Electronic Supporting Information

Reaction Behaviour of Arylamines with Nitroalkenes in the Presence of Bismuth(III) Triflate: An Easy Access to 2,3-Dialkylquinolines

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Theoretical Calculations

All quantum chemical studies were performed using Gaussian09 suite[1] software. The geometry and transition states were optimization without any symmetry constraints using B3LYP method. Bi and I were optimized using LANL2DZ basis set and all other atoms were optimized at 6-311+G(d,p) basis set.[2] Frequencies were calculated at the same level to confirm the zero imaginary frequency for all geometries and one imaginary frequency for all transition states. Natural Bond Orbital (NBO) analysis was performed on the same level of theory to calculate the NBO charges on the atoms.

Table. List of Gibbs free energy the intermediates, substrates and transition state obtained at B3LYP/LANL2DZ-6-311+G(d,p) level of theory.

Geometry name	Gibbs free energy (a. u.)	Imaginary frequency (cm^{-1})		Geometry name	Gibbs free energy (a. u.)	Imaginary frequency (cm^{-1})
1A (aniline)	-287.591460	0		**$IN2_{C–C}$**	-3539.701940	0
2	-361.757450	0		**$IN2_{C–N}$**	-3539.692394	0
2A	-3252.112001	0		**$IN3_{C–N}$**	-649.337655	0
$Bi(OTf)_3$	-2890.352483	0		**$IN4_{C–N}$**	-404.288719	0
CH_3NO_2	-245.069404	0		**$IN4'_{C–N}$**	-404.286710	0
$IN1_{C–C}$	-3539.699971	0		**$IN5_{C–N}$**	-808.560616	0
$IN1_{C–N}$	-3539.690831	0		**$IN6_{C–N}$**	-808.572945	0
$IN1'_{C–N}$	-3539.706161	0		**$IN7_{C–N}$**	-520.993155	0
$TS_{C–C}$	-3539.678511	-782.66		**TS2**	-649.276296	-230.57
TS1	-649.300839	-263.68		**$IN3_{C–C}$**	-649.347404	0

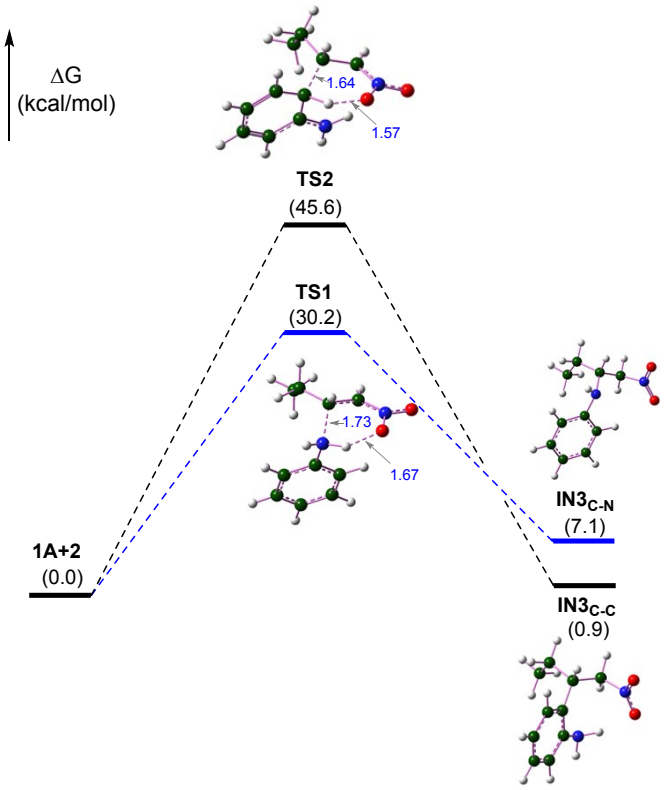


Figure S1. Potential energy diagram for the formation of intermediate $\mathbf{IN3_{C-N}}$ *via* C–N bond formation and $\mathbf{IN3_{C-C}}$ *via* C–C bond formation without $Bi(OTf)_3$.

List of co-ordinates

1A

0 1

C	3.06449700	0.23909800	0.53754000
C	2.08602500	-0.38746200	-0.47138300
H	3.10627100	1.32592800	0.42647600
C	0.70074100	0.16035300	-0.33301600
C	-0.37592700	-0.57658100	-0.07972700
H	0.56413700	1.23368200	-0.43767100
H	-0.41074700	-1.64785600	0.05482200
N	-1.70140100	0.03300300	0.04761300
O	-2.62367700	-0.74190100	0.28496000
O	-1.82052100	1.24524400	-0.08401400

H	2.76583600	0.01680400	1.56471200
H	4.07225300	-0.15335000	0.38395100
H	2.43701700	-0.16966500	-1.48787500
H	2.07660500	-1.47575800	-0.36575600

2

0 1

C	-1.15506900	1.21959500	0.00000300
C	0.23837400	1.19248300	-0.00000500
C	0.92633100	-0.02655400	0.00000100
C	0.19490500	-1.21532200	-0.00001200
C	-1.19956500	-1.18976200	-0.00001000
C	-1.87826300	0.02718700	0.00001500
H	-1.67538600	2.17110700	0.00000800
H	0.80029000	2.12122100	0.00000100
H	0.73739300	-2.15320200	-0.00002500
H	-1.75456100	-2.12136600	-0.00001400
H	-2.96218900	0.04782100	0.00002300
N	2.36708700	-0.11333600	-0.00002000
H	2.76228000	0.34121000	-0.81735800
H	2.76227900	0.34079800	0.81754800

2A

0 1

C	6.53565700	-0.49837000	-3.71449900
C	6.05874300	0.39240600	-2.55203000
H	6.45971100	-1.55841100	-3.45941400
C	4.65277100	0.09161900	-2.15350300
C	3.66848200	0.99134700	-2.14021200
H	4.41431600	-0.92738400	-1.85981300
H	3.73792300	2.03825600	-2.39516800

N	2.33404200	0.62079300	-1.73002000
O	1.48890500	1.51728500	-1.69694400
O	2.07757900	-0.54642200	-1.42151800
H	5.94268500	-0.32228100	-4.61475900
H	7.58006100	-0.28207500	-3.94751600
H	6.69741500	0.20704400	-1.67899400
H	6.16685100	1.44936500	-2.80819500
O	-0.62882300	-2.60111400	-0.56559500
O	-2.12803500	1.58577200	-1.19323200
O	1.78545100	0.89527800	1.30361000
S	-2.02868700	-2.65152500	-0.04890100
O	-2.30566400	-1.20574300	0.42569900
S	1.45984800	0.03038200	2.46842400
O	0.18649500	-0.74188100	2.03934800
S	-2.36263200	2.33404300	0.07500900
O	-1.44581300	1.63013300	1.10692400
Bi	-0.43524600	-0.04285500	0.02186300
O	-2.43484700	-3.69645000	0.85521400
O	1.42729300	0.57693400	3.80097200
O	-3.70344400	2.61028200	0.52262700
C	2.75714000	-1.33947200	2.47319700
C	-3.12052400	-2.77972300	-1.58120900
C	-1.50124800	3.99730000	-0.14713200
F	3.95422400	-0.79716000	2.70238900
F	2.77576500	-1.94902500	1.28631800
F	2.48213600	-2.22399900	3.42243900
F	-1.57590200	4.69682600	0.97885600
F	-0.22156500	3.79869000	-0.46486400
F	-2.10032200	4.66704700	-1.12889400
F	-2.78717100	-1.81311800	-2.44069400
F	-4.39632900	-2.65117200	-1.24186200

F	-2.92719100	-3.96394200	-2.15564700

$Bi(OTf)_3$

0 1

O	-0.29361600	2.62443200	-0.70091800
O	2.42918500	-1.04795600	-0.68025200
O	-2.12859200	-1.57376000	-0.69071000
S	0.57704800	2.86517200	0.48331300
O	0.96784500	1.42876900	0.95346100
S	-2.77264800	-0.93169600	0.48867800
O	-1.72558800	0.13052400	0.94964200
S	2.19236700	-1.93158900	0.49499300
O	0.74812700	-1.55742500	0.95478900
Bi	-0.00042100	-0.00172500	-0.39189500
O	0.16906400	3.75851200	1.53395700
O	-3.34013500	-1.72403600	1.54635600
O	3.15997800	-2.03221700	1.55411600
C	-4.14211300	0.16649400	-0.20609600
C	2.21741300	3.49773600	-0.20472500
C	1.92914800	-3.66258400	-0.21119500
F	-5.08201900	-0.60405100	-0.74032500
F	-3.62489700	0.95748800	-1.14918000
F	-4.66076000	0.90589800	0.76255300
F	1.55712300	-4.49155600	0.75224800
F	0.98013700	-3.60689000	-1.14890700
F	3.06546600	-4.08133800	-0.75541200
F	2.65243600	2.64655100	-1.13675200
F	3.10955600	3.58756900	0.76991000
F	2.02182400	4.69170300	-0.75146000

CH_3NO_2

0 1

C	-1.32845000	-0.00936600	-0.00307400
H	-1.66200500	-0.95153900	-0.42759600
N	0.17479500	-0.00001800	-0.01004600
O	0.74167300	-1.08116100	0.00266800
O	0.72253000	1.09109600	0.00264800
H	-1.67022100	0.85457200	-0.56618900
H	-1.63427000	0.07381300	1.04001900

IN1$_{C–C}$

0 1

O	-0.32020100	1.50567100	-2.10877300
O	-1.53942800	1.28345000	2.22240400
O	-0.63005200	-2.64881000	-0.16811500
S	-1.60922500	2.25955400	-2.07920900
O	-2.38687100	1.62488800	-0.90152800
S	-1.58504700	-2.74339200	-1.30489600
O	-2.01283700	-1.27682500	-1.57560400
S	-2.72974600	0.42120300	2.47323800
O	-2.77684400	-0.52941000	1.25038900
Bi	-1.05656400	0.03397500	-0.06243400
O	-2.36256500	2.46285500	-3.28956000
O	-2.66040300	-3.70128000	-1.28106300
O	-3.98978800	1.00660900	2.85208700
C	-0.54057400	-3.13105300	-2.82796200
C	-1.17202200	3.96185200	-1.39379500
C	-2.22069900	-0.74955200	3.86123700
F	0.01392600	-4.33279600	-2.67057700
F	0.42426800	-2.21873000	-2.95854800
F	-1.30269100	-3.13083400	-3.91310800
F	-3.17423200	-1.64944400	4.06736800

F	-1.08749500	-1.36947900	3.52554100
F	-2.02418100	-0.04432600	4.97221000
F	-0.50216000	3.81460800	-0.24821000
F	-2.27748500	4.66127900	-1.17595100
F	-0.40409200	4.59972800	-2.27323700
C	4.41675000	-0.99432400	1.36472700
C	3.40430000	-1.83466400	0.56630200
H	3.19211300	-2.76410600	1.09537700
N	2.07947200	-1.12664000	0.48498900
O	1.72940200	-0.66404100	-0.60328600
O	1.41181700	-1.01756300	1.50042200
C	4.68234300	0.43947400	0.89696600
C	4.83839500	0.87727800	-0.43804300
C	4.89576600	1.37273900	1.92274900
C	5.26228300	2.19369800	-0.67587600
C	5.30823200	2.67682900	1.67701700
H	4.75228900	1.05245300	2.95019400
C	5.51011600	3.08304200	0.36084600
H	5.38222400	2.52075100	-1.70415100
H	5.46936600	3.36217900	2.50036500
H	5.83603800	4.09271500	0.13871500
N	4.62148300	0.01043900	-1.54234000
H	3.64926100	-0.26563600	-1.63680100
H	4.90678700	0.44532000	-2.41148700
H	3.98302200	-0.90378900	2.36514800
C	5.72344400	-1.81754400	1.55197800
C	6.54355700	-2.11737500	0.29473000
H	5.46093900	-2.75639800	2.05498400
H	6.34220100	-1.25683500	2.25847200
H	7.45719500	-2.65064500	0.57004400
H	6.00142800	-2.74433900	-0.41745300

H	6.82809900	-1.20158100	-0.22462300
H	3.70955900	-2.03127300	-0.45506600

IN1$_{C–N}$

0 1

C	-3.28793600	2.17890200	-1.07943300
C	-2.24184800	1.39287500	-1.82602700
H	-2.18018800	1.33124900	-2.90337600
N	-1.30193800	0.77817900	-1.19806200
O	-0.32843900	0.10387500	-1.82528400
O	-1.15743700	0.76089300	0.11966900
H	-2.72866300	2.73951600	-0.32151400
C	-3.96456900	3.22957500	-1.99071400
C	-4.78091300	2.72337800	-3.18405600
H	-3.17308200	3.90194600	-2.34392400
H	-4.60630200	3.83824400	-1.34506000
H	-5.17413800	3.57423700	-3.74611200
H	-4.17971700	2.13089600	-3.87993600
H	-5.62544500	2.10944500	-2.87120500
O	1.61288200	1.93342500	-0.41442800
O	2.27850100	-0.76061000	-1.97184600
O	-2.70162600	-0.87180300	1.48819500
S	1.52904400	2.71668700	0.93145000
O	1.27068100	1.70731700	1.97760800
S	-1.74958200	-2.05887700	1.91363900
O	-0.47298600	-1.95947500	1.18727000
S	3.73846300	-1.07770900	-1.56184100
O	3.81570000	-0.82958800	-0.10448200
Bi	1.07745700	-0.18607500	-0.16041900
O	0.72050900	3.91229700	0.84606000
O	-2.48440500	-3.29462900	1.94596400

O	4.73852300	-0.54266000	-2.45351300
C	-1.34916500	-1.57284000	3.69479000
C	3.31761100	3.27860300	1.14836400
C	3.76891700	-2.95195700	-1.75450800
F	-2.46405600	-1.54611300	4.41346100
F	-0.77910100	-0.37095900	3.70212000
F	-0.50869800	-2.47049400	4.19870300
F	4.94141400	-3.42420200	-1.34199600
F	2.79285600	-3.48506400	-1.00560200
F	3.57577500	-3.29058000	-3.02501700
F	4.12334300	2.22202000	1.15352900
F	3.42080200	3.92366200	2.30918600
F	3.65541200	4.09577700	0.15604600
N	-4.17167800	1.30975800	-0.28841400
H	-2.22159700	-0.15893100	0.95415200
H	-4.55213600	1.81483400	0.50010300
C	-5.09584900	0.38263800	-0.81430900
C	-6.36028900	0.27330400	-0.21484700
C	-4.77782100	-0.49784600	-1.85834300
C	-7.27713000	-0.67730300	-0.65026800
H	-6.62302600	0.94152500	0.59978600
C	-5.70880500	-1.43386100	-2.30151300
H	-3.80113600	-0.47070200	-2.32462600
C	-6.96308200	-1.53410300	-1.70388600
H	-8.24562400	-0.74061500	-0.16686300
H	-5.43979900	-2.10097700	-3.11288200
H	-7.67921700	-2.27053400	-2.04748900

IN1′$_{C–N}$

0 1

C	3.10417300	-2.52110900	-0.14090300

C	2.21367900	-1.74459100	-1.04078200
H	2.44685500	-1.45733600	-2.05280700
N	1.06150400	-1.33632900	-0.58410100
O	0.25991200	-0.58804800	-1.32035700
O	0.61037100	-1.58574400	0.60197300
H	2.49825000	-2.87588200	0.69344500
C	3.81671900	-3.71805300	-0.79184500
C	4.34419800	-3.54697900	-2.22159100
H	3.08247300	-4.52911300	-0.78423800
H	4.62314700	-4.04866100	-0.12765100
H	4.83772500	-4.46878900	-2.53702200
H	3.53006700	-3.36252500	-2.92592100
H	5.06789100	-2.73639700	-2.31318400
O	-2.26078600	-1.93105200	-0.48370600
O	-1.92303600	1.03087500	-1.59122900
O	2.76325900	0.59059700	1.55372300
S	-2.64149400	-2.87131900	0.68182100
O	-2.30696800	-2.16694600	1.93583500
S	2.00720800	1.70601700	0.91995700
O	0.52474300	1.47101800	0.93042000
S	-3.23847100	1.81675400	-1.36057200
O	-3.64263000	1.57255900	0.03796100
Bi	-1.23755400	-0.05307000	0.23814600
O	-2.22049400	-4.24314000	0.48727400
O	2.55153500	2.18062400	-0.34869800
O	-4.19330700	1.68532500	-2.43645700
C	2.18621700	3.11718600	2.15280500
C	-4.52254000	-2.86902200	0.56809900
C	-2.61442600	3.59467900	-1.41101700
F	3.48198200	3.40680000	2.30497200
F	1.67814200	2.76610100	3.33430400

F	1.54832300	4.19539200	1.70273900
F	-3.63006600	4.42390200	-1.17132400
F	-1.67709900	3.77019800	-0.47480900
F	-2.09607500	3.86947400	-2.60566500
F	-4.97936300	-1.62074200	0.66099300
F	-5.02096400	-3.59479200	1.57070200
F	-4.91217400	-3.39713400	-0.58999300
N	4.09688000	-1.54351000	0.58075400
H	3.53193700	-0.72293600	0.94195200
H	4.43682800	-2.03164100	1.41101500
C	5.25992700	-1.03270600	-0.16453000
C	6.48965800	-1.66557900	-0.00802300
C	5.10928000	0.08038600	-0.98547900
C	7.59236700	-1.18866400	-0.71209400
H	6.59476400	-2.51733100	0.65596900
C	6.22109200	0.54375700	-1.68746000
H	4.16374400	0.60498100	-1.05809400
C	7.45589000	-0.08917900	-1.55806100
H	8.55413300	-1.67289800	-0.59389100
H	6.11717100	1.41421100	-2.32373800
H	8.31489700	0.28268900	-2.10374000

$TS_{C–C}$

0 1

C	-2.96276300	-2.80389600	-1.62363000
C	-1.60680100	-2.80684600	-0.97553900
H	-1.27028500	-3.56232300	-0.28122500
N	-0.75013700	-1.86986900	-1.22863800
O	0.44295900	-1.82443400	-0.67052400
O	-1.02403800	-0.82789200	-2.01158000
C	-3.54653900	-1.36786100	-1.80555900

C	-3.82730800	-0.44382400	-0.70713100
C	-4.33414500	-1.19594000	-3.01564300
C	-4.66302200	0.68054400	-0.97600500
C	-5.15868200	-0.13235300	-3.21501100
H	-4.20038800	-1.92999500	-3.80322800
C	-5.30554100	0.82360500	-2.17460500
H	-4.80125900	1.41215100	-0.18832200
H	-5.69215000	-0.00869500	-4.14867100
H	-5.94438200	1.68602700	-2.32962300
N	-3.25512400	-0.52879200	0.49428100
H	-2.61439600	-1.25887900	0.78880400
H	-3.22517800	0.30160100	1.07003400
H	-2.78868400	-3.13247200	-2.65846300
C	-3.91134800	-3.85909100	-1.00903500
C	-4.31782800	-3.67422600	0.45580300
H	-3.42182900	-4.83255600	-1.12737800
H	-4.80779200	-3.89399500	-1.63572500
H	-4.93173700	-4.51997700	0.77435400
H	-3.45332800	-3.62979900	1.12350800
H	-4.90753800	-2.76832700	0.60661300
H	-2.41374000	-0.84737300	-2.08477800
O	-1.29796300	1.74744100	0.17790900
O	3.05701200	0.52305500	-2.14572700
O	-1.22085100	-1.96260100	1.94564000
S	-0.59575800	2.91024700	0.82489800
O	0.88014300	2.59757200	0.79652200
S	0.08400600	-1.49428600	2.44040000
O	0.52536700	-0.20777300	1.69928400
S	3.95296500	0.05186800	-1.06180500
O	3.03805800	-0.17369000	0.16889200
Bi	0.93145700	0.38949400	-0.33012100

O	-1.15143500	3.41998300	2.05998400
O	1.14480000	-2.45938400	2.62783900
O	5.17925700	0.75670600	-0.77503500
C	-0.27596000	-0.71051900	4.11855400
C	-0.77198800	4.29021900	-0.44438500
C	4.44147300	-1.71340400	-1.51527200
F	-0.68581700	-1.67051200	4.95083000
F	-1.24212400	0.20119000	3.99783400
F	0.81666400	-0.13895200	4.60756300
F	5.13326000	-2.26210400	-0.52262100
F	3.35156400	-2.44260800	-1.75315200
F	5.19521400	-1.68036500	-2.61464000
F	-0.25348500	3.89409700	-1.61494600
F	-0.13861100	5.38521900	-0.03632700
F	-2.06606200	4.57311100	-0.62366500

IN2$_{C–C}$

0 1

O	-2.04002100	-2.03234500	-1.59649400
O	-2.56117200	2.53281900	-0.59454500
O	2.10788800	-1.56134700	0.81386600
S	-3.25582600	-2.03740800	-0.73563400
O	-3.12580600	-0.80739200	0.17724300
S	0.95485900	-1.61643000	1.74419600
O	-0.34514700	-1.23856300	1.01228900
S	-2.49080100	2.68738100	0.88206400
O	-1.61043400	1.50026200	1.36215900
Bi	-1.14354400	0.22349100	-0.36741500
O	-3.66603400	-3.25803000	-0.08349300
O	1.11307500	-0.99654000	3.04051900
O	-3.68644900	2.90576500	1.65558000

C	0.62087600	-3.45488200	2.01281000
C	-4.66390000	-1.52857700	-1.87928100
C	-1.37162000	4.17301200	1.20463200
F	1.67746200	-3.98255800	2.63135600
F	0.44847200	-4.05644300	0.84025700
F	-0.45938500	-3.61055700	2.76422700
F	-1.09704300	4.25600900	2.50168800
F	-0.23606000	4.05531600	0.51692600
F	-2.00841200	5.27530400	0.81324600
F	-4.35157500	-0.37409000	-2.48098600
F	-5.78641500	-1.37140400	-1.18659800
F	-4.84347400	-2.46683000	-2.80742000
C	4.19273600	1.12555600	-1.79120000
C	3.06086600	1.55387600	-0.90750900
H	3.06817700	2.48895400	-0.36648200
N	1.94723100	0.91288800	-0.80750400
O	0.93041200	1.29390900	-0.07230100
O	1.77473200	-0.29383700	-1.47631100
C	5.09204100	0.03207100	-1.20748500
C	5.28142600	-0.15209000	0.16998000
C	5.81603900	-0.76342100	-2.10358000
C	6.22459200	-1.08612900	0.61505000
C	6.74735800	-1.69279600	-1.65478800
H	5.65598800	-0.64045000	-3.17014300
C	6.96254100	-1.84484500	-0.28600900
H	6.36230500	-1.22379700	1.68240300
H	7.30075600	-2.29308300	-2.36734200
H	7.68673600	-2.56412000	0.07851900
N	4.50172300	0.62620100	1.09051800
H	3.68641300	0.10142700	1.40267100
H	5.03756300	0.86936700	1.91747800

H	1.97452900	-0.97159900	-0.77353900
H	3.73366900	0.69684500	-2.68745500
C	5.00563200	2.37134300	-2.24381000
C	5.80717100	3.07979600	-1.14957700
H	4.31273100	3.07685500	-2.71693100
H	5.68670200	2.03867900	-3.03231700
H	6.34925600	3.92790800	-1.57462700
H	5.17070300	3.46690300	-0.34938600
H	6.53922000	2.40818700	-0.69624700

IN2$_{C–N}$

0 1

O	0.80459200	2.63440400	0.53209800
O	1.65521900	-0.61889600	-2.47388000
O	0.38666400	-1.75471100	1.91741200
S	2.17475100	2.96349400	0.03947700
O	2.76480800	1.59280800	-0.37086400
S	1.39071400	-1.18933900	2.85762200
O	2.04373600	-0.01855500	2.07770900
S	2.72459000	-1.55823600	-2.03228000
O	2.71186700	-1.44969200	-0.48592500
Bi	1.17116100	0.07708600	0.03998100
O	3.04415200	3.81215900	0.81254000
O	2.31321200	-2.05298400	3.54955400
O	4.02748200	-1.52295000	-2.64512000
C	0.40095200	-0.27070800	4.17584900
C	1.91529400	3.79722000	-1.63238200
C	2.03439900	-3.29160400	-2.31113800
F	-0.33547900	-1.15435900	4.85001800
F	-0.40528500	0.61797600	3.59439700
F	1.22265200	0.35169100	5.01032100

