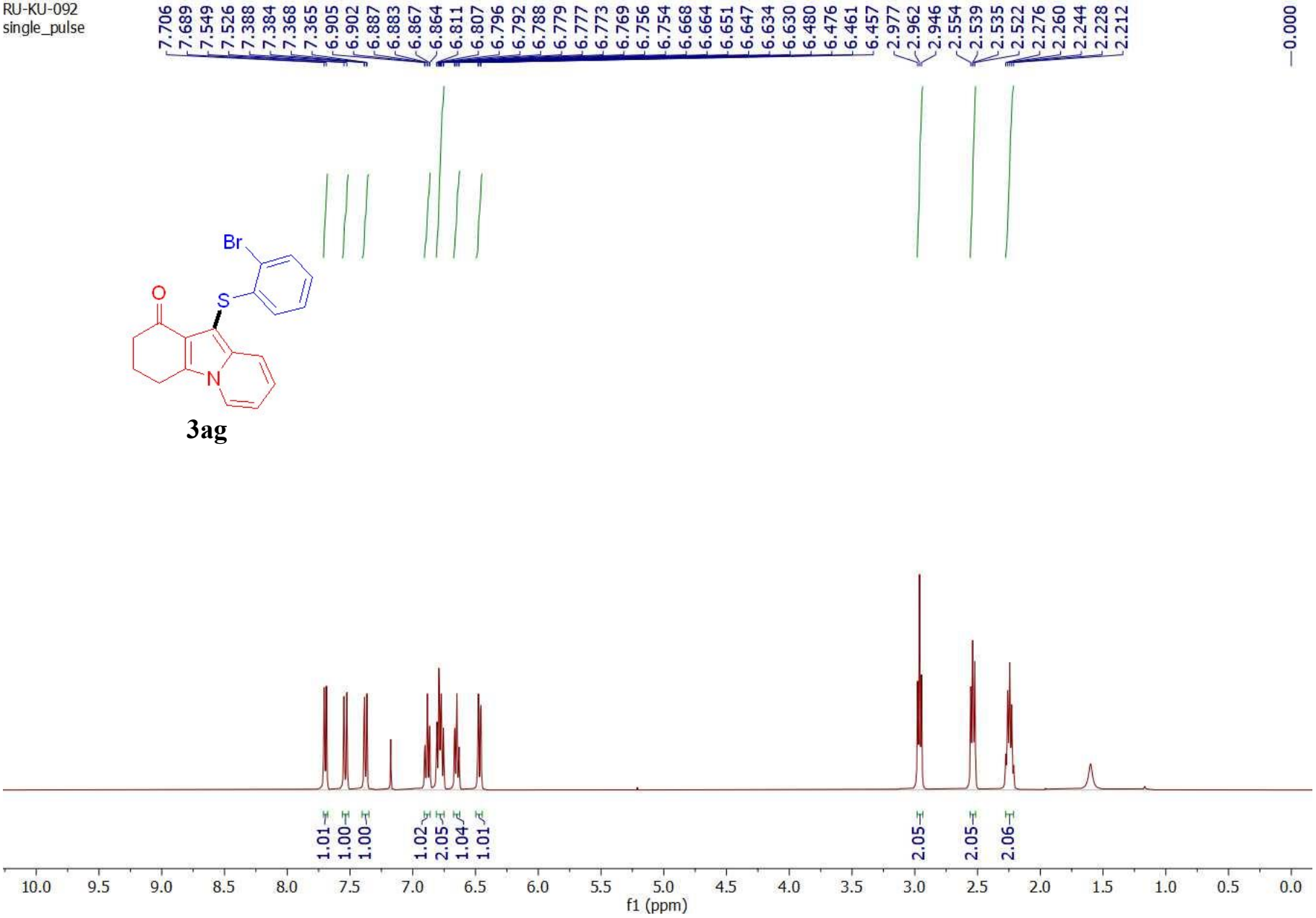
3af

$^{13}C\{H\}$ NMR spectrum of 3af (100 MHz, $CDCl_3$)



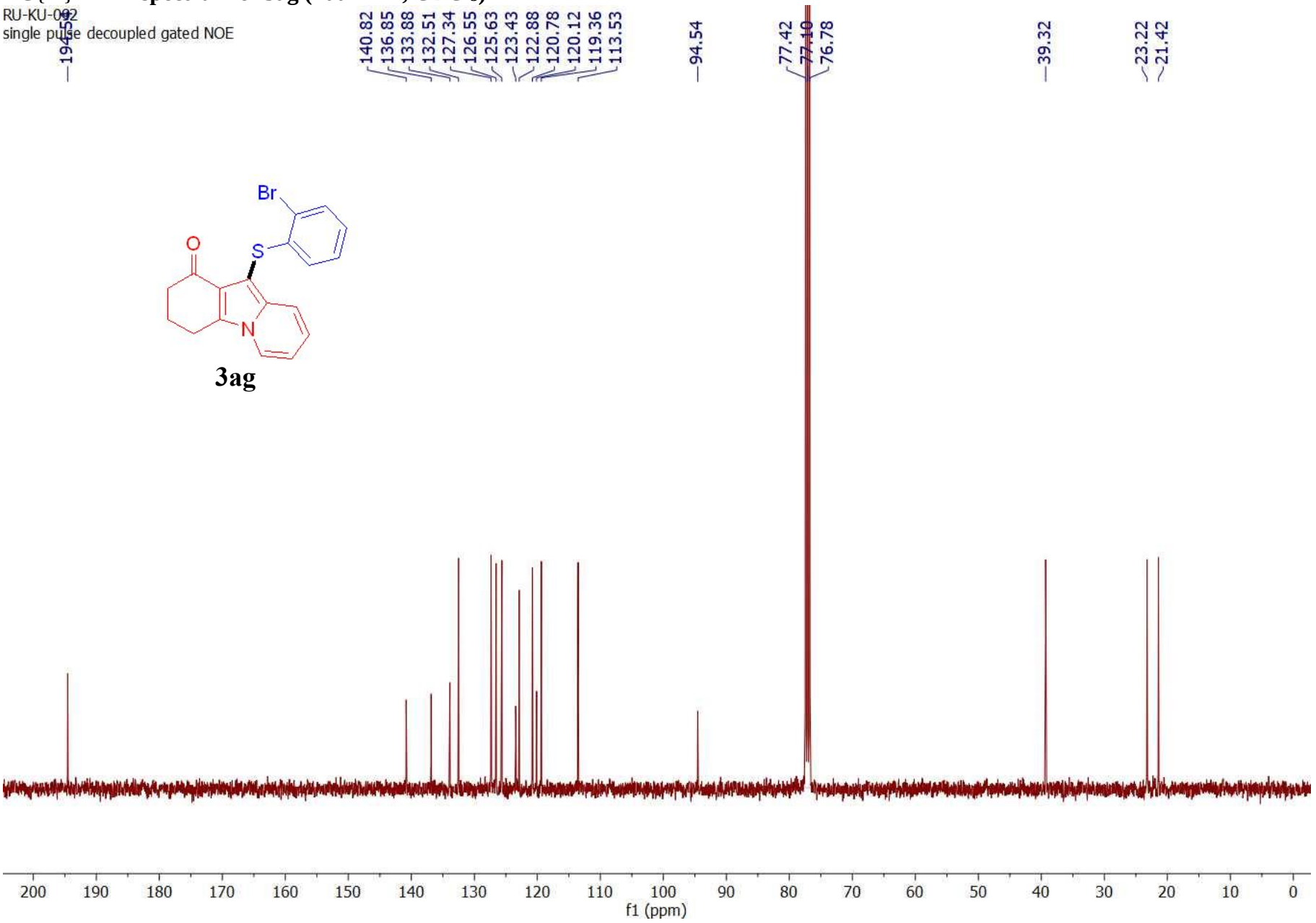
3af

^{1}H NMR spectrum of 3ag (400 MHz, $CDCl_3$)



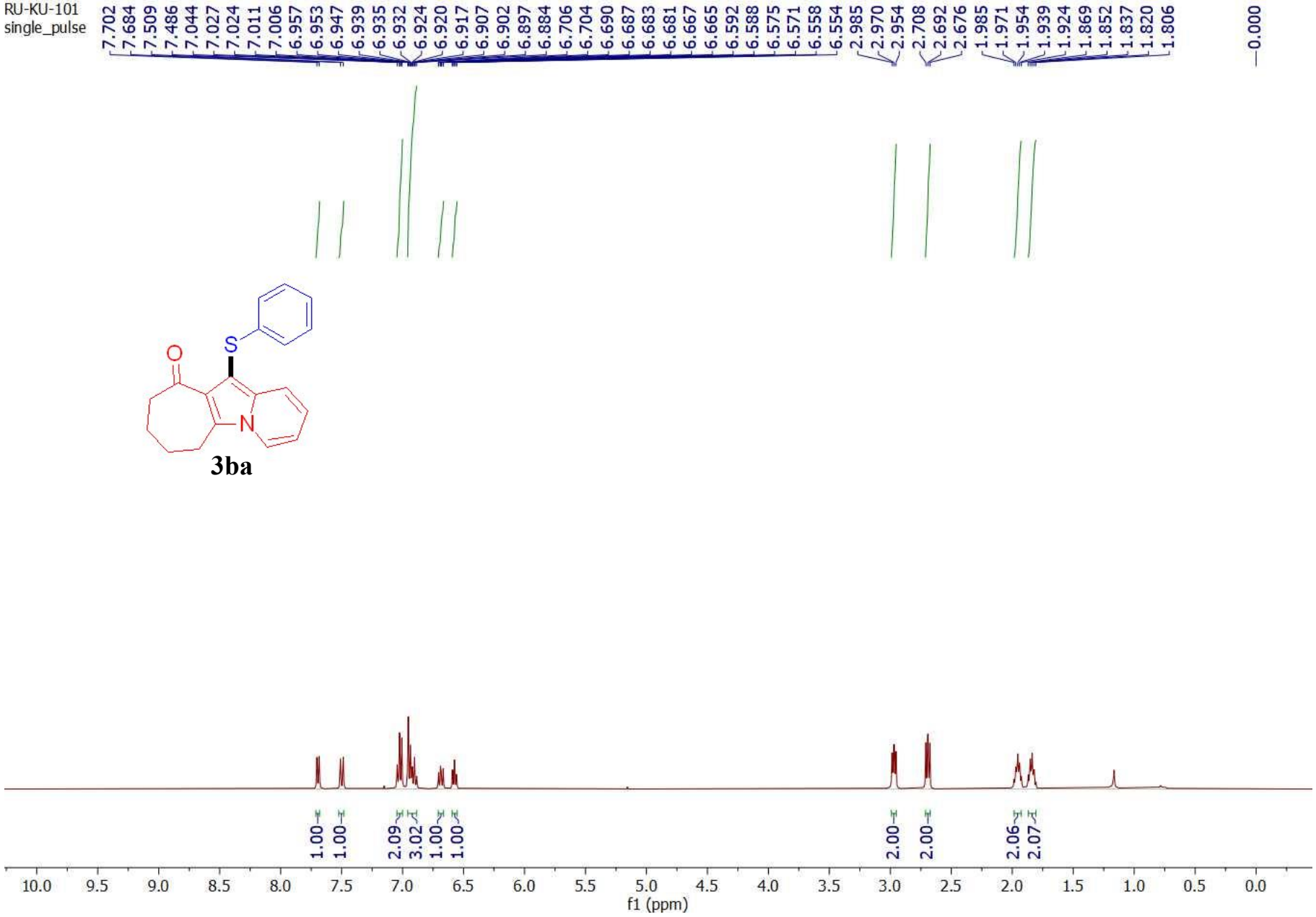
3ag

$^{13}C\{H\}$ NMR spectrum of 3ag (100 MHz, $CDCl_3$)



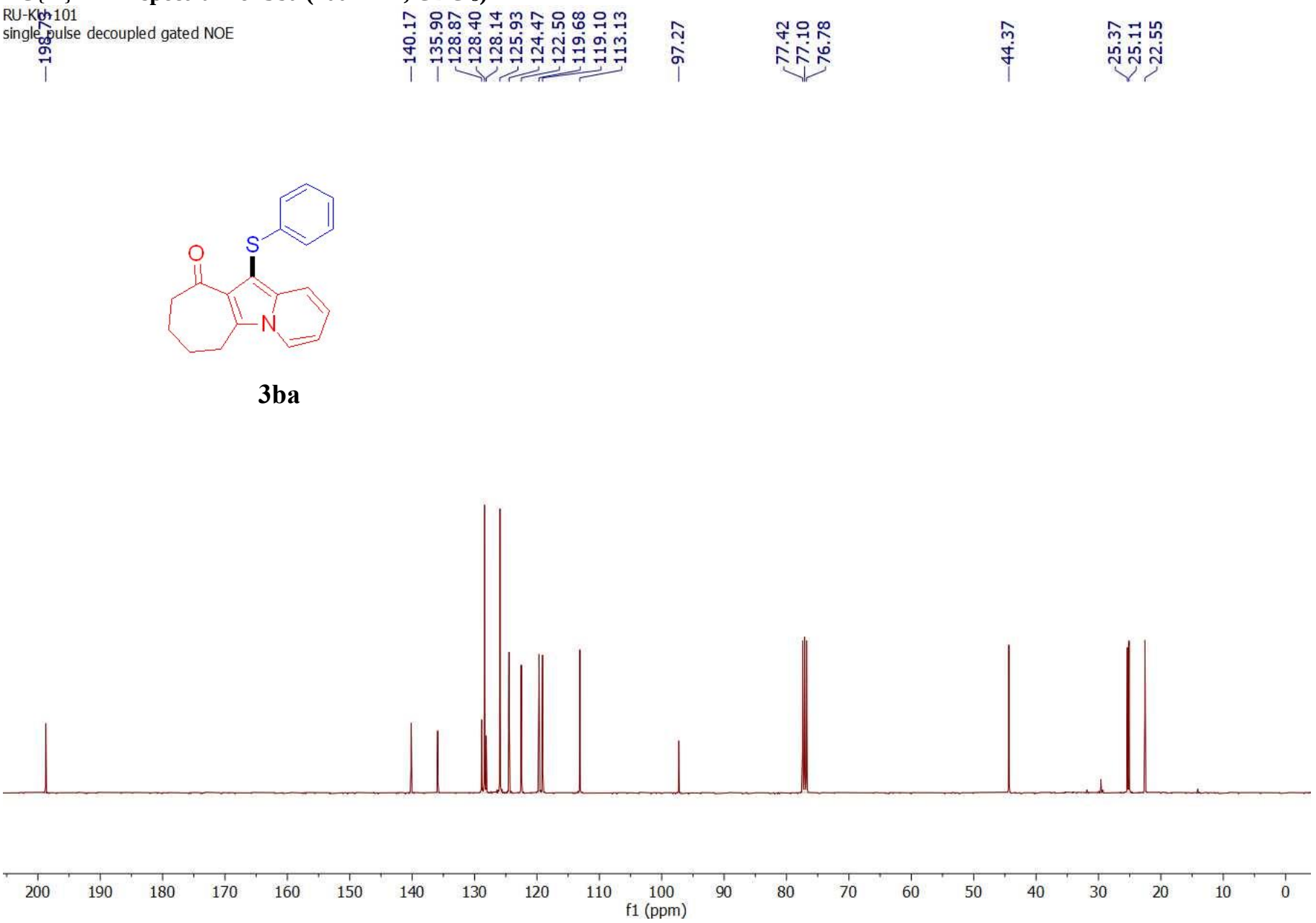
3ag

^{1}H NMR spectrum of 3ba (400 MHz, $CDCl_3$)



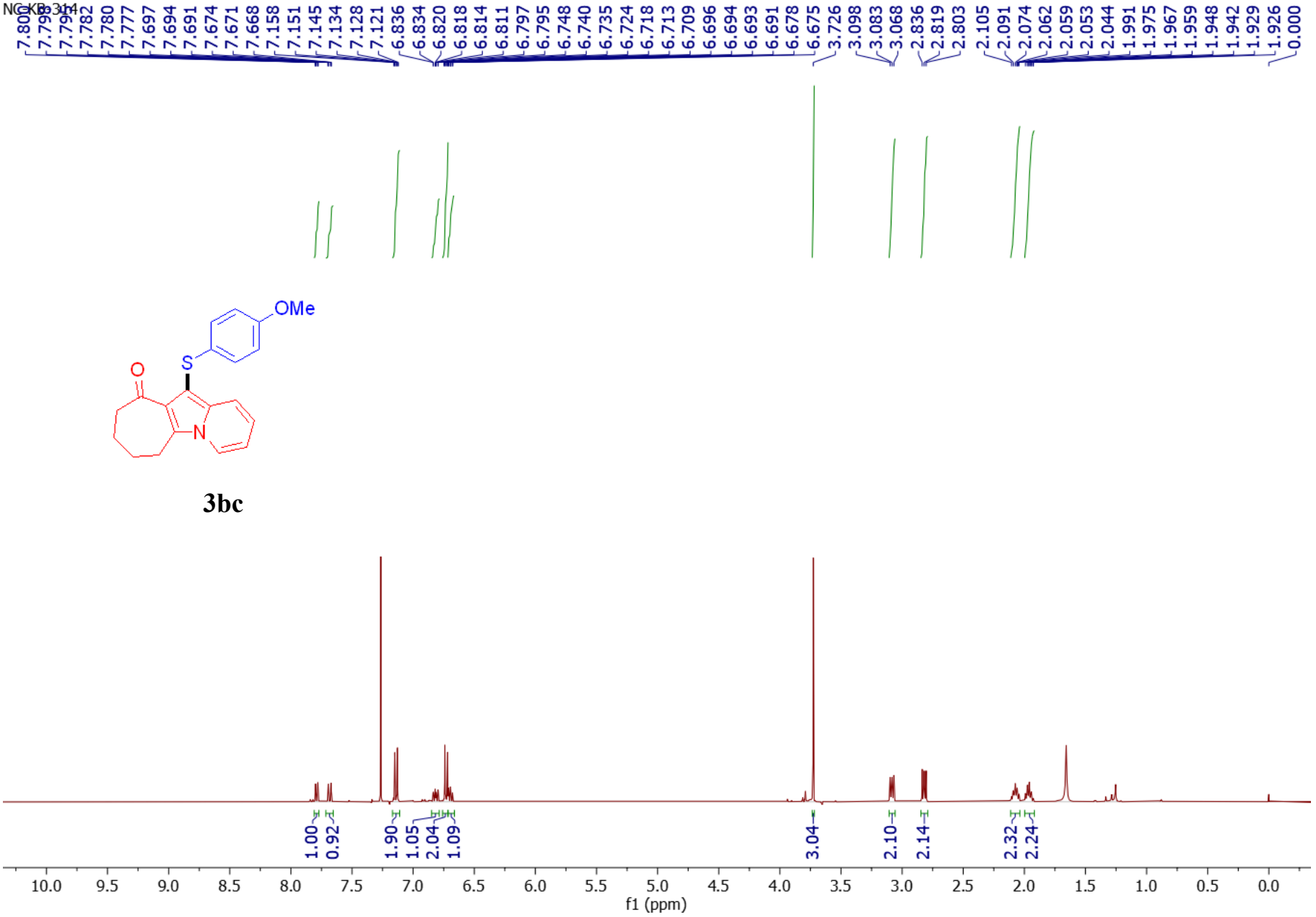
3ba

$^{13}C\{H\}$ NMR spectrum of 3ba (100 MHz, $CDCl_3$)



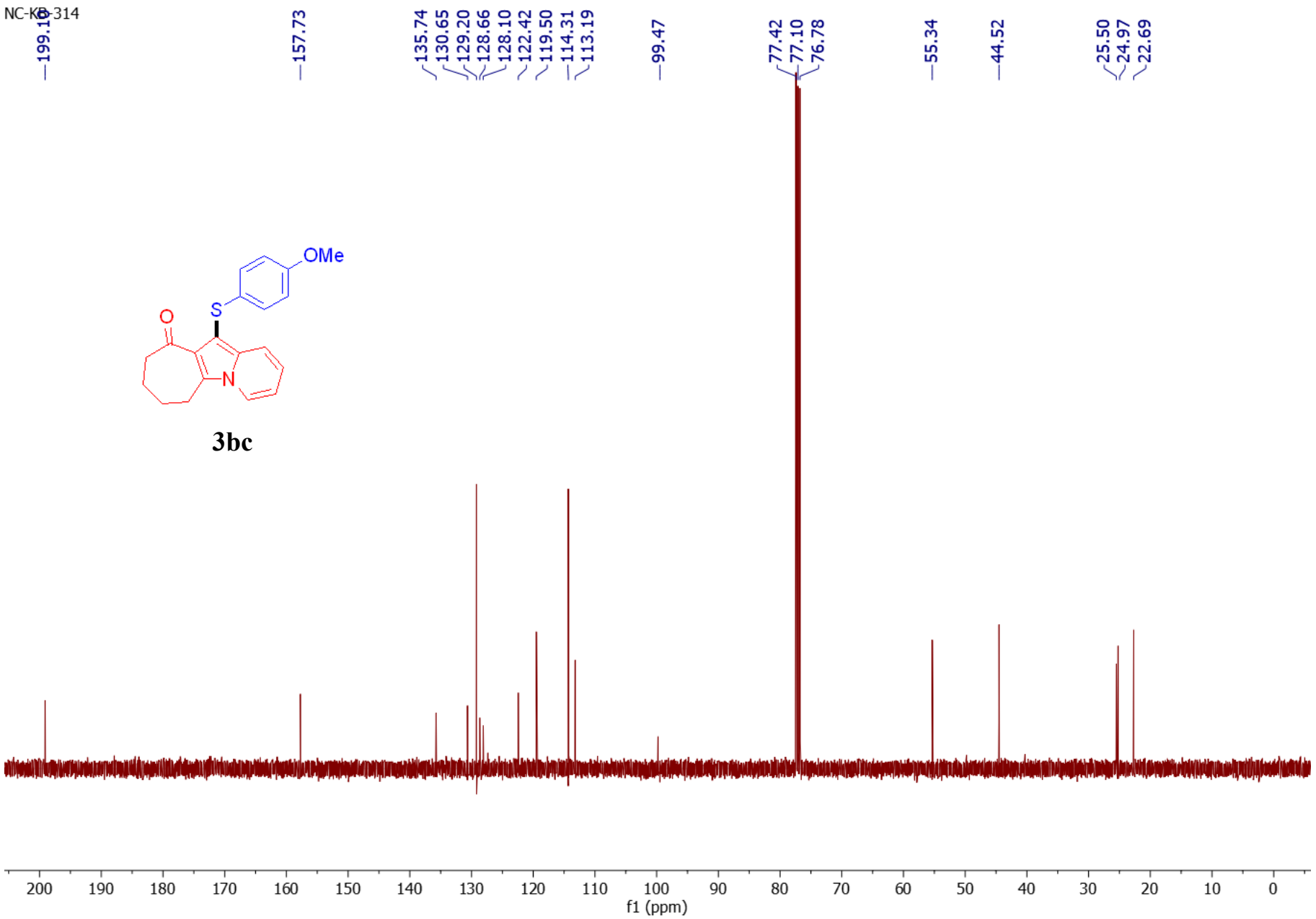
3ba

^{1}H NMR spectrum of 3bc (400 MHz, $CDCl_3$)



3bc

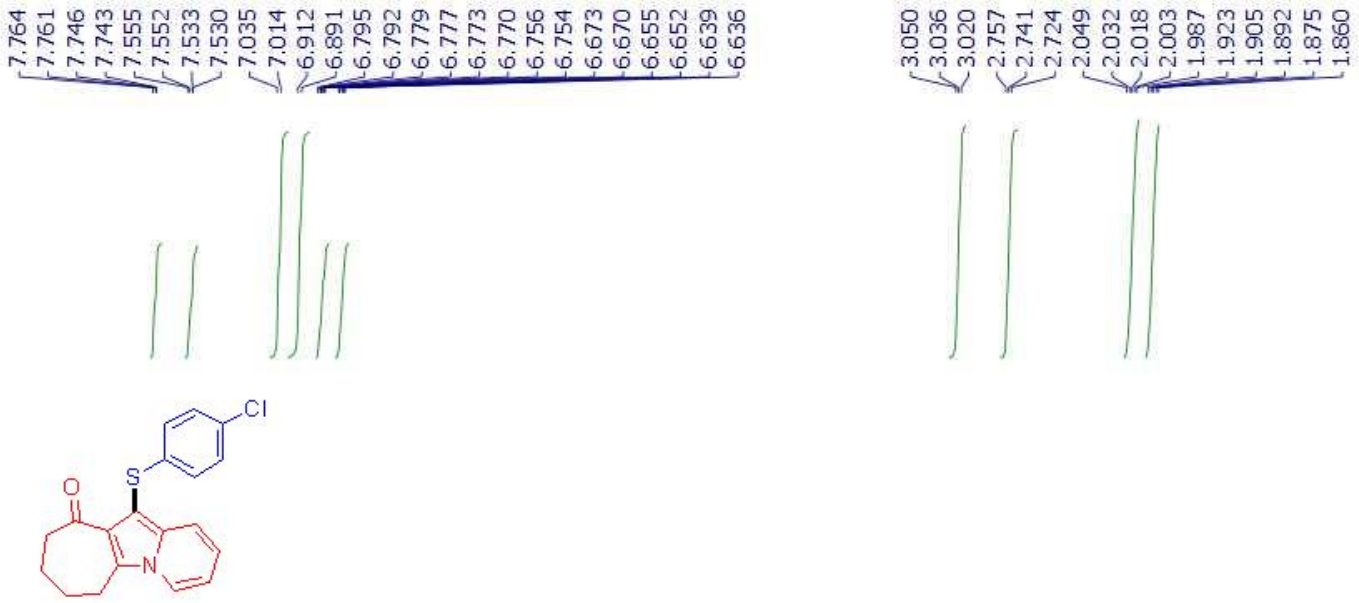
$^{13}C\{H\}$ NMR spectrum of 3bc (100 MHz, $CDCl_3$)



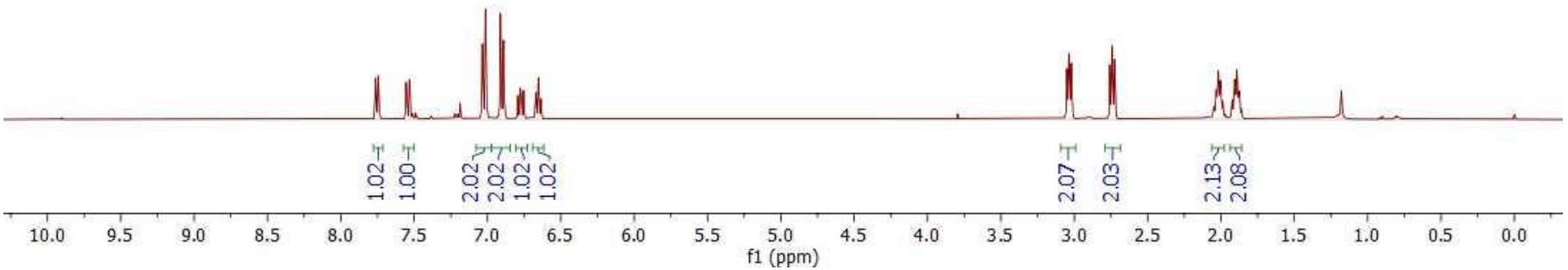
3bc

^{1}H NMR spectrum of 3bd (400 MHz, $CDCl_3$)