F	2.89140700	-4.19703700	-1.85505800
F	0.86983600	-3.41989100	-1.67406200
F	1.84449000	-3.47498400	-3.61600600
F	1.14535900	3.01811100	-2.39688900
F	3.08393100	3.98930600	-2.22982600
F	1.30987500	4.96660500	-1.44619100
C	-4.15903000	-1.71506000	-0.88057600
C	-3.36334900	-1.57333000	0.42300600
H	-3.13132400	-2.55249400	0.84527900
N	-2.02967200	-0.93499200	0.14855100
O	-1.75532700	0.11590700	0.71532400
O	-1.26993900	-1.50062100	-0.62813600
H	-3.52137200	-2.28702600	-1.55911700
C	-5.43520200	-2.56554800	-0.65018800
C	-6.35755700	-2.17679400	0.51223200
H	-5.11124200	-3.60458900	-0.51597900
H	-6.00033100	-2.54680800	-1.58774800
H	-7.21860700	-2.84944000	0.53877600
H	-5.85718400	-2.26443100	1.48116100
H	-6.73520600	-1.15848400	0.41807200
H	-3.84457000	-0.94546600	1.16573200
N	-4.32277700	-0.41191500	-1.55241800
H	-4.40912900	-0.56884200	-2.54848700
C	-5.28402900	0.55120800	-1.12356900
C	-6.42370200	0.80831000	-1.89674500
C	-5.07118100	1.31312100	0.03335800
C	-7.33915500	1.78592800	-1.51331100
H	-6.59339700	0.23558600	-2.80337800
C	-6.00299200	2.26994100	0.42726300
H	-4.15784500	1.19076700	0.60155600
C	-7.14155000	2.51165100	-0.34045000

H	-8.21184300	1.97243000	-2.12913600
H	-5.82161400	2.84965300	1.32537400
H	-7.85662000	3.26694400	-0.03666100

IN3$_{C–N}$

0 1

C	-1.22579700	1.02313900	-0.44109900
C	-1.94344700	0.21544100	0.64223900
H	-1.28473300	-0.16295700	1.41712000
N	-2.63469200	-0.99283200	0.04855800
O	-2.32810100	-2.09076000	0.48761100
O	-3.46404800	-0.78652100	-0.82307600
H	-1.98392100	1.23882400	-1.19810900
C	-0.75127400	2.39162600	0.11299600
C	0.09685700	2.38809300	1.39139900
H	-1.64623400	3.00366400	0.27954600
H	-0.19602200	2.88641400	-0.69108800
H	0.38135200	3.41143000	1.65050800
H	-0.45267800	1.98289400	2.24603500
H	1.01264000	1.80767400	1.27551500
N	-0.22129000	0.21883800	-1.16305900
H	-0.09597500	0.60663600	-2.08892900
C	1.03509300	-0.14583300	-0.60800800
C	2.22103700	0.38751900	-1.13324500
C	1.12810000	-1.10727600	0.40945700
C	3.46278800	-0.00963000	-0.64289100
H	2.16644600	1.12194600	-1.93126800
C	2.37093600	-1.47956900	0.91461200
H	0.23389400	-1.59915700	0.77054100
C	3.54519700	-0.93431600	0.39604400
H	4.36585100	0.41364300	-1.06884100

H	2.42106300	-2.22491600	1.70077400
H	4.50986700	-1.23832500	0.78503800
H	-2.73941900	0.81327600	1.08935800

IN4$_{C–N}$

0 1

C	-1.69859400	-0.54856800	0.47010000
H	-1.28185400	-1.34200100	1.10909300
C	-3.19719600	-0.48933100	0.39837900
C	-3.76655300	0.61306600	-0.49138000
H	-3.57359200	-0.39311200	1.42635300
H	-4.85898200	0.58141100	-0.48526400
H	-3.44682800	1.59861000	-0.14750900
H	-3.42280900	0.50273300	-1.52177500
N	-0.94395500	0.26353700	-0.14945200
C	0.45781400	0.11923600	-0.07992300
C	1.23464000	1.26928800	0.11500800
C	1.09952700	-1.11453200	-0.25857800
C	2.62077600	1.17803300	0.17831300
H	0.73255400	2.22365000	0.22236700
C	2.48989800	-1.19593300	-0.21191900
H	0.50861300	-2.00047500	-0.46245800
C	3.25592100	-0.05426000	0.01456700
H	3.20945000	2.07354400	0.34418500
H	2.97490100	-2.15447200	-0.36122300
H	4.33726000	-0.12026000	0.04893600
H	-3.54843300	-1.47638200	0.06605400

IN4′$_{C–N}$

0 1

C	1.86272600	-0.72758800	-0.28419700

H	1.44803400	-1.67580800	-0.60207900
C	3.18934700	-0.59555200	-0.13110600
C	3.90120100	0.65232700	0.31034600
H	3.79621200	-1.46099100	-0.37059700
H	4.79853200	0.40621400	0.88427100
H	4.22802500	1.26777500	-0.53812900
H	3.27447200	1.28197700	0.95088200
N	0.92493300	0.28062200	-0.10529600
H	1.26912900	1.22592000	-0.04876100
C	-0.45918800	0.13042100	-0.03964700
C	-1.27015700	1.27647900	-0.11792700
C	-1.07917300	-1.12010200	0.11173700
C	-2.65347000	1.17269400	-0.05473700
H	-0.80515800	2.25059200	-0.23645700
C	-2.46827200	-1.21089900	0.16037700
H	-0.48440400	-2.01849000	0.21406800
C	-3.26800400	-0.07333600	0.07860600
H	-3.25576300	2.07238700	-0.11737000
H	-2.92628500	-2.18704000	0.27762200
H	-4.34737600	-0.15356000	0.12291800

IN5$_{C–N}$

0 1

C	1.02764000	1.31565700	-0.42929700
C	0.74396100	2.71934200	-0.99029200
C	-0.73319900	3.06969400	-1.18732400
H	1.21453500	3.47135500	-0.34434300
H	-1.27979000	3.11325600	-0.24148500
H	-0.82888000	4.05004500	-1.66161800
H	-1.23377600	2.33868200	-1.82764700
N	2.47281000	1.12534500	-0.43119700

H	3.00977400	1.91974300	-0.11563800
C	3.10452800	-0.10278100	-0.26860300
C	4.47944900	-0.13391200	0.03784200
C	2.43506800	-1.32765300	-0.44147800
C	5.15757900	-1.33938000	0.15399200
H	5.01333600	0.80207400	0.17499800
C	3.12987400	-2.53017600	-0.32112000
H	1.37721500	-1.34825300	-0.67076800
C	4.49017700	-2.55299400	-0.02519200
H	6.21680700	-1.33094300	0.38789300
H	2.59107800	-3.46125600	-0.46127300
H	5.02042800	-3.49320800	0.06696300
C	-1.06549600	0.64706500	0.88850300
H	-1.76408500	1.19946800	1.53491100
C	0.39765100	1.01775100	0.97813700
N	-1.46849900	-0.29226400	0.13221000
C	-2.84060100	-0.60989100	0.05405500
C	-3.20032700	-1.96396400	0.01042400
C	-3.84510200	0.36485800	-0.03541100
C	-4.53841700	-2.33352400	-0.06953900
H	-2.41629200	-2.71096700	0.05045100
C	-5.18285500	-0.01262400	-0.13345600
H	-3.57473600	1.41432200	-0.05606800
C	-5.53654600	-1.36040300	-0.14234100
H	-4.80378500	-3.38480500	-0.08696900
H	-5.94964100	0.75042300	-0.21131400
H	-6.57789500	-1.65094900	-0.21969100
H	0.59433000	0.58579100	-1.11789700
H	1.25892600	2.78252700	-1.95357200
H	0.90224600	0.10578600	1.31818300
C	0.65047100	2.10936200	2.02442600

H	1.71613400	2.33820200	2.10330000
H	0.12277100	3.03869900	1.79180100
H	0.31800000	1.77987100	3.01274000

IN6$_{C–N}$

0 1

C	1.99315300	-1.35595500	0.22735300
C	2.90220500	-2.59959200	0.13125200
C	2.41528600	-3.81628700	0.92630000
H	3.05276500	-2.86106800	-0.92165100
H	1.43725600	-4.16863800	0.59465700
H	3.11833700	-4.64762200	0.82518300
H	2.33490000	-3.57872600	1.99156500
N	2.83712100	-0.15835100	0.19406900
H	3.65590600	-0.20075800	0.78363700
C	2.27626300	1.10634100	0.07066500
C	3.04510600	2.25228800	0.35150500
C	0.95138900	1.26471200	-0.37888300
C	2.51226900	3.52125600	0.18571700
H	4.06860100	2.13157200	0.69364300
C	0.43812800	2.55556800	-0.54301600
C	1.19977700	3.68500200	-0.26722700
H	3.12369300	4.38905000	0.40790300
H	-0.58438800	2.66714000	-0.89076400
H	0.78266100	4.67556900	-0.40263000
C	0.08640500	0.04701600	-0.65502500
C	0.95808100	-1.21155500	-0.90835600
N	-0.87844300	-0.14735500	0.44537900
C	-2.26428200	-0.08494100	0.29626200
C	-3.05338200	0.26527500	1.41008800
C	-2.92498800	-0.39537600	-0.90463000

C	-4.43831100	0.30307700	1.32387000
H	-2.56435900	0.51056000	2.34824500
C	-4.31573700	-0.34400000	-0.98148800
H	-2.36218700	-0.69110900	-1.78004700
C	-5.08692500	0.00204600	0.12468600
H	-5.01580800	0.57775900	2.20008800
H	-4.79777100	-0.58694800	-1.92251800
H	-6.16758900	0.03561600	0.05712500
H	1.44041200	-1.41004100	1.18165000
H	3.89396700	-2.32462100	0.50843000
H	1.53499200	-1.00920900	-1.82080100
C	0.09985600	-2.45562500	-1.14622200
H	0.71125100	-3.32004400	-1.41231100
H	-0.49509800	-2.70584600	-0.26508400
H	-0.59176200	-2.28612400	-1.97577600
H	-0.56379300	0.26791000	1.31028400
H	-0.48848400	0.24000500	-1.56407800

IN7$_{C–N}$

0 1

C	-1.40810500	-0.42518400	0.25039800
C	-2.63798700	-1.04976800	-0.45471700
C	-3.95848200	-0.96026500	0.31755700
H	-2.73830000	-0.61712800	-1.45503000
H	-4.29231100	0.06752900	0.46722600
H	-4.75048500	-1.48633600	-0.22230500
H	-3.86715500	-1.42508900	1.30430600
N	-0.21981400	-1.17024200	-0.18484400
H	-0.30033500	-2.16947500	-0.06320000
C	1.06682200	-0.67400000	-0.04344200
C	2.18593700	-1.51360300	0.00767700

C	1.24555400	0.72635100	-0.03229100
C	3.46737400	-0.97108200	0.06961300
H	2.05019700	-2.59089100	-0.00739400
C	2.54055300	1.24787100	0.02874500
C	3.65371900	0.41164700	0.08282500
H	4.32384800	-1.63507300	0.11065700
H	2.66999400	2.32579100	0.03158700
H	4.65163600	0.83047200	0.13255200
C	0.05138500	1.55427000	-0.11053200
C	-1.19530700	1.06382900	-0.00602700
H	-1.56429500	-0.55014900	1.34212000
H	-2.41376400	-2.11028400	-0.61494300
C	-2.39337800	1.97141000	-0.01715600
H	-3.10348300	1.71041800	-0.80830500
H	-2.94121900	1.92127100	0.93175100
H	-2.08645800	3.00766500	-0.17079300
H	0.19231300	2.62412000	-0.24022600

IN3$_{C–C}$

0 1

C	-0.72340400	0.81245100	-0.68477700
C	-1.98653900	0.34816500	0.05550200
H	-2.85541500	0.86286800	-0.35539300
N	-2.25449600	-1.12107200	-0.18230600
O	-2.08351600	-1.89107300	0.75836300
O	-2.61227000	-1.45213500	-1.29885700
C	0.60248000	0.10215100	-0.39187600
C	1.06342400	-0.35393900	0.86445800
C	1.47856900	0.00650300	-1.48325400
C	2.38566500	-0.81383900	0.97674400
C	2.78276700	-0.45868400	-1.36528000
H	1.12239100	0.32778000	-2.45738500
C	3.24377700	-0.85629500	-0.11306400

H	2.73209200	-1.15880400	1.94642900
H	3.42552000	-0.50936700	-2.23601500
H	4.25747500	-1.21970200	0.01262300
N	0.24899400	-0.32205700	2.02231500
H	-0.58953900	-0.88808100	1.92979800
H	0.75726700	-0.63576000	2.83982300
H	-0.93111600	0.62396900	-1.74251000
C	-0.59586600	2.35724500	-0.55204800
C	-0.31059100	2.90753600	0.84833200
H	-1.51624100	2.80756000	-0.94442700
H	0.20669300	2.66765100	-1.22736200
H	-0.19822500	3.99424000	0.80359800
H	-1.11716900	2.69066600	1.55319600
H	0.60822100	2.48986400	1.26336000
H	-1.93883700	0.48690700	1.12973400

TS1

0 1

C	1.35316900	1.14090300	0.43005300
C	1.94493400	0.26732800	-0.54883000
H	1.93155200	0.43113900	-1.61185500
N	2.49357500	-0.90378400	-0.13086200
O	3.08182000	-1.66977400	-0.91207700
O	2.32876800	-1.23310800	1.11494300
H	1.99539100	1.29291400	1.30258800
C	0.77278200	2.46425100	-0.05249100
C	-0.00235900	2.45526500	-1.37497000
H	1.62367600	3.14949000	-0.13909700
H	0.14451400	2.88134000	0.74320000
H	-0.39379300	3.45517100	-1.57927400
H	0.63837800	2.17904000	-2.21445000
H	-0.84545900	1.76354300	-1.35439600
H	0.85681200	-0.54825900	1.51331200
N	0.17467300	0.24119400	1.31698700
H	-0.01812000	0.75421300	2.17458200
C	-1.03842200	-0.19834400	0.68040000
C	-2.23415000	0.48135200	0.91889100

C	-0.99846100	-1.28660800	-0.19189900
C	-3.39814700	0.07276600	0.27564400
H	-2.25560800	1.32316200	1.60388200
C	-2.16971400	-1.68120700	-0.83693900
H	-0.07358900	-1.82632800	-0.35153800
C	-3.36661600	-1.00574000	-0.60905200
H	-4.32805700	0.59558000	0.46634400
H	-2.14257400	-2.52692800	-1.51386600
H	-4.27366700	-1.32268700	-1.11007900

TS2

0 1

C	-0.62953400	0.86608400	-0.77921100
C	-1.89814900	0.58807900	-0.07633600
H	-2.40815300	1.28274200	0.57243800
N	-2.48664300	-0.60995000	-0.23265400
O	-3.54435200	-0.93229200	0.35602100
O	-1.86235000	-1.48987100	-0.97796100
C	0.47040400	-0.31735000	-0.50252900
C	0.87203300	-0.60772000	0.87552400
C	1.54913900	-0.29822300	-1.47649500
C	2.23877600	-0.82447900	1.18533700
C	2.84992200	-0.54839300	-1.15867500
H	1.27353000	-0.07823800	-2.50332800
C	3.19084400	-0.80210700	0.19658100
H	2.51986700	-1.02868100	2.21330700
H	3.62168900	-0.54520300	-1.91832300
H	4.22767700	-0.98288800	0.45894600
N	-0.05560500	-0.74310700	1.83306600
H	-1.02578000	-0.52136400	1.64192700
H	0.21637000	-0.92190100	2.78709300
H	-0.77993800	0.73098900	-1.85771900
C	-0.09224400	2.29016100	-0.55576200
C	0.24625500	2.69138300	0.88367200

H	-0.85145500	2.97571700	-0.94928300
H	0.79463000	2.42483800	-1.18308400
H	0.56520200	3.73648800	0.91688100
H	-0.61293300	2.58989500	1.55139000
H	1.06317500	2.09026900	1.29083400
H	-0.33918600	-1.12856300	-0.80107400

Figure: S2. ORTEP Diagram of compound 3k with 40% ellipsoid probability

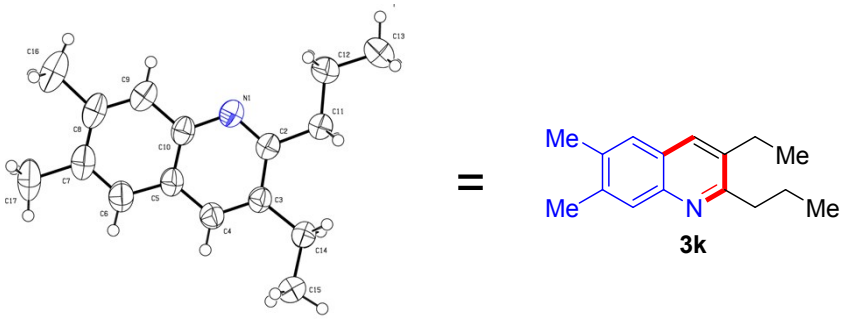
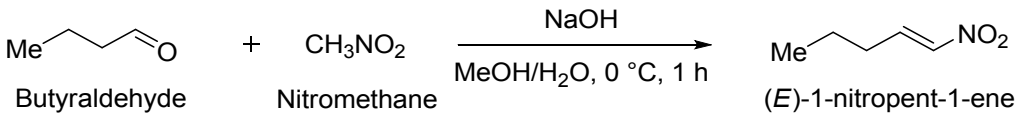


Table S2. Crystal data and structure refinement for compound 3k:

Entry	Identification code	Compound 3k
01	Empirical formula	$C_{16}H_{21}N$
02	Formula weight	227.34
03	Temperature	293(2)K
04	Wavelength	0.71073
05	Radiation type	MoK\a
06	Radiation source	'fine-focus sealed tube'
07	Crystal system	Triclinic
08	Space group	P-1
09	Cell length	a=7.4928(7)b=8.7755(11)c=11.1633(11)
10	Cell Angle	α 84.247(9)β 78.666(8)δ 76.675(10)
11	Cell Volume	699.17(13)
12	Density	1.080
13	Completeness to theta	0.999-25.046
14	Absorption correction	multi-scan
15	Refinement method	Full-matrix least-squares on F2
16	Index ranges	$-11 \leq h \leq 11$, $-11 \leq k \leq 11$, $-14 \leq l \leq 16$
17	Reflection number	4702
18	Theta range	2.840-25.046
19	Cell formula units Z	4
20	CCDC no	1859531

1. General Procedure for (E)-1-nitropent-1-ene[3]



A mixture of butyraldehyde (1.72 g, 14.95 mmol) and nitromethane (1.22 g, 20 mmol) was dissolved in 5 mL of methanol into 25 mL round bottomed flask and it was cooled in ice-bath Then a solution of NaOH was added drop-wise manner into it by dissolving 1 g of NaOH in 2 mL of water. Subsequently, 2 mL of methanol was added into it and the resulting yellow slurry stirred at same temperature for another 1h. After that 15 mL of water was added and the clear yellow solution was poured into hydrochloric acid solution (10 mL conc. HCl in 15mL H_2O) and stirred for 10 min. The resulting mixture was extracted with CH_2Cl_2 (3 x 20 mL), the combined organic layers were dried over anhydrous Na_2SO_4 and the solvent removed under reduced pressure. The residue was purified by column chromatography (*n*-hexane/EtOAc, 25:1, v/v) to give the product as a pale-yellow liquid (0.532 g, 32%).

References

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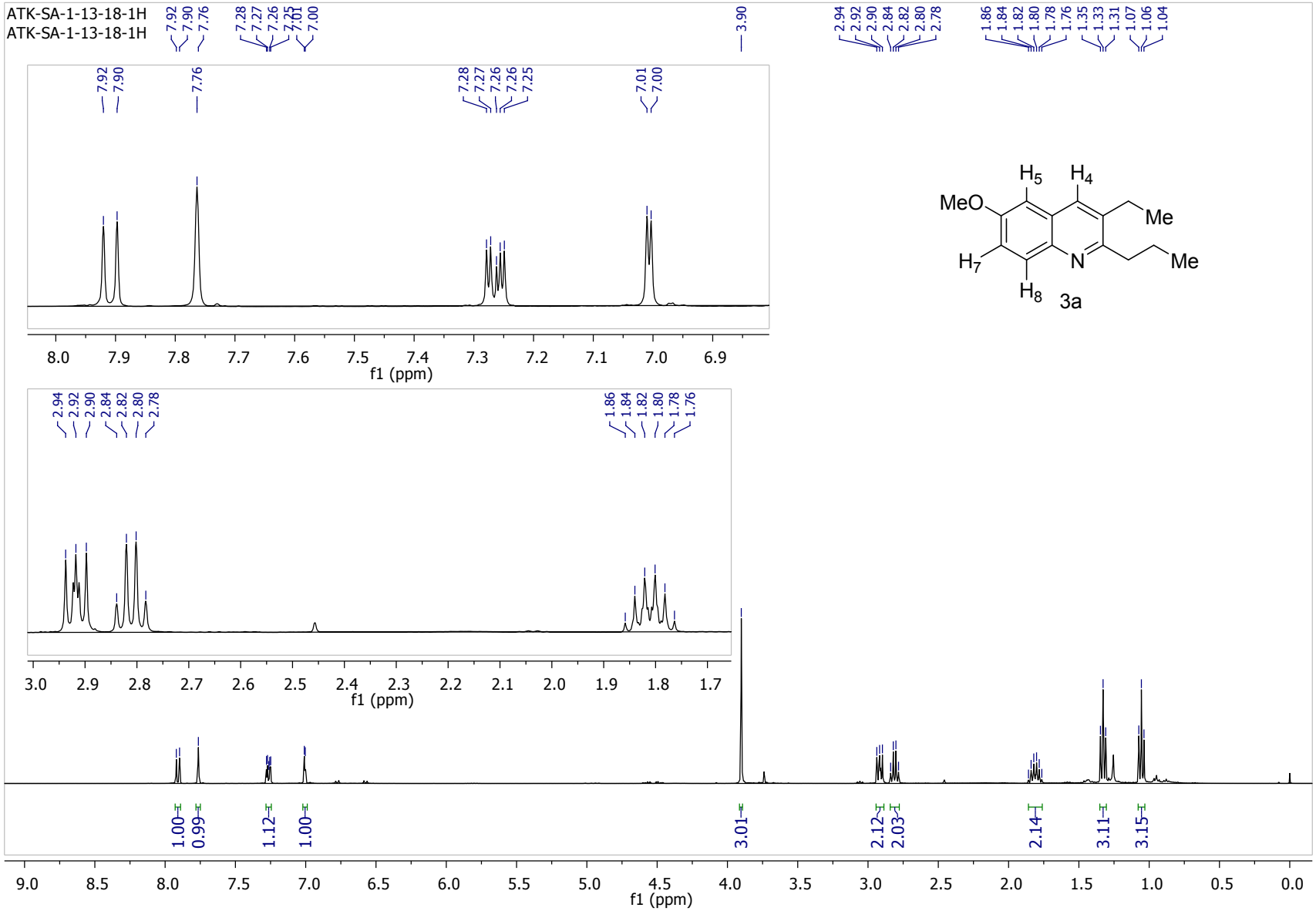
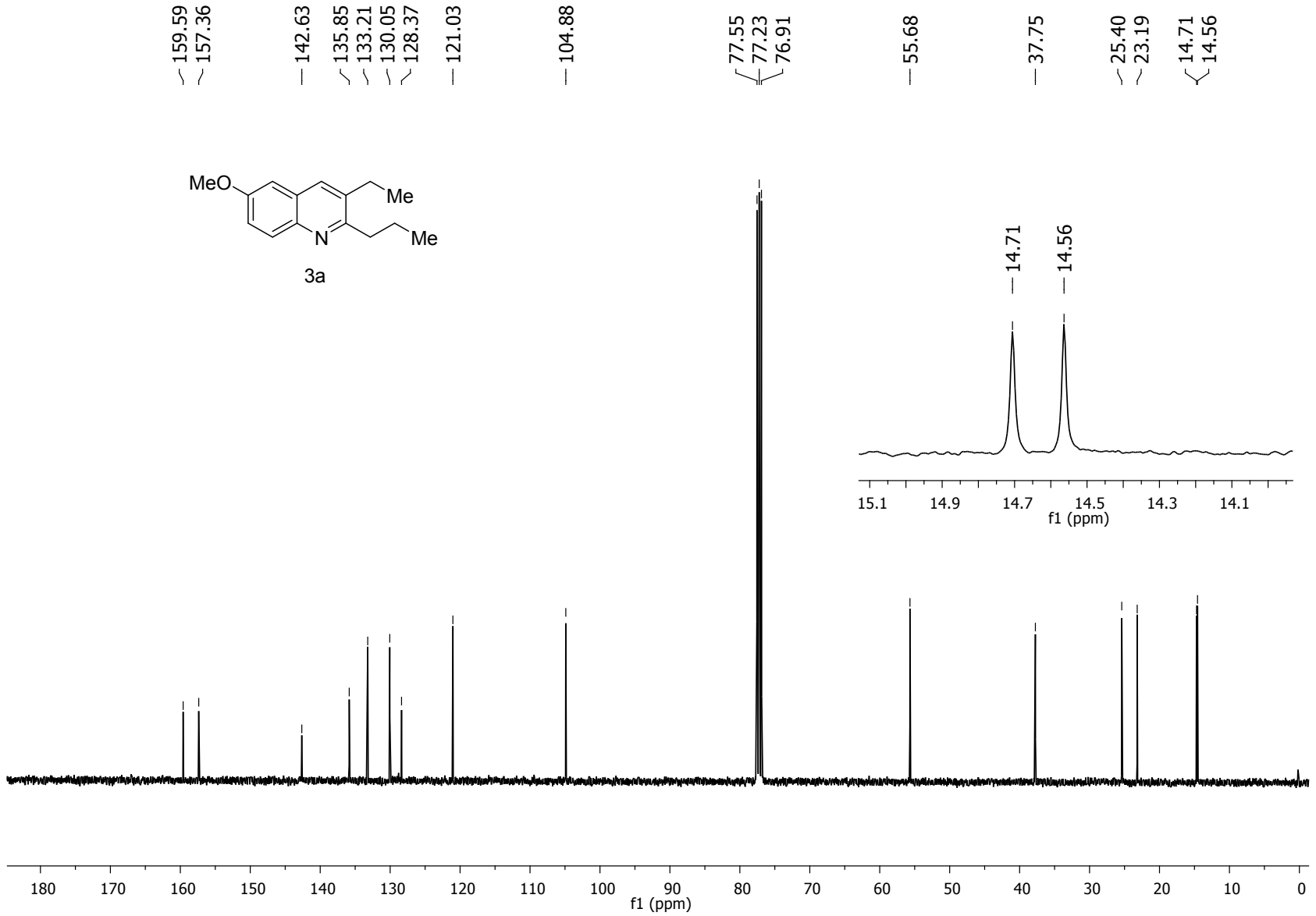
2. (a) W. Kohn, A. D. Becke, R. G. Parr, *J. Phys. Chem.,* 1996, **100**, 12974-12980; (b) C. Lee, W. Yang, R. G. Parr, *Phys. Re*V. *B.,* 1988, **37**, 785-789; (c) W. R. Wadt, P. J. Hay, *J. Chem. Phys*., **1978, 82**, 284-298.

3. G. Zhang, *Org. Biomol. Chem*., 2012, 10, 2534.

^{1}H NMR spectra of compound: 3a



^{13}C NMR spectra of compound: 3a



HRMS spectra of compound: 3a

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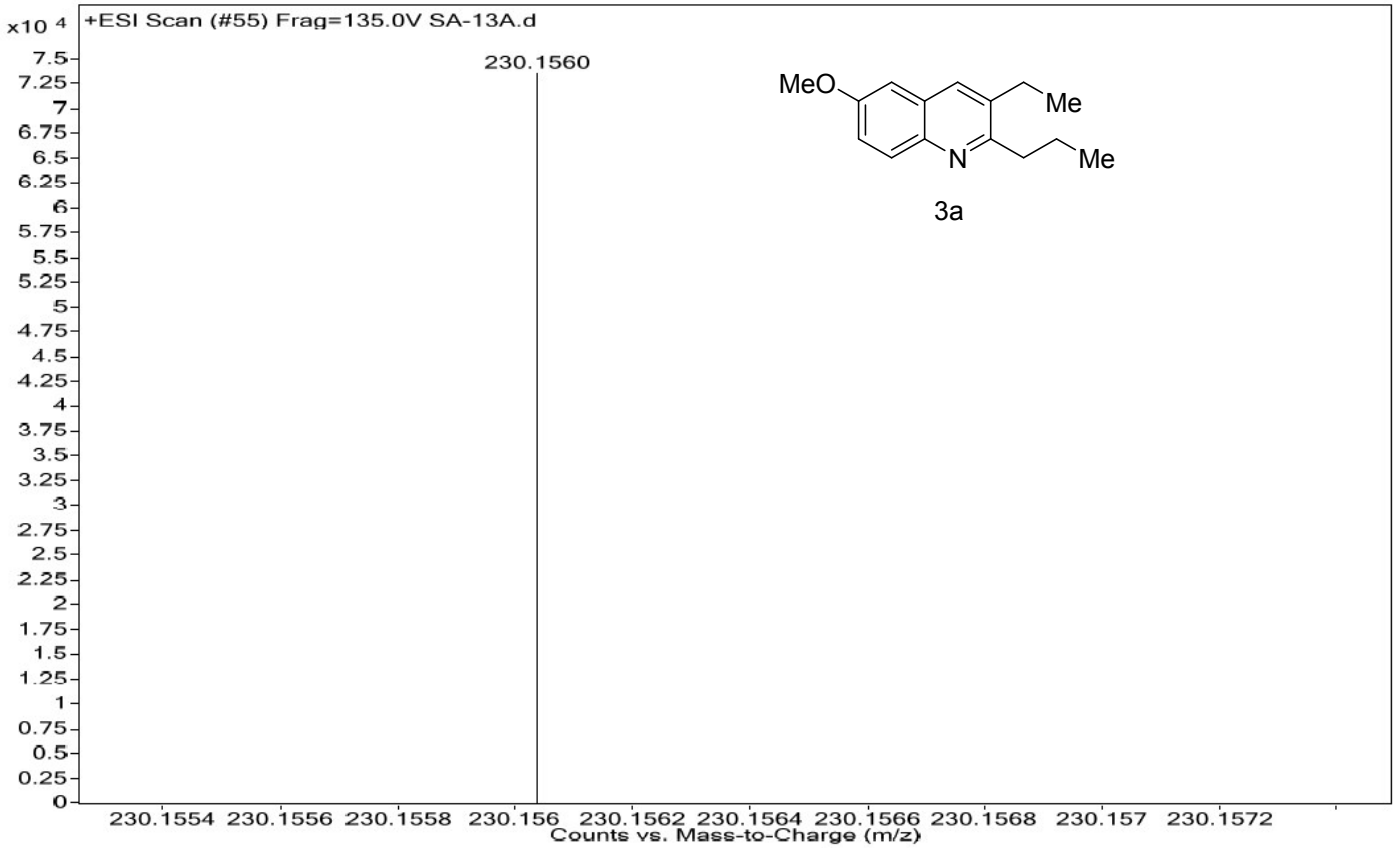
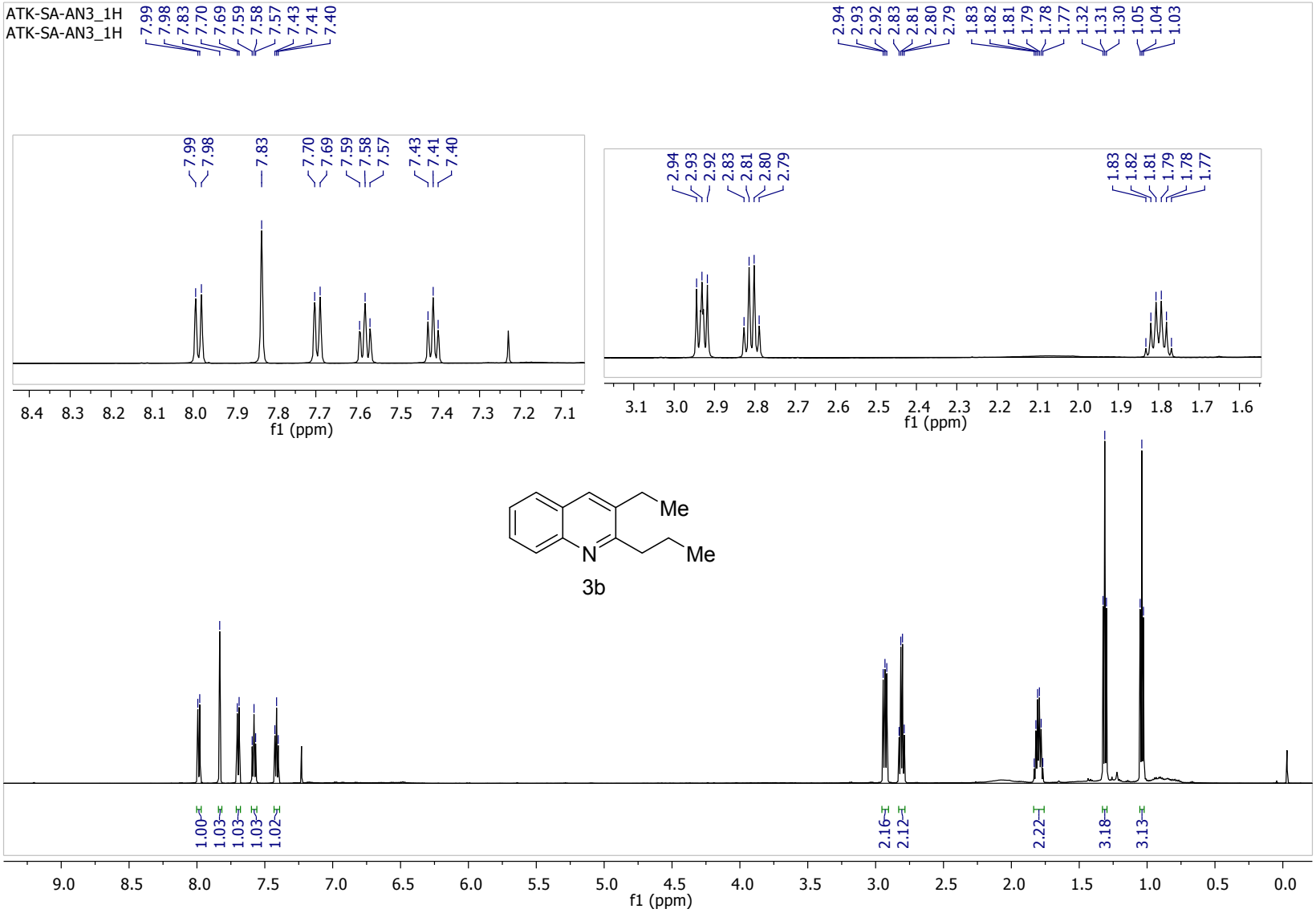
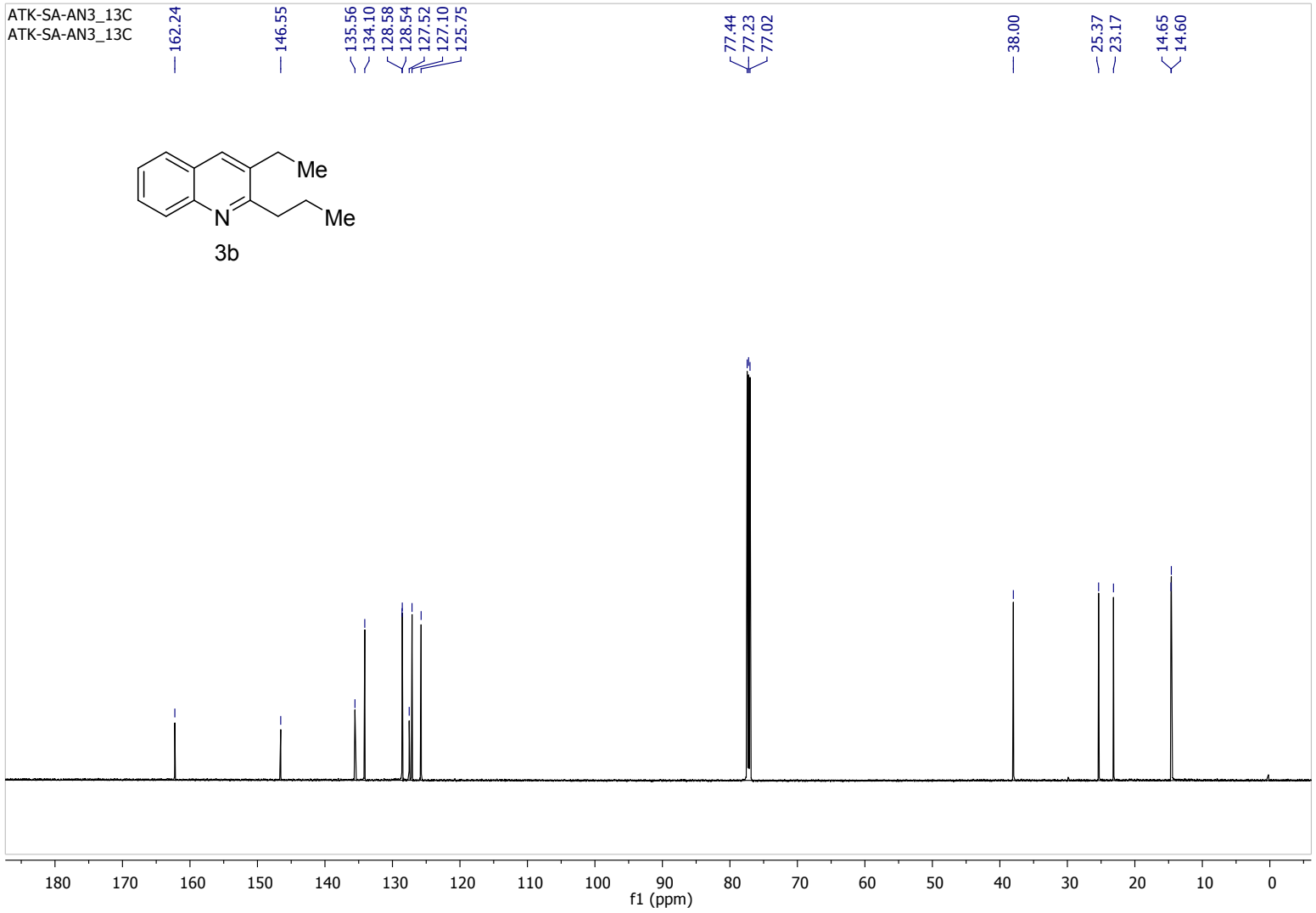


^{1}H NMR spectra of compound: 3b



^{13}C NMR spectra of compound: 3b



HRMS spectra of compound: 3b

Sample Name	SA-AN3	Position	Vial 1	Instrument Name	QTOF	User Name	
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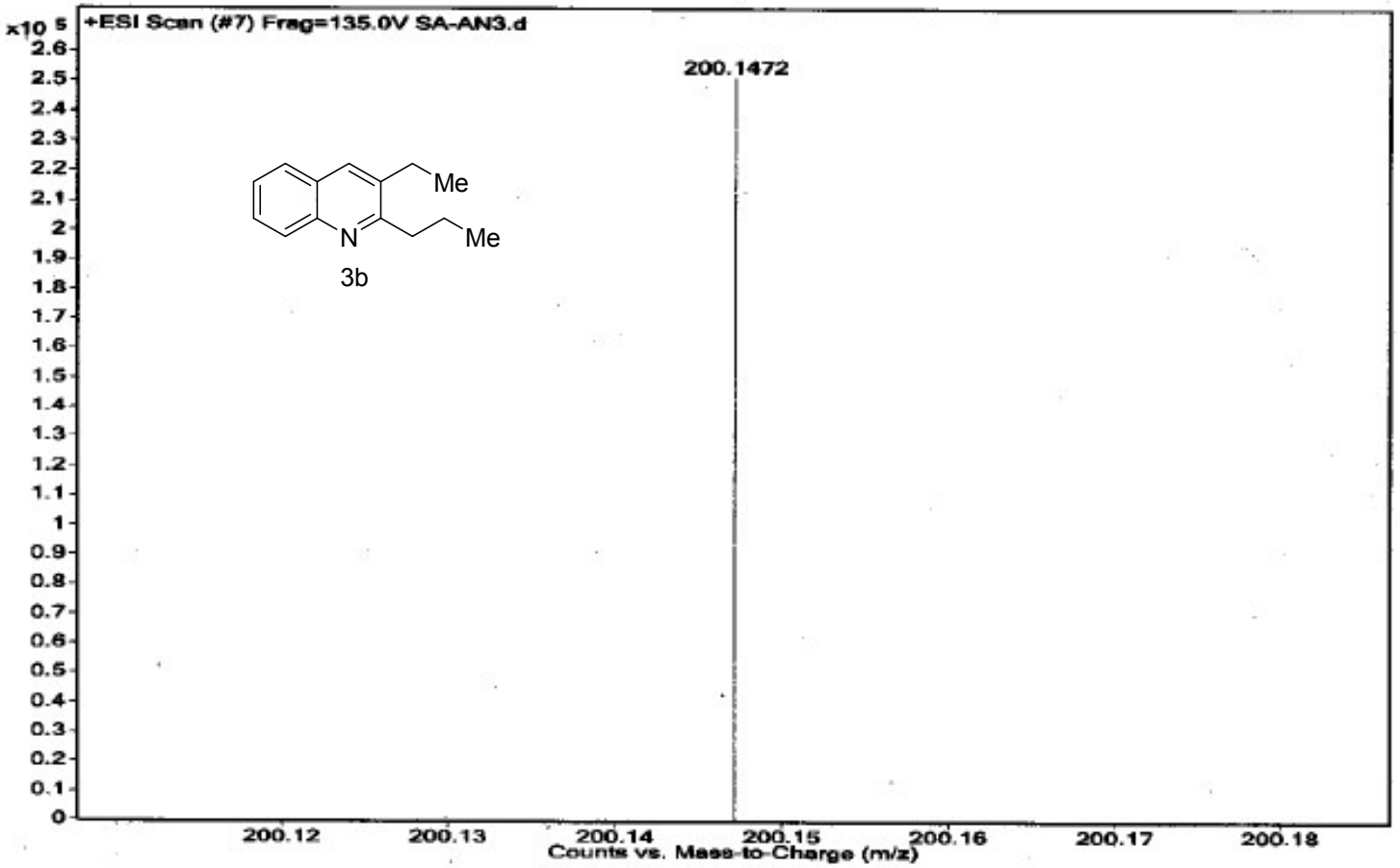
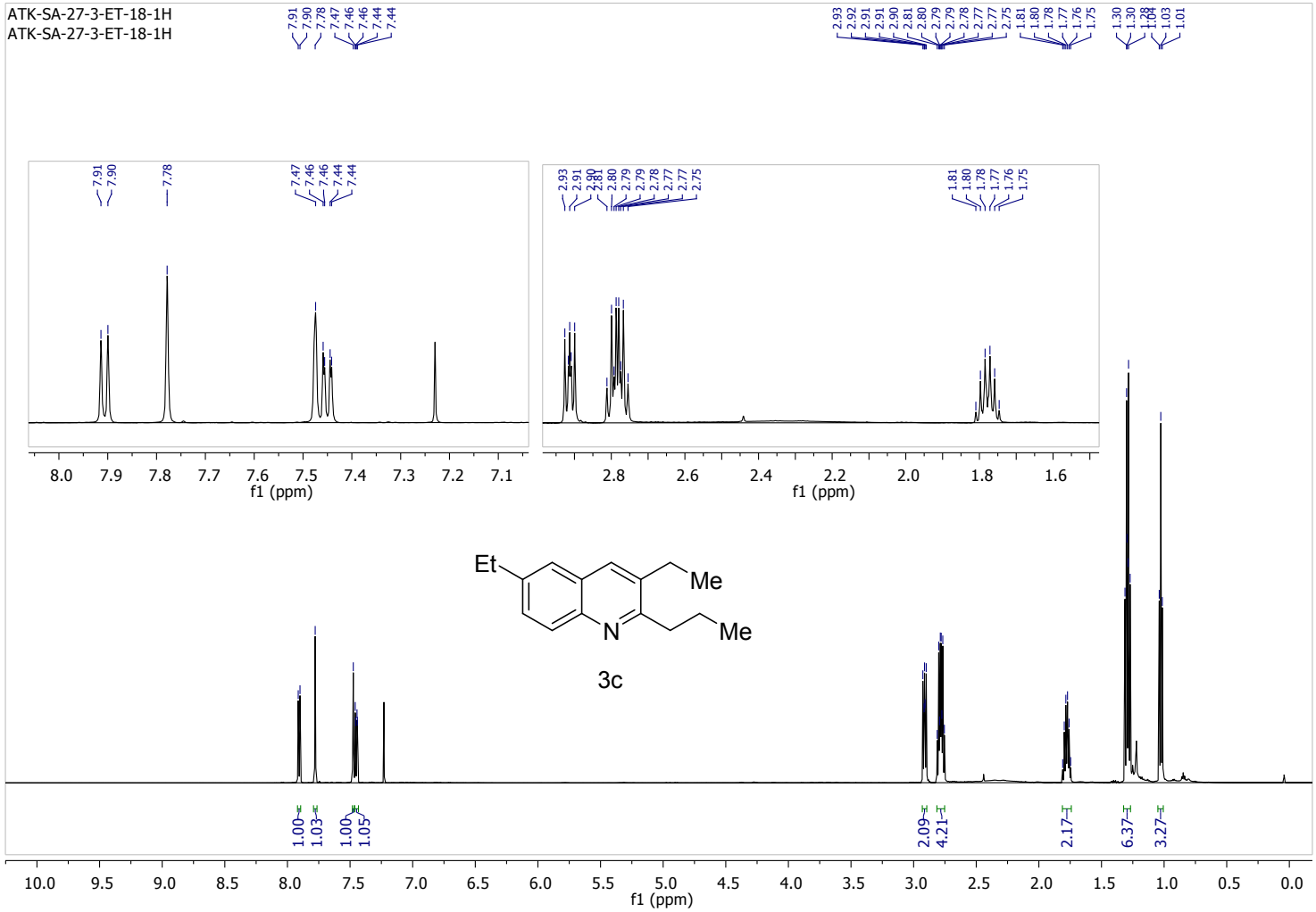
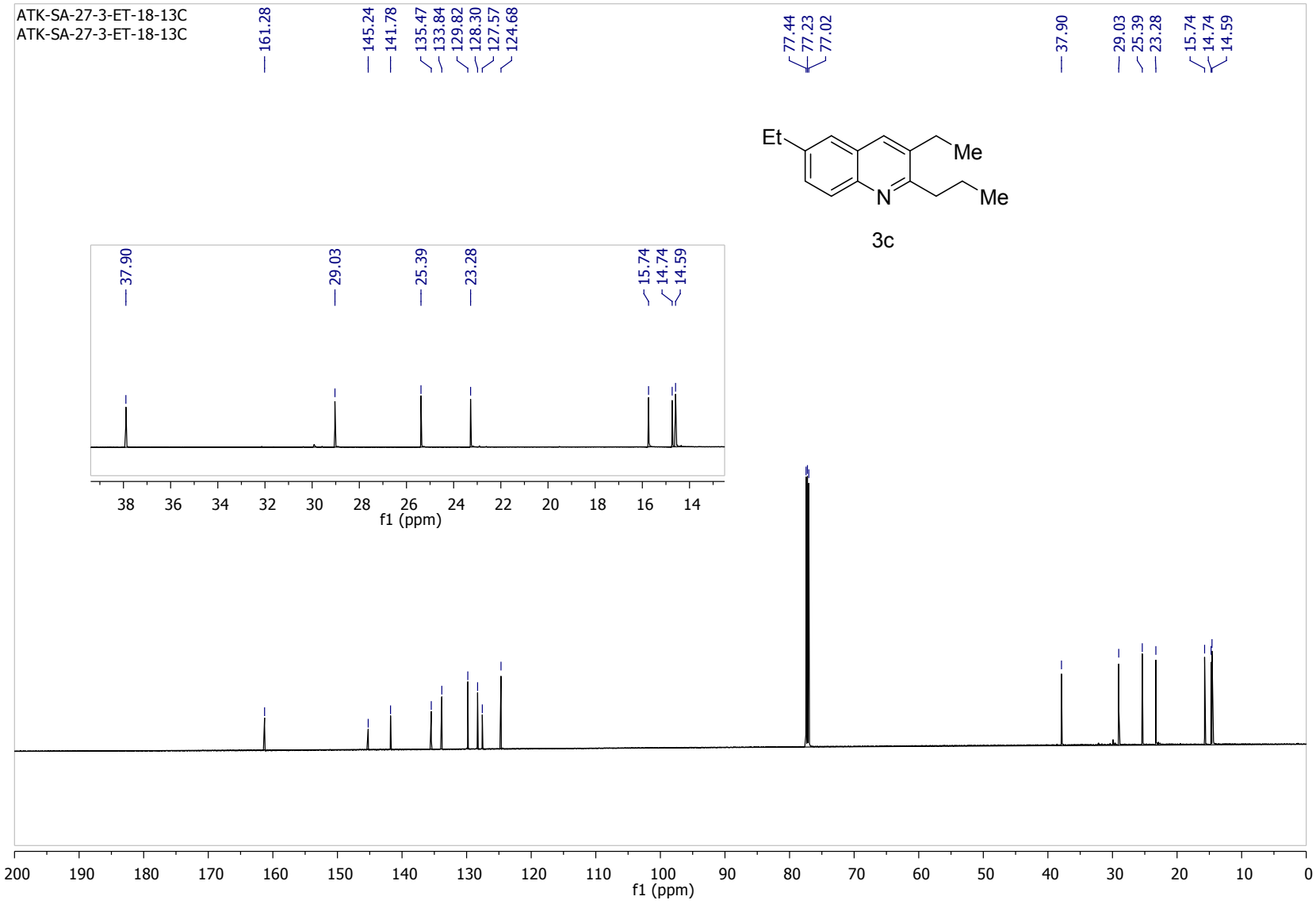
Data Filename	SA-AN3.d	ACQ Method		Comment		Acquired Time	7/26/2018 10:21:23 AM