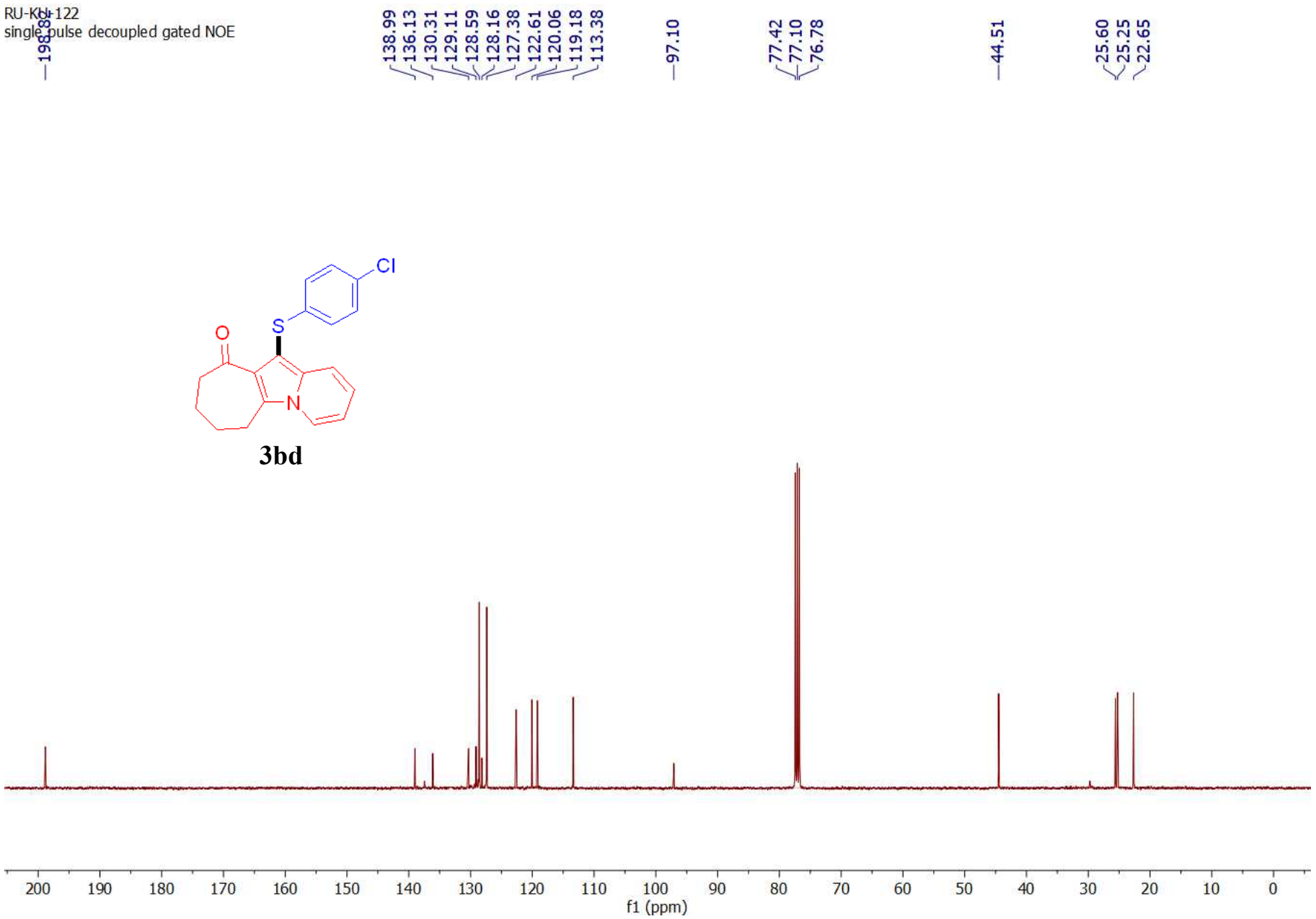
RU-KU-122
single_pulse



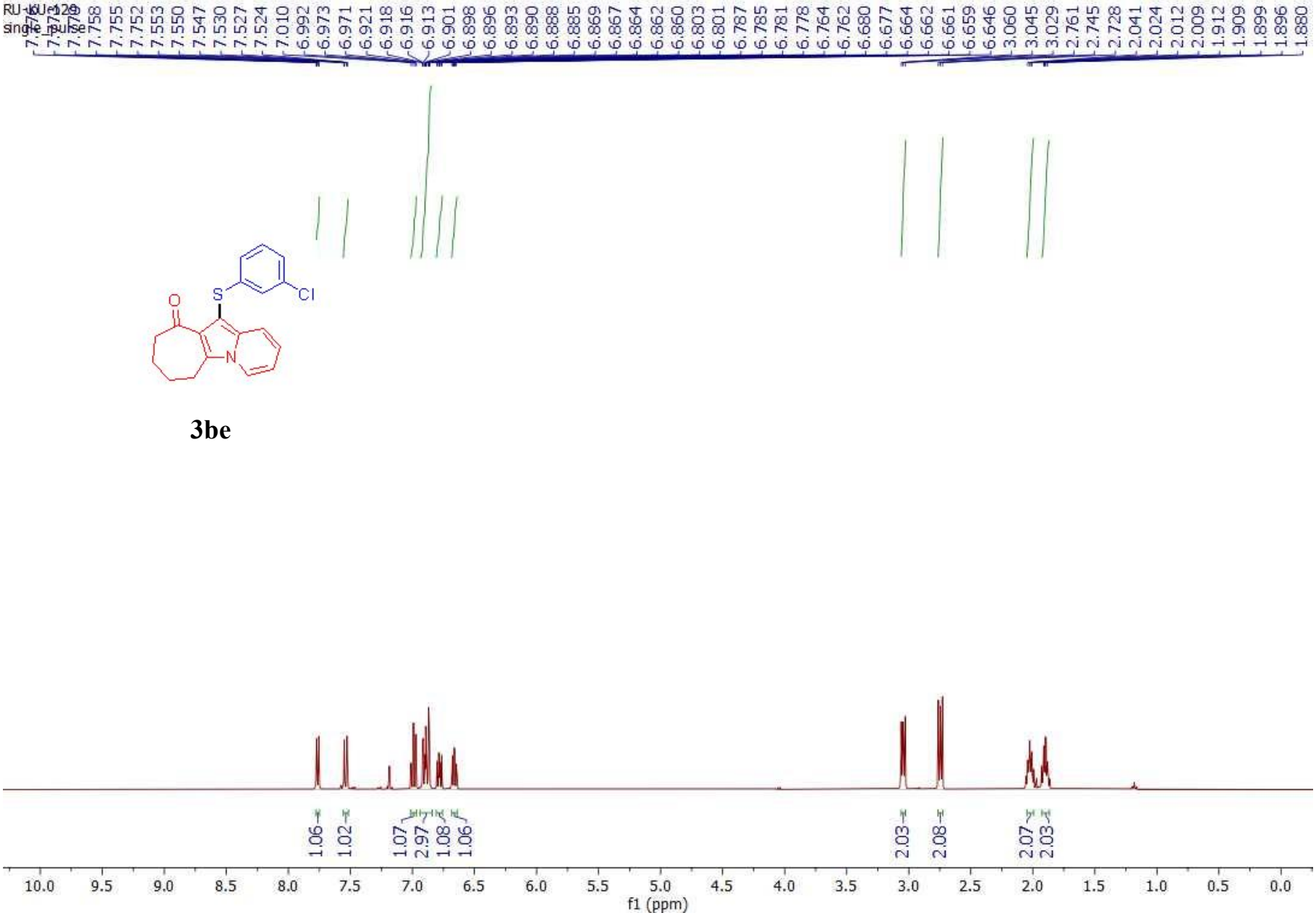
3bd



$^{13}C\{H\}$ NMR spectrum of 3bd (100 MHz, $CDCl_3$)

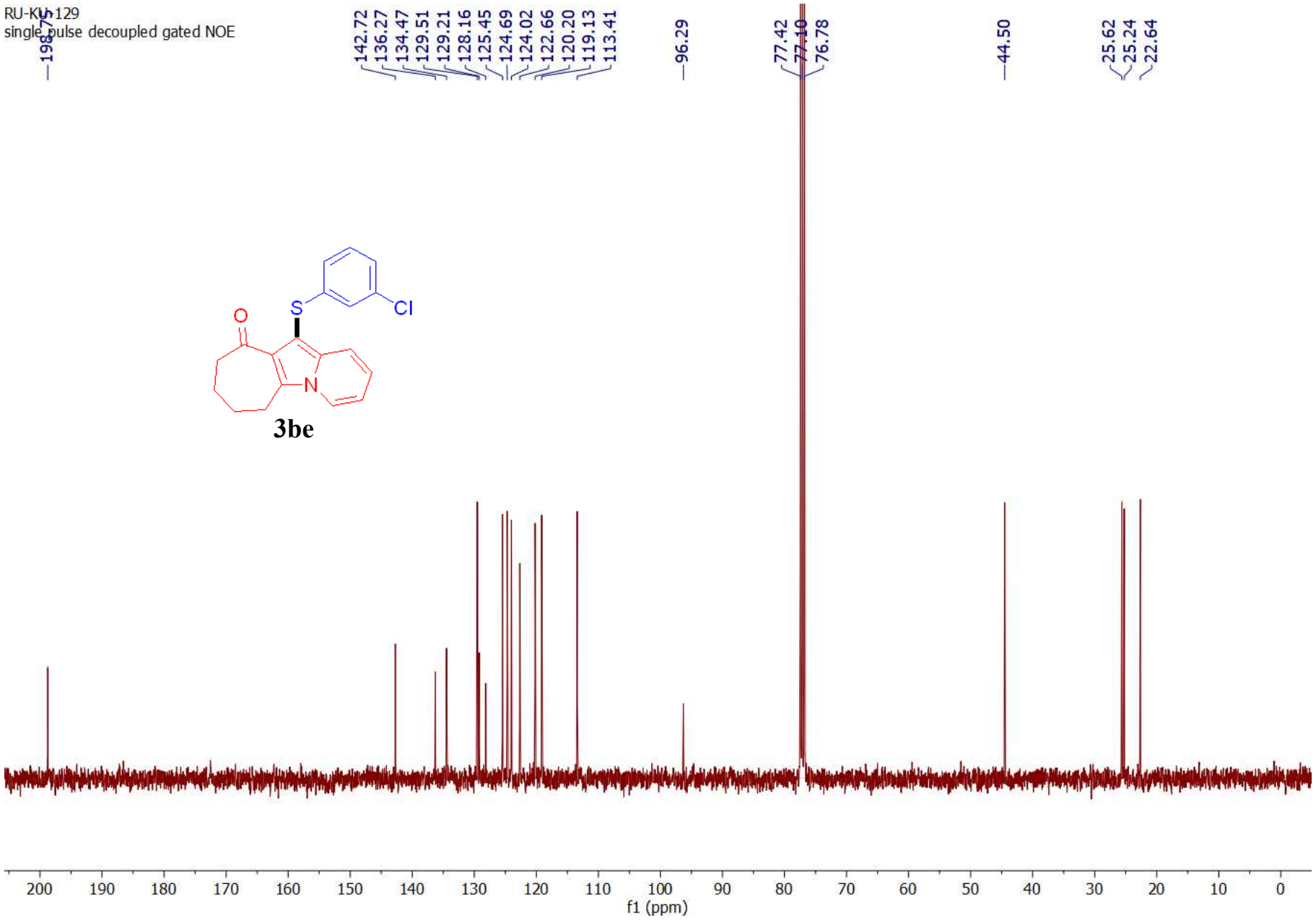


^{1}H NMR spectrum of 3be (400 MHz, $CDCl_3$)

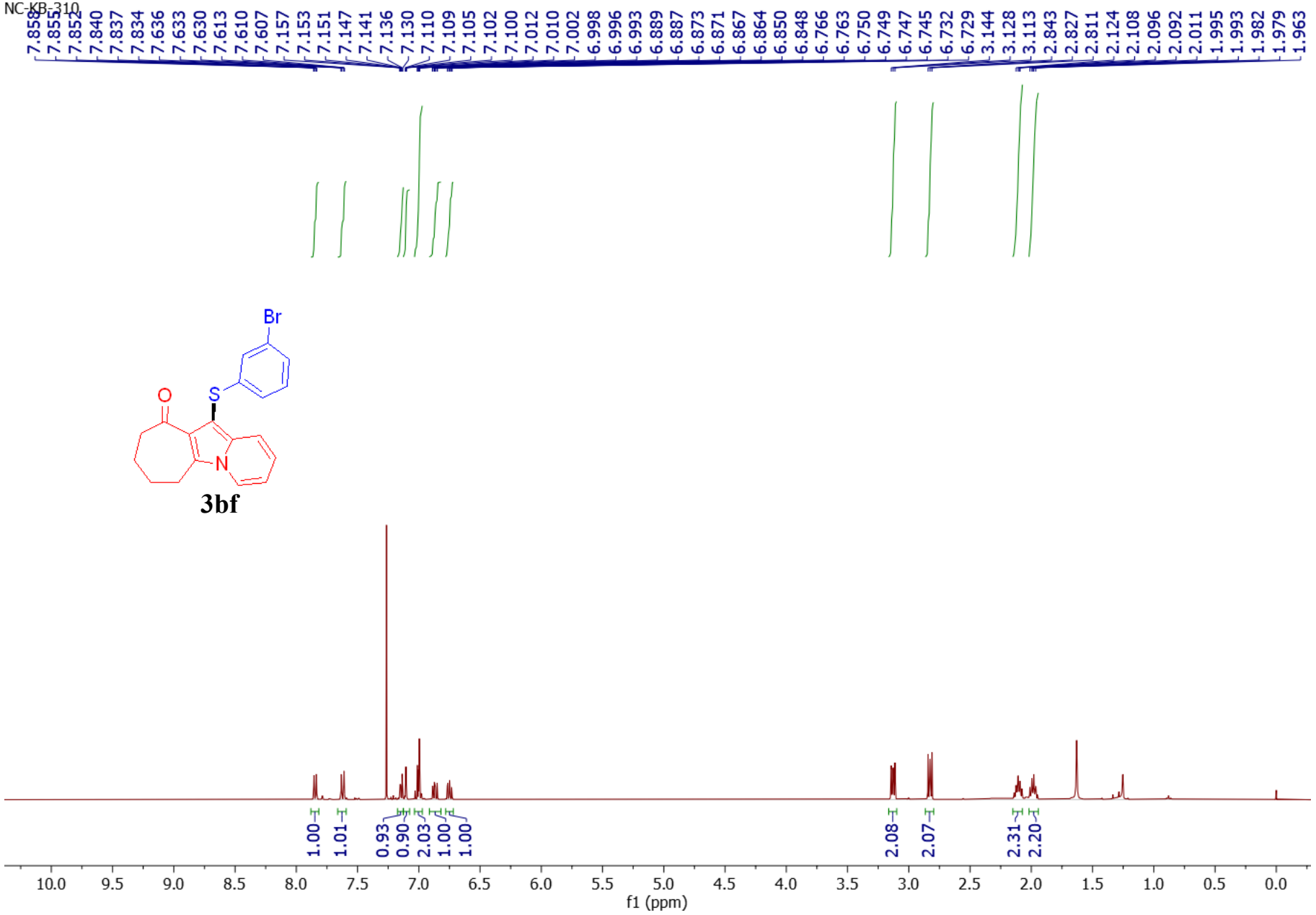


3be

$^{13}C\{H\}$ NMR spectrum of 3be (100 MHz, $CDCl_3$)

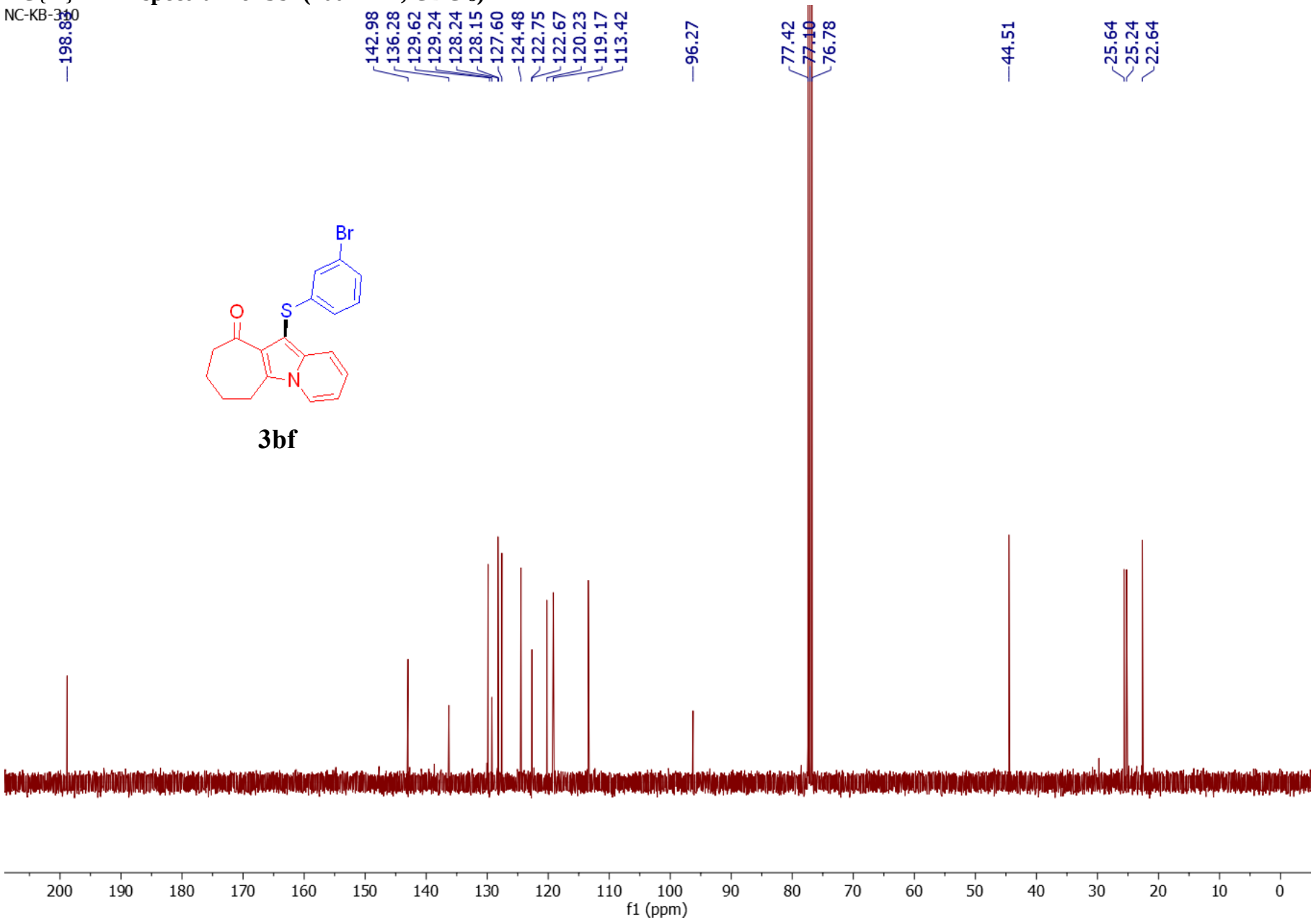


^{1}H NMR spectrum of 3bf (400 MHz, $CDCl_3$)



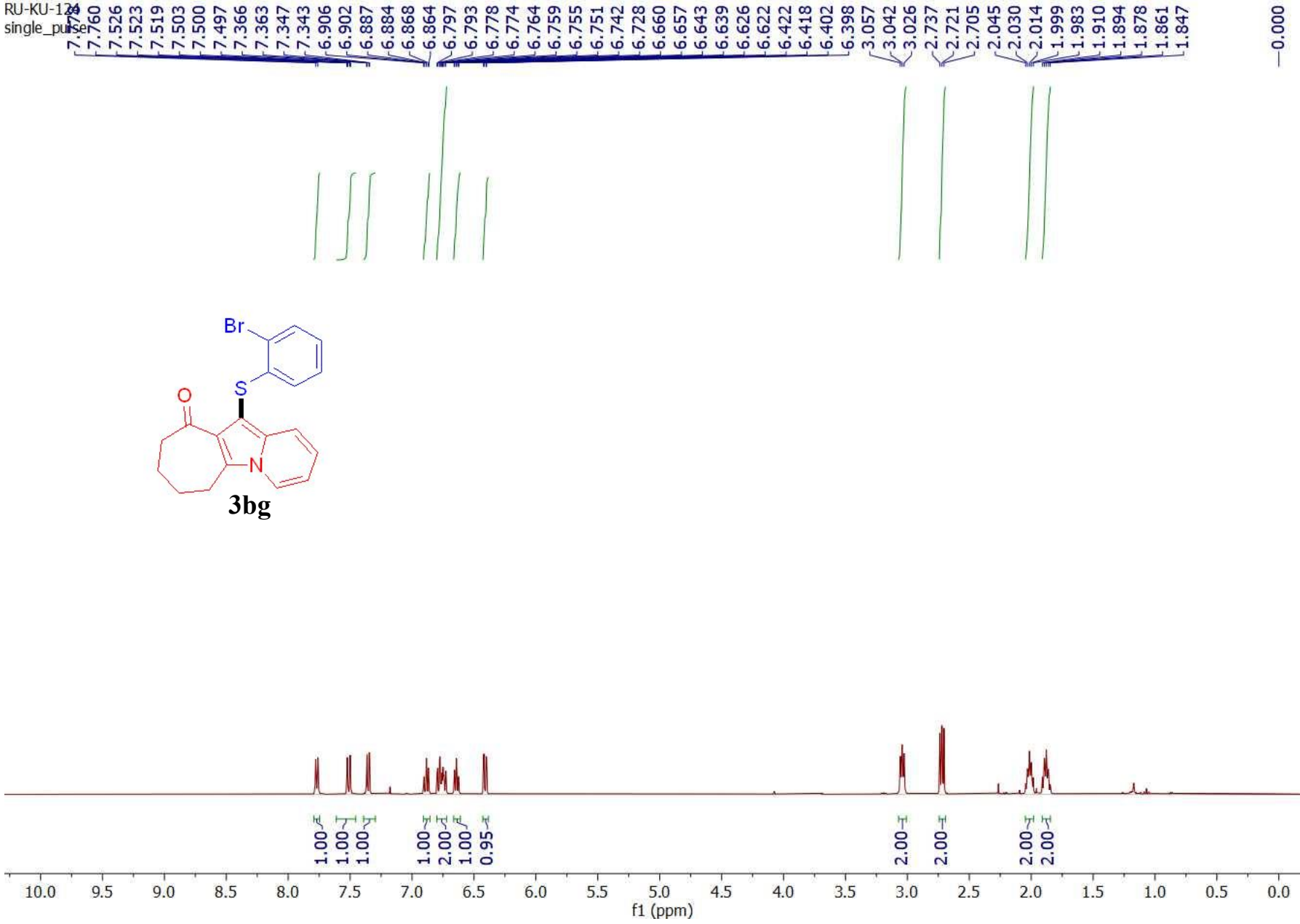
3bf

$^{13}C\{H\}$ NMR spectrum of 3bf (100 MHz, $CDCl_3$)



3bf

^{1}H NMR spectrum of 3bg (400 MHz, $CDCl_3$)



$^{13}C\{H\}$ NMR spectrum of 3bg (100 MHz, $CDCl_3$)

RU-KU-124
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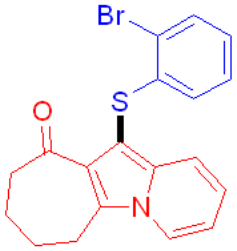
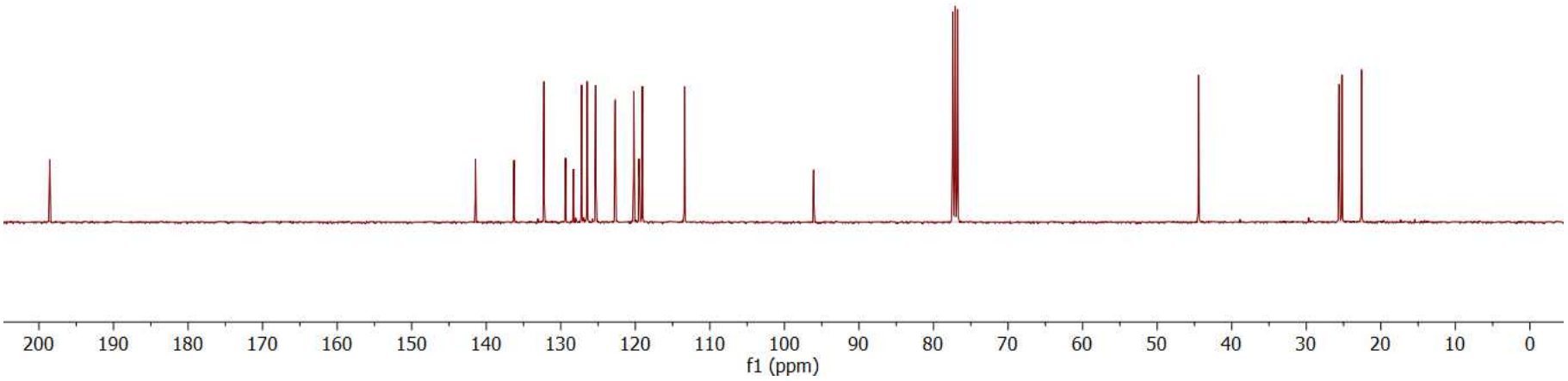
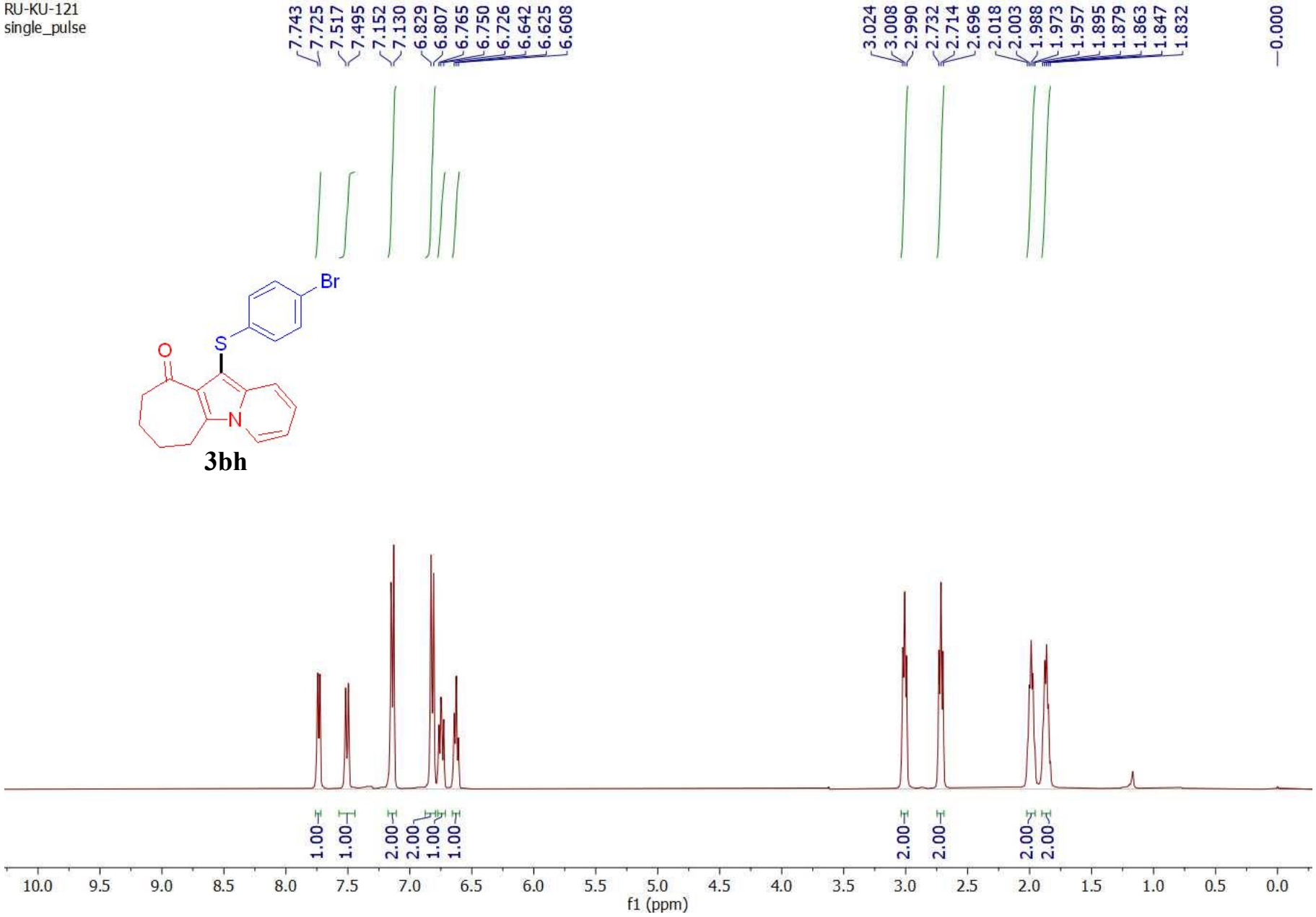


3bg

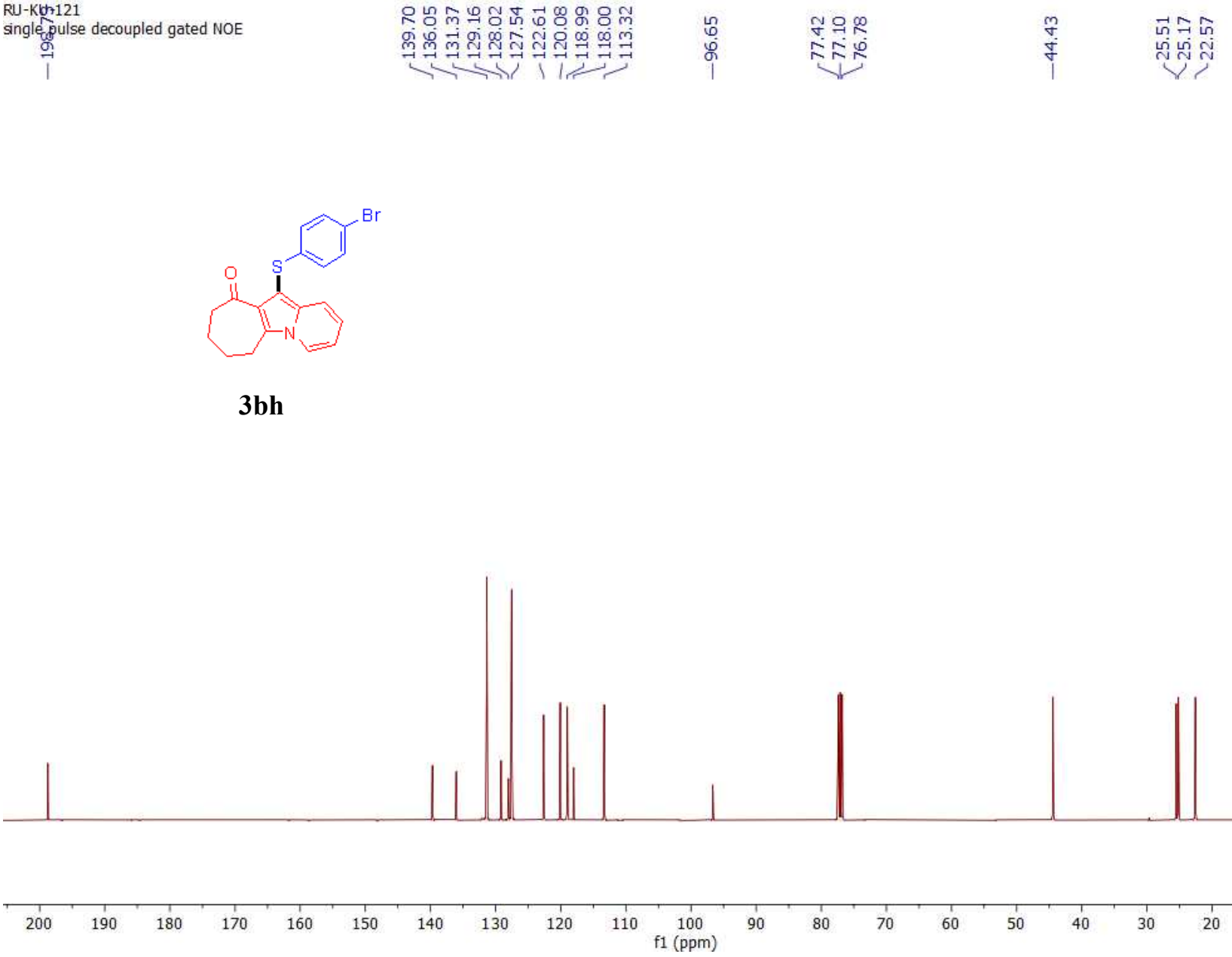


^{1}H NMR spectrum of 3bh (400 MHz, $CDCl_3$)