1H NMR spectra of compound: 3c



^{13}C NMR spectra of compound: 3c



HRMS spectra of compound: 3c

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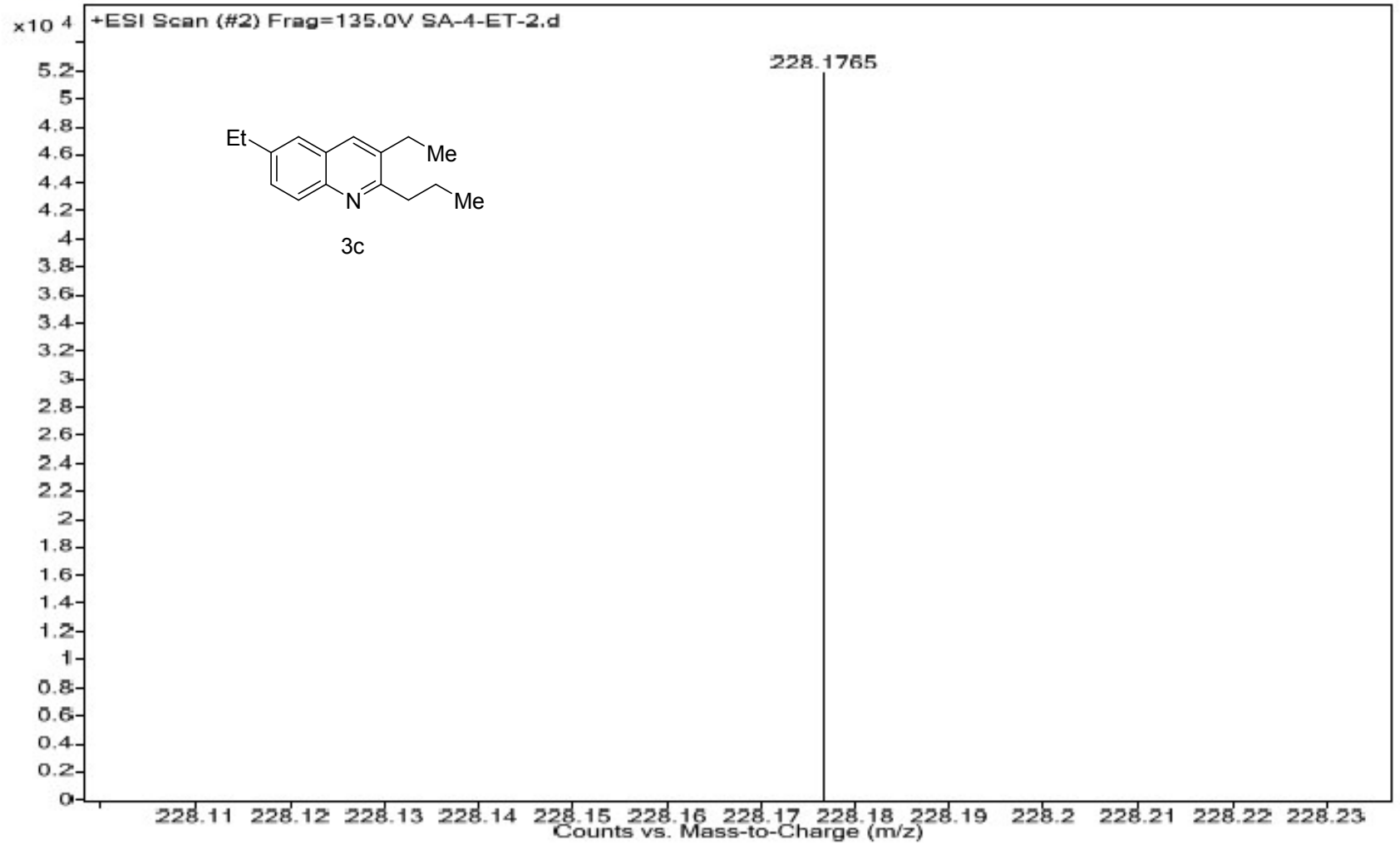
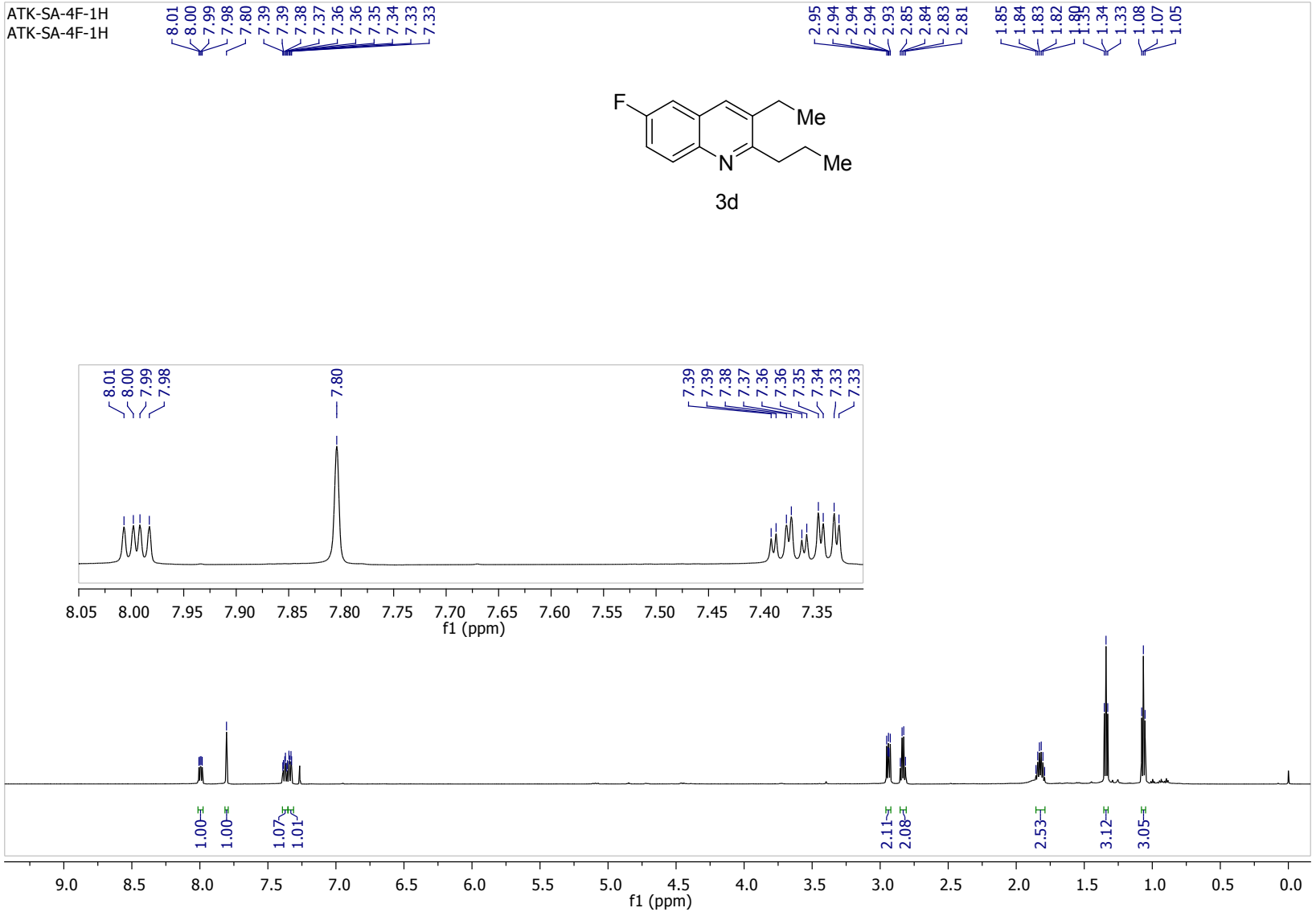
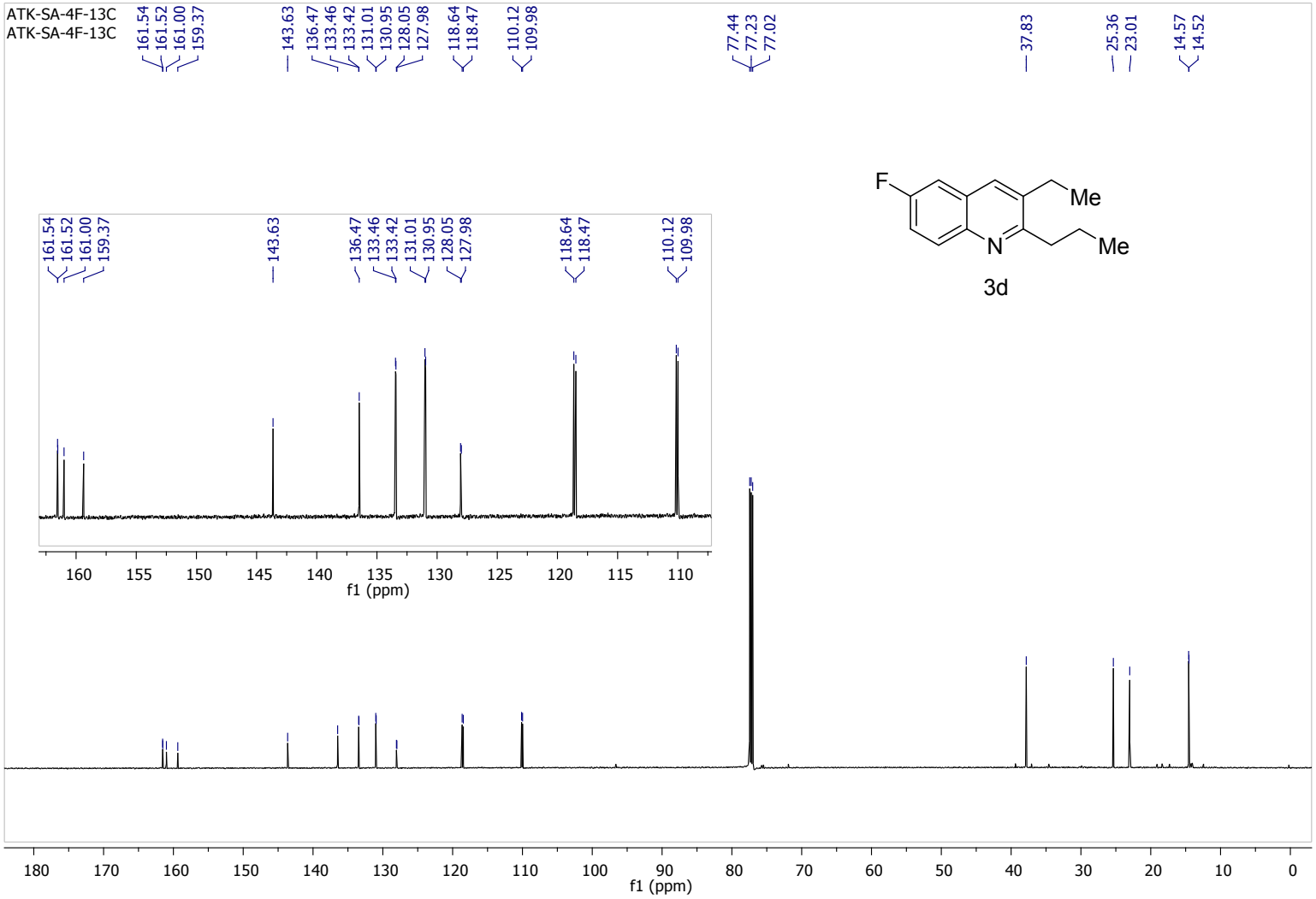


^{1}H NMR spectra of compound: 3d



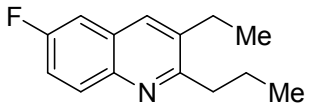
^{13}C NMR spectra of compound: 3d



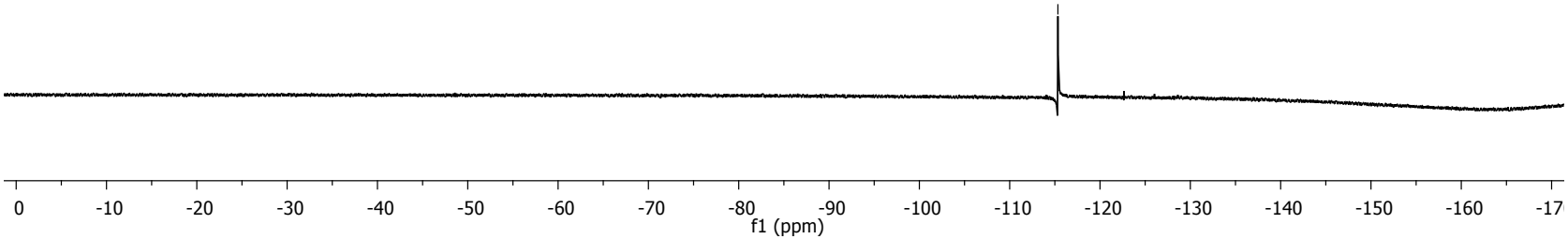
^{19}F NMR spectra of compound: 3d

ATK-SA-4F-BUT-19F
ATK-SA-4F-BUT-19F

-115.34



3d



HRMS spectra of compound: 3d

Sample Name	SA-4F-2	**Position**	Vial 1	**Instrument Name**	QTOF	**User Name**	
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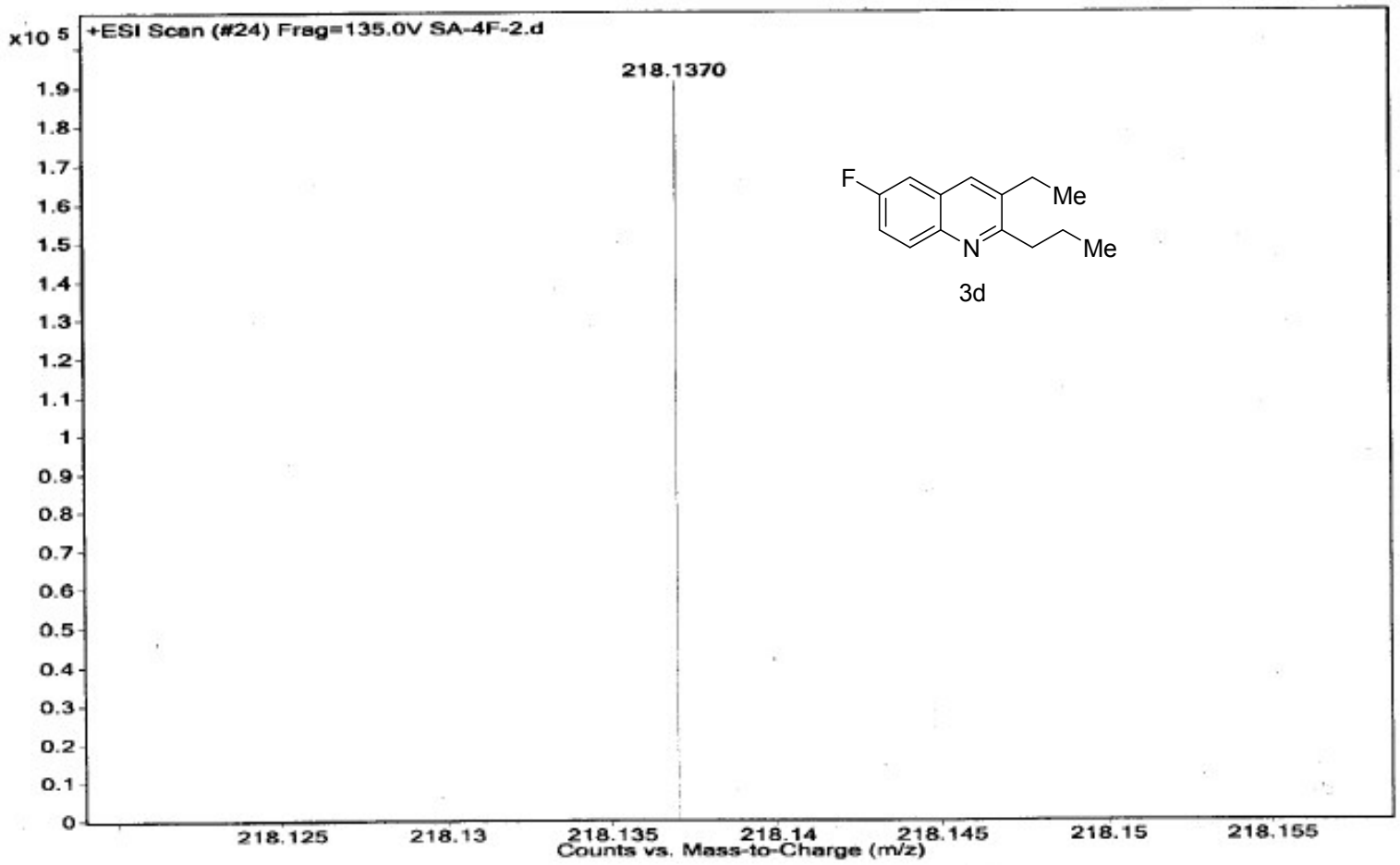
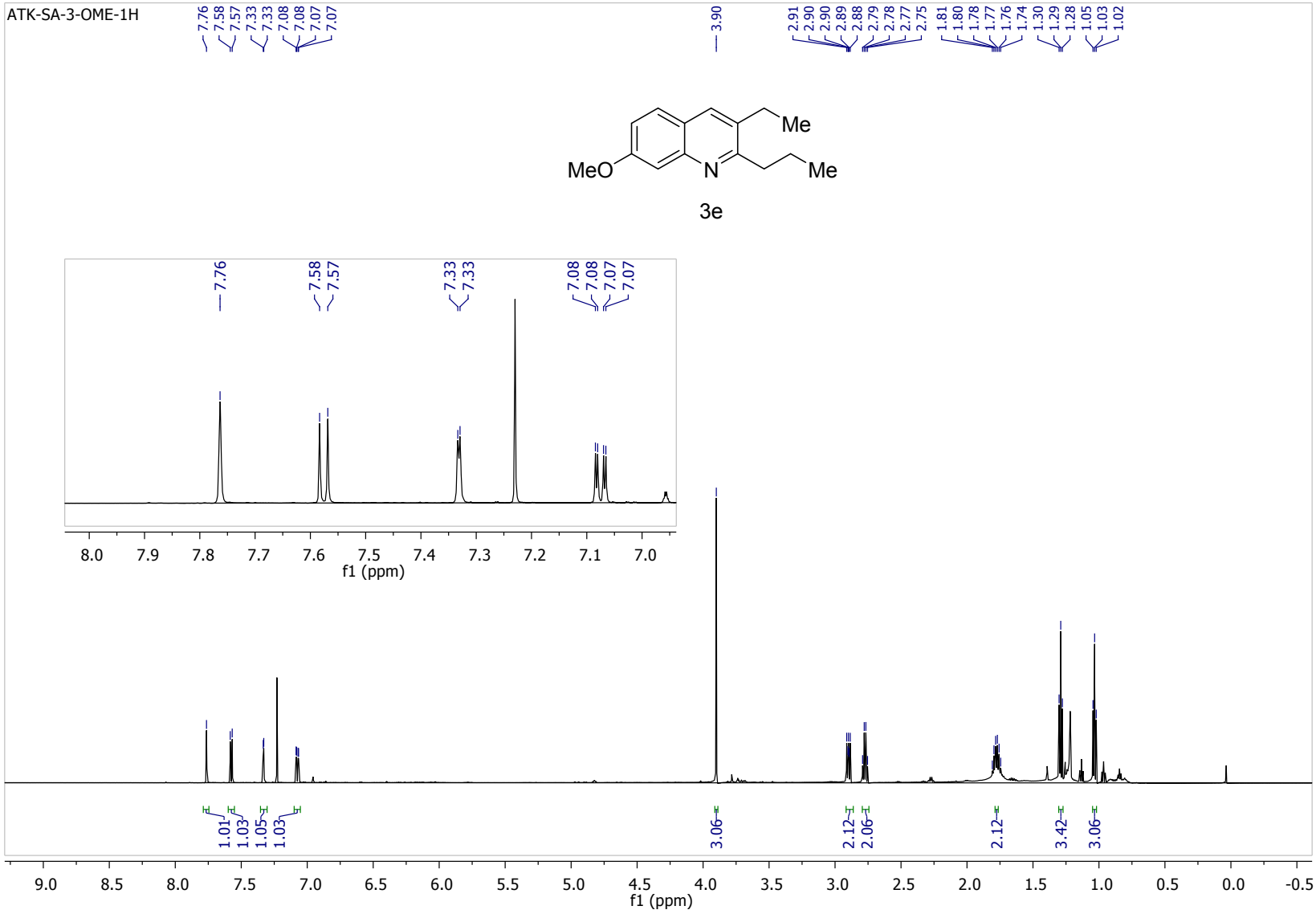
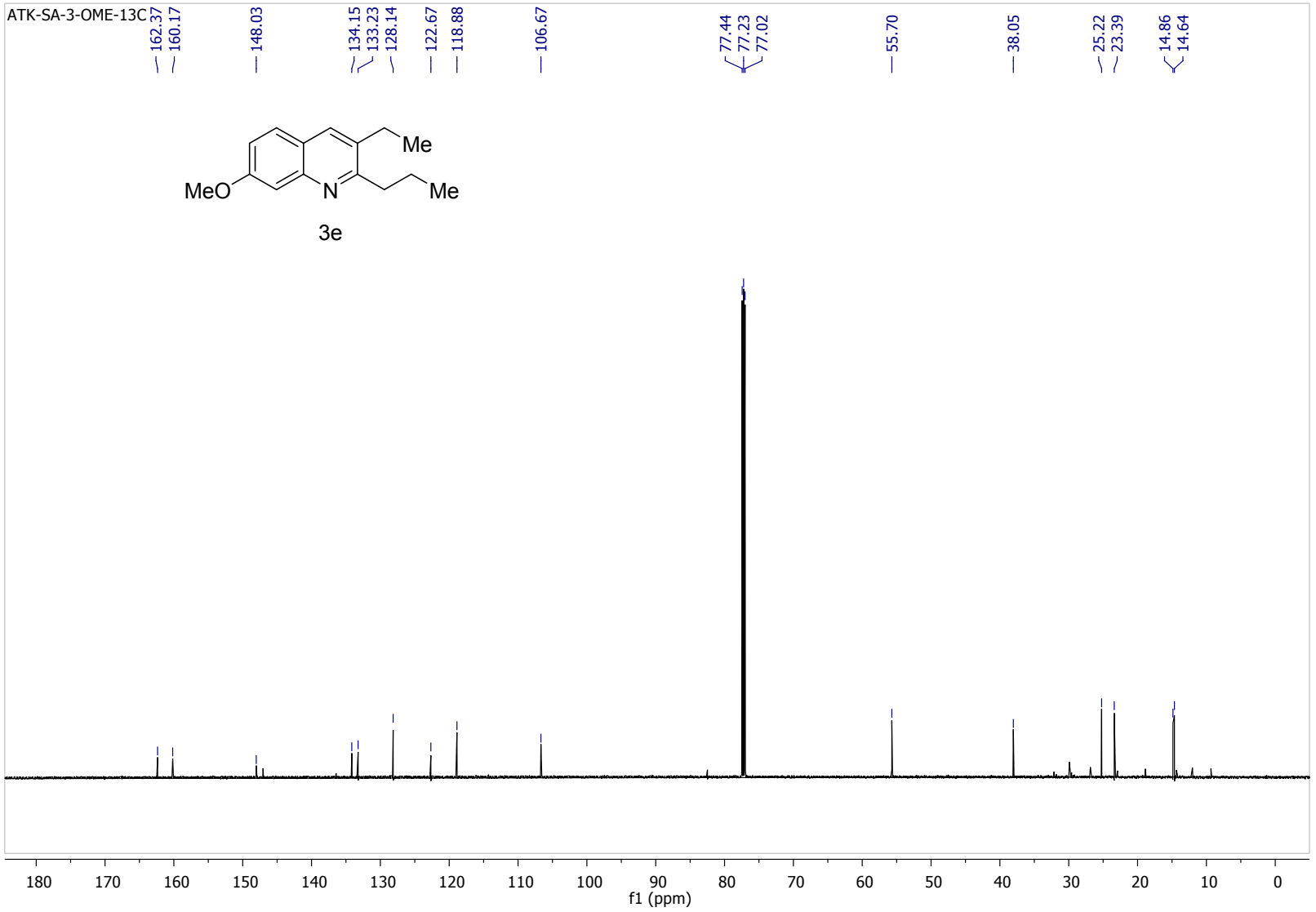