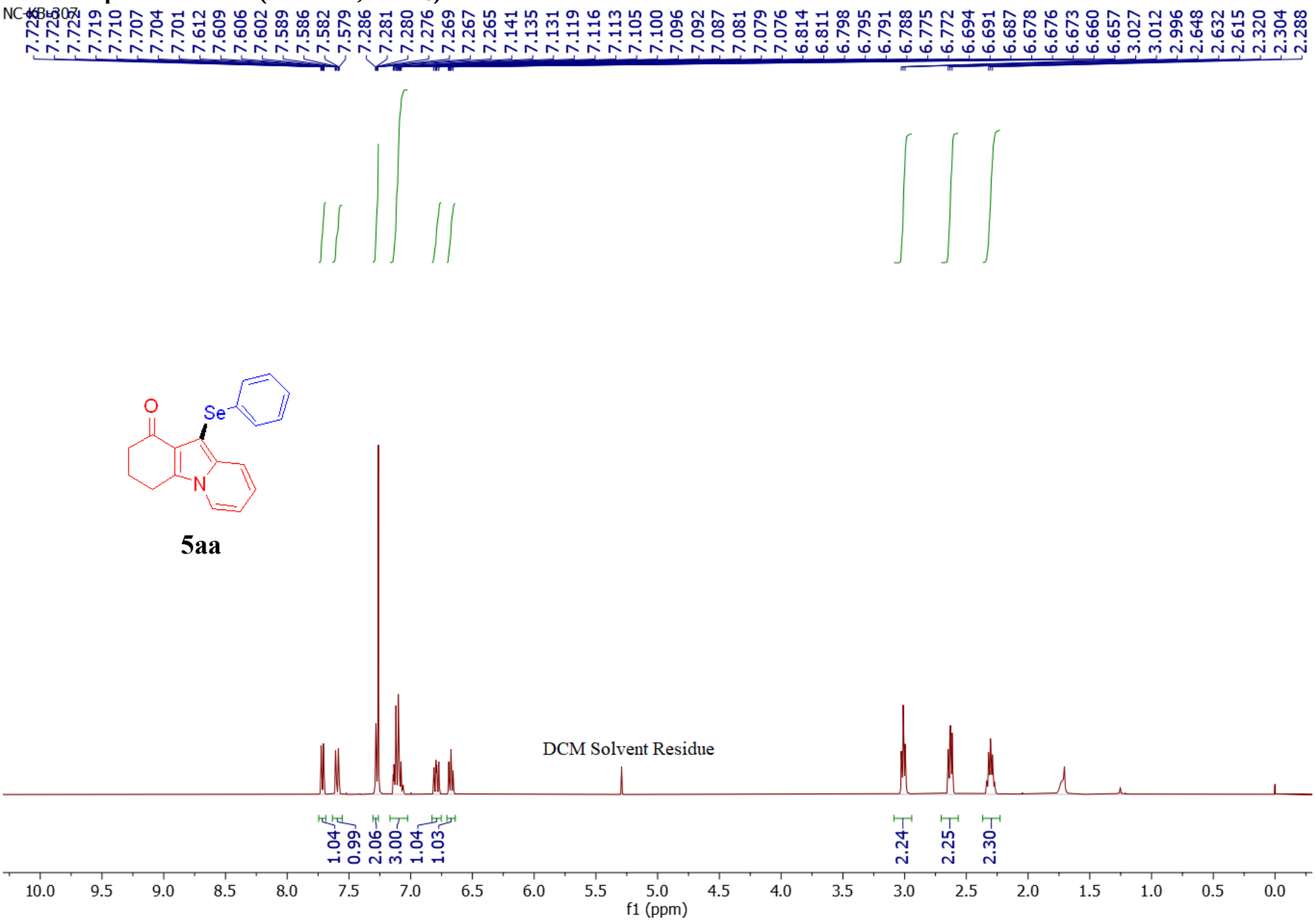
3bh

$^{13}C\{H\}$ NMR spectrum of 3bh (100 MHz, $CDCl_3$)

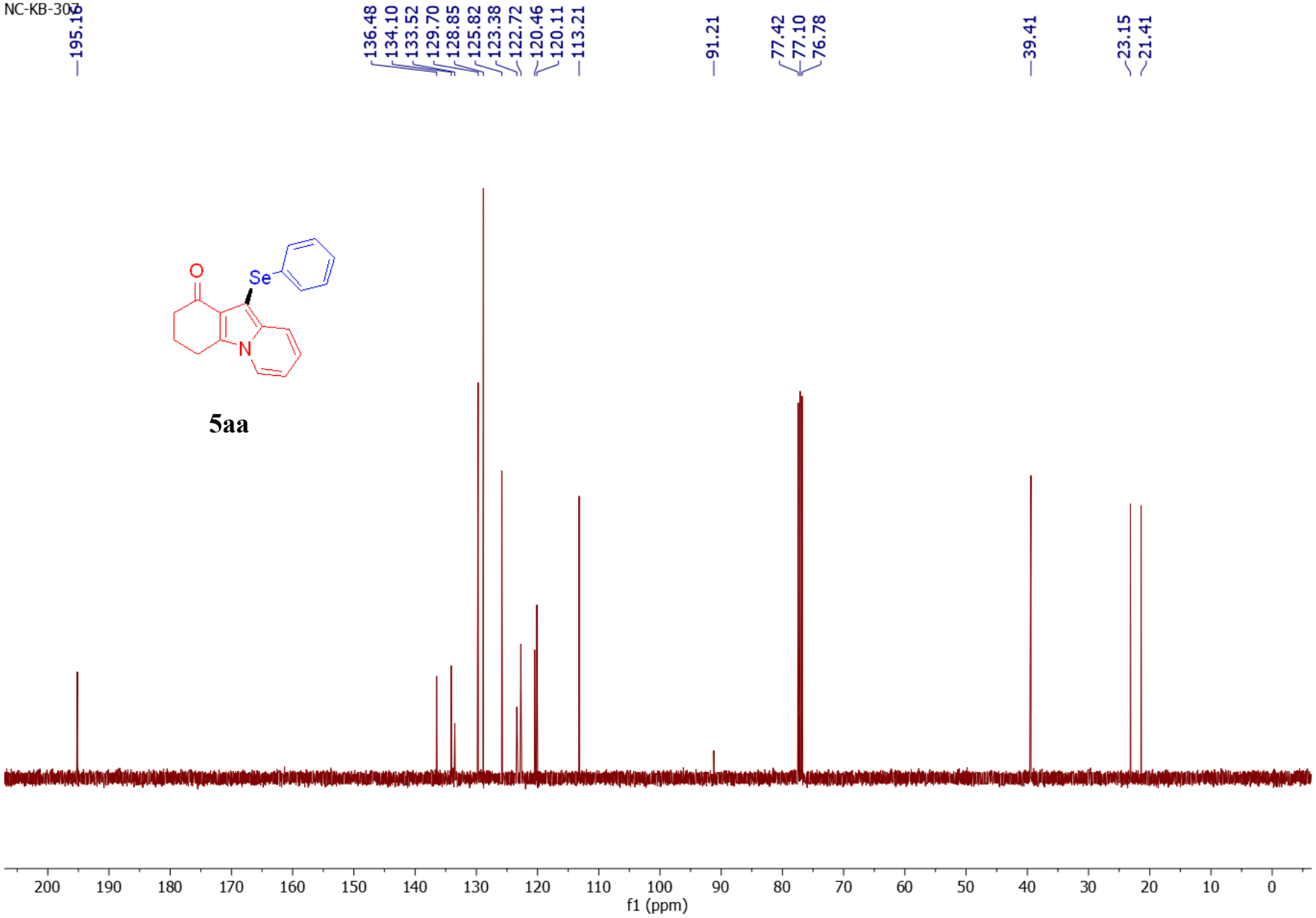


3bh

^{1}H NMR spectrum of 5aa (400 MHz, $CDCl_3$)



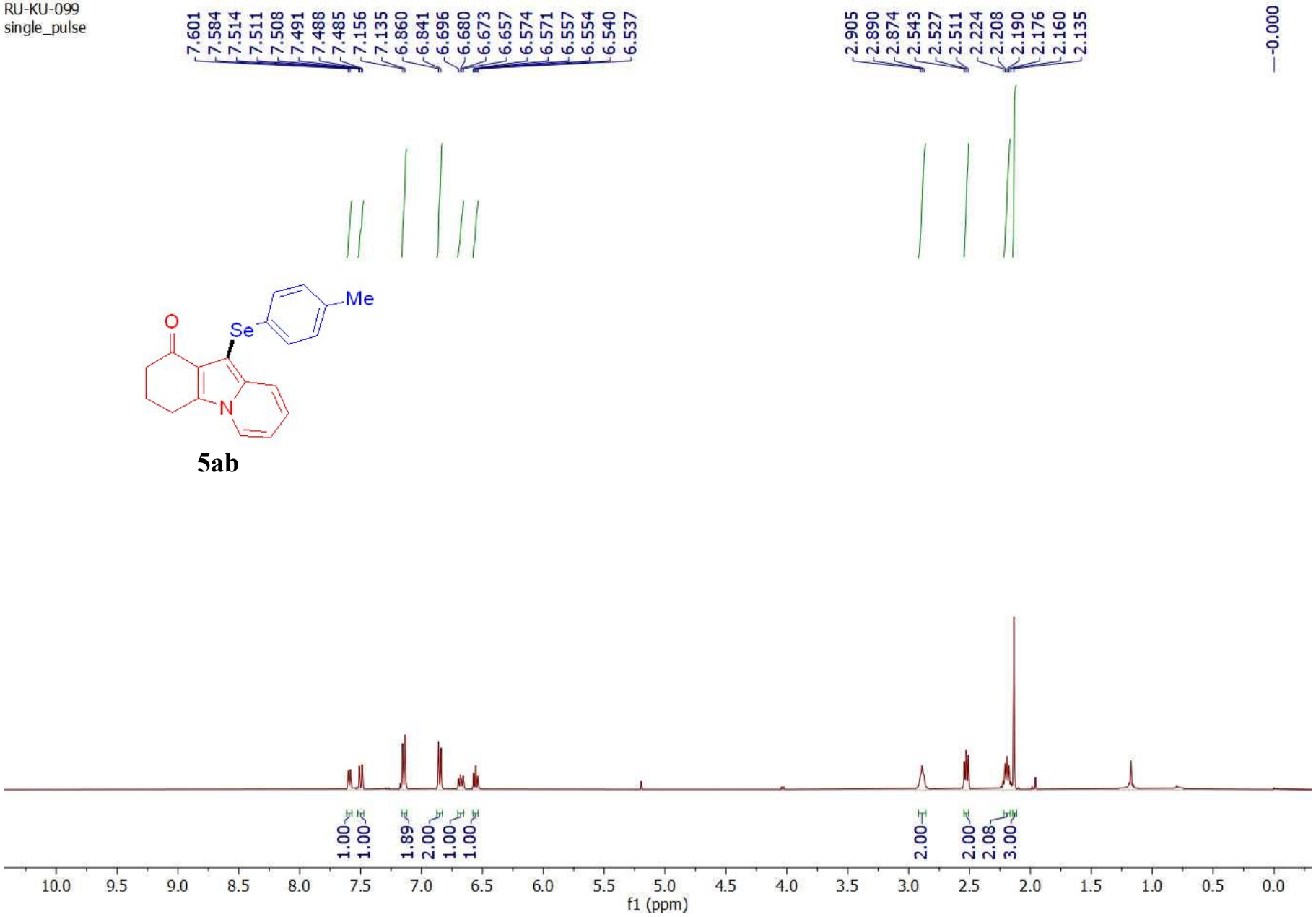
$^{13}C\{H\}$ NMR spectrum of 5aa (100 MHz, $CDCl_3$)



5aa

^{1}H NMR spectrum of 5ab (400 MHz, $CDCl_3$)

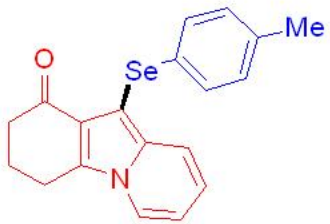
RU-KU-099
single_pulse



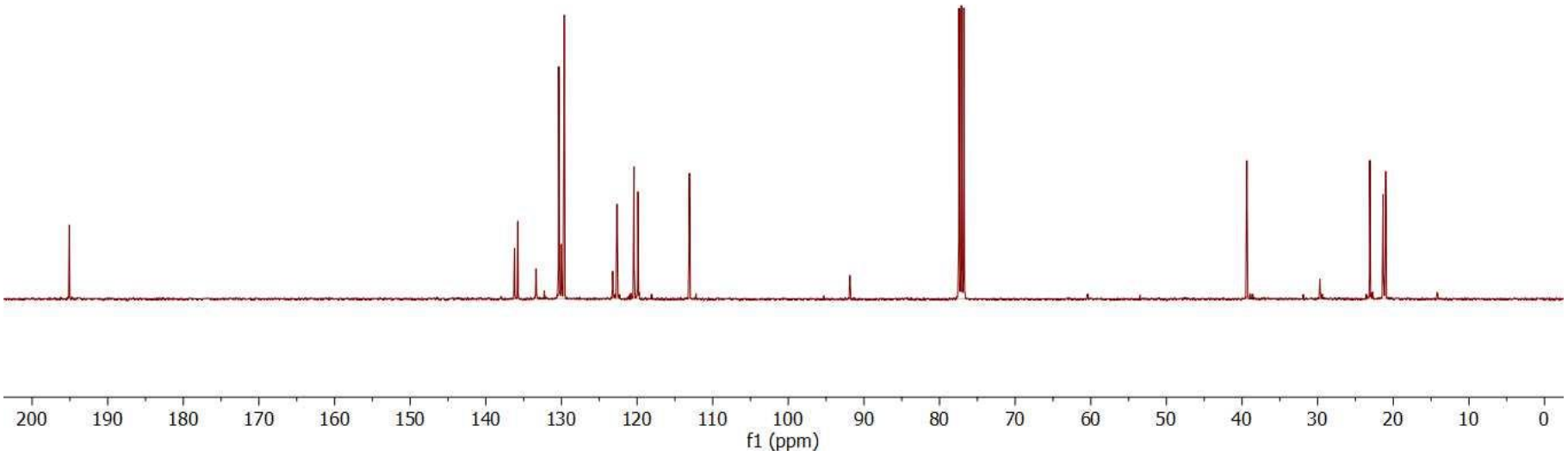
5ab

$^{13}C\{H\}$ NMR spectrum of 5ab (100 MHz, $CDCl_3$)

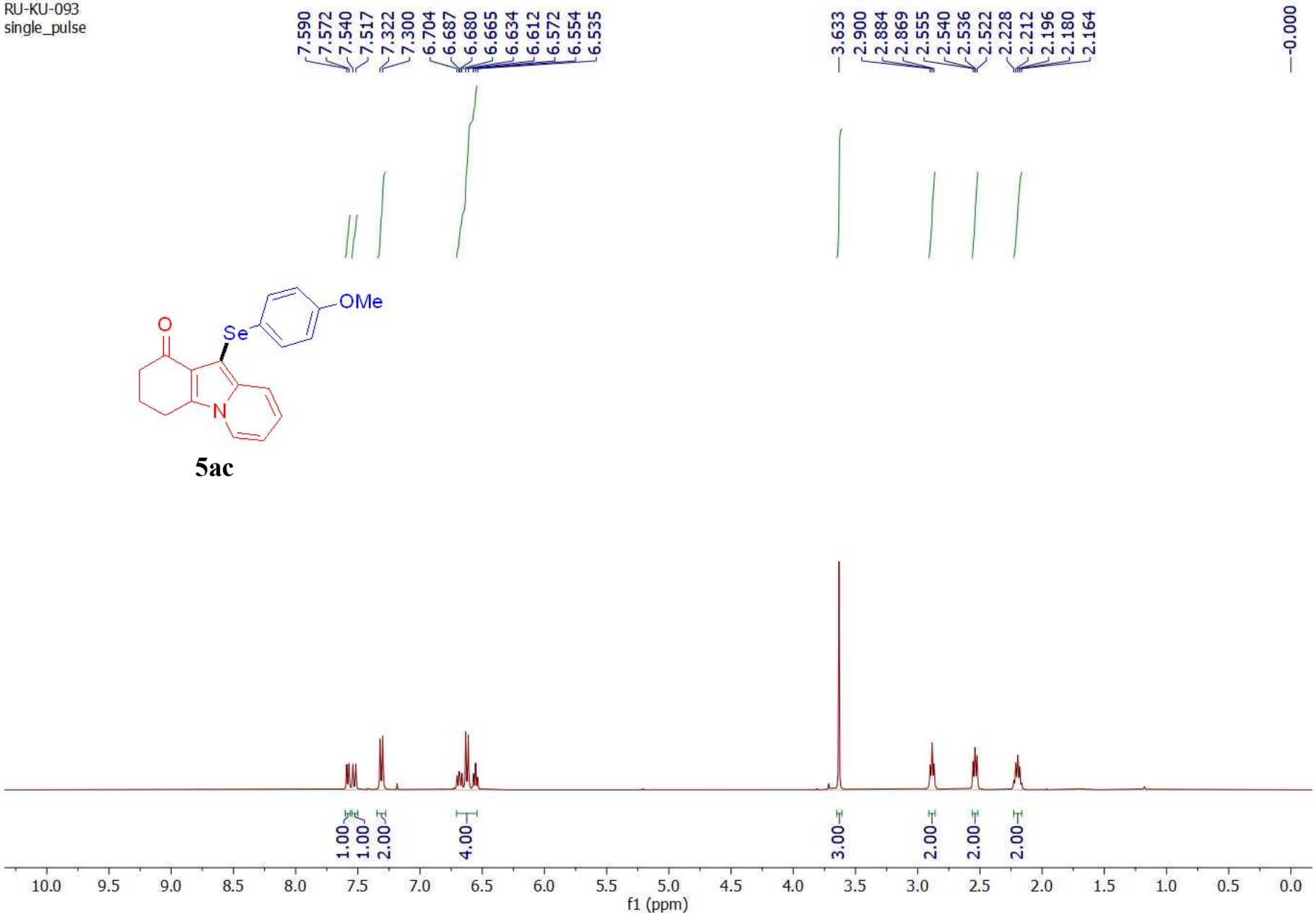
RU-KU-099
single pulse decoupled gated NOE



5ab



^{1}H NMR spectrum of 5ac (400 MHz, $CDCl_3$)



5ac

$^{13}C\{H\}$ NMR spectrum of 5ac (100 MHz, $CDCl_3$)

RU-KU-093
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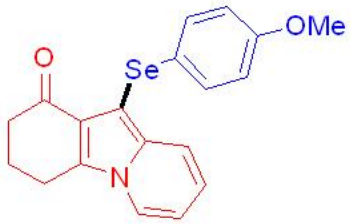
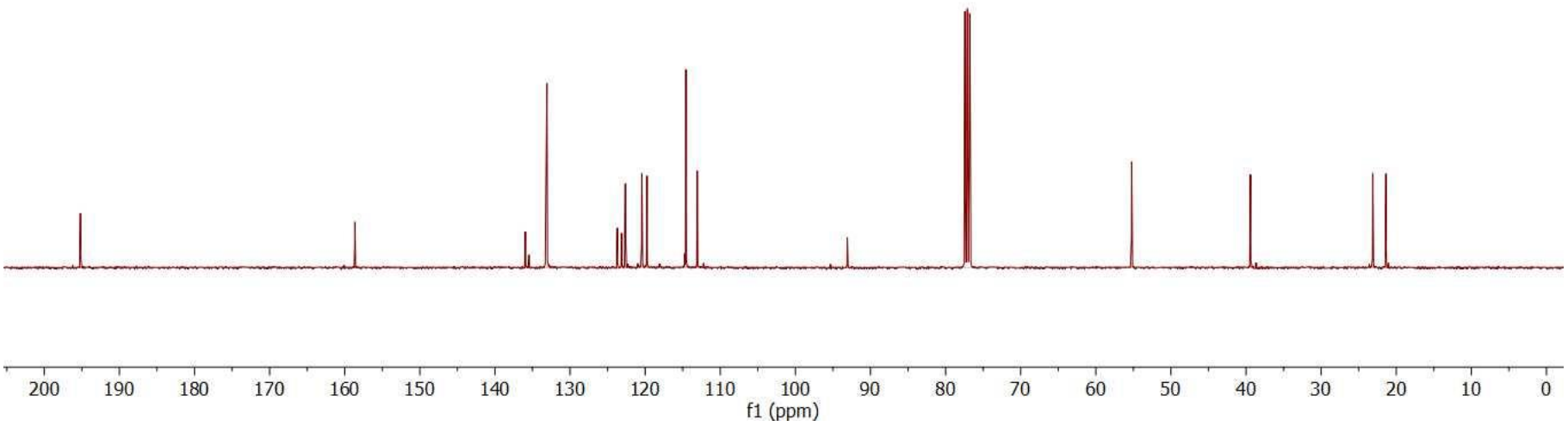
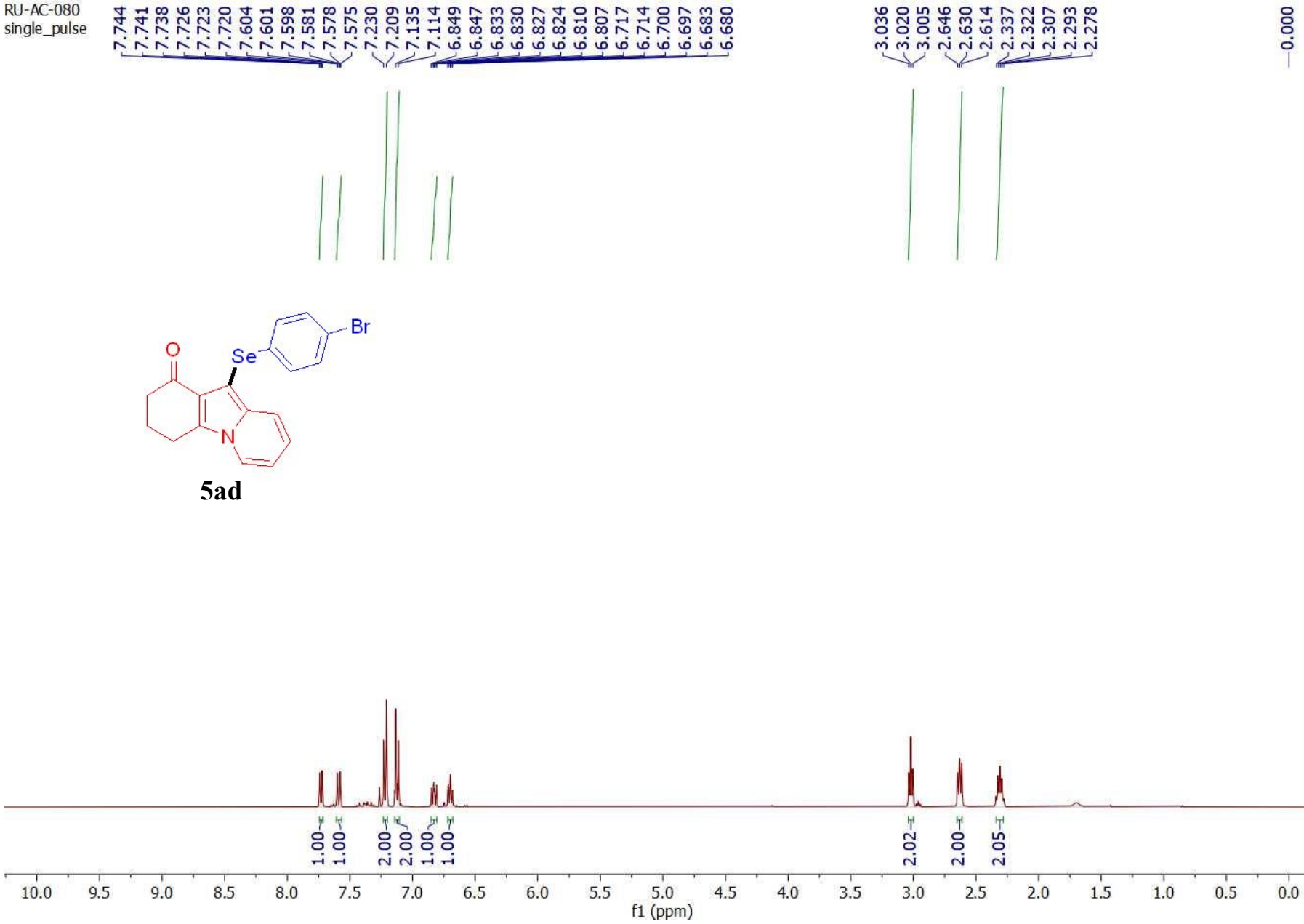


5ac

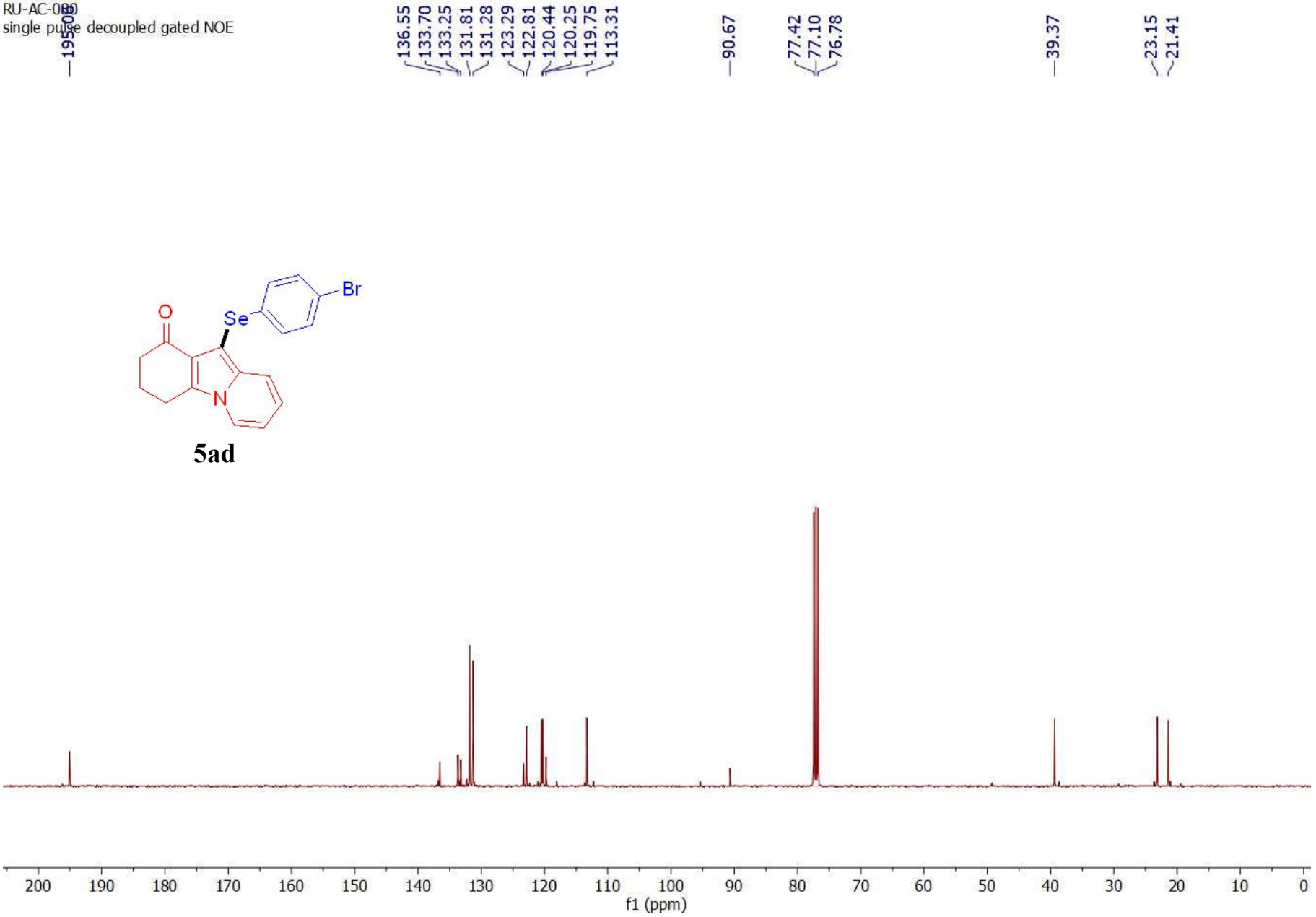


^{1}H NMR spectrum of 5ad (400 MHz, $CDCl_3$)