3d

^{1}H NMR spectra of compound: 3e

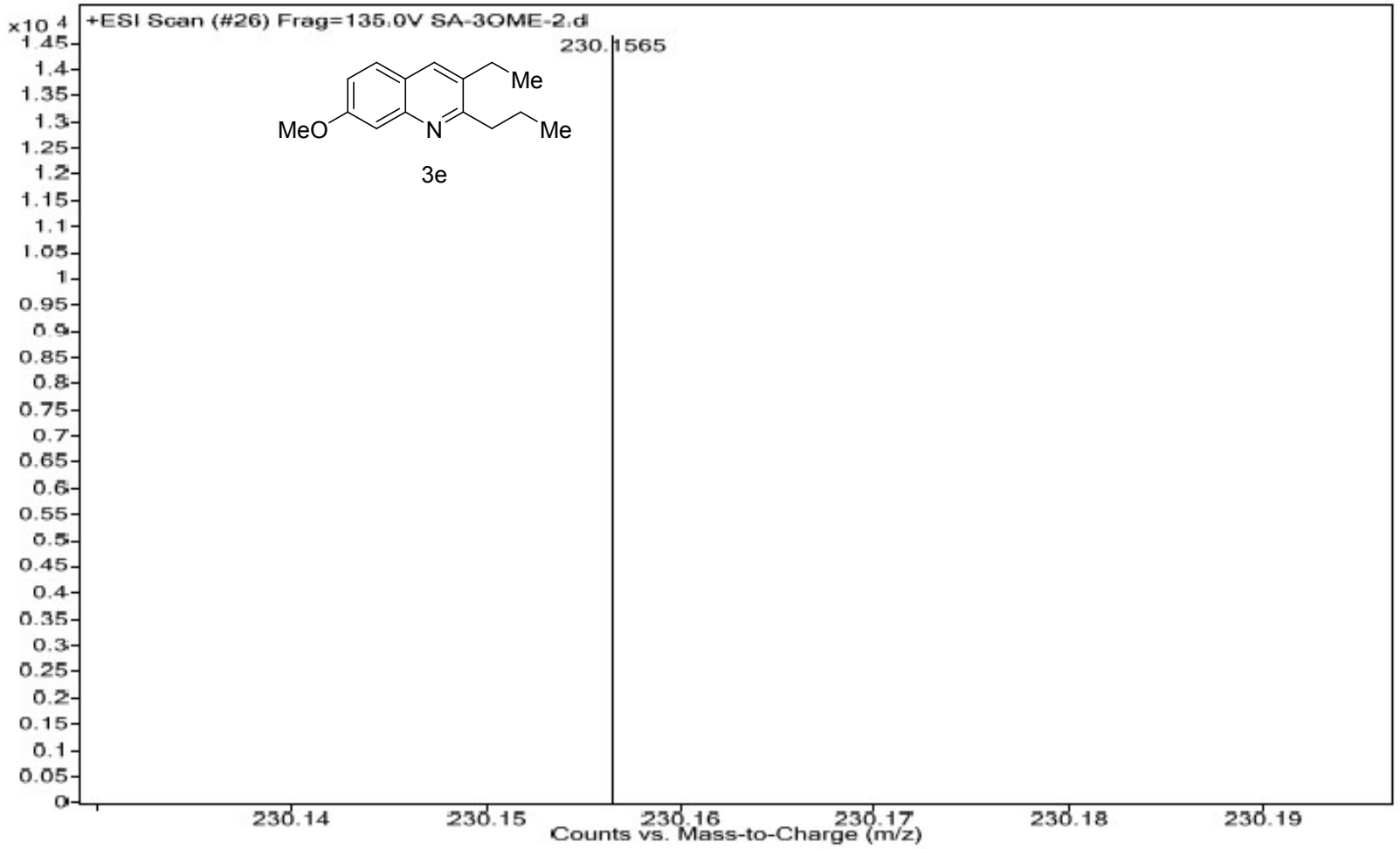


^{13}C NMR spectra of compound: 3e

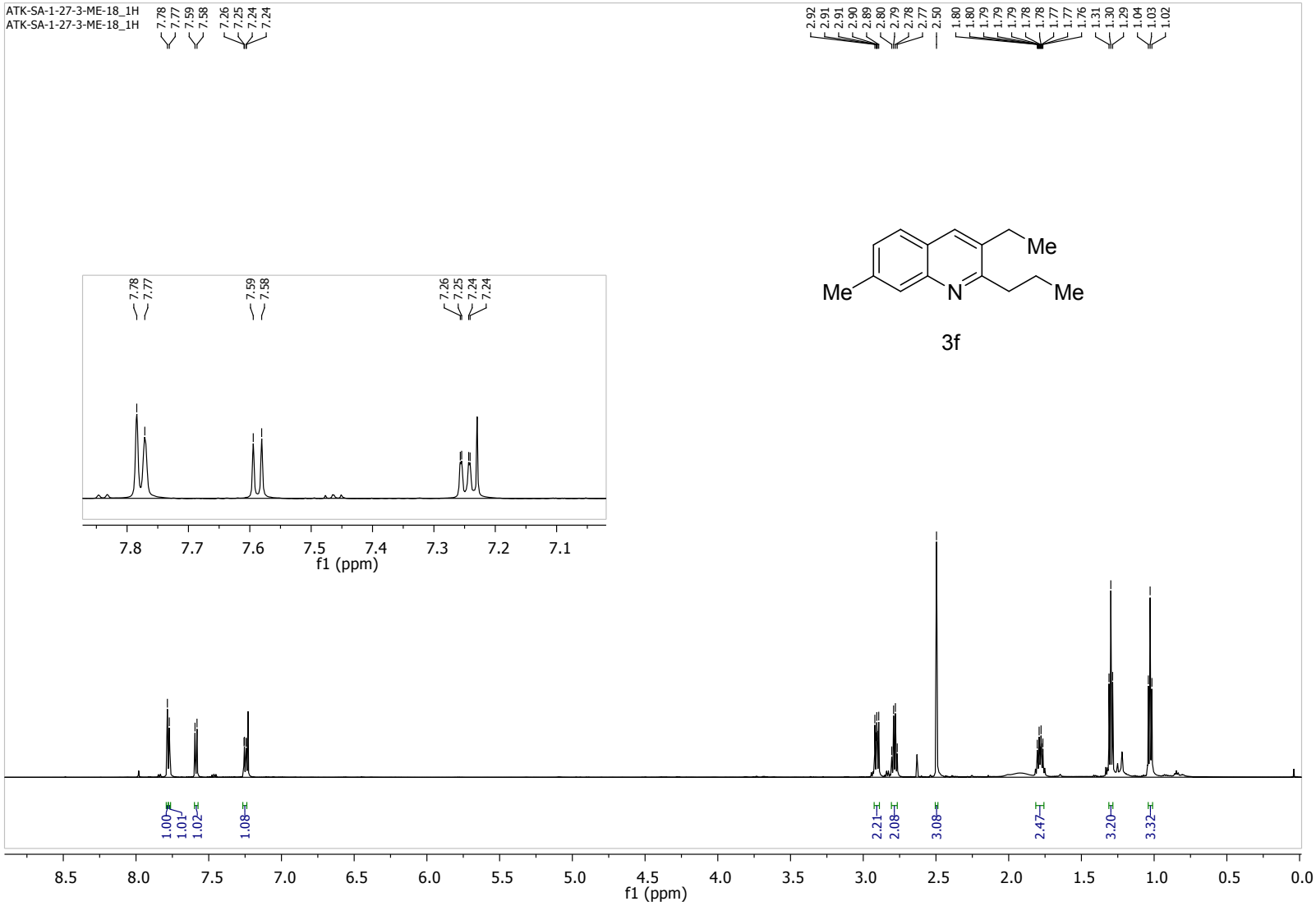


HRMS spectra of compound: 3e

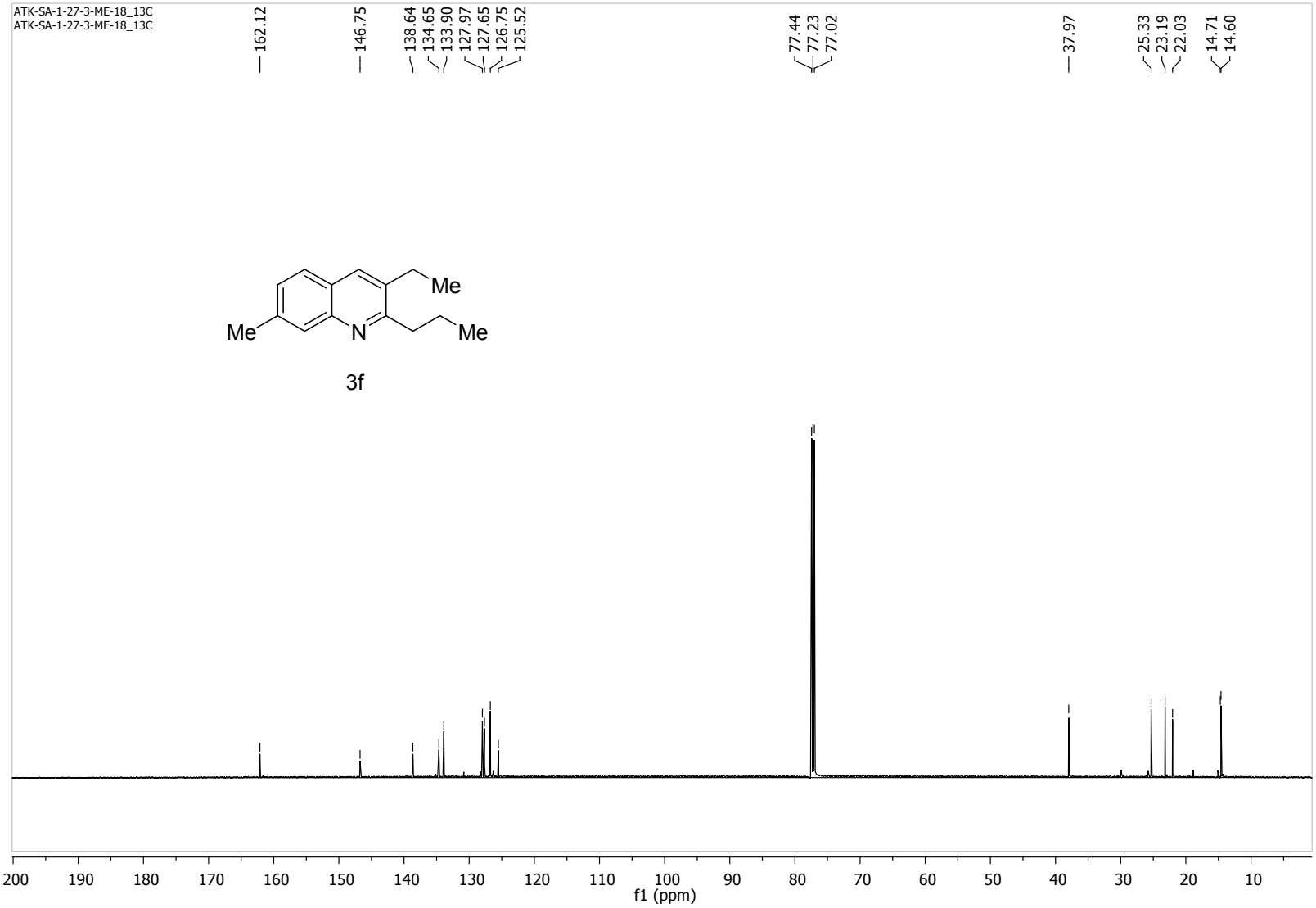
Sample Name	**Position**	**Instrument Name**	**User Name**
Inj Vol	**InjPosition**	**SampleType**	**IRM Calibration Status**
Data Filename	**ACQ Method**	**Comment**	**Acquired Time**



1H NMR spectra of compound: 3f



^{13}C NMR spectra of compound: 3f



HRMS spectra of compound: 3f

Sample Name	SA-3-ME	**Position**	Vial 1	**Instrument Name**	QTOF	**User Name**	
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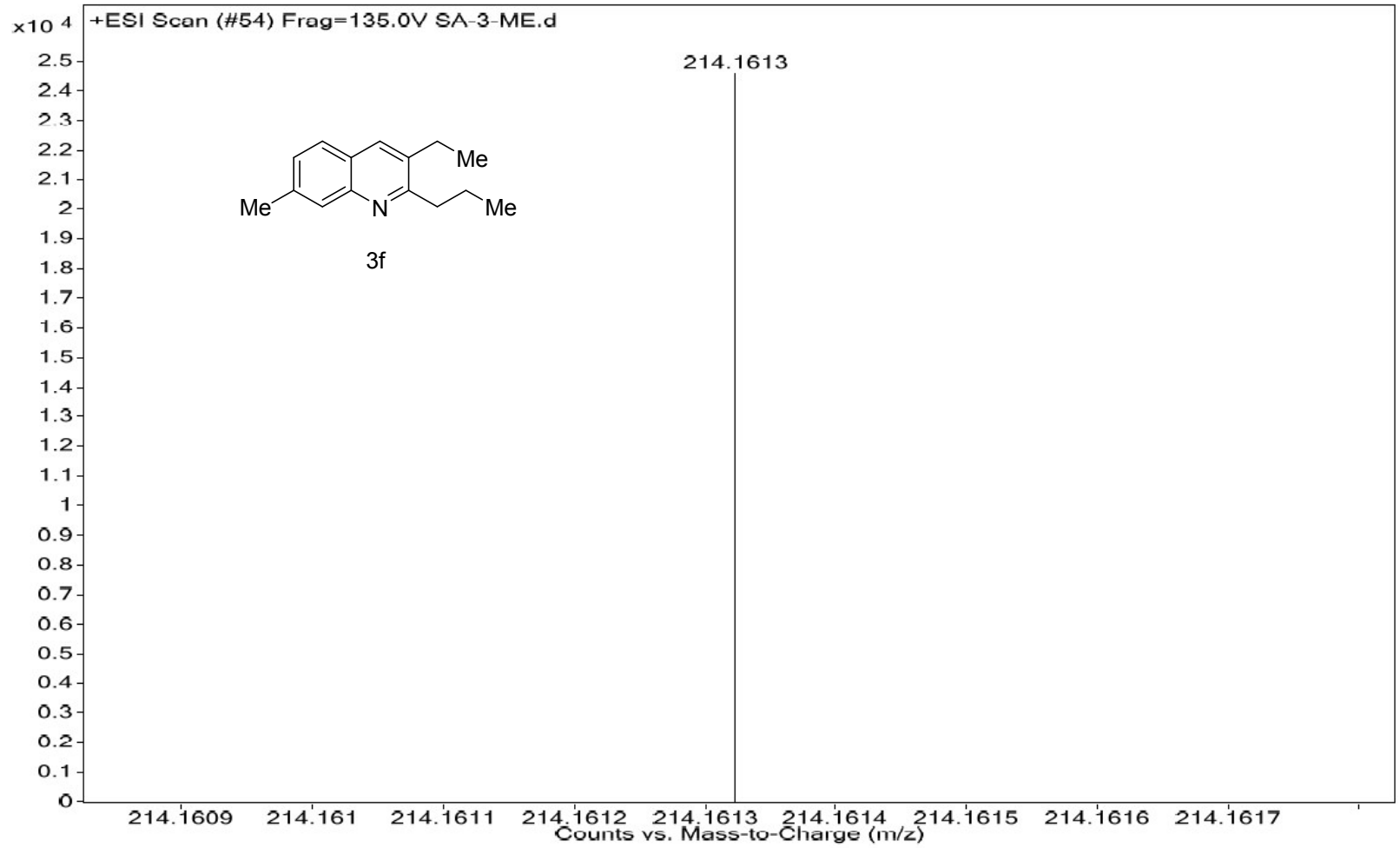
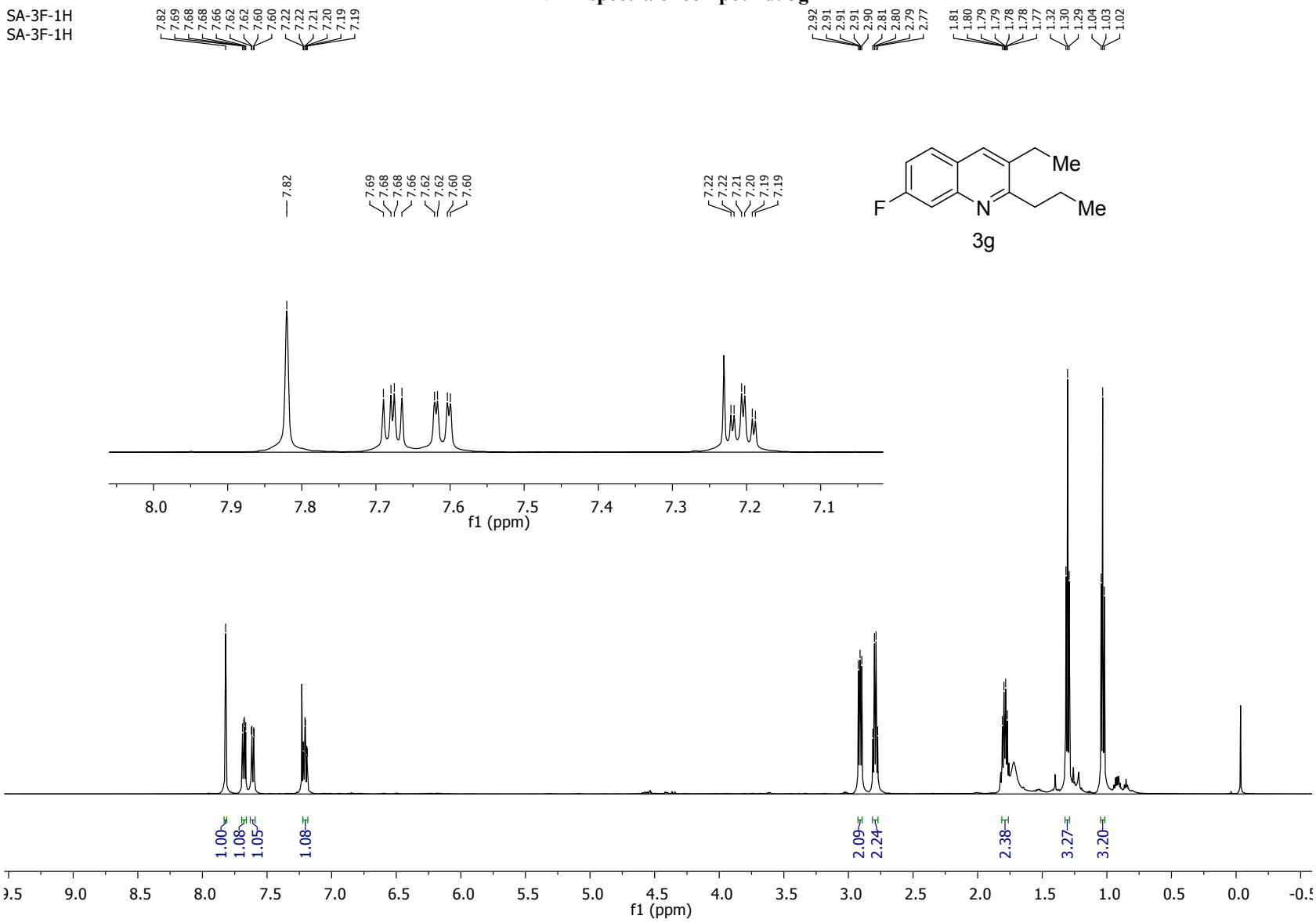
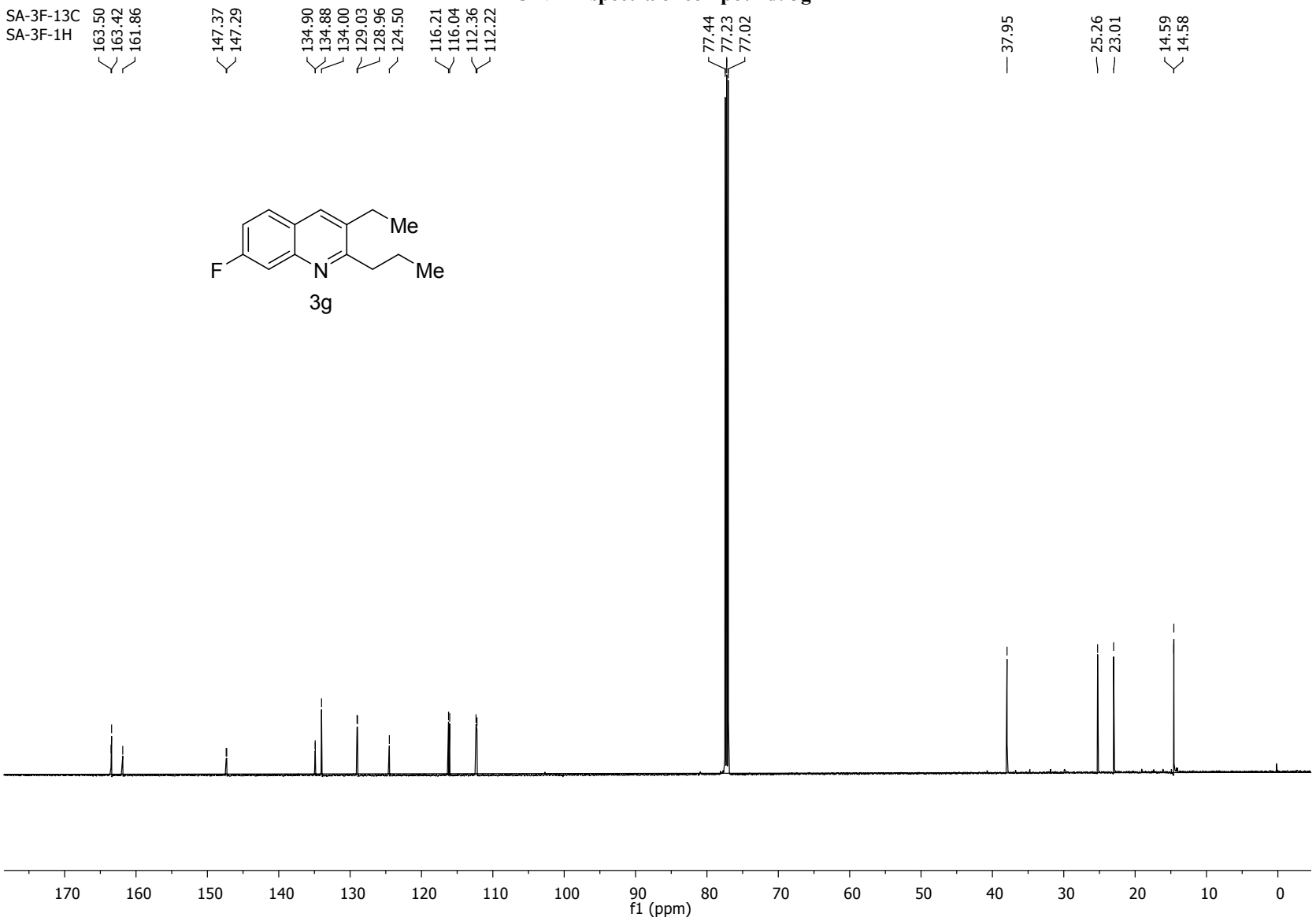