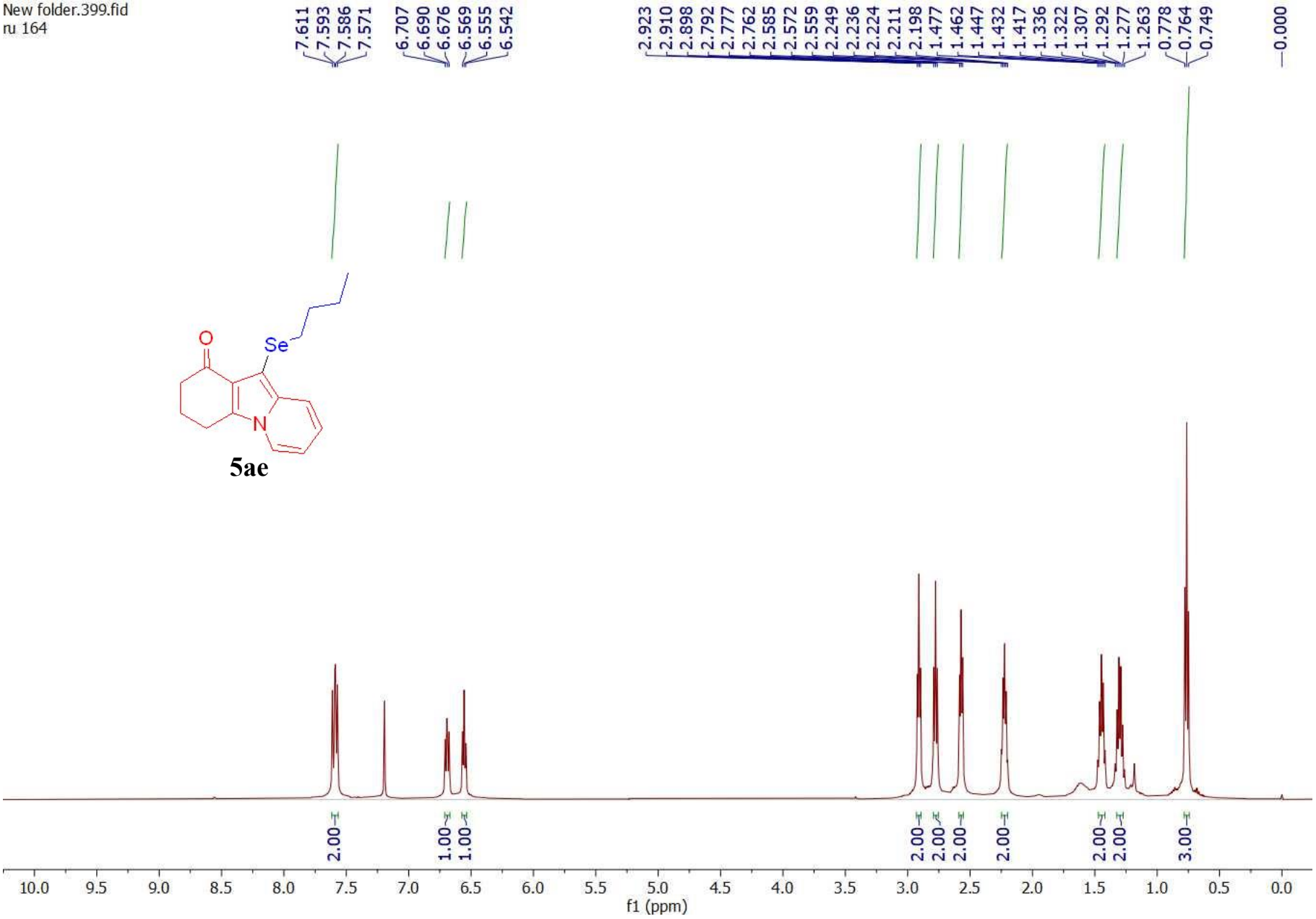
5ad

$^{13}C\{H\}$ NMR spectrum of 5ad (100 MHz, $CDCl_3$)



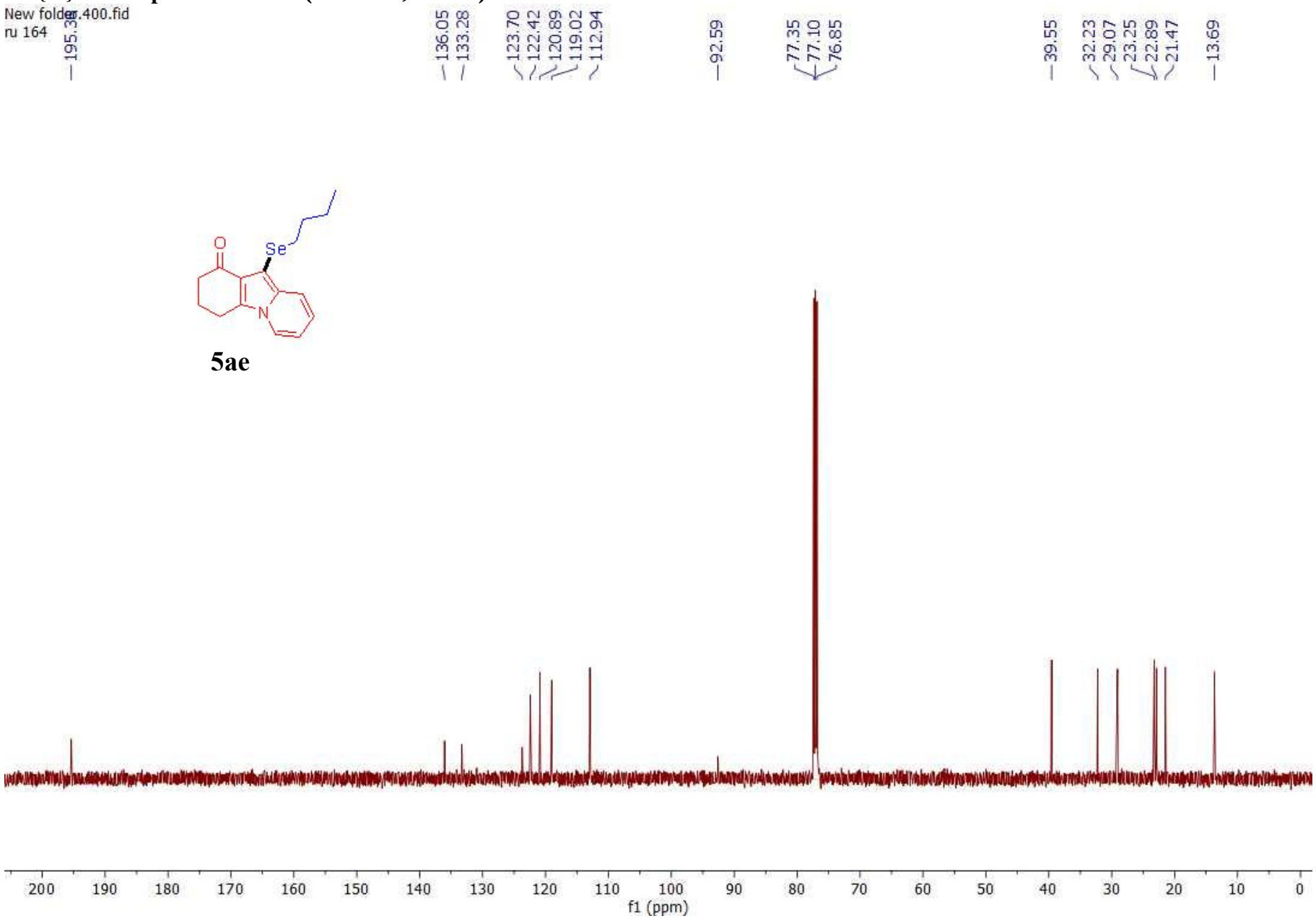
5ad

^{1}H NMR spectrum of 5ae (400 MHz, $CDCl_3$)



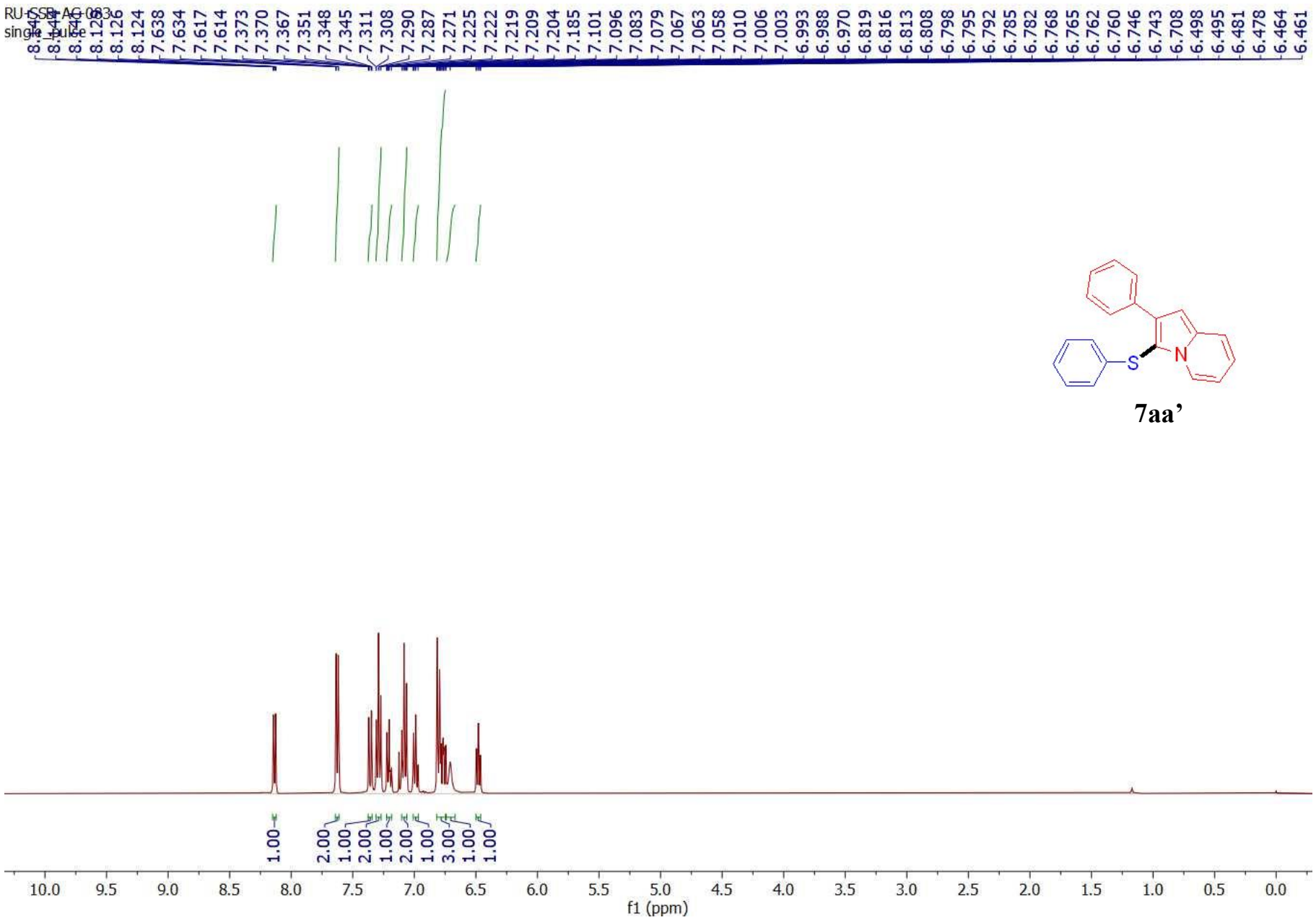
5ae

$^{13}C\{H\}$ NMR spectrum of 5ae (100 MHz, $CDCl_3$)



5ae

^{1}H NMR spectrum of 7aa' (400 MHz, $CDCl_3$)

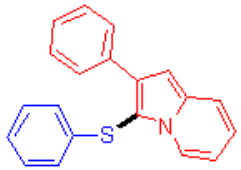


7aa'

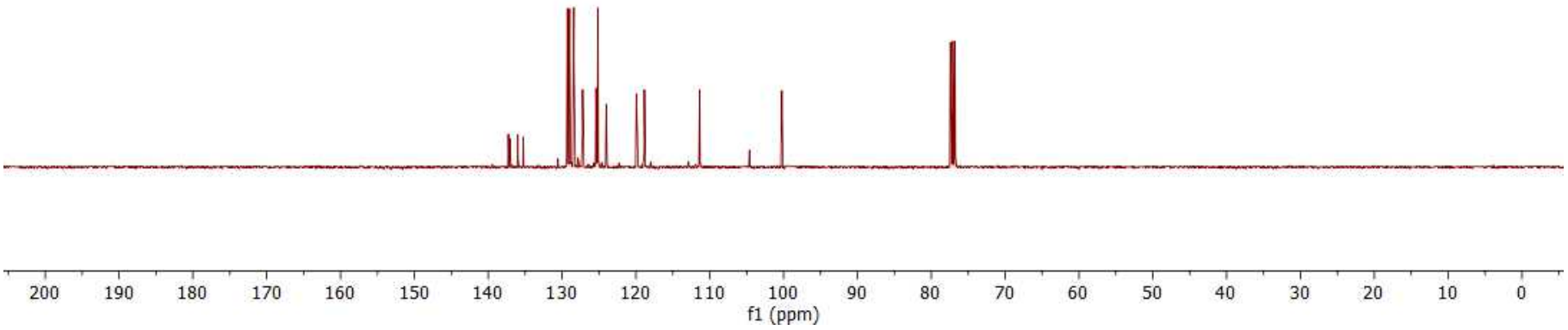
$^{13}C\{H\}$ NMR spectrum of 7aa' (100 MHz, $CDCl_3$)

RU-SSB-AC-083
single pulse decoupled gated NOE

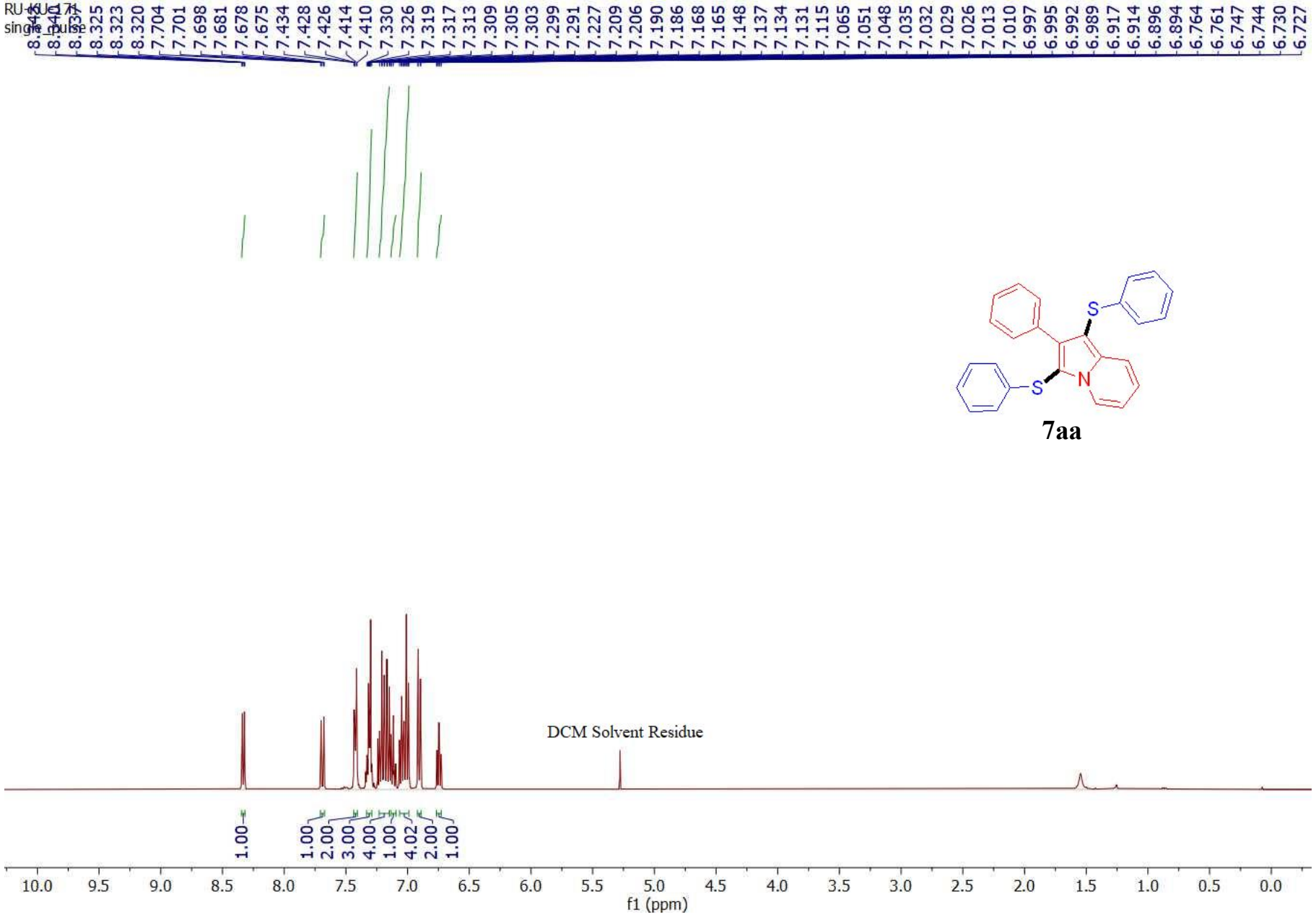
137.28
137.05
135.99
135.24
129.28
128.97
128.40
127.21
125.41
125.15
124.02
119.95
118.85
111.35
104.61
100.23
77.42
77.10
76.78



7aa'

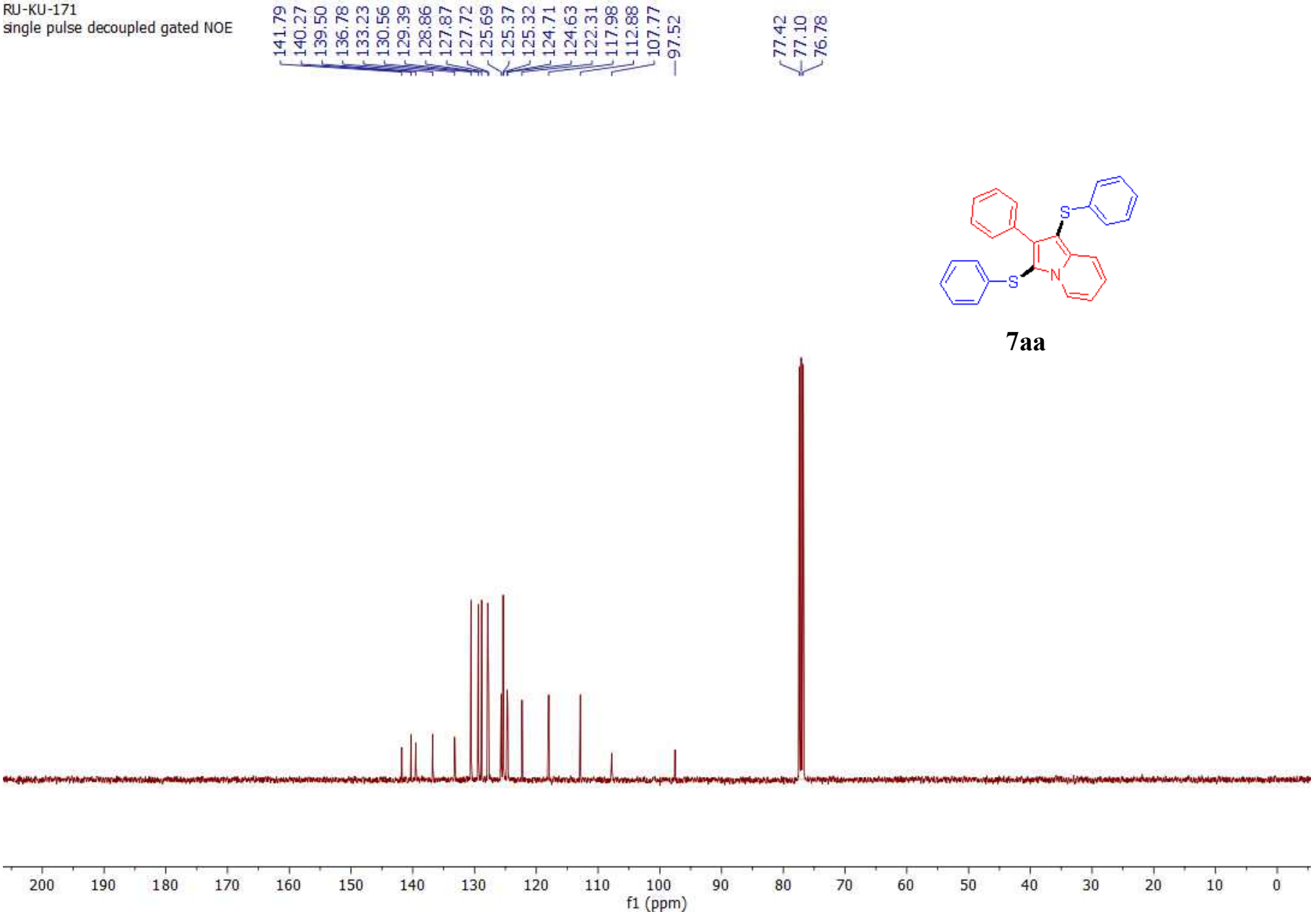


^{1}H NMR spectrum of 7aa (400 MHz, $CDCl_3$)



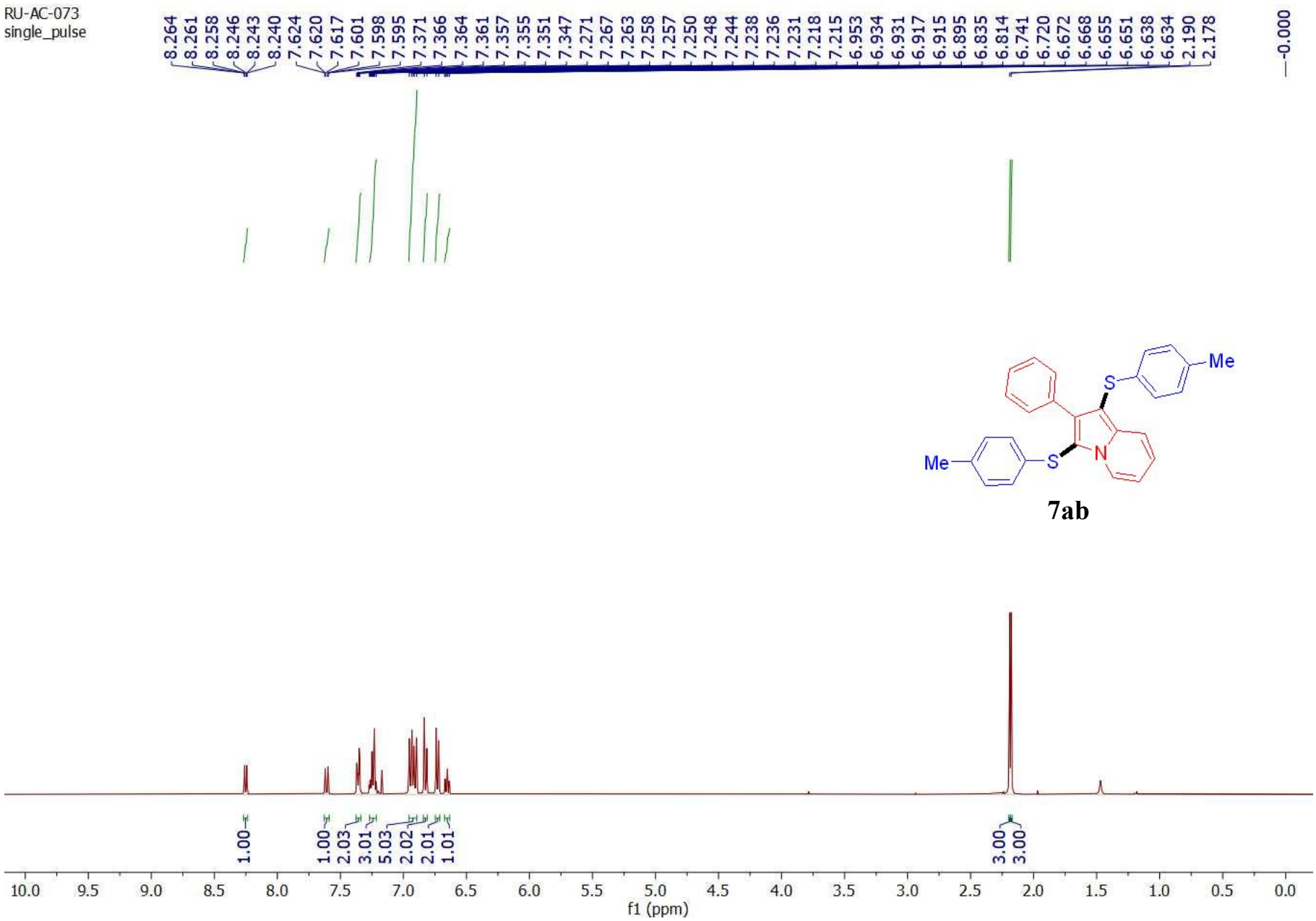
$^{13}C\{H\}$ NMR spectrum of 7aa (100 MHz, $CDCl_3$)

RU-KU-171
single pulse decoupled gated NOE



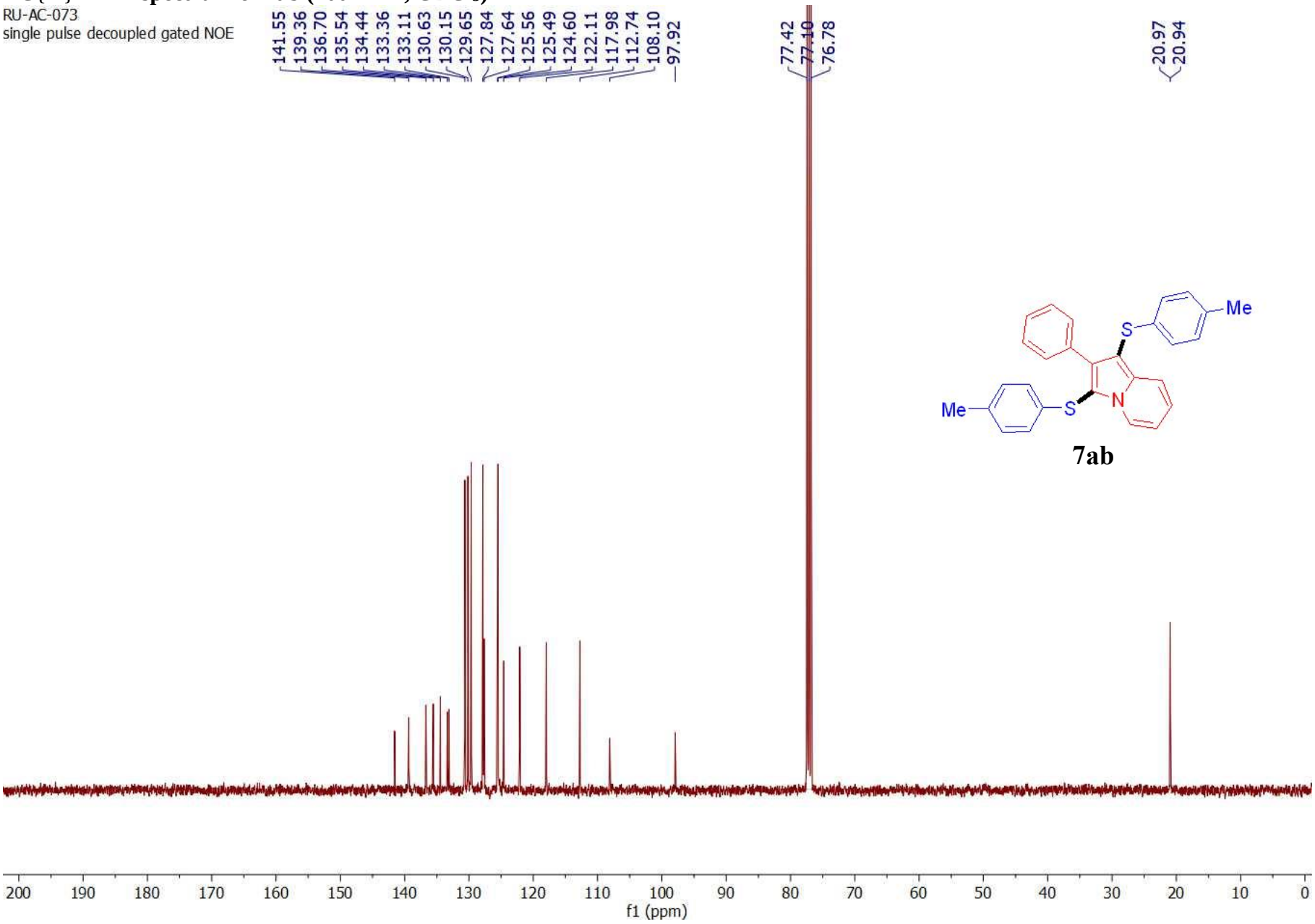
7aa

^{1}H NMR spectrum of 7ab (400 MHz, $CDCl_3$)



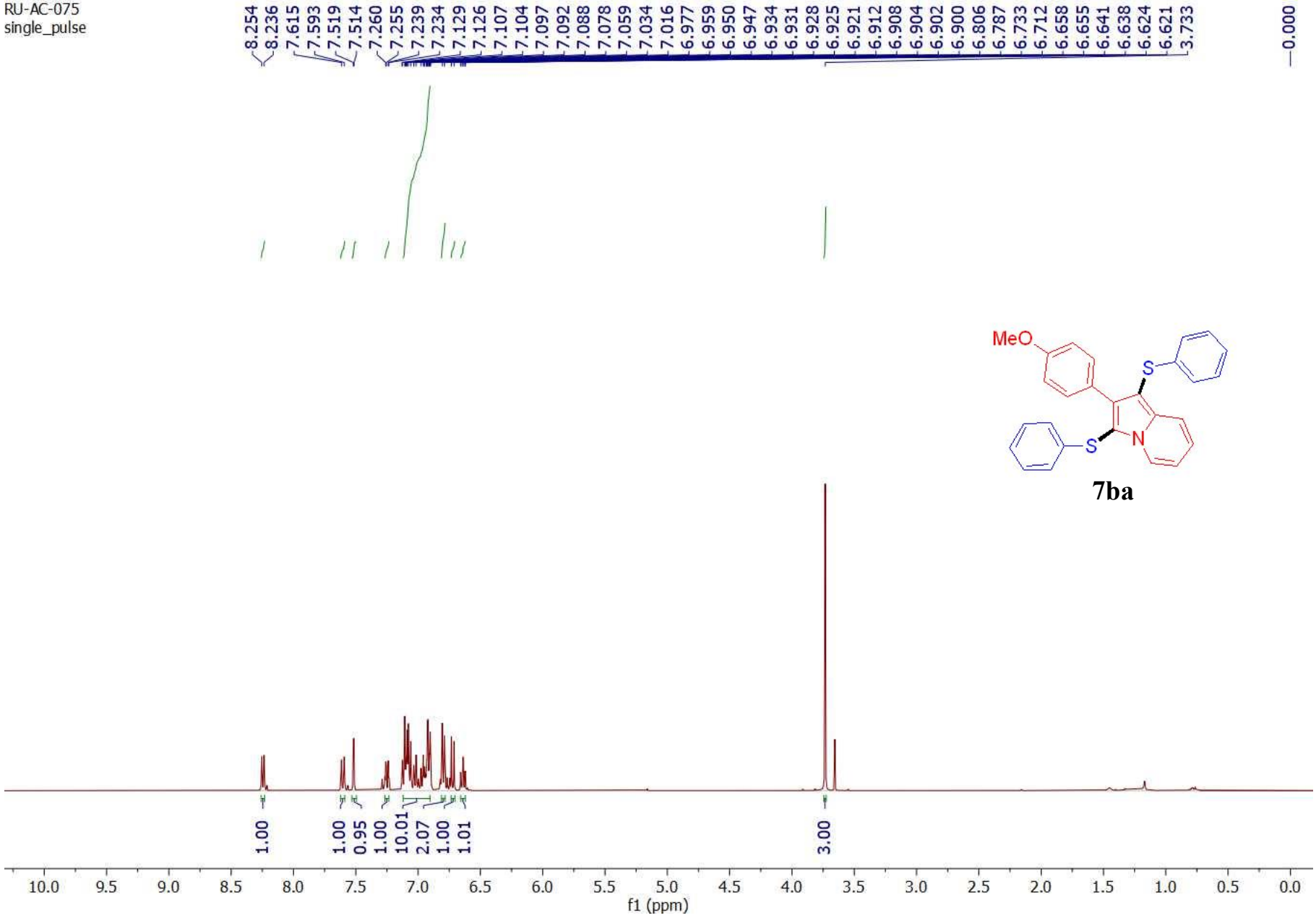
$^{13}C\{H\}$ NMR spectrum of 7ab (100 MHz, $CDCl_3$)

RU-AC-073
single pulse decoupled gated NOE



7ab

^{1}H NMR spectrum of 7ba (400 MHz, $CDCl_3$)

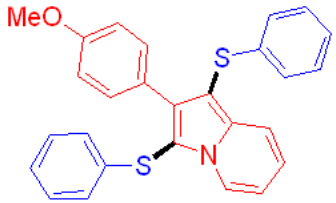


7ba

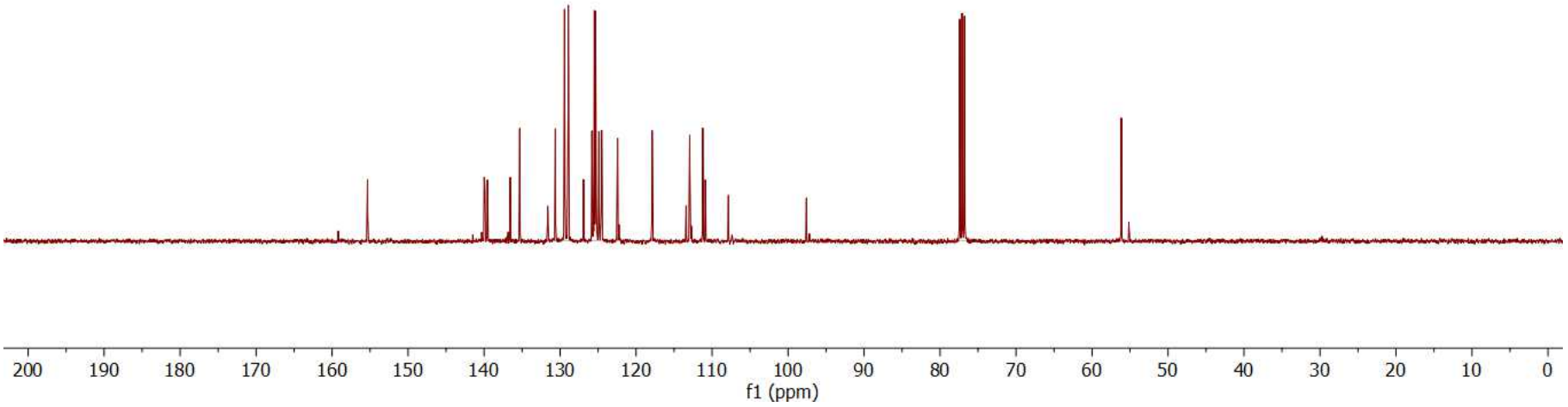
$^{13}C\{H\}$ NMR spectrum of 7ba (100 MHz, $CDCl_3$)

RU-AC-075

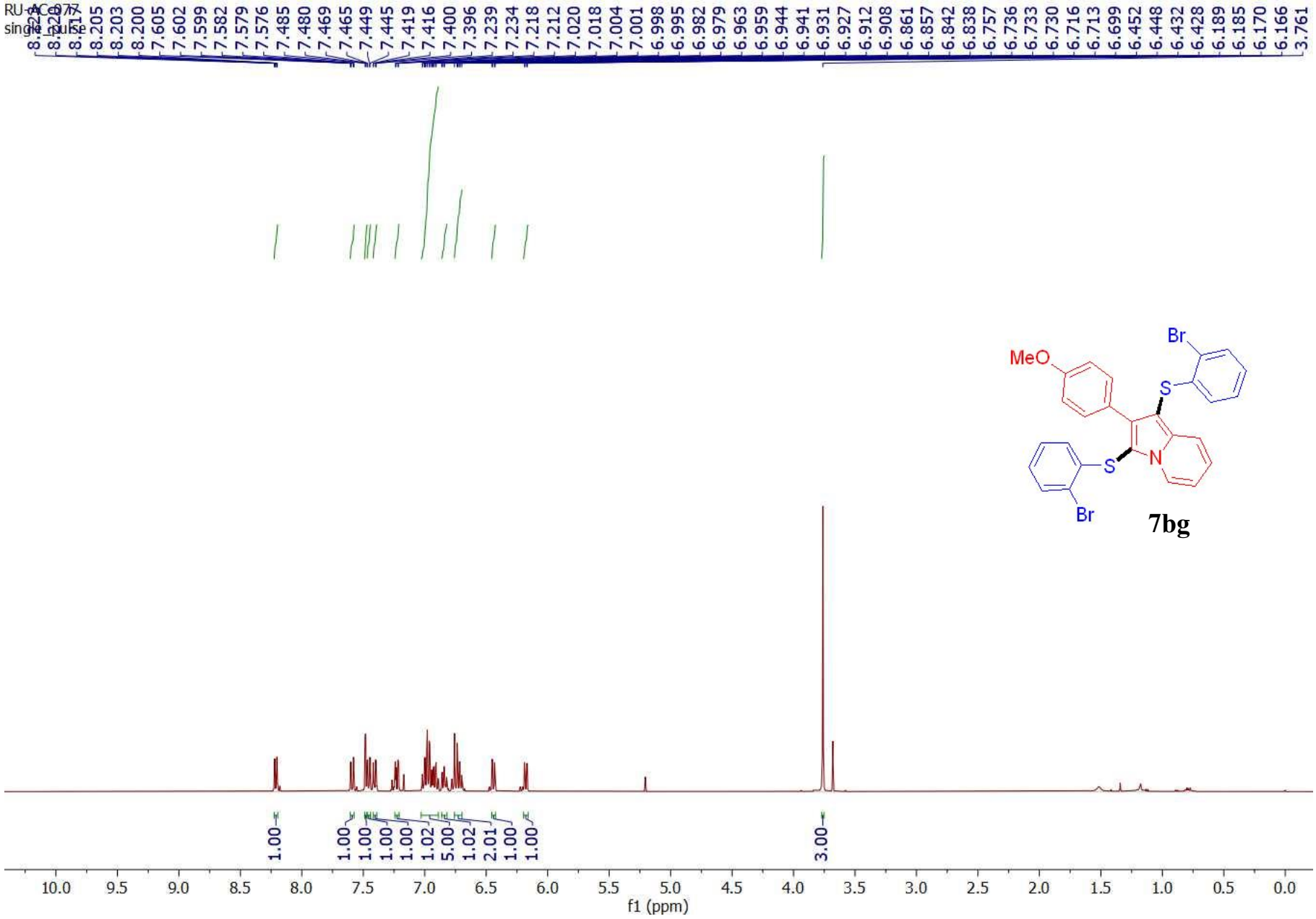
single pulse decoupled gated NOE



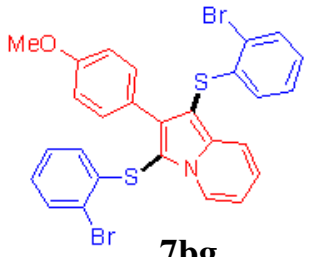
7ba



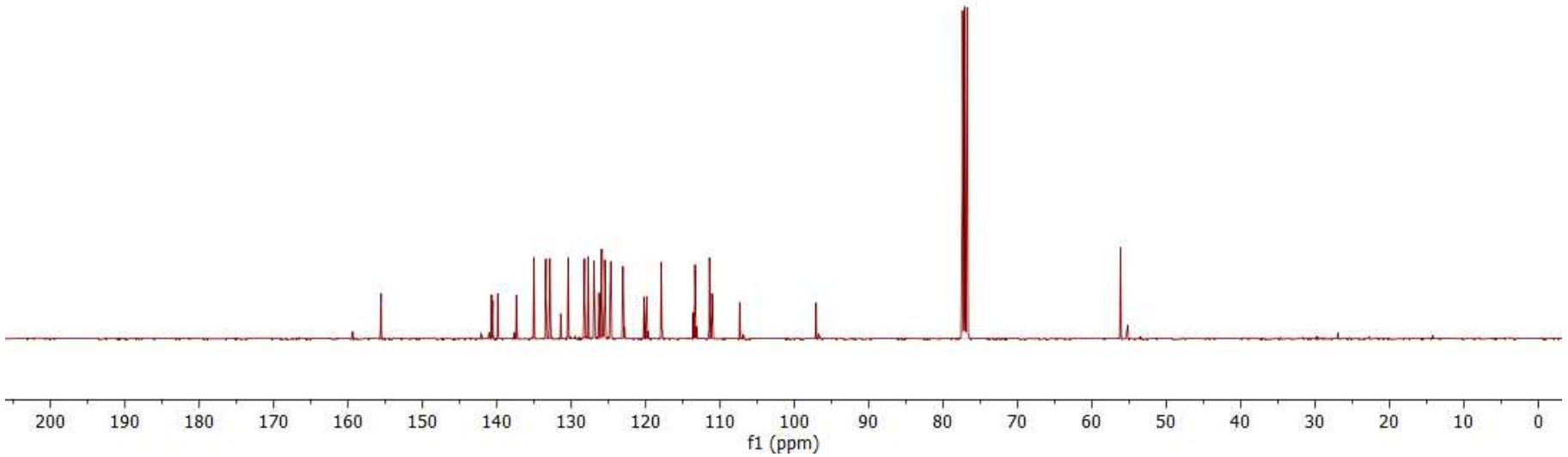
^{1}H NMR spectrum of 7bg (400 MHz, $CDCl_3$)



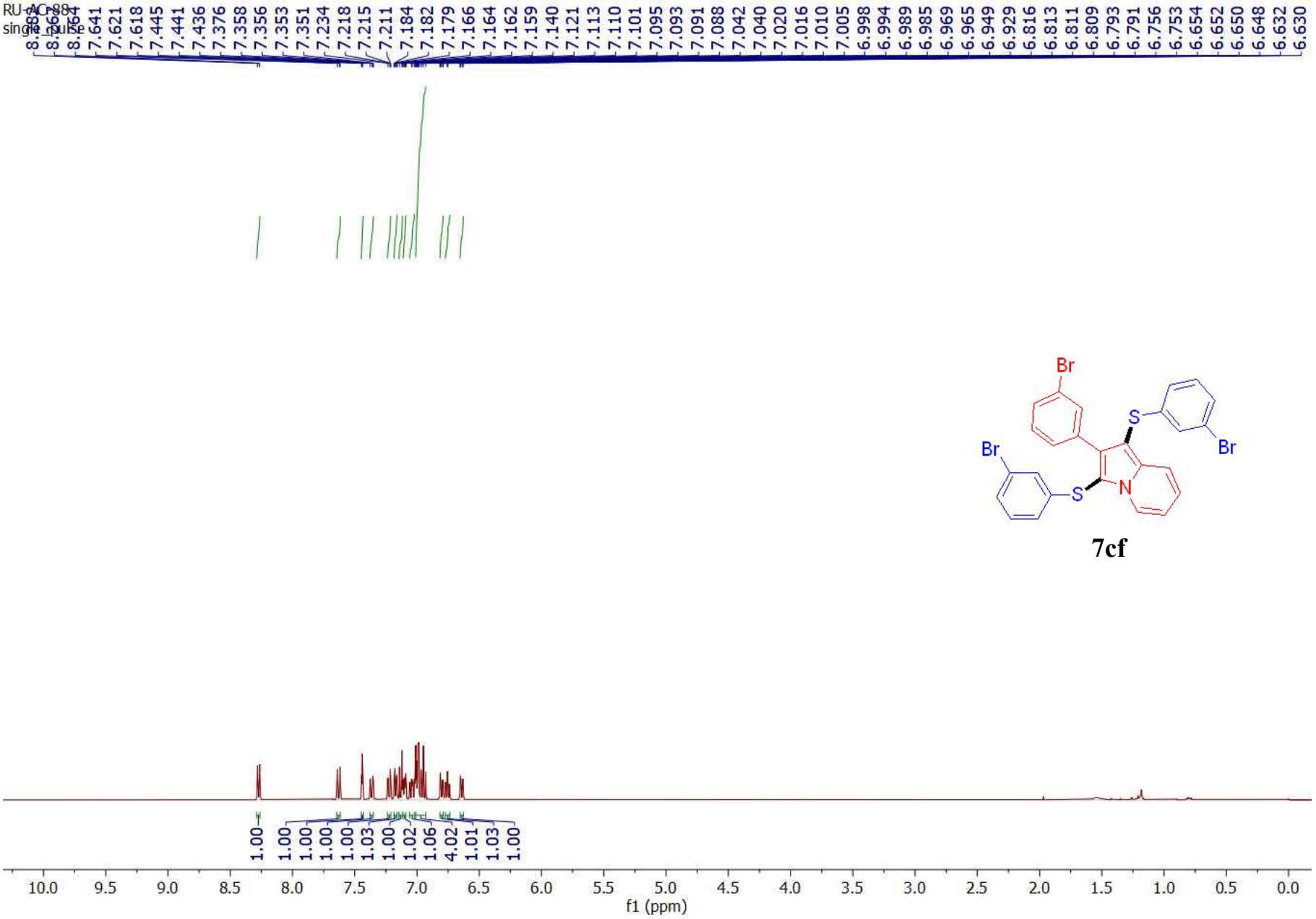
$^{13}C\{H\}$ NMR spectrum of 7bg (100 MHz, $CDCl_3$)



7bg

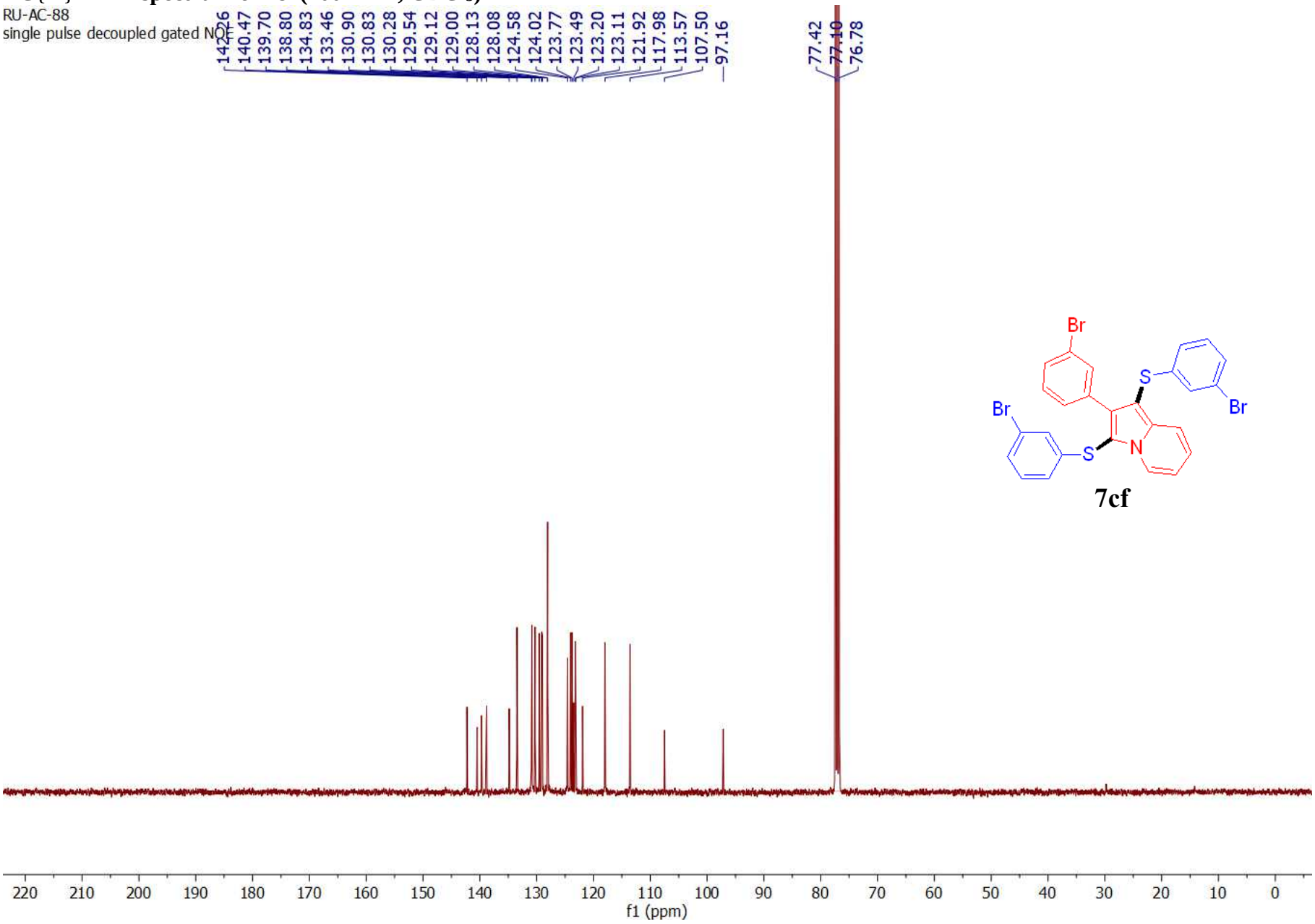


^{1}H NMR spectrum of 7cf (400 MHz, $CDCl_3$)



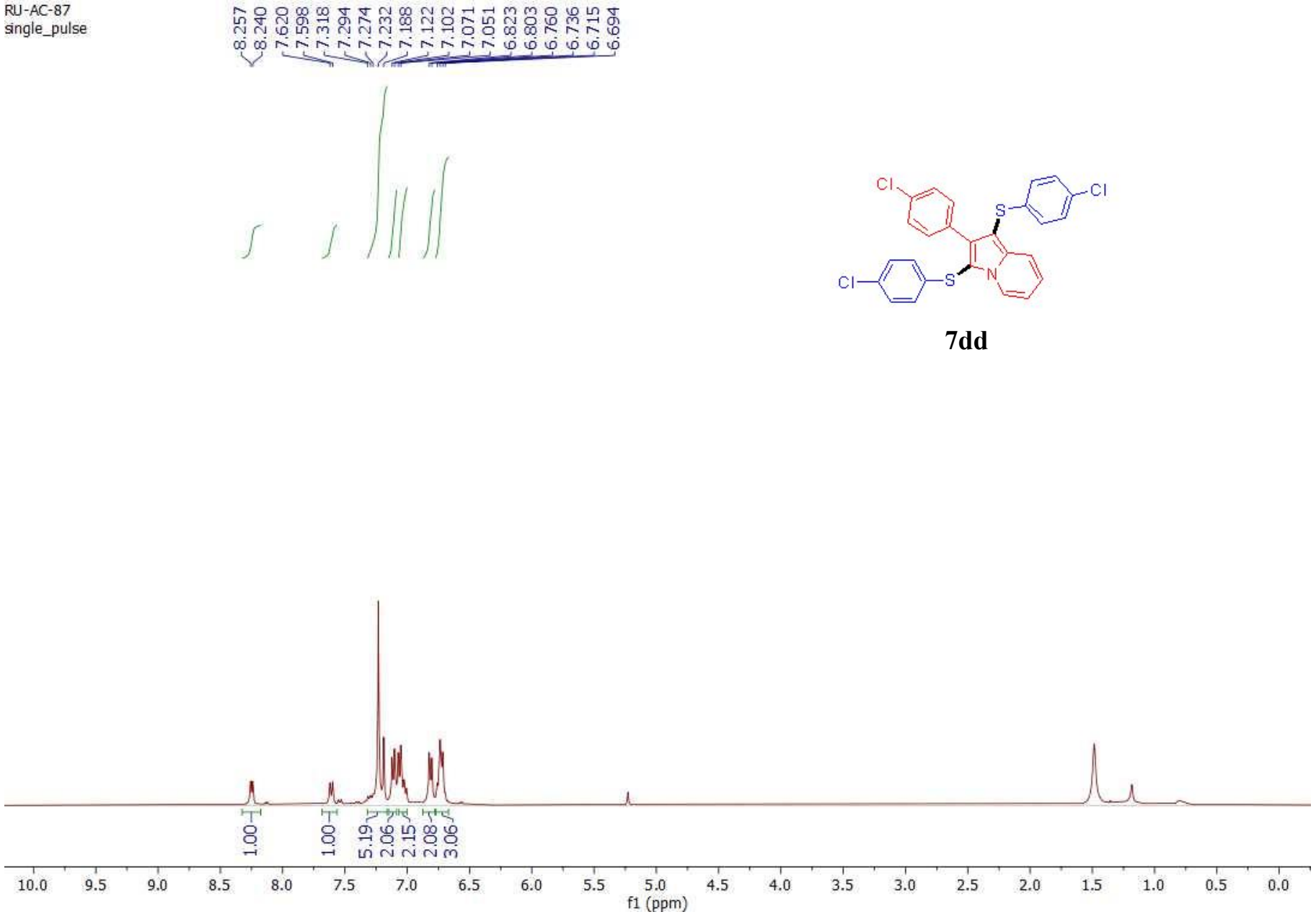
7cf

$^{13}C\{H\}$ NMR spectrum of 7cf (100 MHz, $CDCl_3$)



7cf

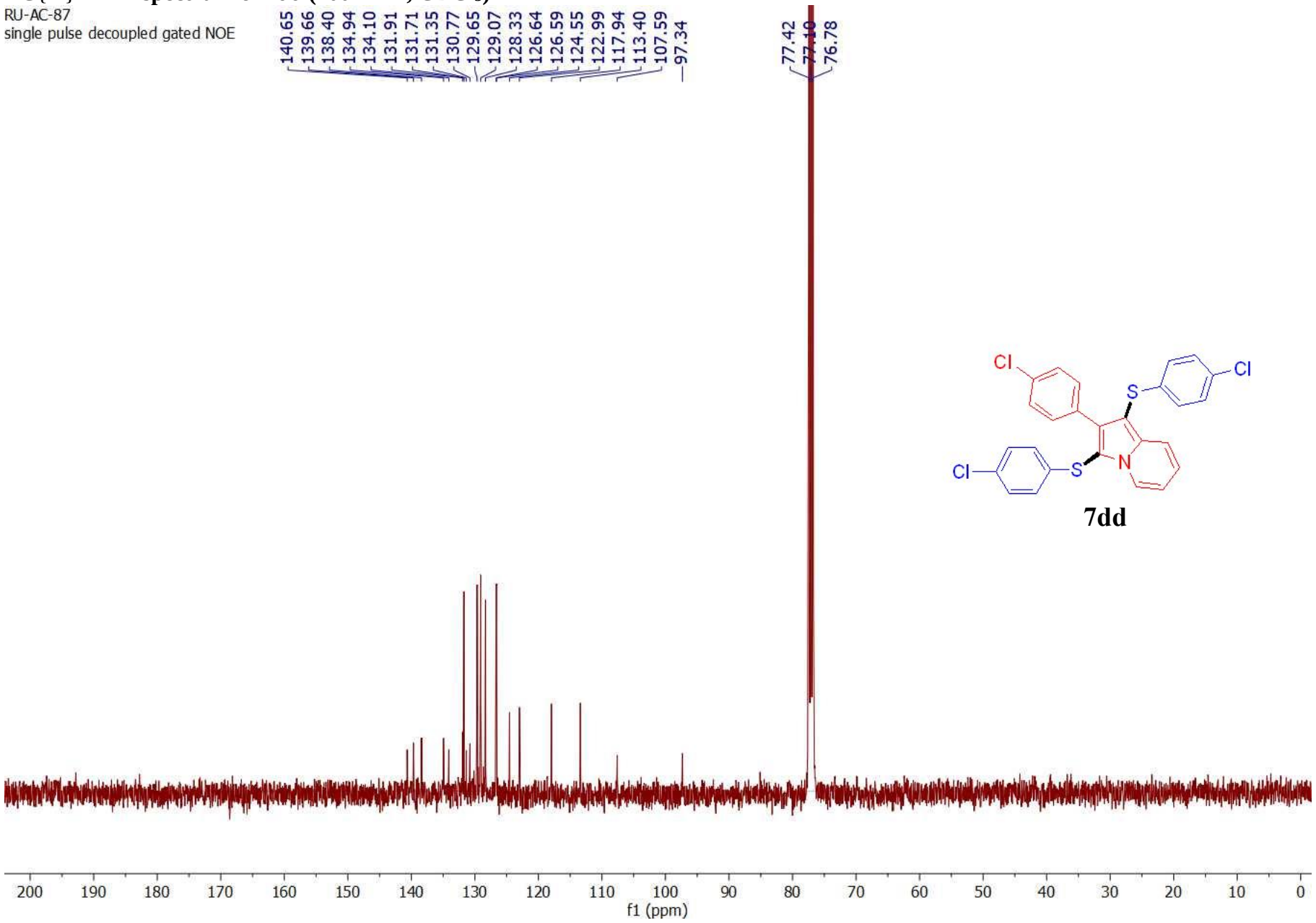
^{1}H NMR spectrum of 7dd (400 MHz, $CDCl_3$)