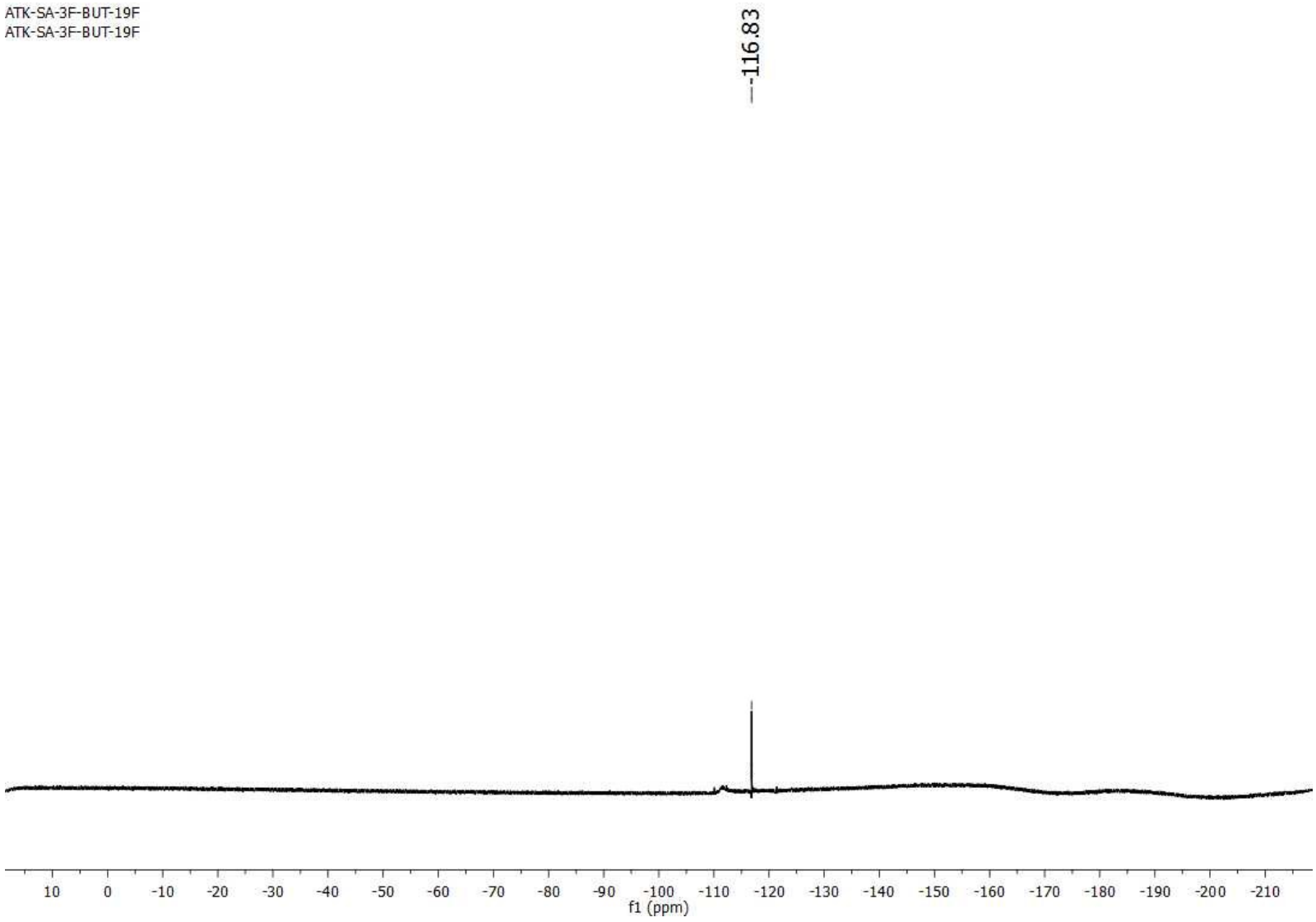
^{1}H NMR spectra of compound: 3g



^{13}C NMR spectra of compound: 3g



^{19}F NMR spectra of compound: 3g



HRMS spectra of compound: 3g

Sample Name	SA-3F-2	**Position**	Vial 1	**Instrument Name**	QTOF	**User Name**	
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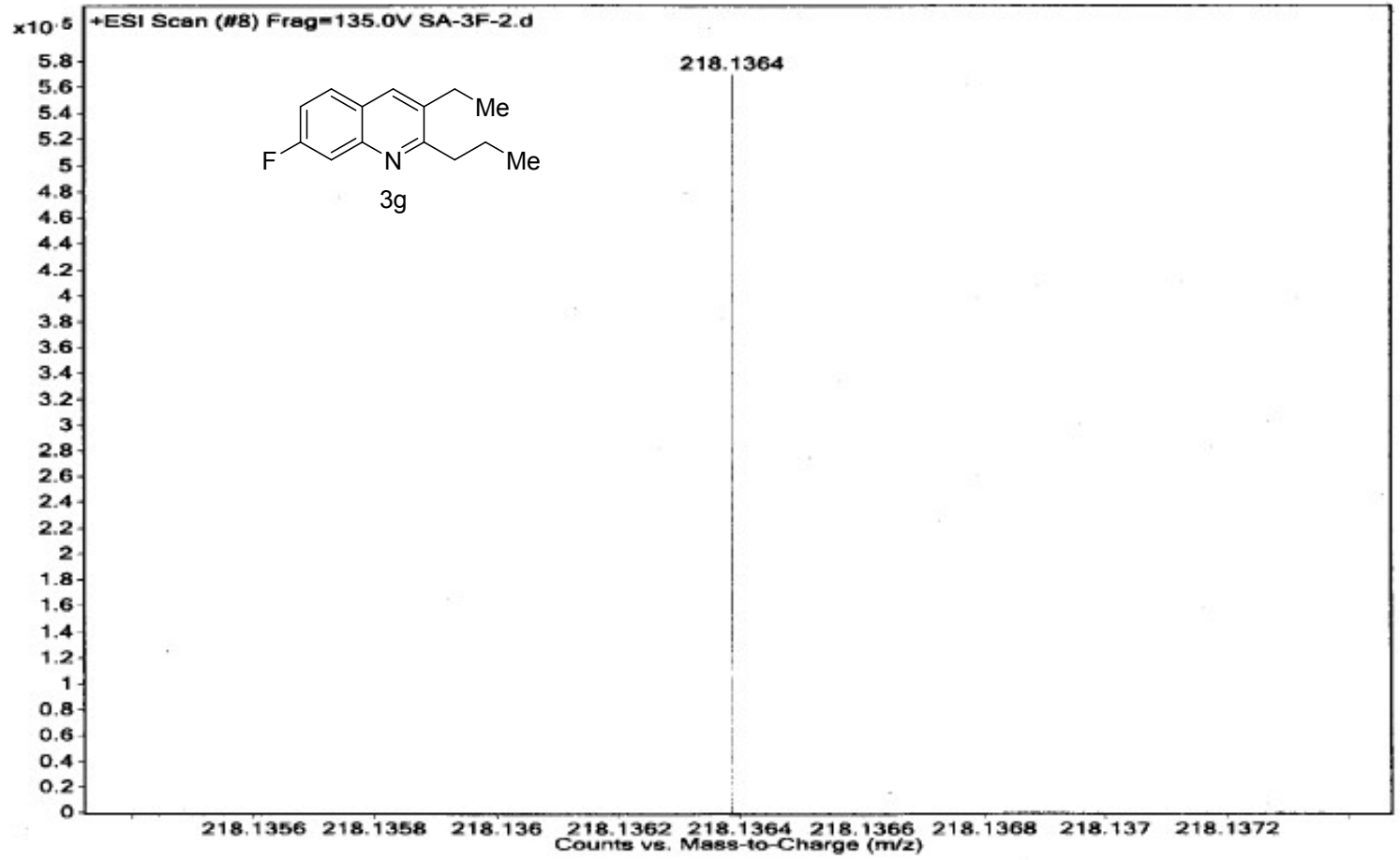
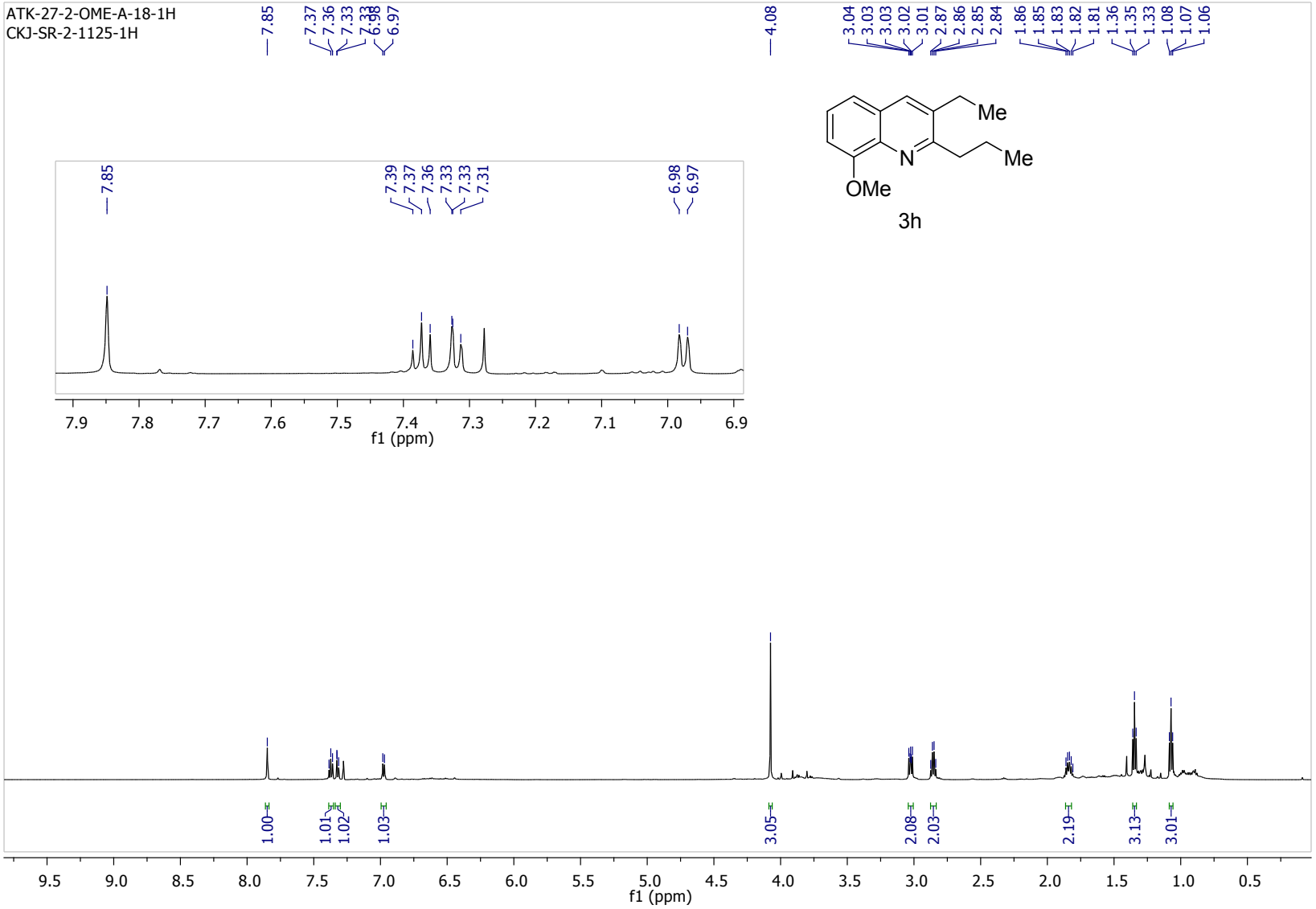
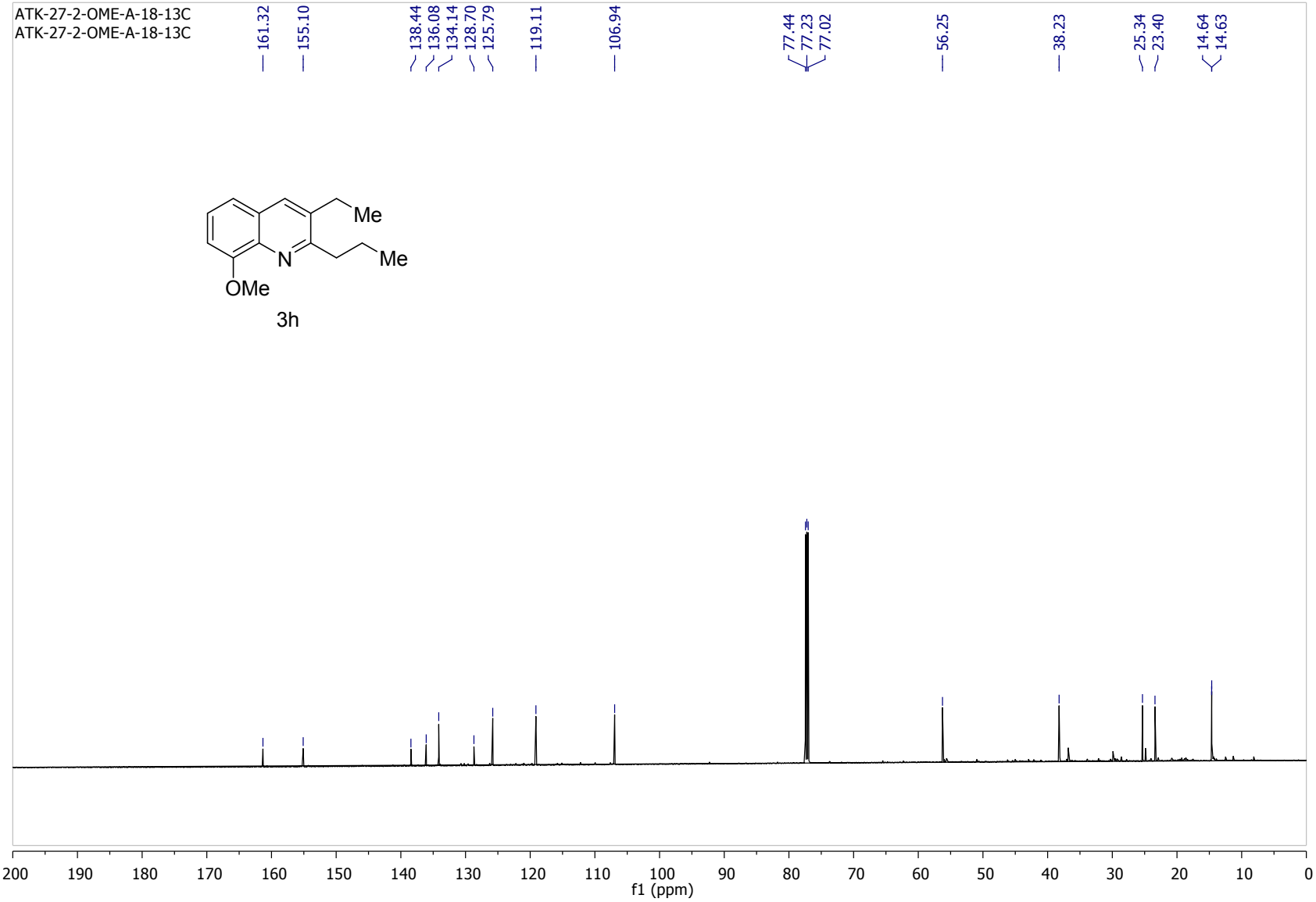