7dd

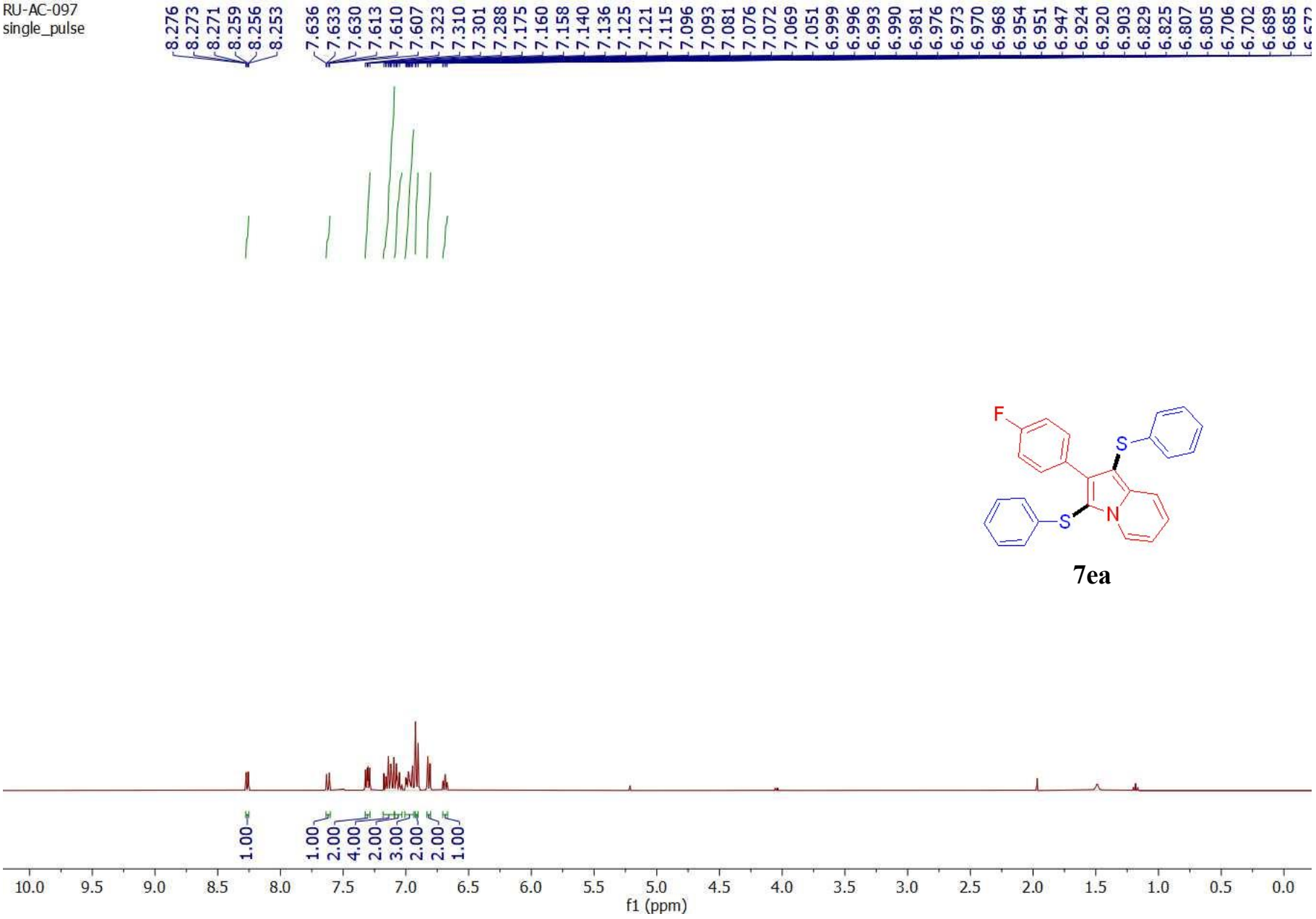
$^{13}C\{H\}$ NMR spectrum of 7dd (100 MHz, $CDCl_3$)

RU-AC-87
single pulse decoupled gated NOE



7dd

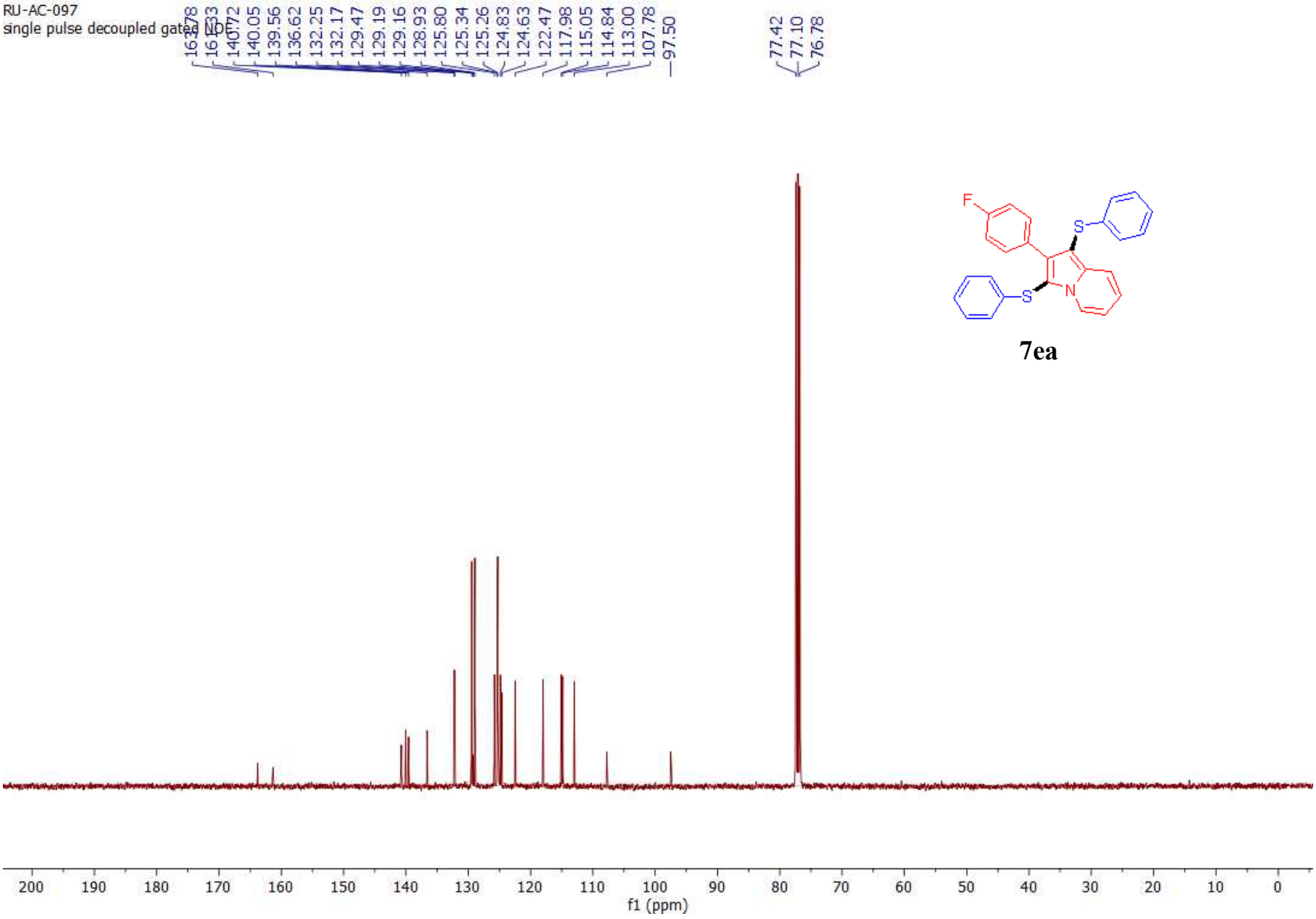
^{1}H NMR spectrum of 7ea (400 MHz, $CDCl_3$)



7ea

$^{13}C\{H\}$ NMR spectrum of 7ea (100 MHz, $CDCl_3$)

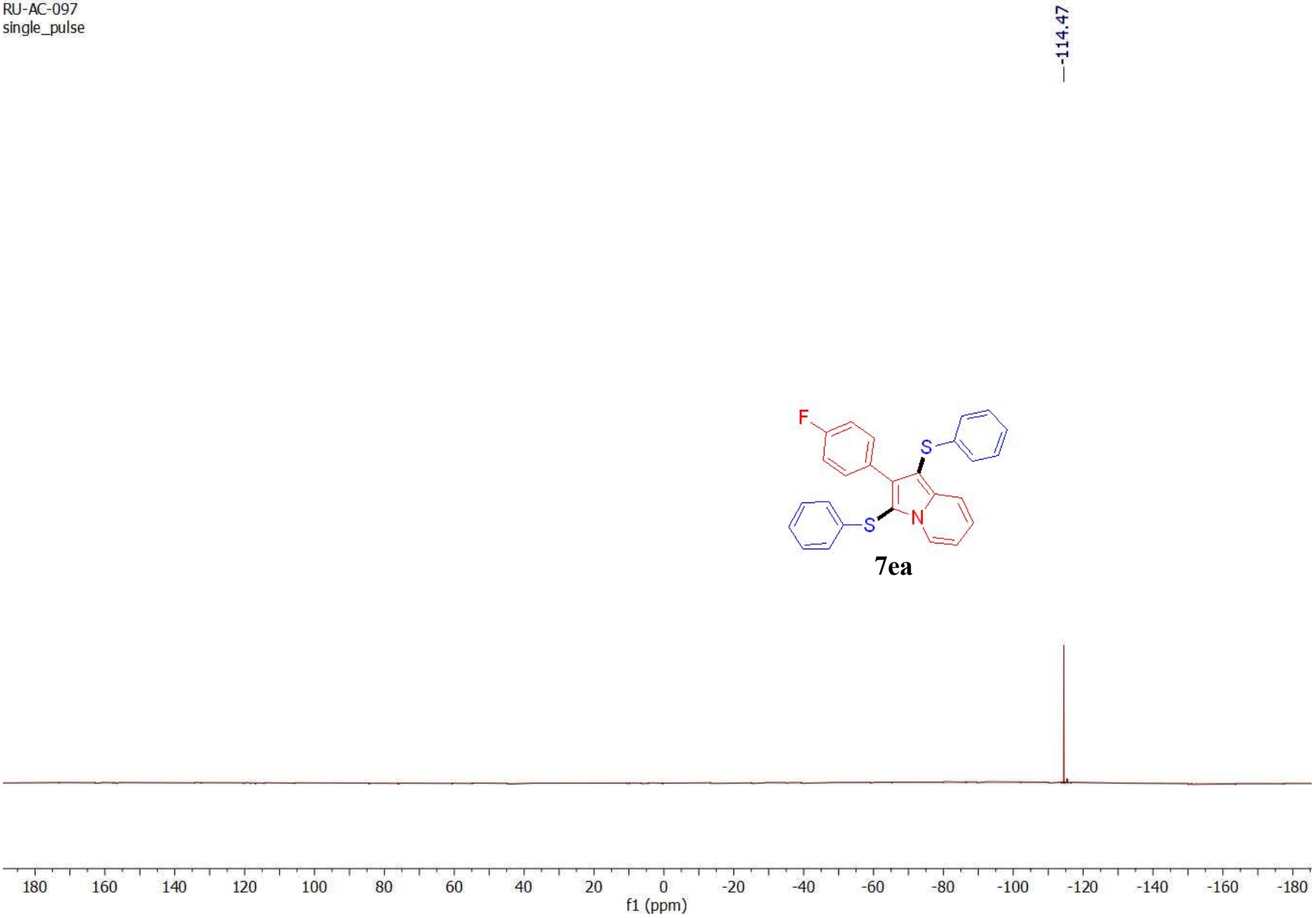
RU-AC-097
single pulse decoupled gated NOE



7ea

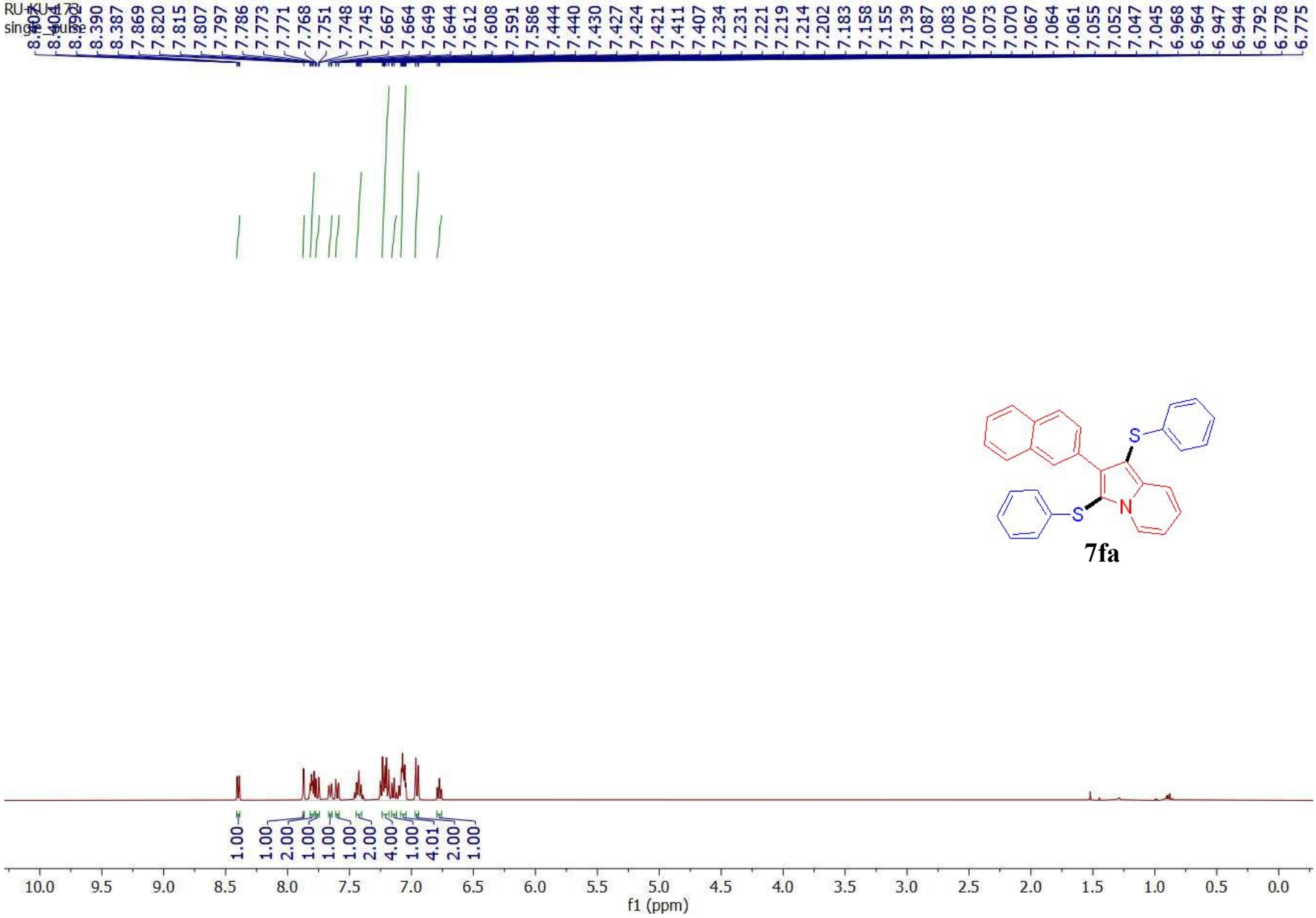
^{19}F NMR spectrum of 7ea (376 MHz, $CDCl_3$)

RU-AC-097
single_pulse



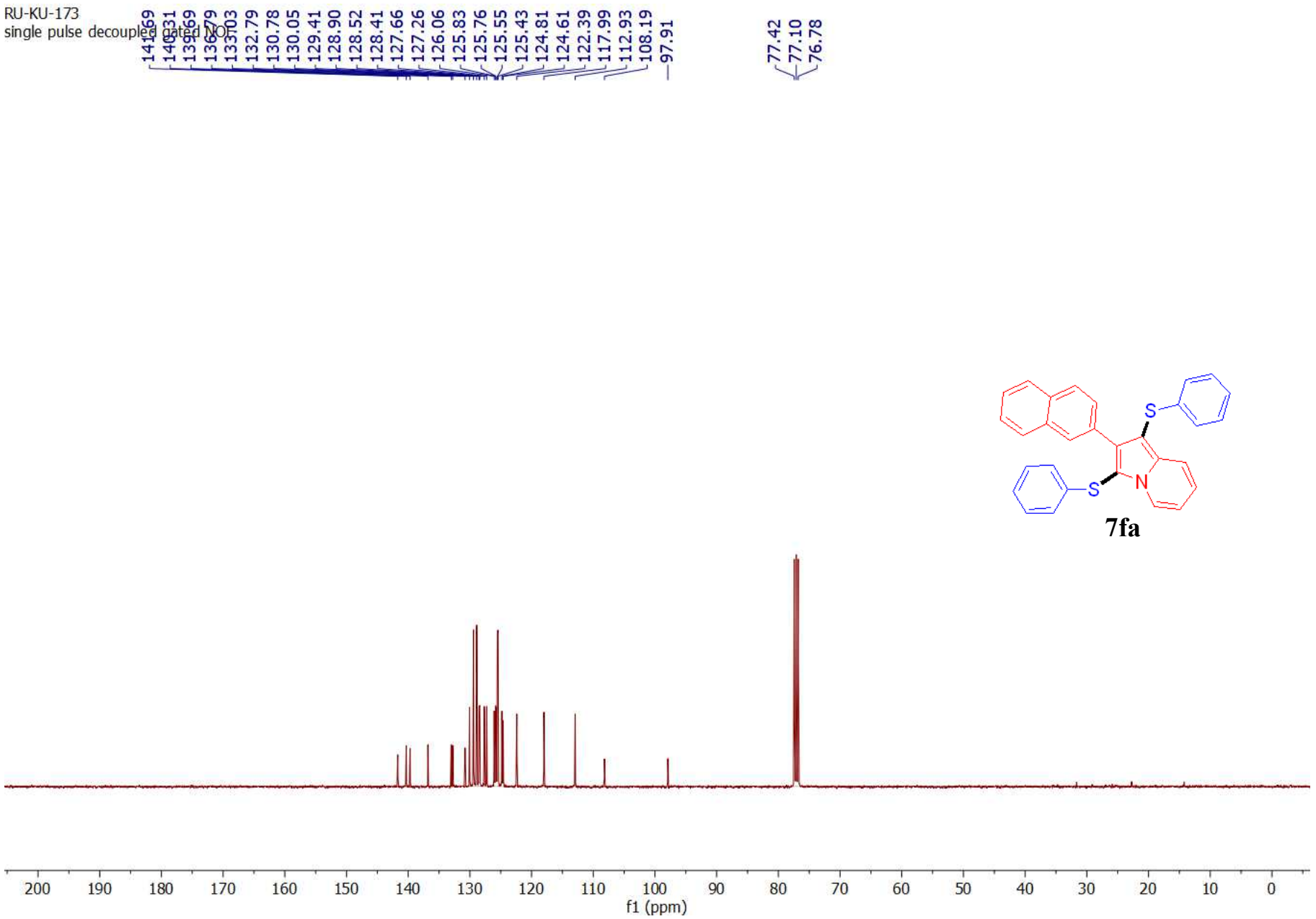
7ea

^{1}H NMR spectrum of 7fa (400 MHz, $CDCl_3$)

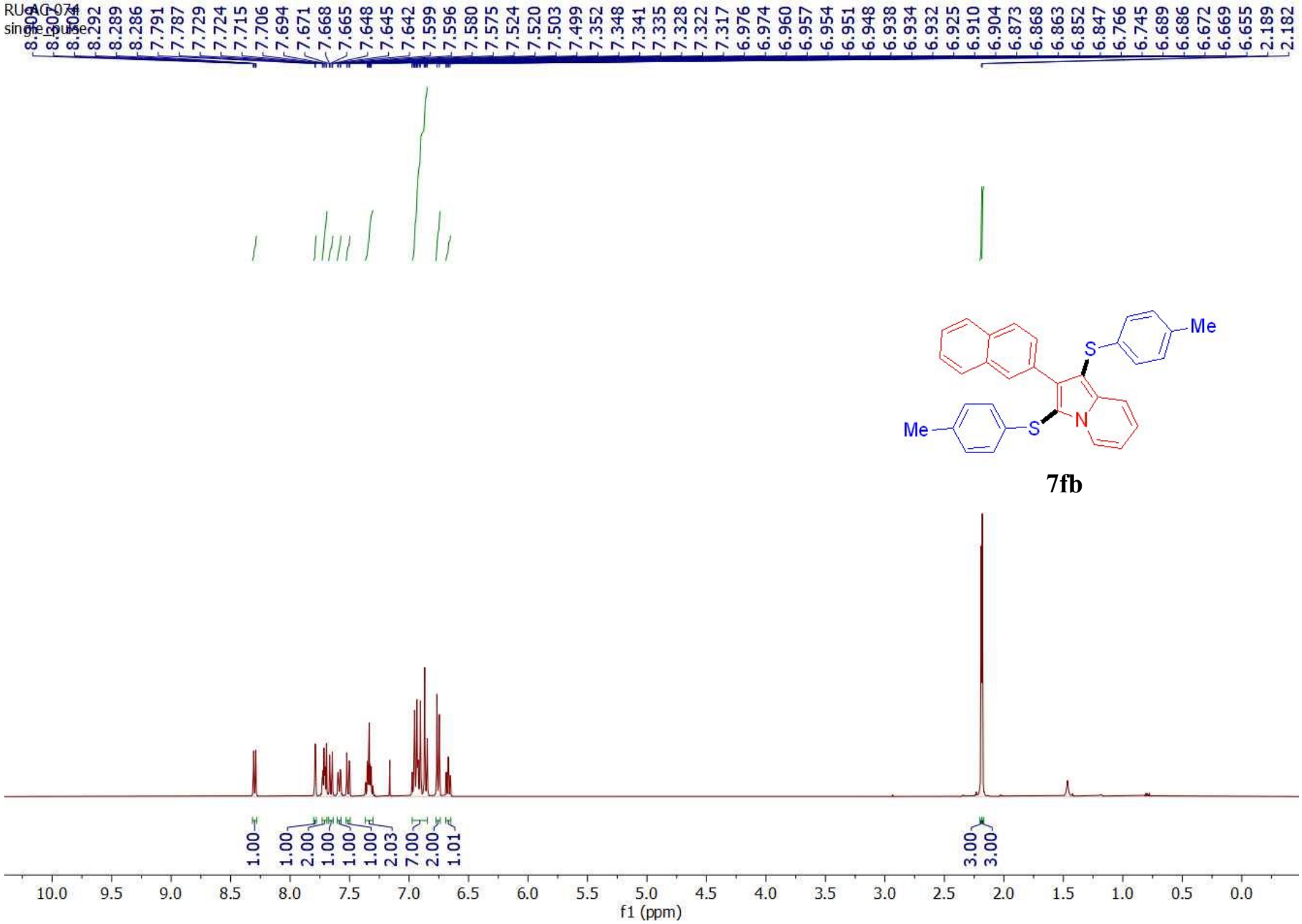


7fa

$^{13}C\{H\}$ NMR spectrum of 7fa (100 MHz, $CDCl_3$)

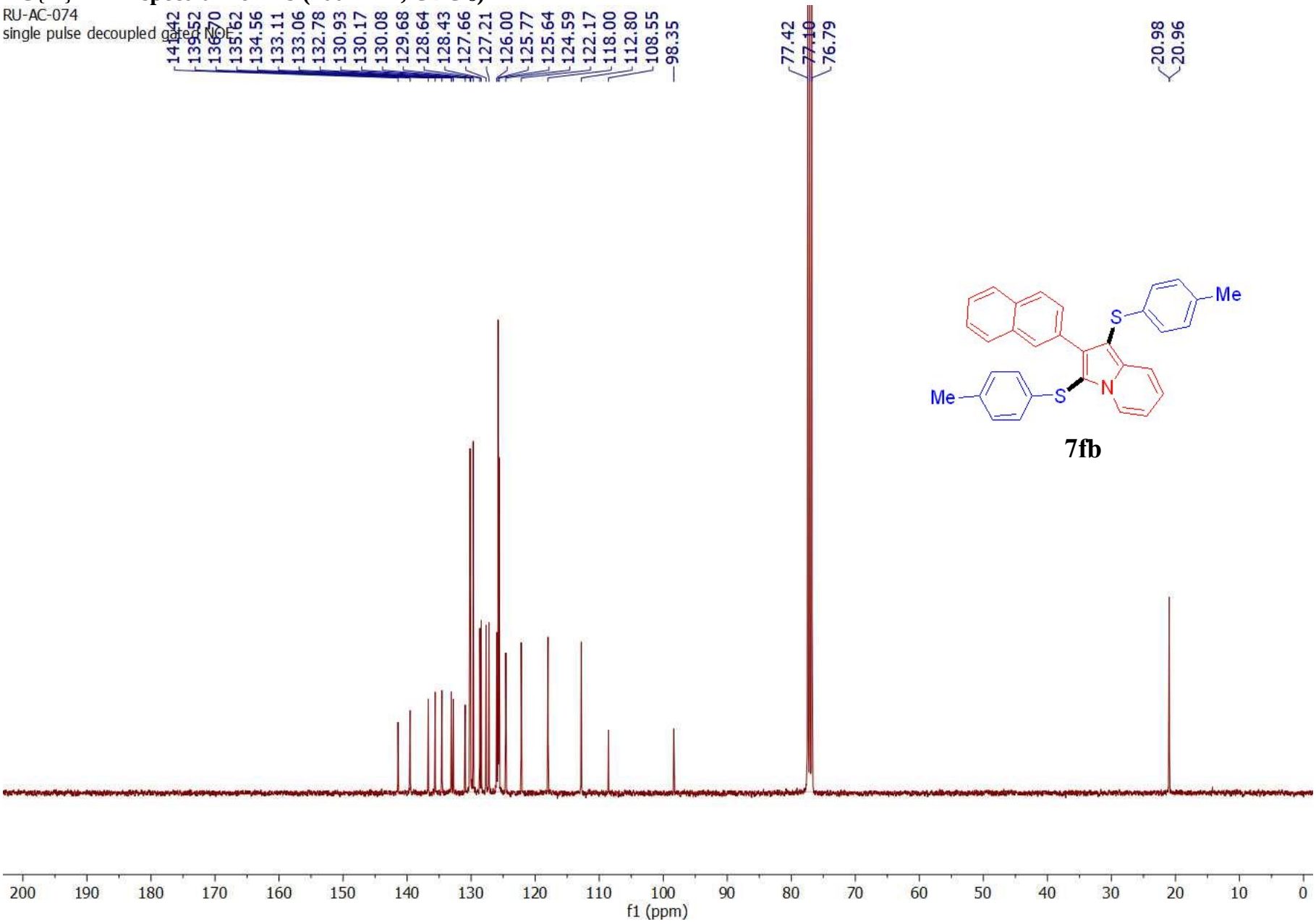


^{1}H NMR spectrum of 7fb (400 MHz, $CDCl_3$)



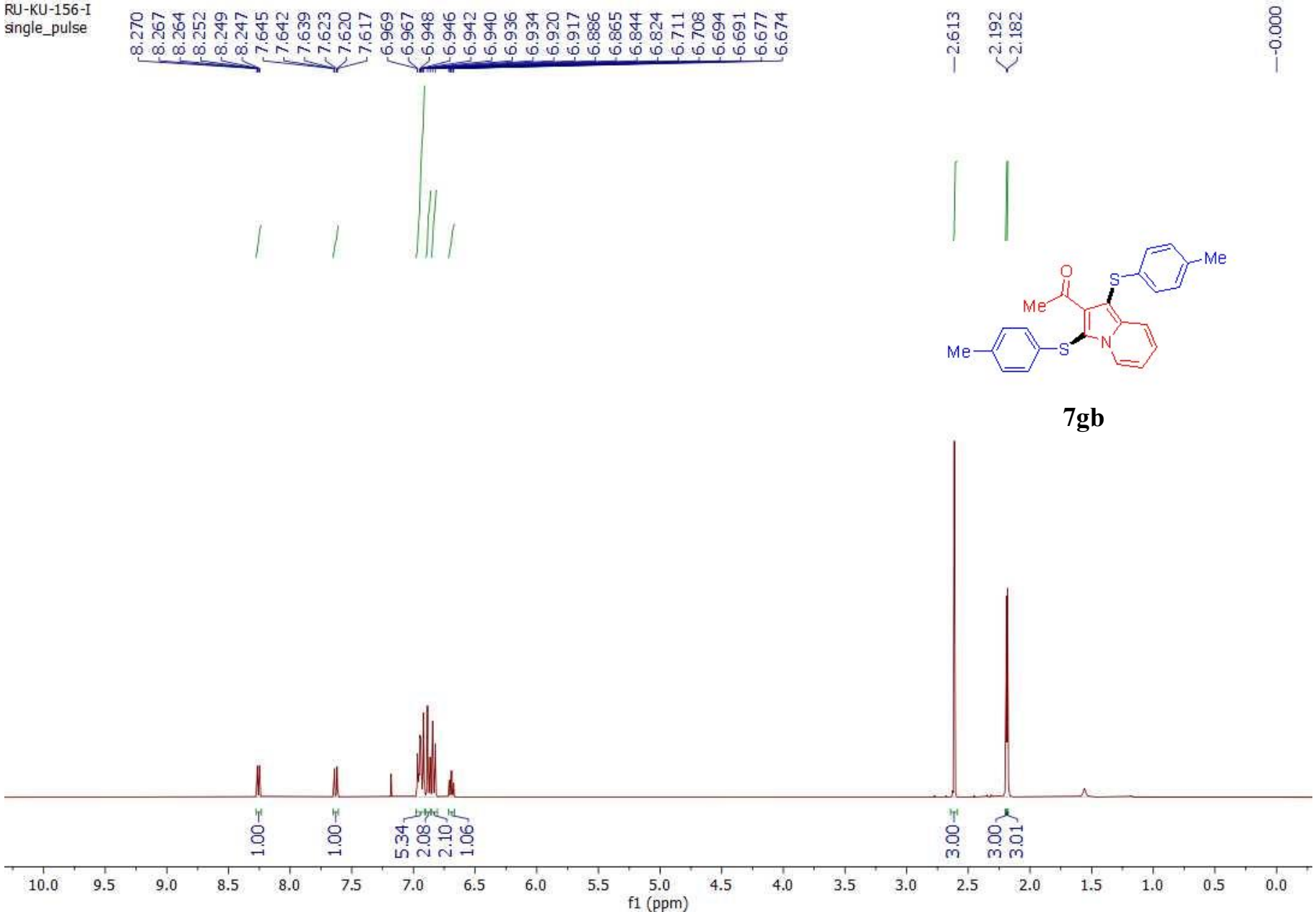
7fb

$^{13}C\{H\}$ NMR spectrum of 7fb (100 MHz, $CDCl_3$)



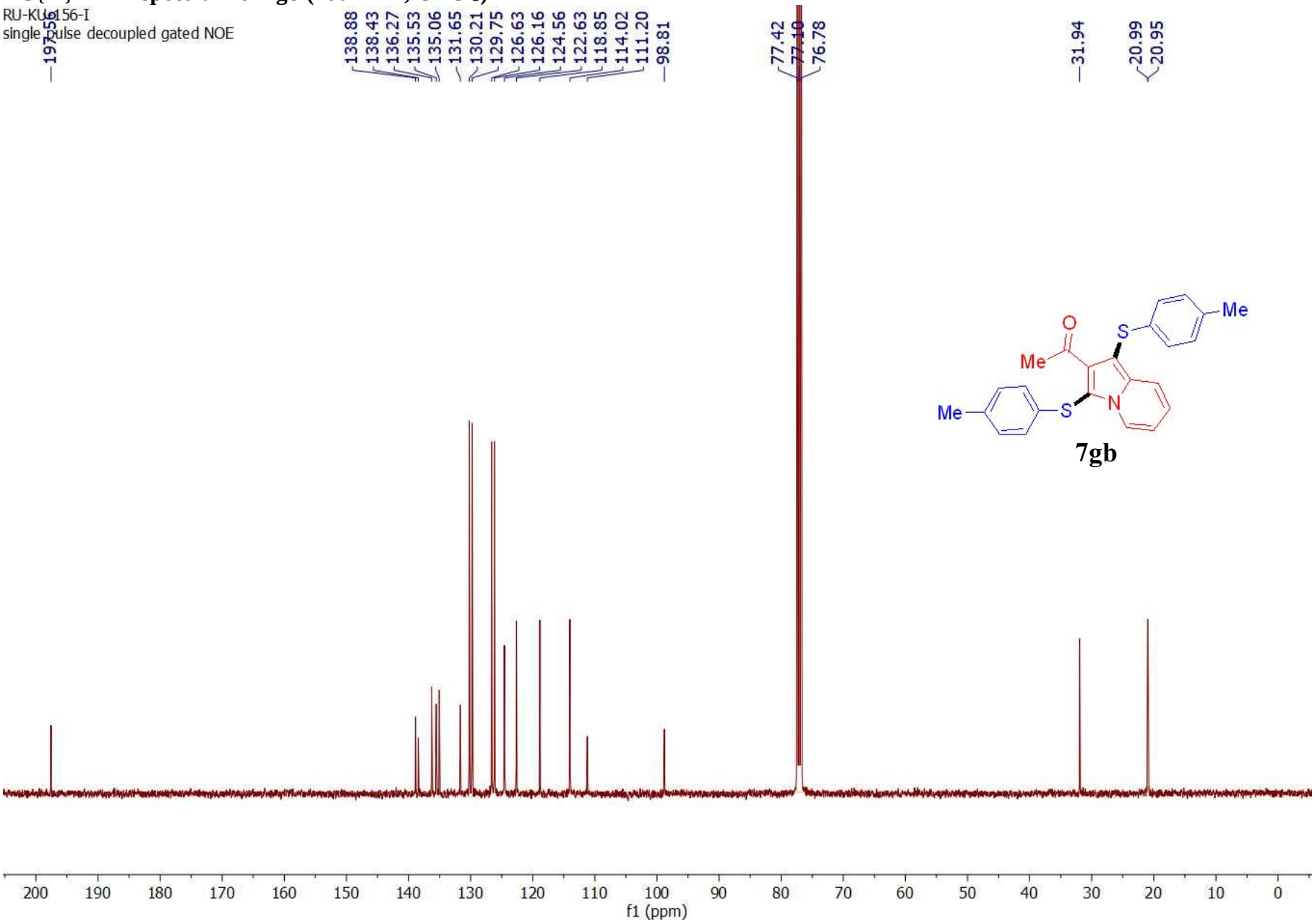
7fb

^{1}H NMR spectrum of 7gb (400 MHz, $CDCl_3$)



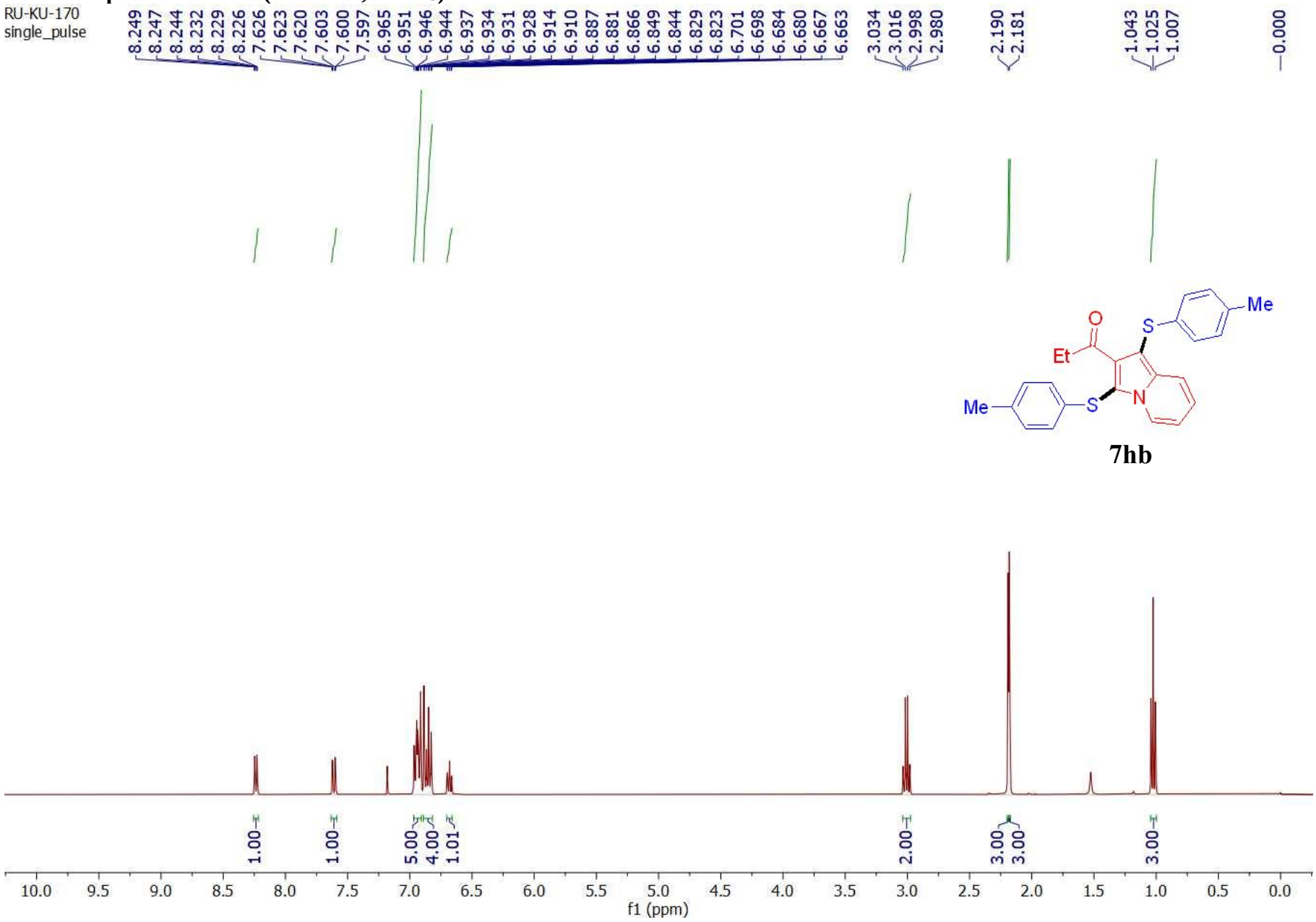
7gb

$^{13}C\{H\}$ NMR spectrum of 7gb (100 MHz, $CDCl_3$)



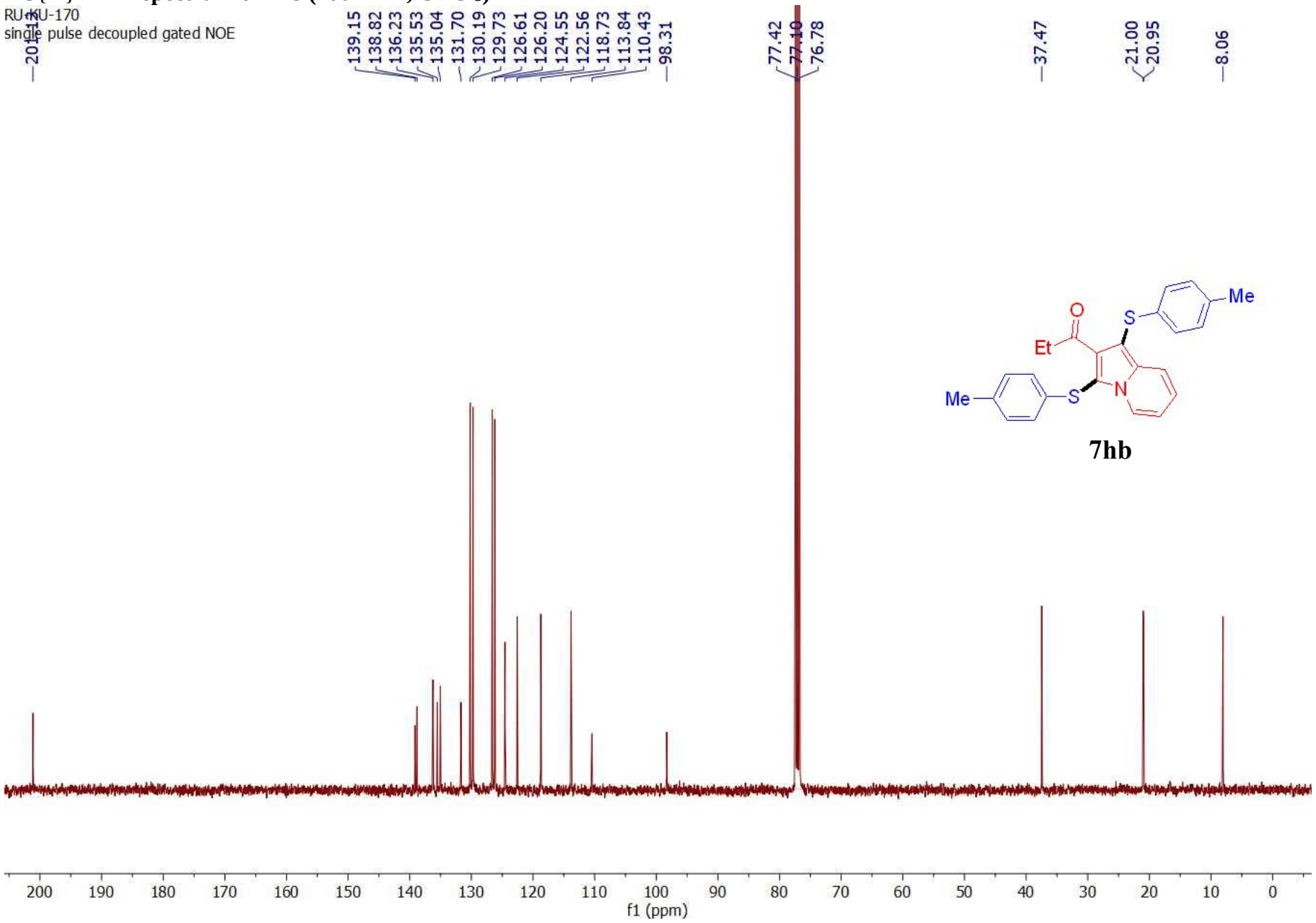
7gb

^{1}H NMR spectrum of 7hb (400 MHz, $CDCl_3$)



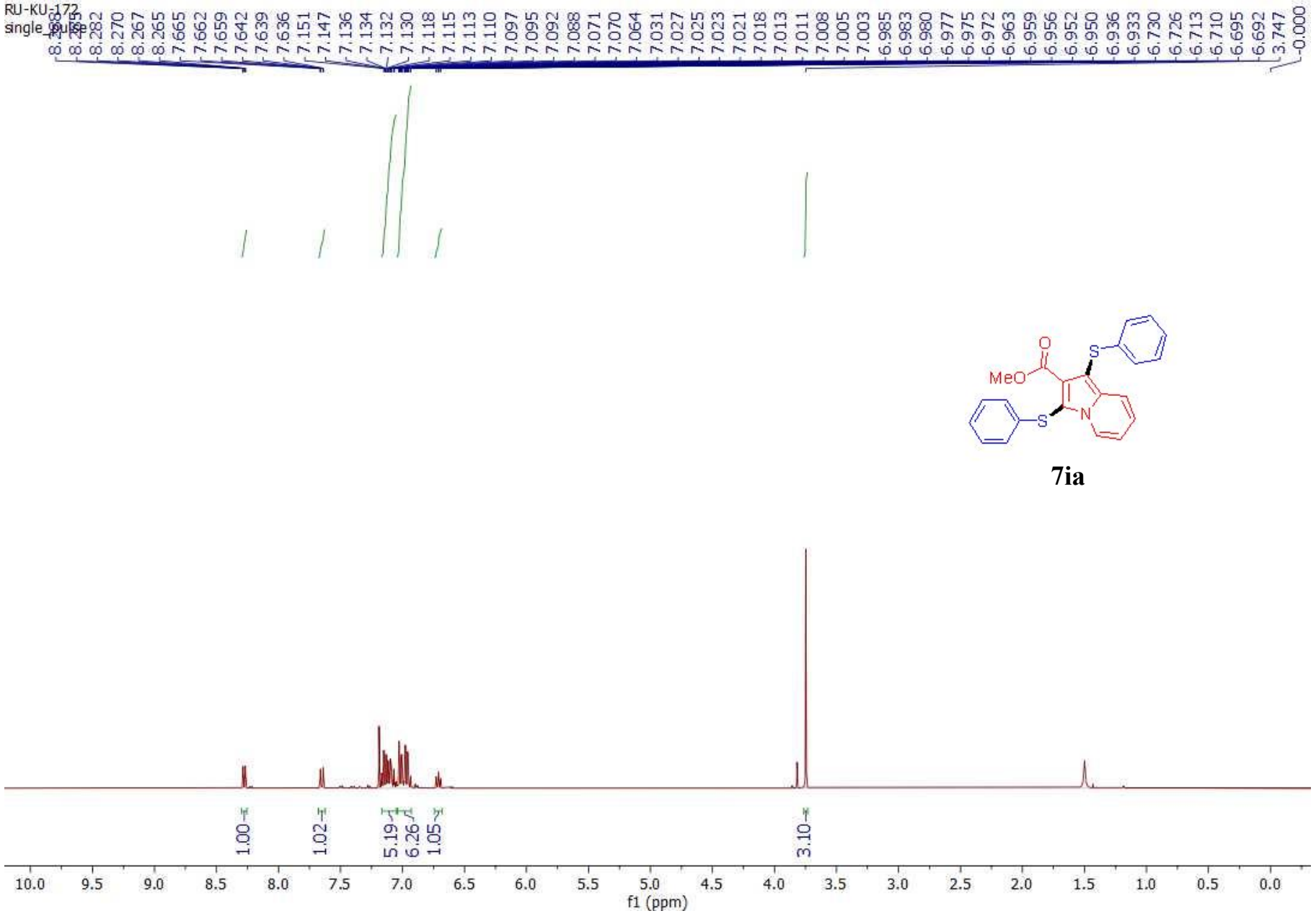
7hb

$^{13}C\{H\}$ NMR spectrum of 7hb (100 MHz, $CDCl_3$)



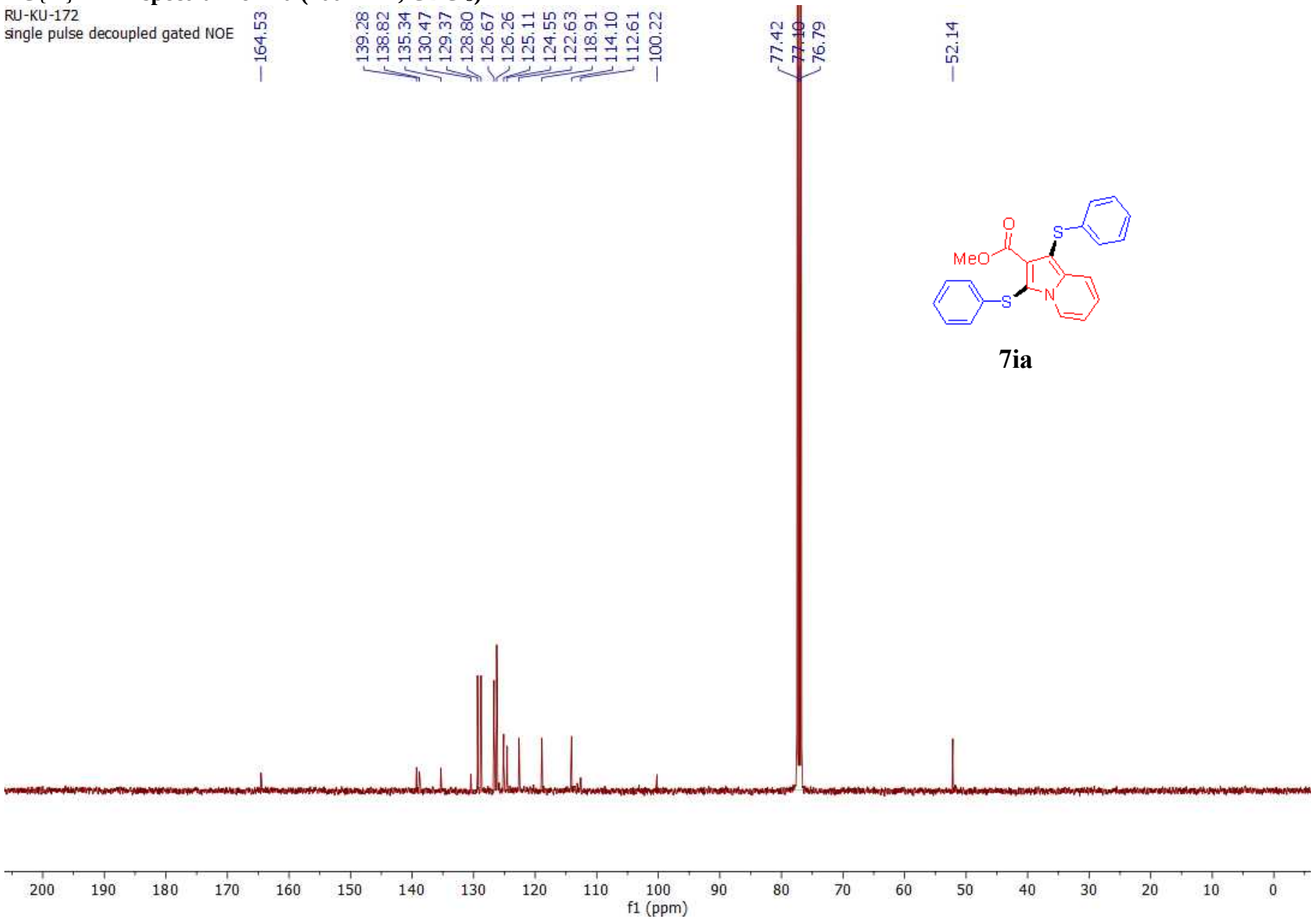
7hb

^{1}H NMR spectrum of 7ia (400 MHz, $CDCl_3$)



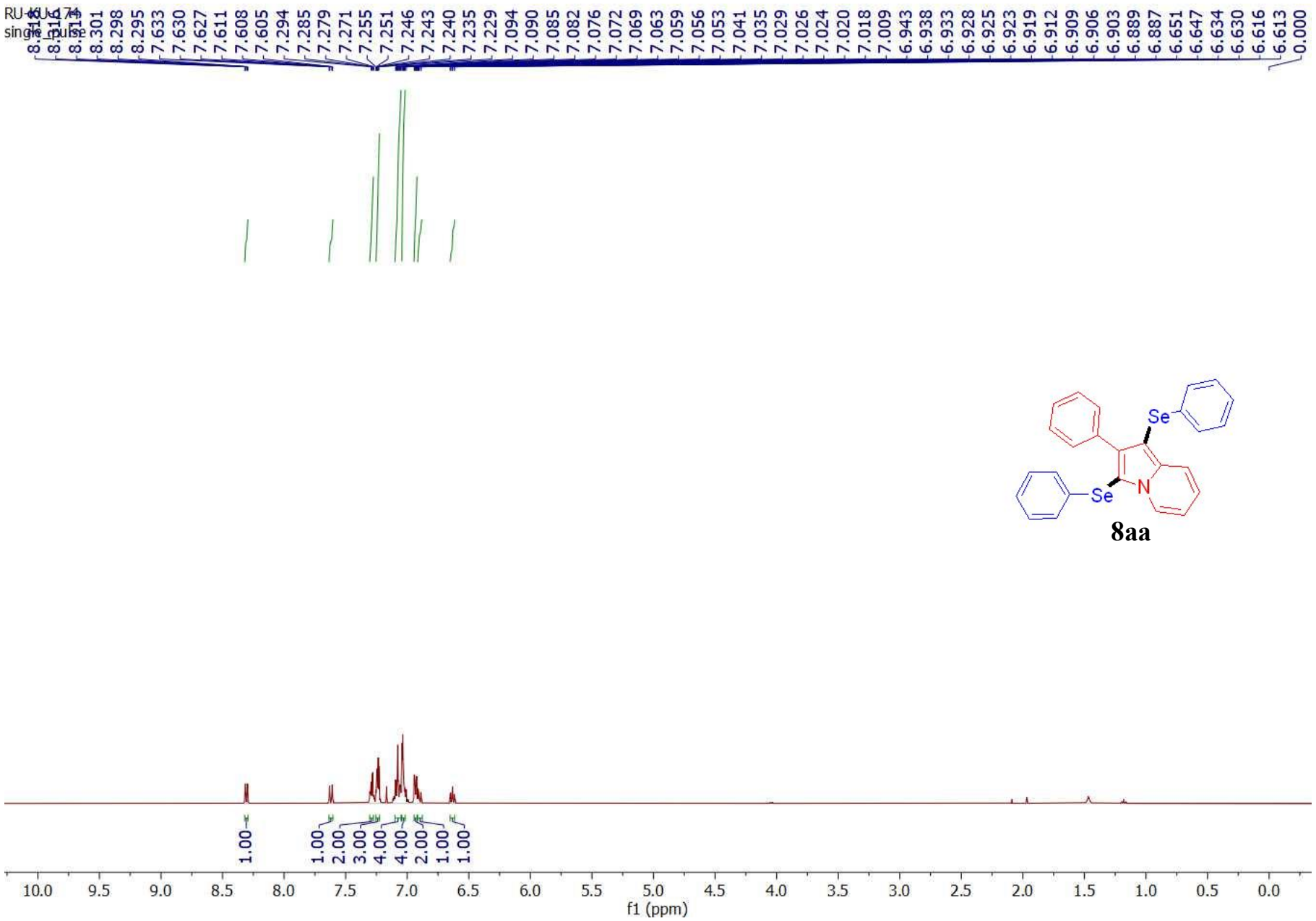
7ia

$^{13}C\{H\}$ NMR spectrum of 7ia (100 MHz, $CDCl_3$)



7ia

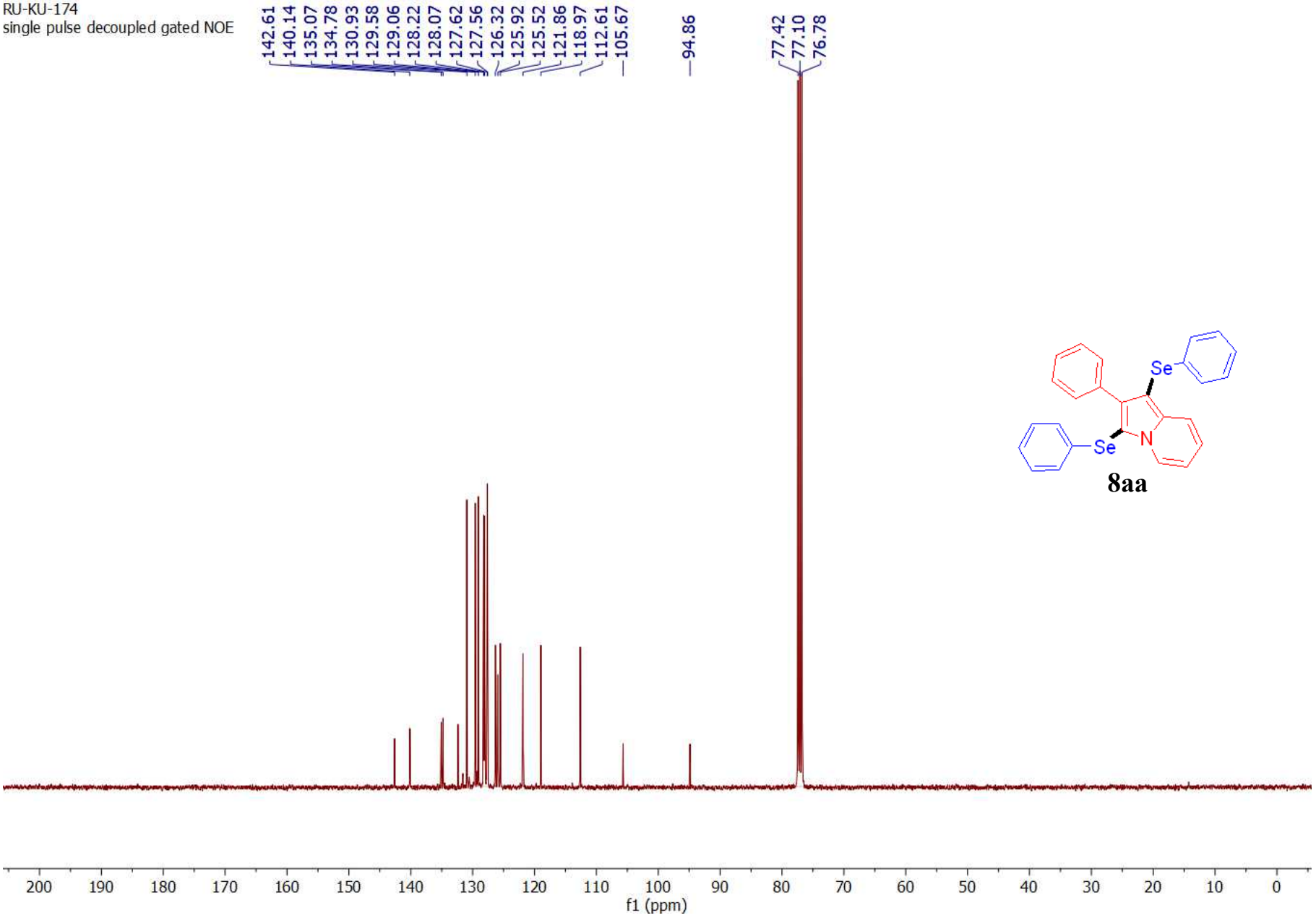
^{1}H NMR spectrum of 8aa (400 MHz, $CDCl_3$)