^{1}H NMR spectra of compound: 3h

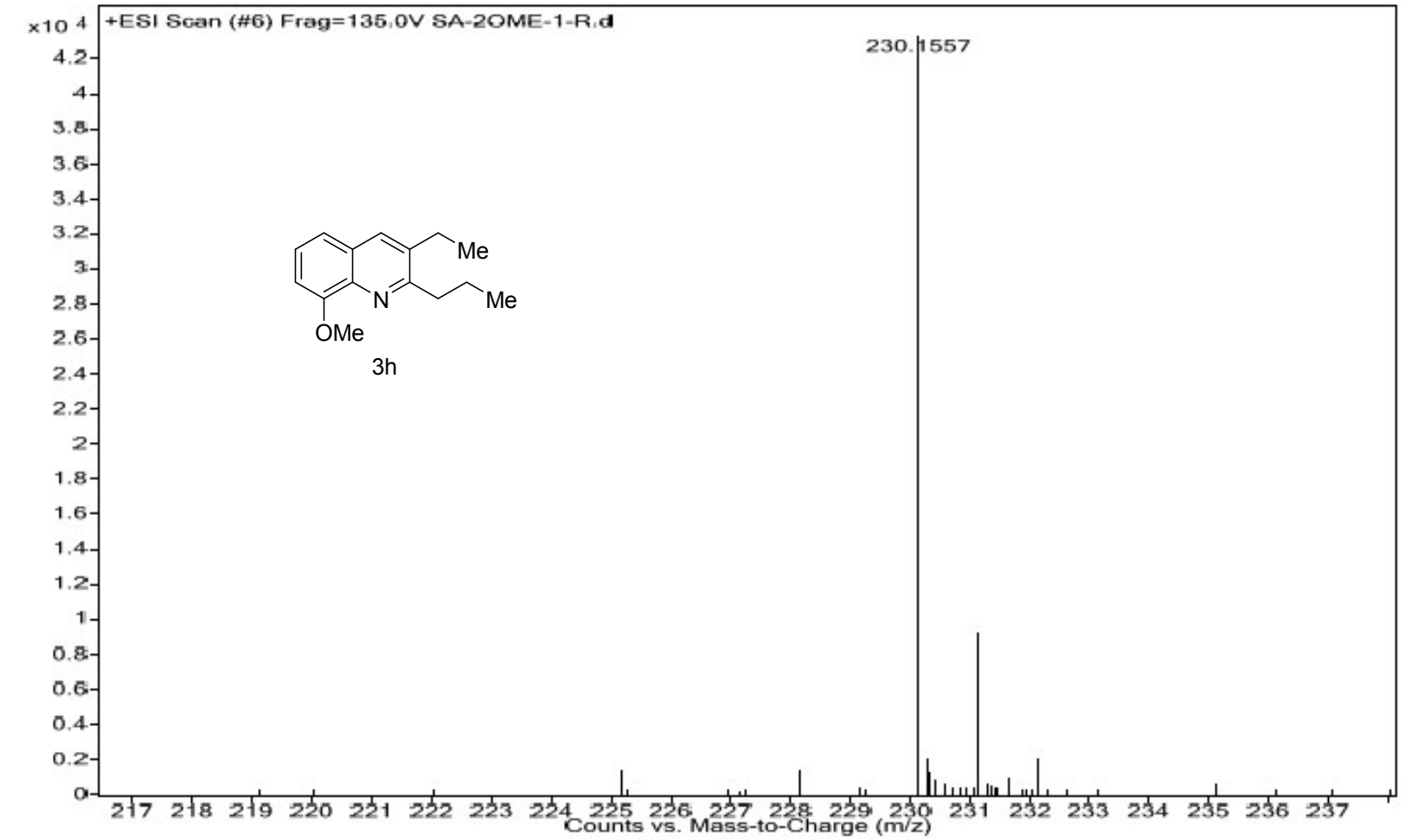


^{13}C NMR spectra of compound: 3h

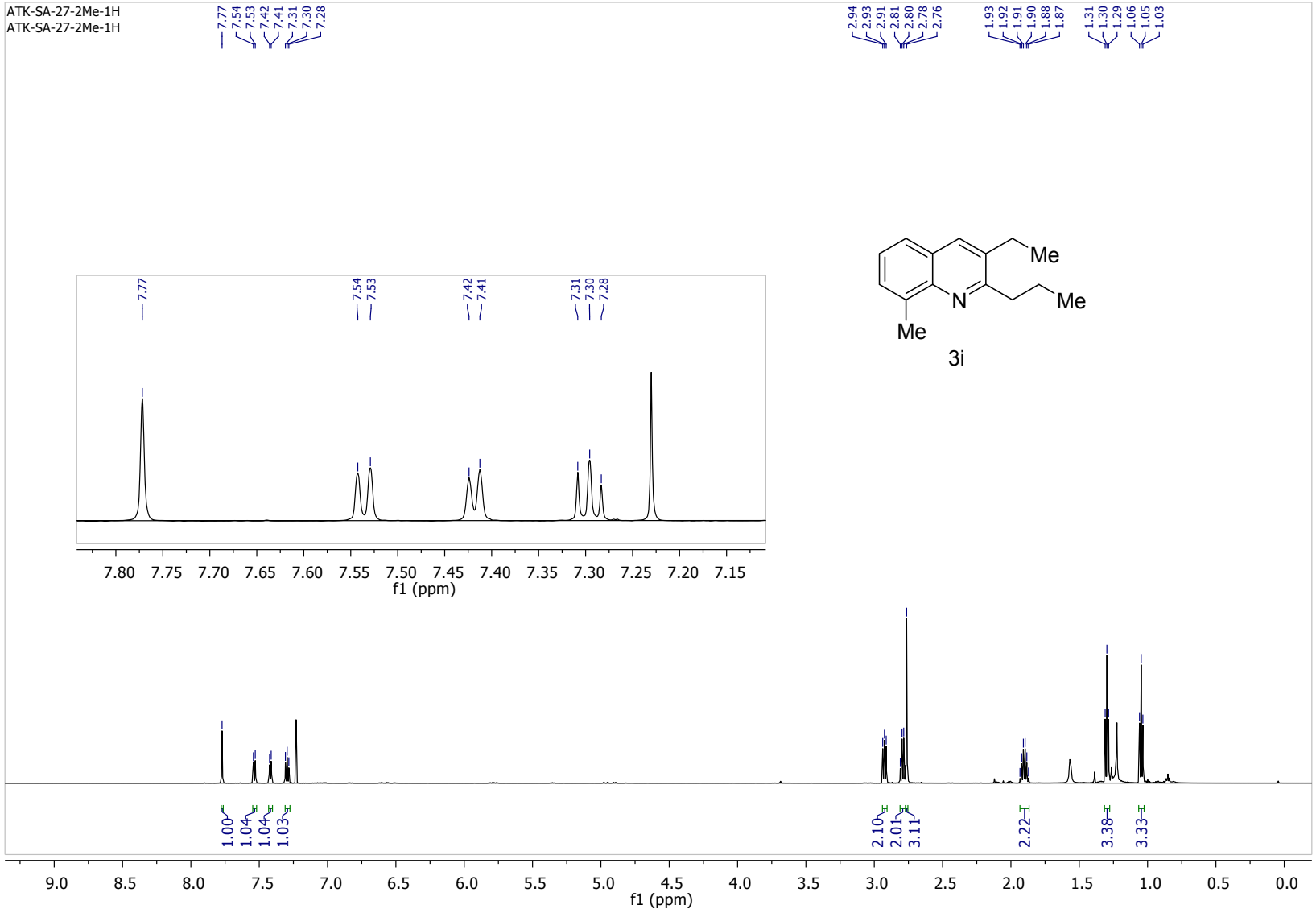


HRMS spectra of compound: 3h

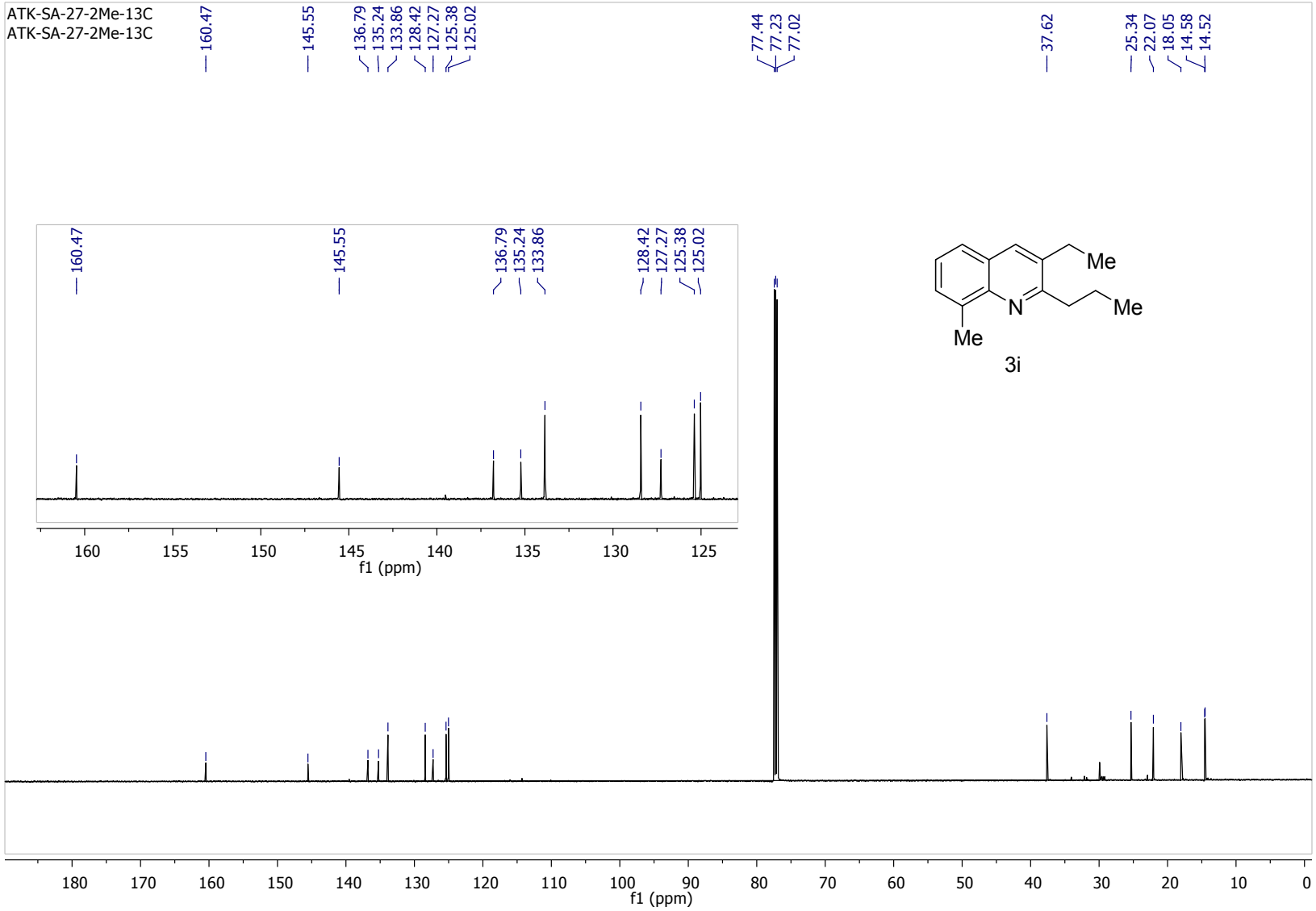
Sample Name	**Position**	**Instrument Name**	**User Name**
Inj Vol	**InjPosition**	**SampleType**	**IRM Calibration Status**
Data Filename	**ACQ Method**	**Comment**	**Acquired Time**



^{1}H NMR spectra of compound: 3i

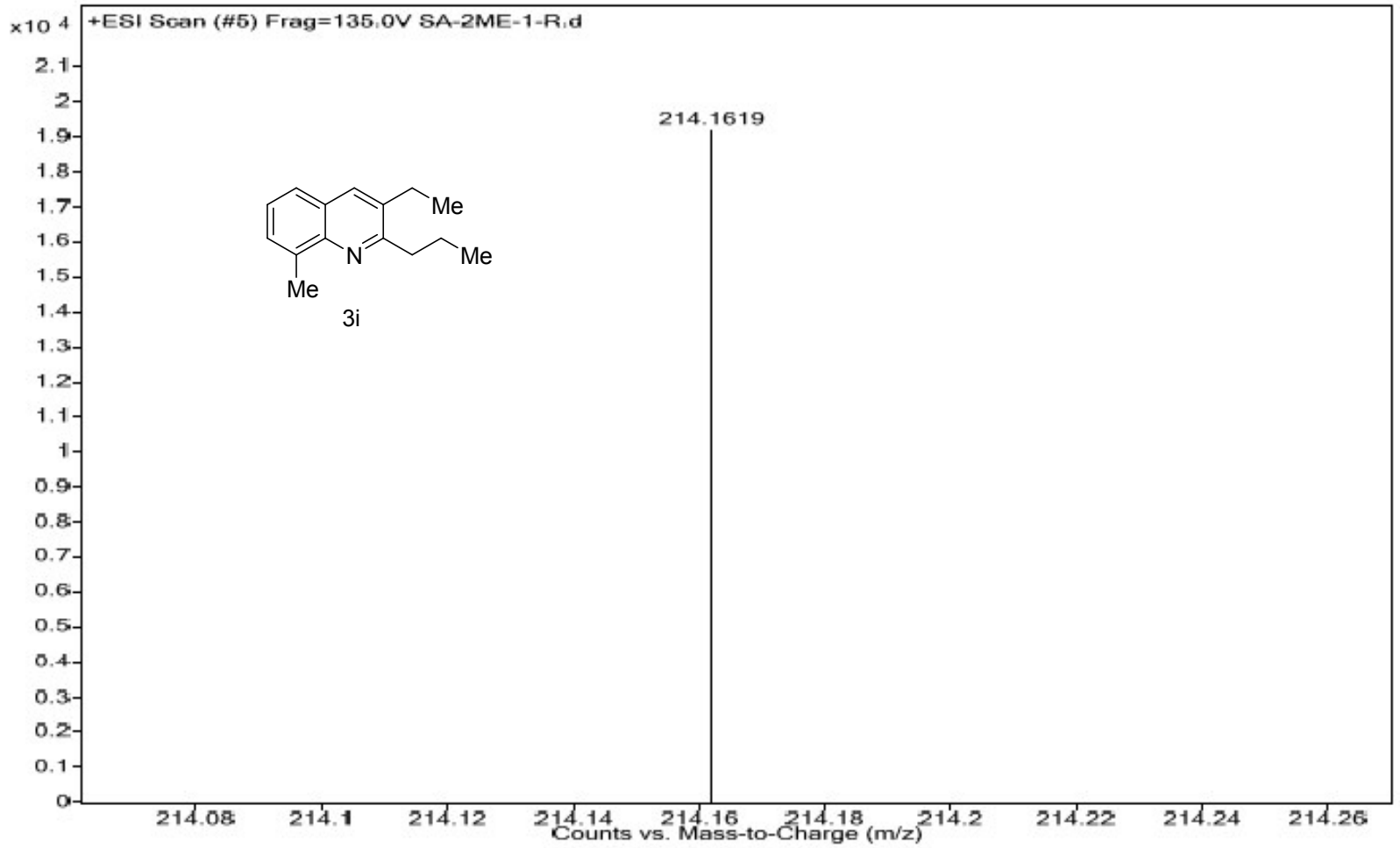


^{13}C NMR spectra of compound: 3i

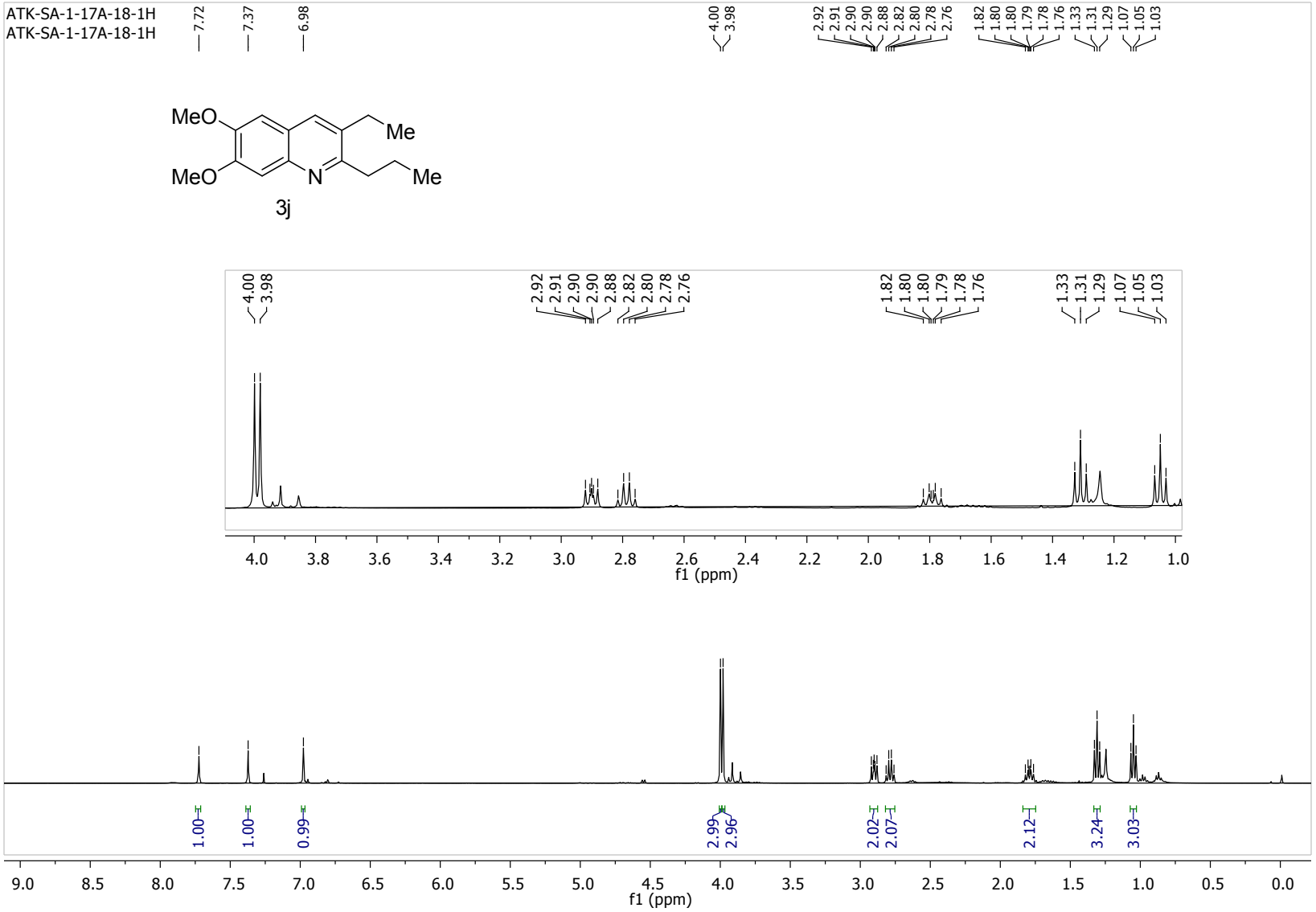


HRMS spectra of compound: 3i

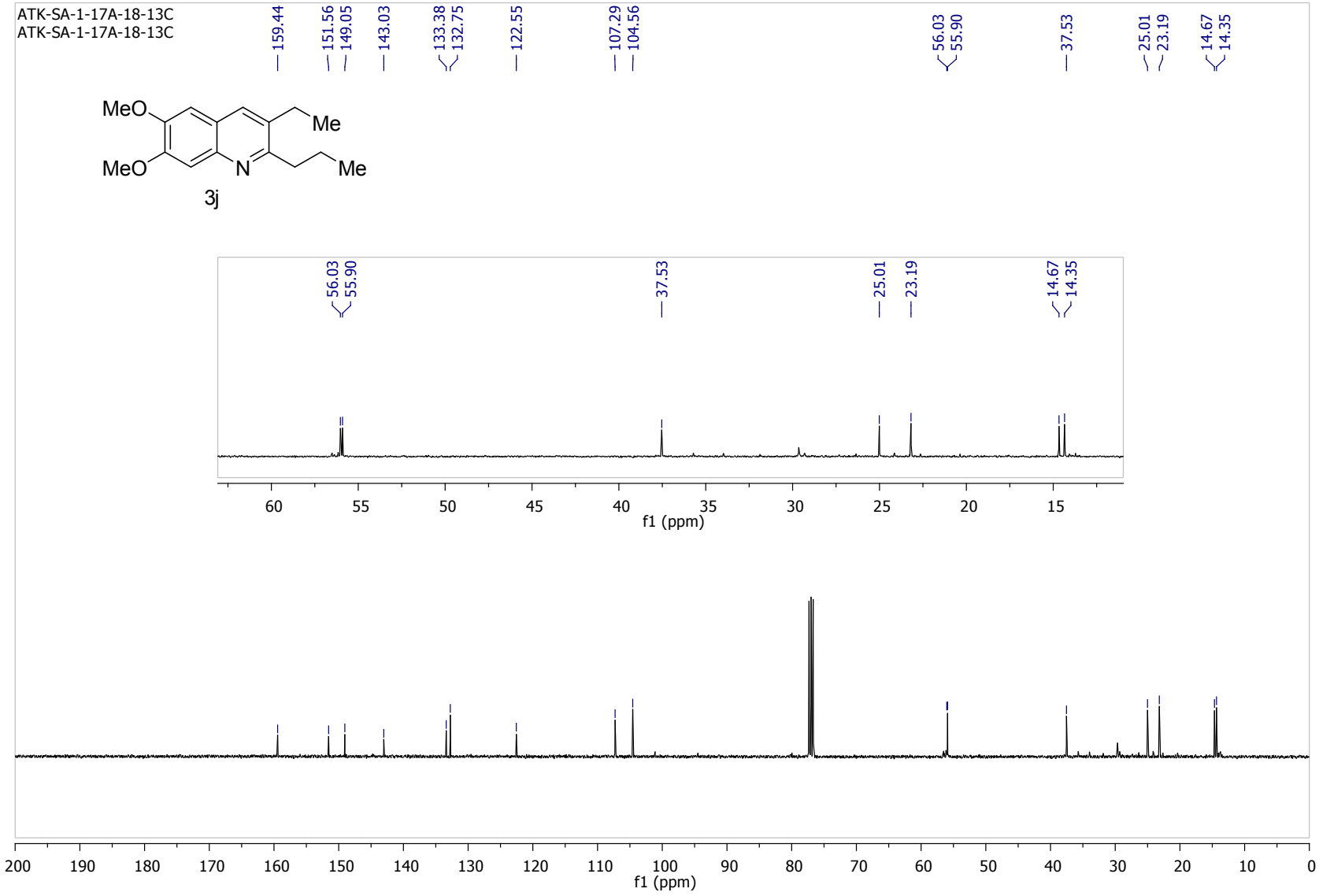
Sample Name	**Position**	**Instrument Name**	**User Name**
Inj Vol	**InjPosition**	**SampleType**	**IRM Calibration Status**
Data Filename	**ACQ Method**	**Comment**	**Acquired Time**