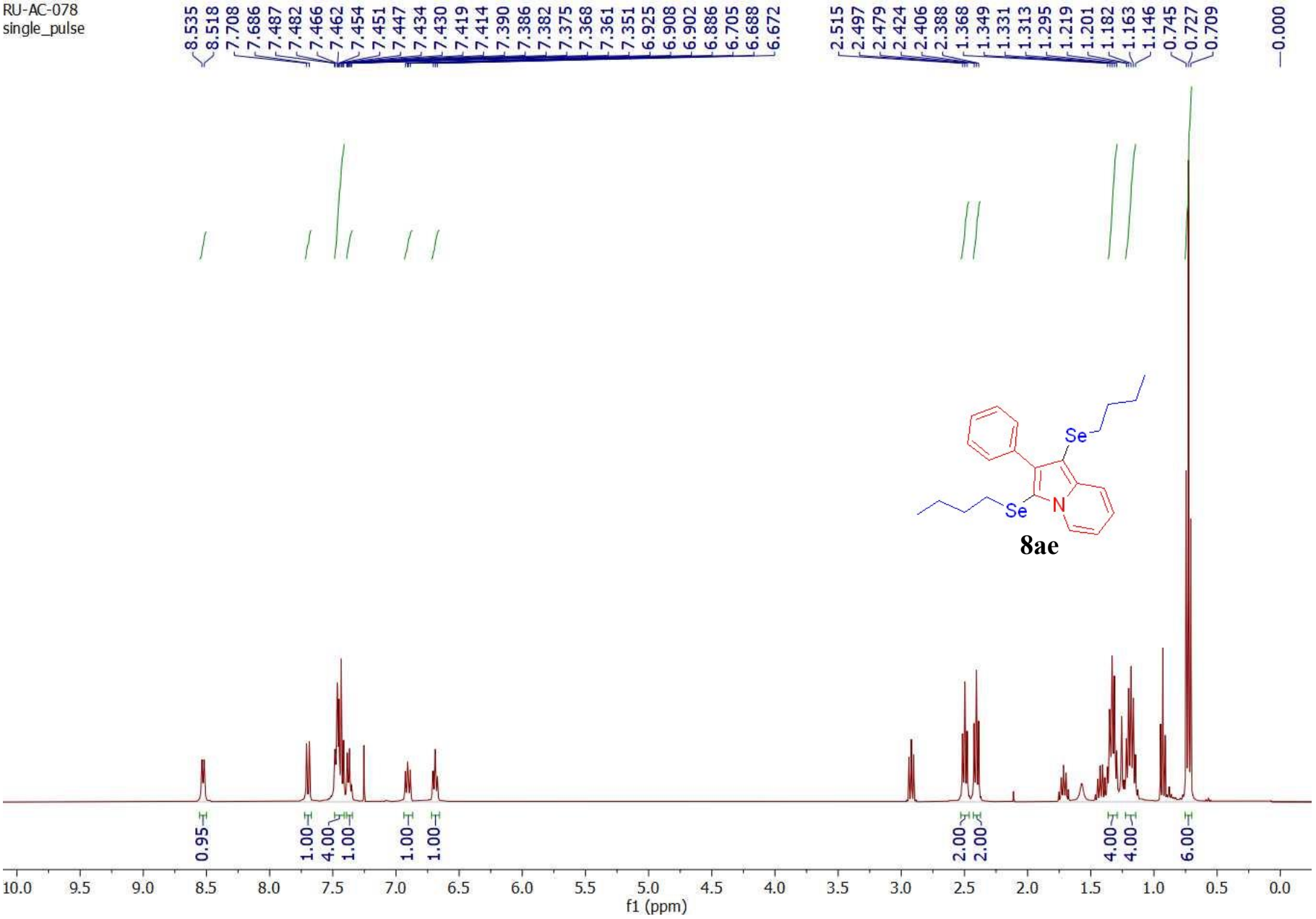
8aa

$^{13}C\{H\}$ NMR spectrum of 7ia (100 MHz, $CDCl_3$)

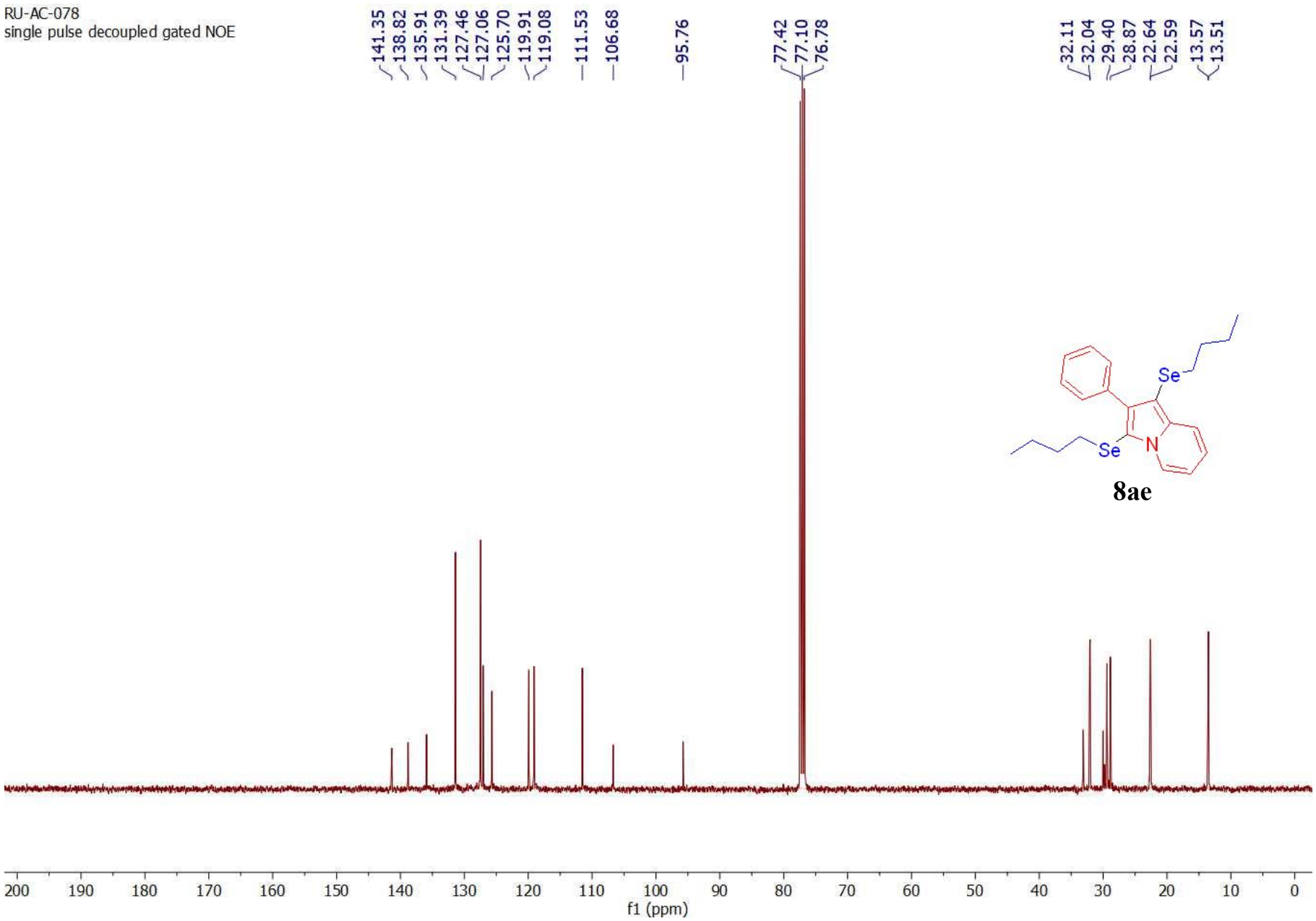
RU-KU-174
single pulse decoupled gated NOE



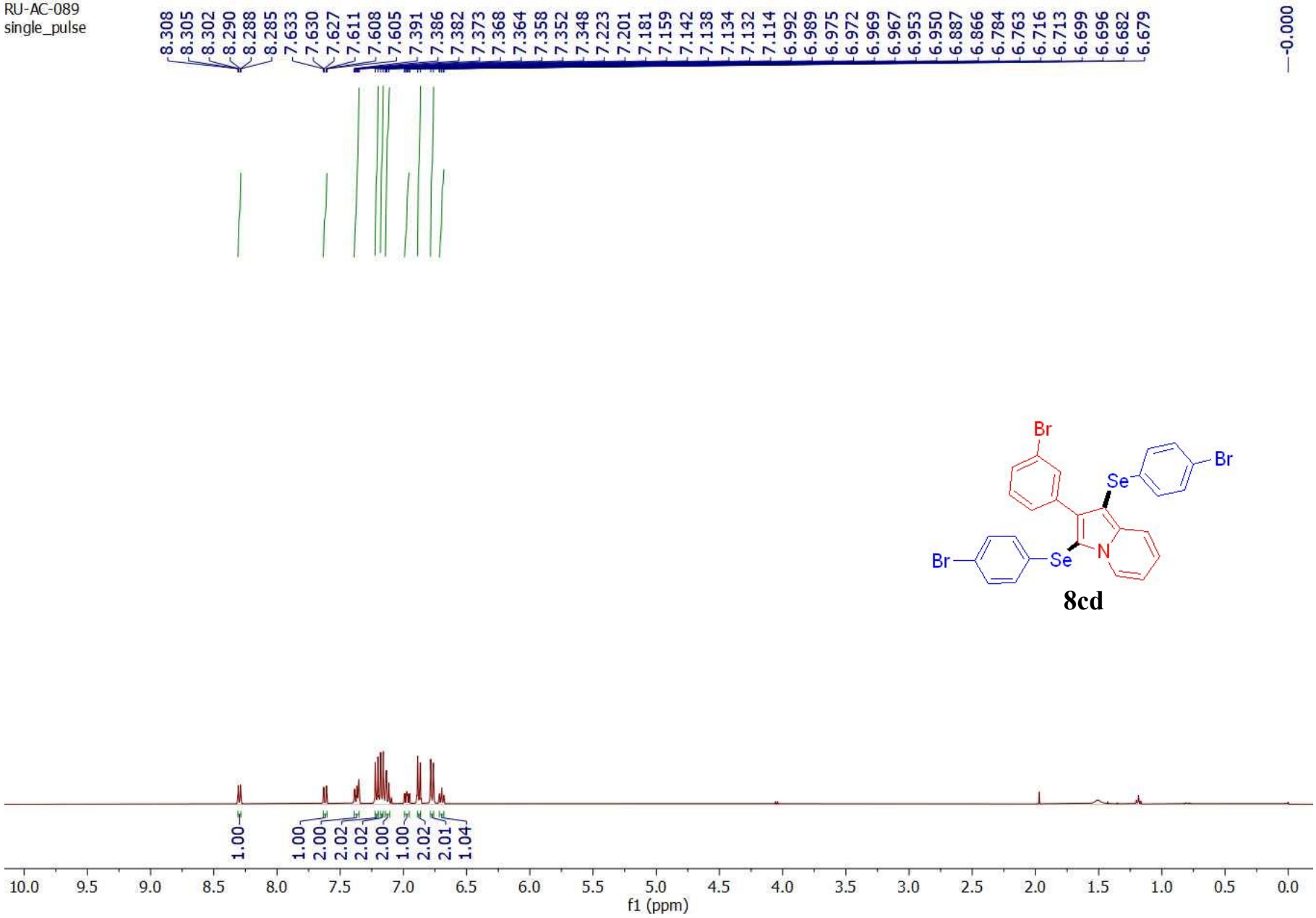
^{1}H NMR spectrum of 8ae (400 MHz, $CDCl_3$)



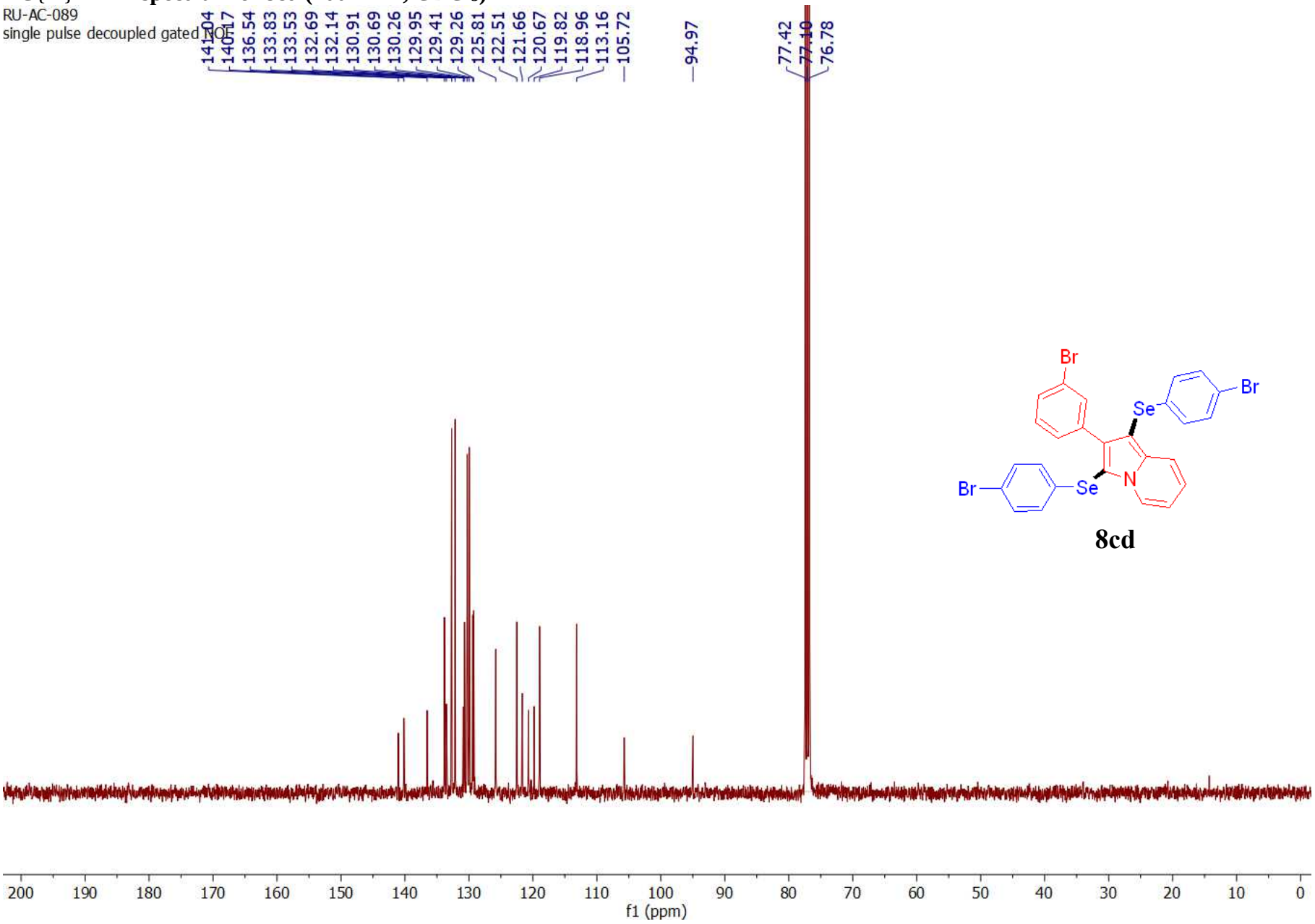
$^{13}C\{H\}$ NMR spectrum of 8ae (100 MHz, $CDCl_3$)



^{1}H NMR spectrum of 8cd (400 MHz, $CDCl_3$)

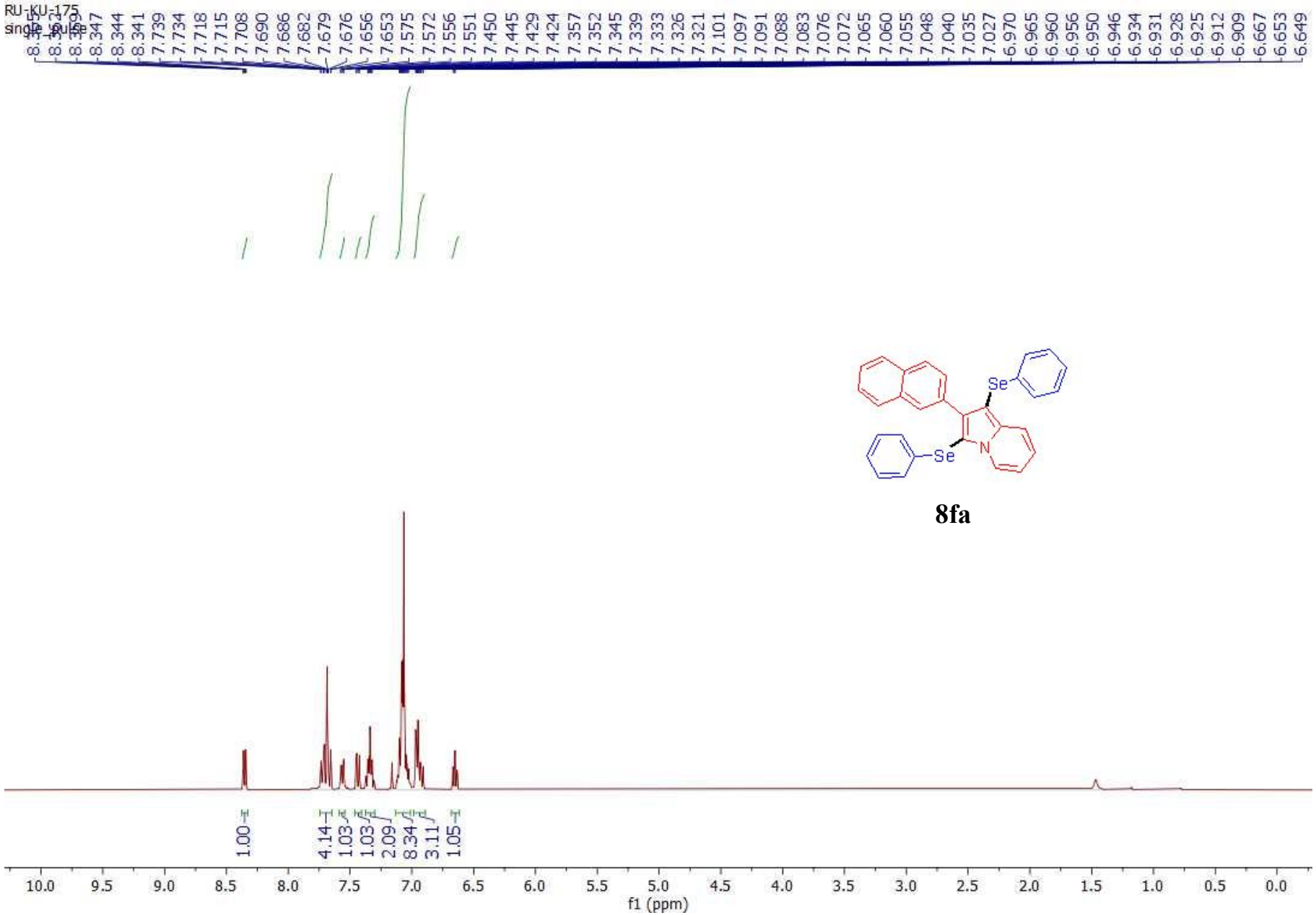


$^{13}C\{H\}$ NMR spectrum of 8cd (100 MHz, $CDCl_3$)



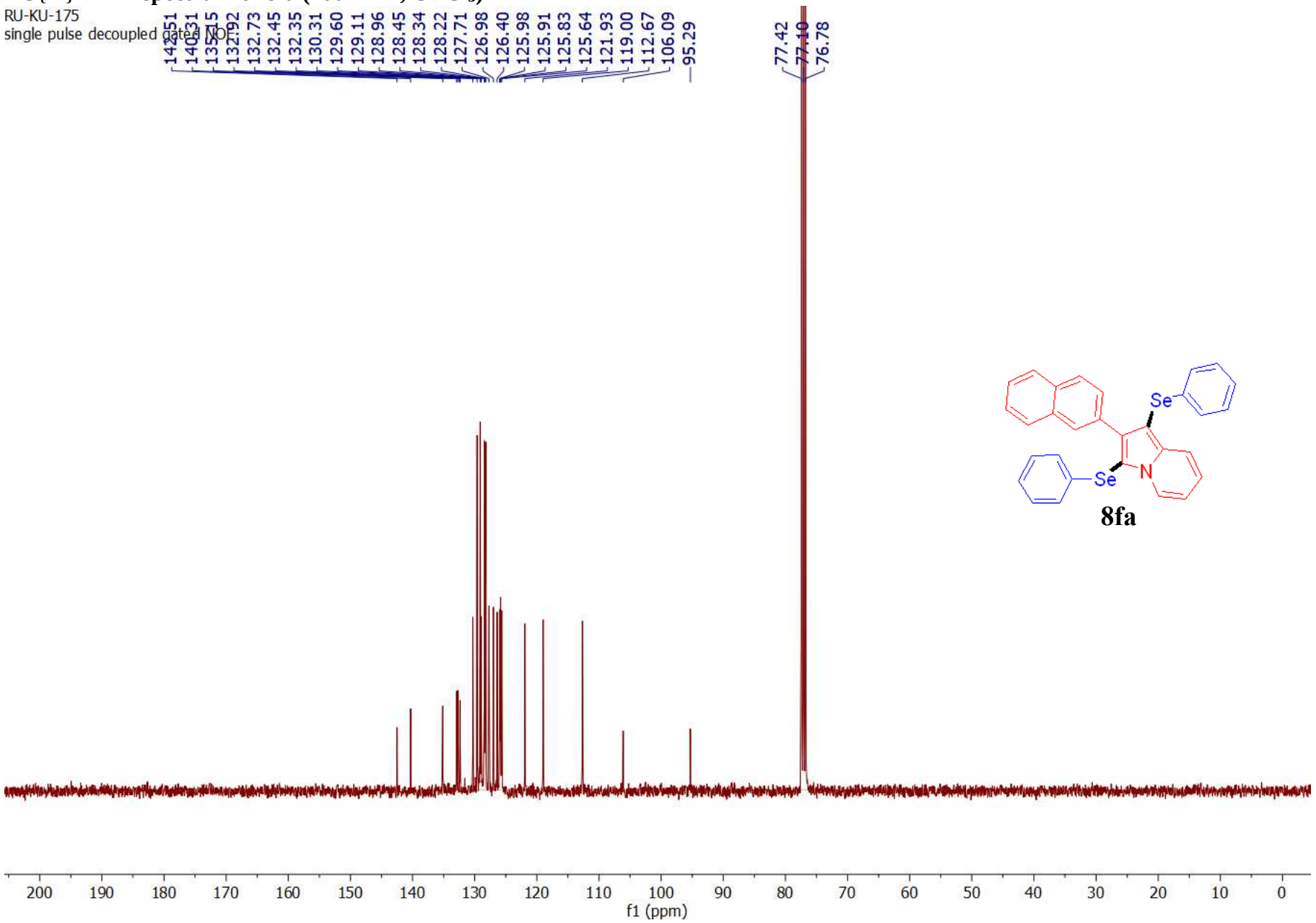
8cd

^{1}H NMR spectrum of 8fa (400 MHz, $CDCl_3$)

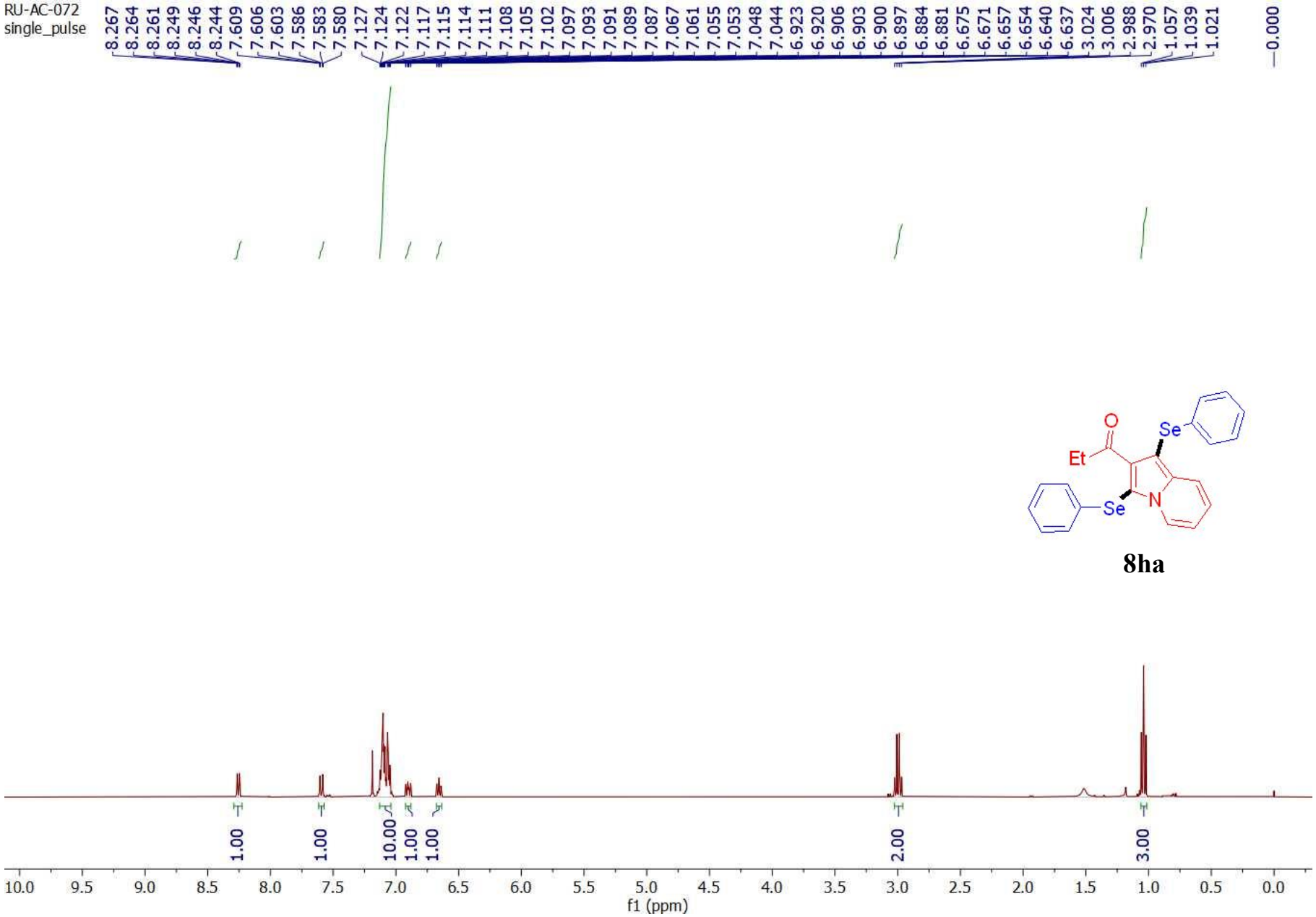


8fa

$^{13}C\{H\}$ NMR spectrum of 8fa (100 MHz, $CDCl_3$)

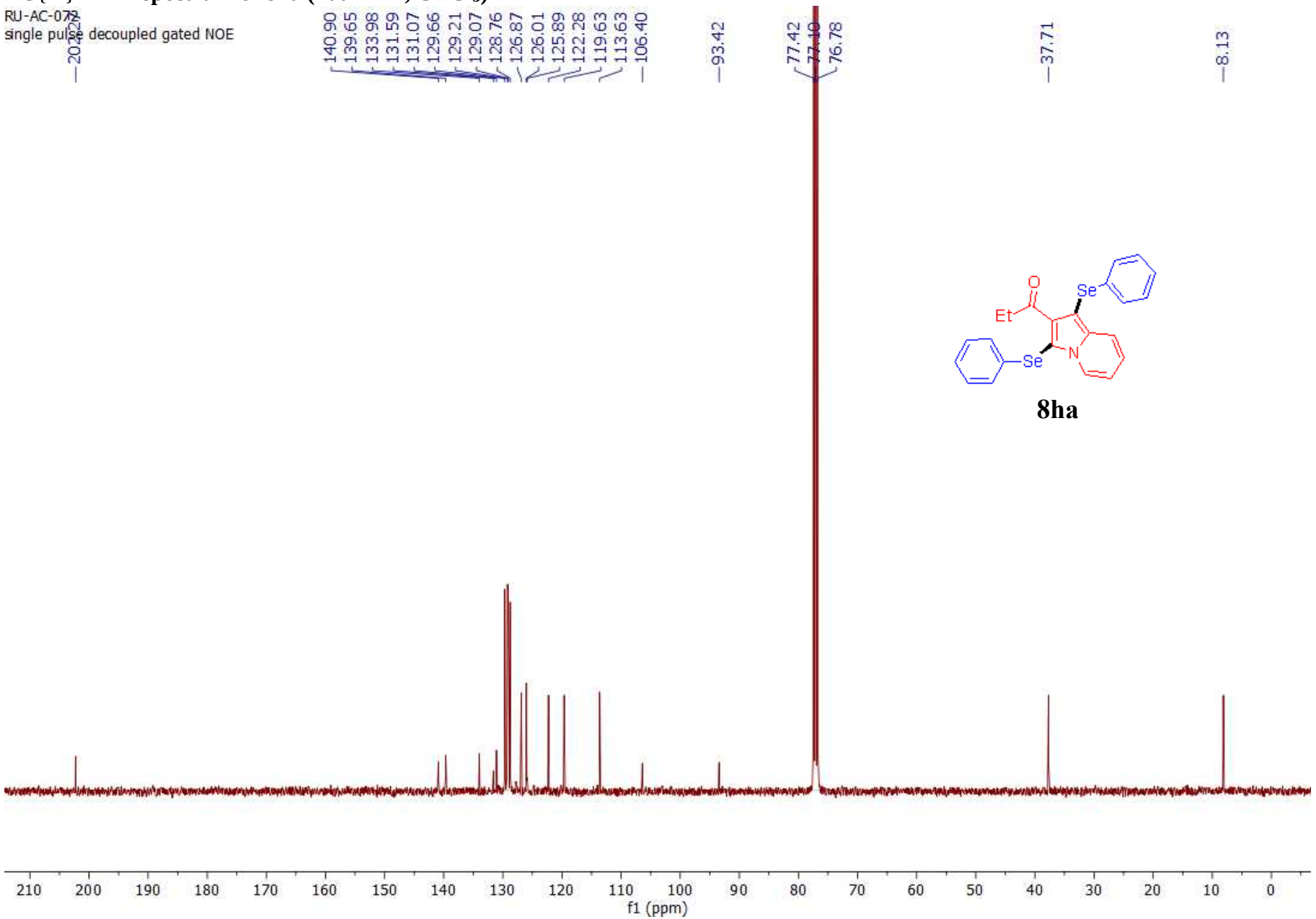


^{1}H NMR spectrum of 8ha (400 MHz, $CDCl_3$)



8ha

$^{13}C\{H\}$ NMR spectrum of 8ha (100 MHz, $CDCl_3$)



8ha