^{1}H NMR spectra of compound: 3j

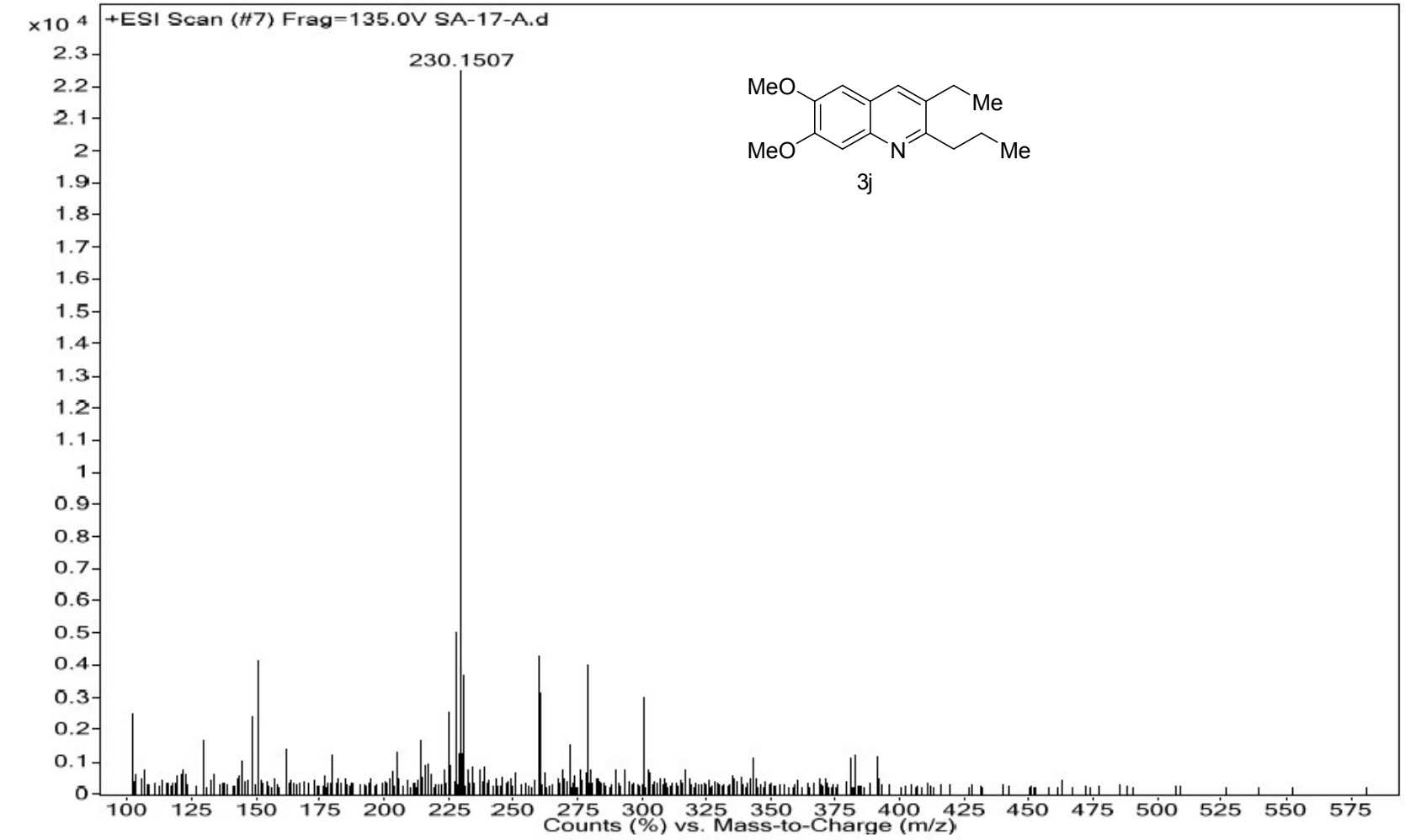


^{13}C NMR spectra of compound: 3j

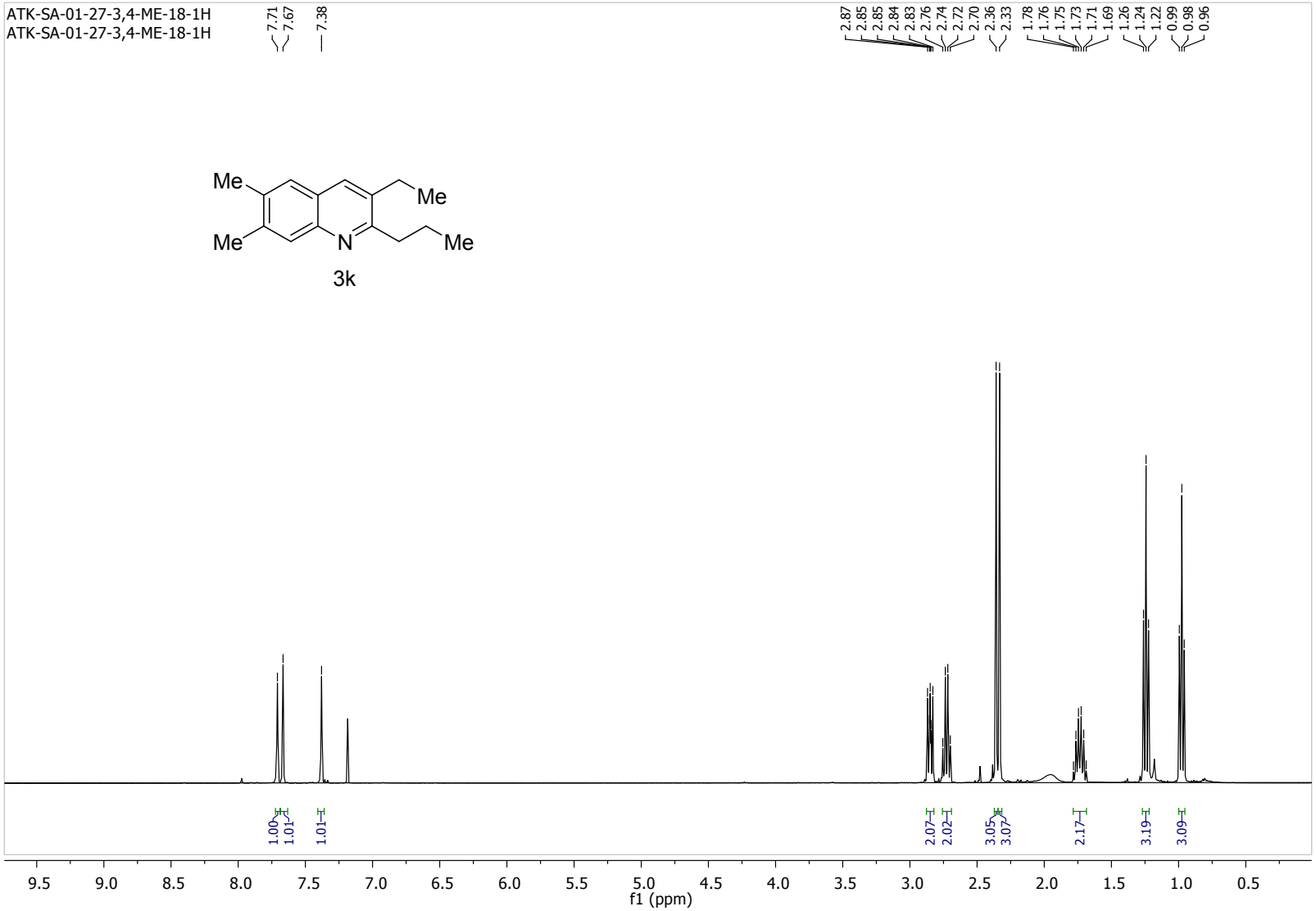


HRMS spectra of compound: 3j

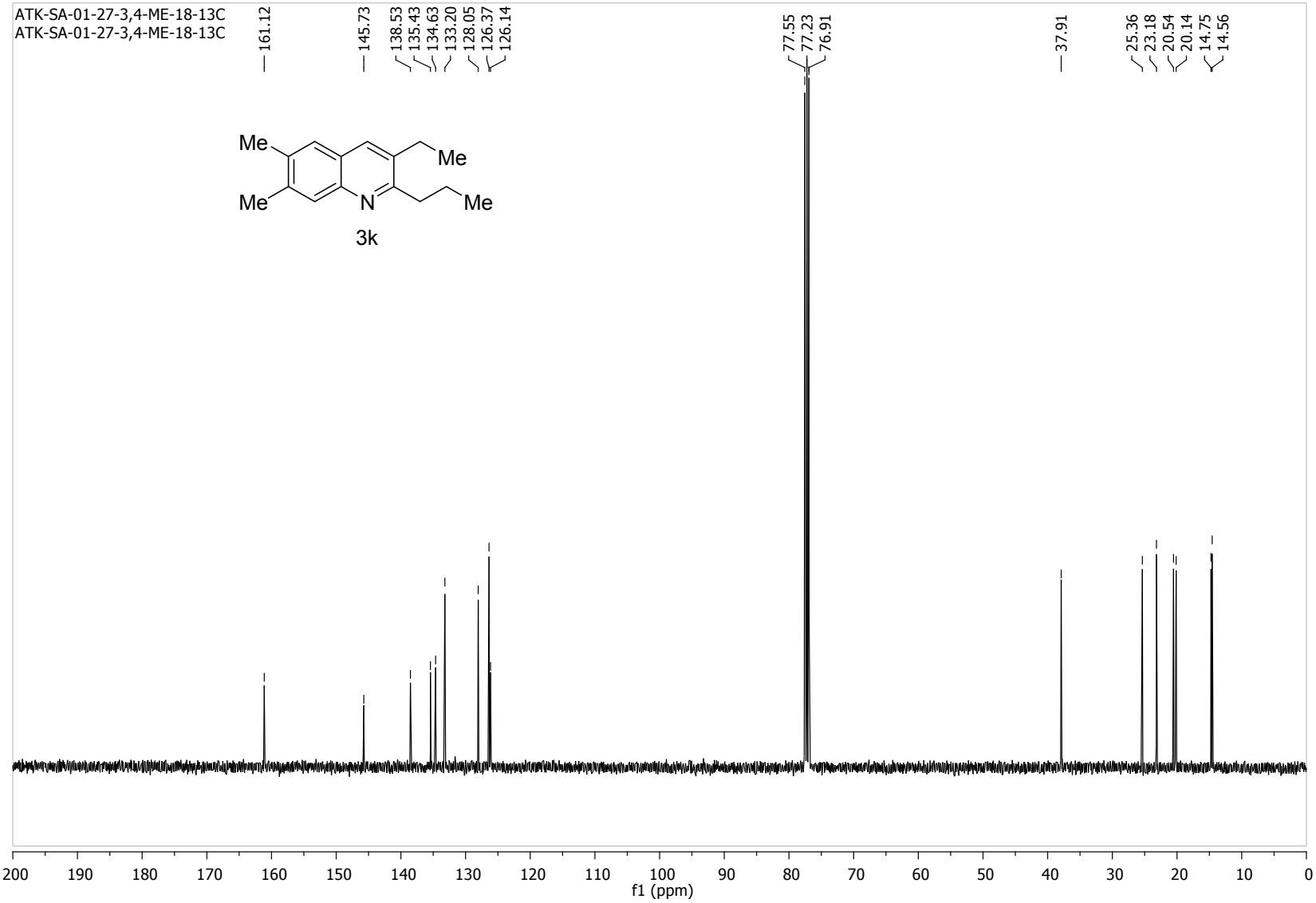
Sample Name	**Position**	**Instrument Name**	**User Name**
Inj Vol	**InjPosition**	**SampleType**	**IRM Calibration Status**
Data Filename	**ACQ Method**	**Comment**	**Acquired Time**



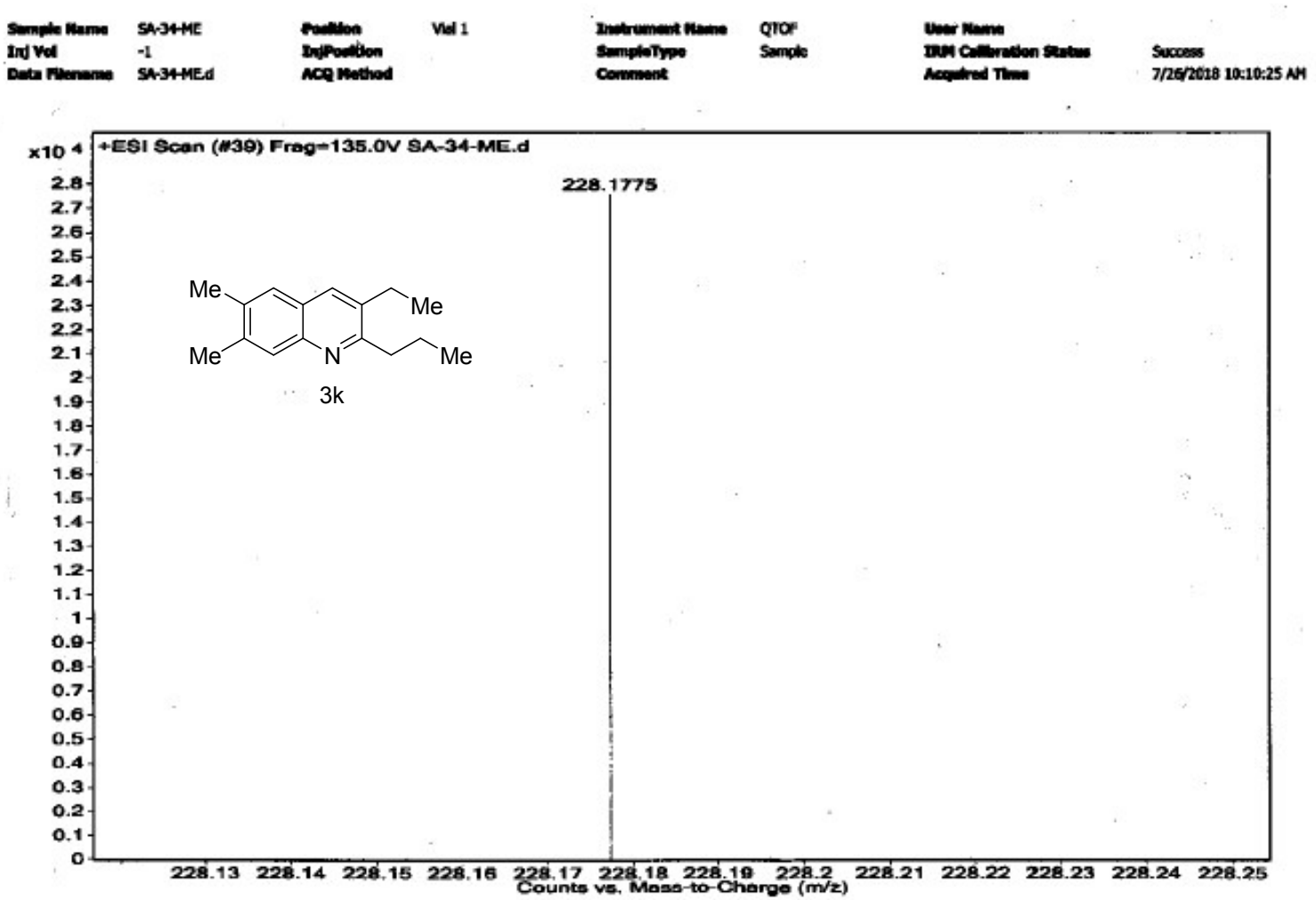
^{1}H NMR spectra compound: 3k



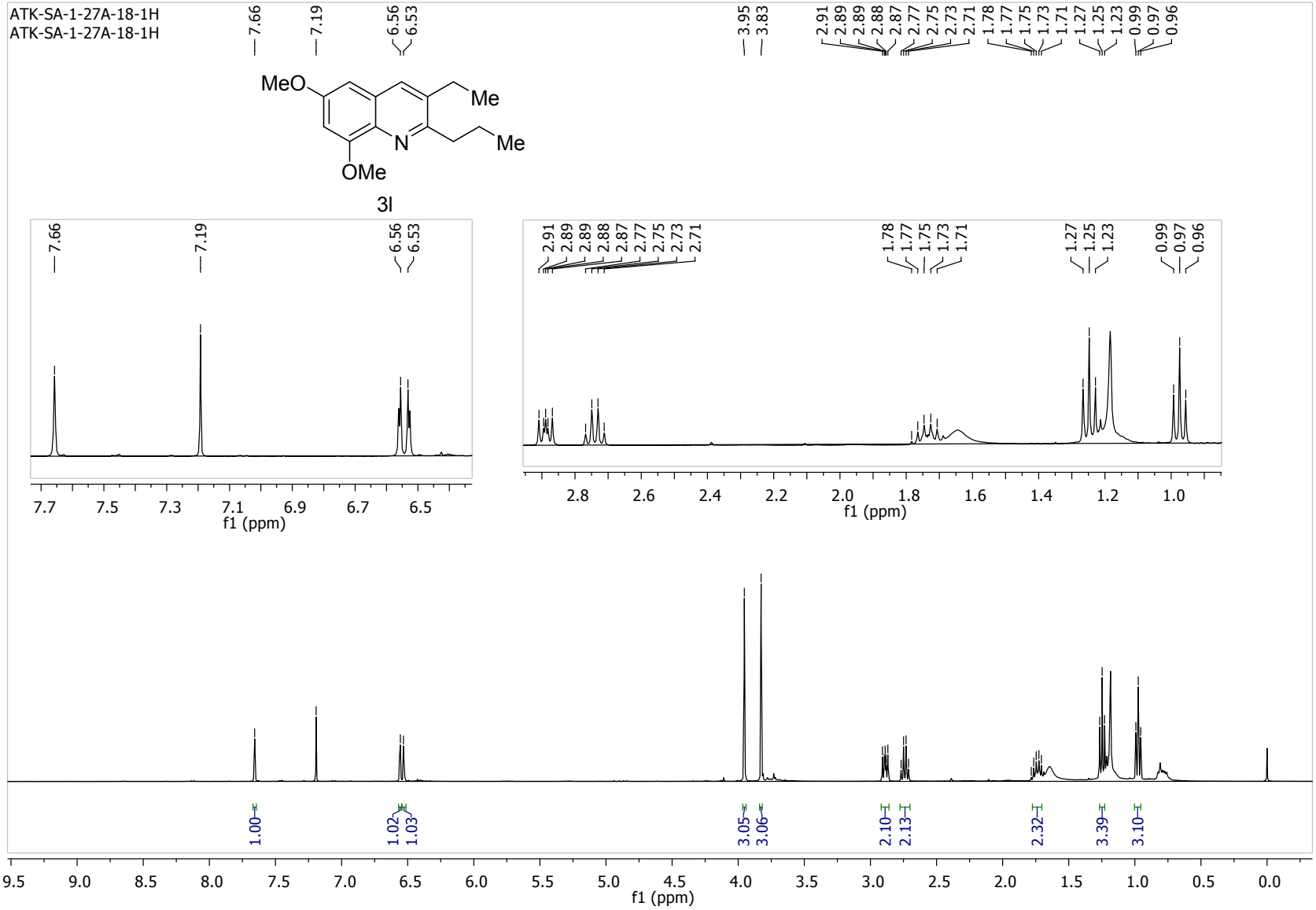
^{13}C NMR spectra of compound: 3k



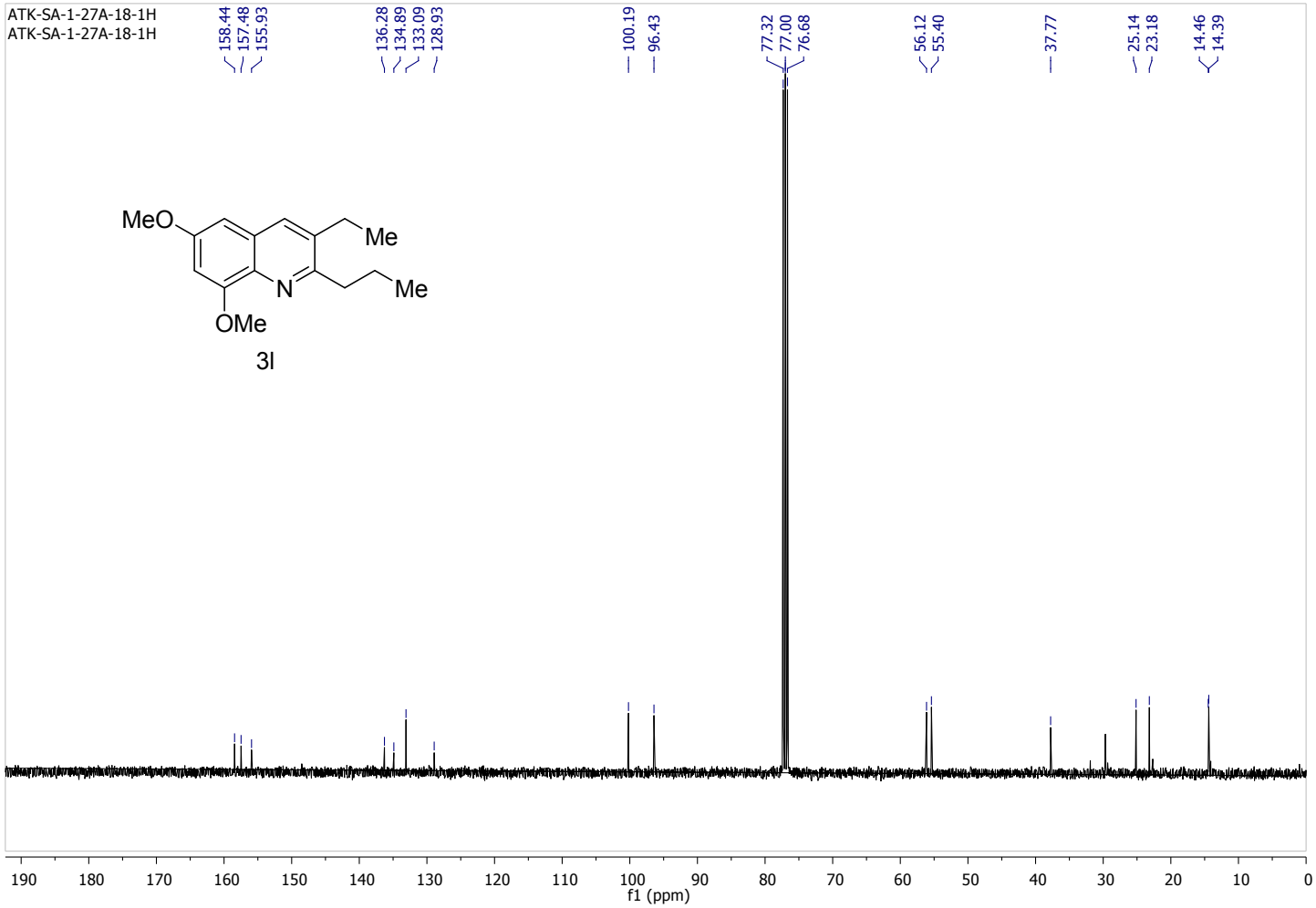
HRMS spectra of compound: 3k



^{1}H NMR spectra of compound: 3l

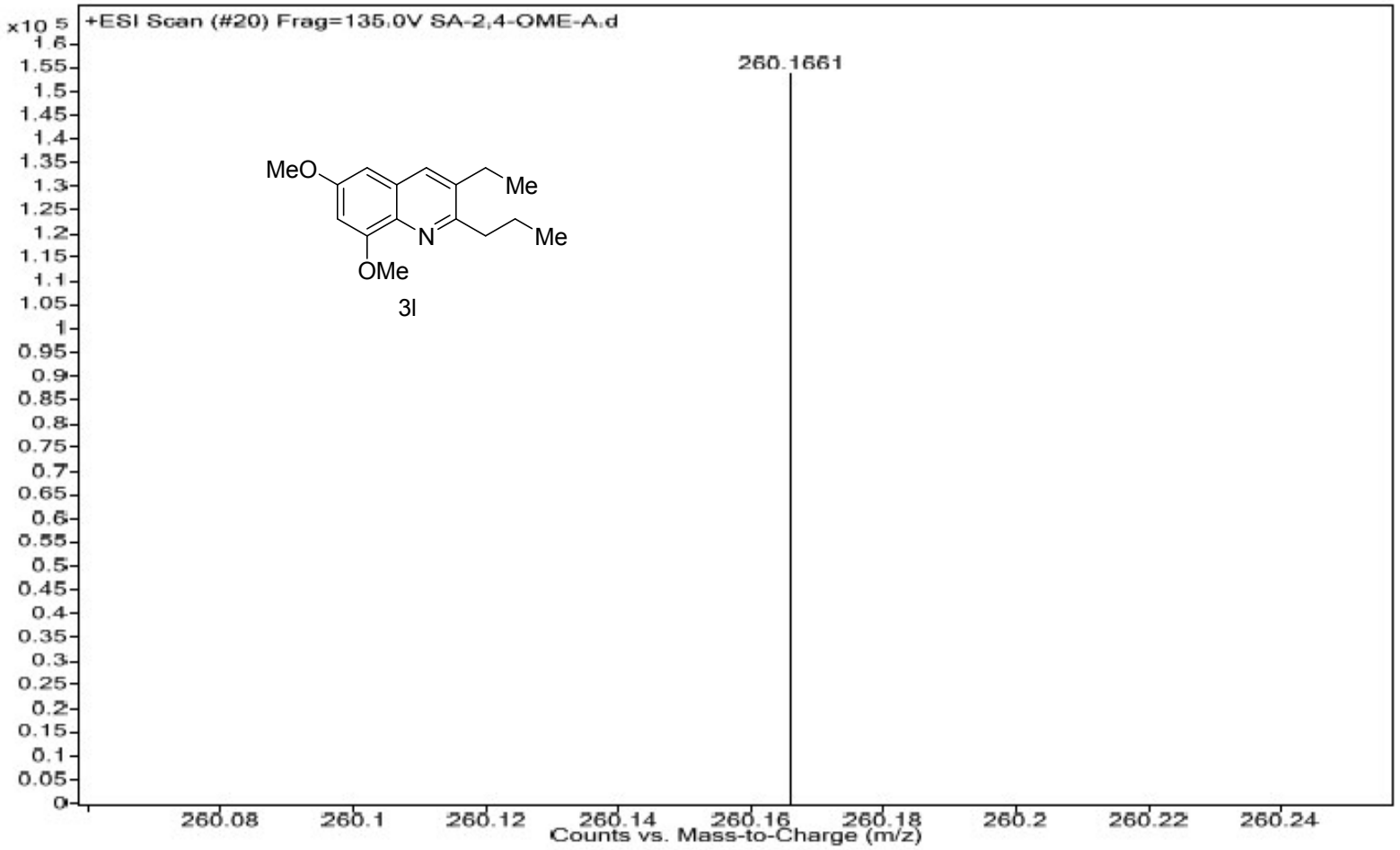


^{13}C NMR spectra of compound: 3l

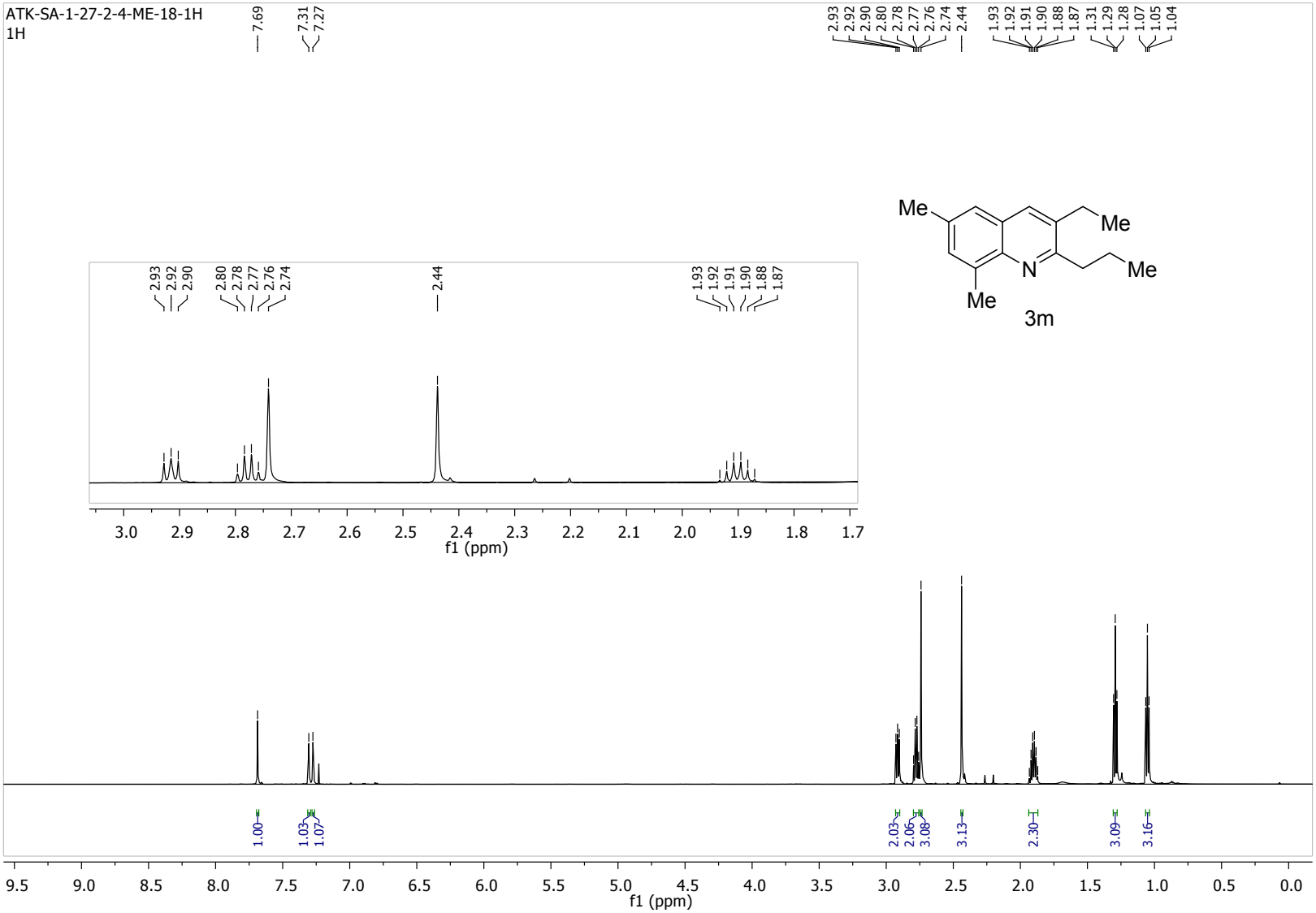


HRMS spectra of compound: 3l

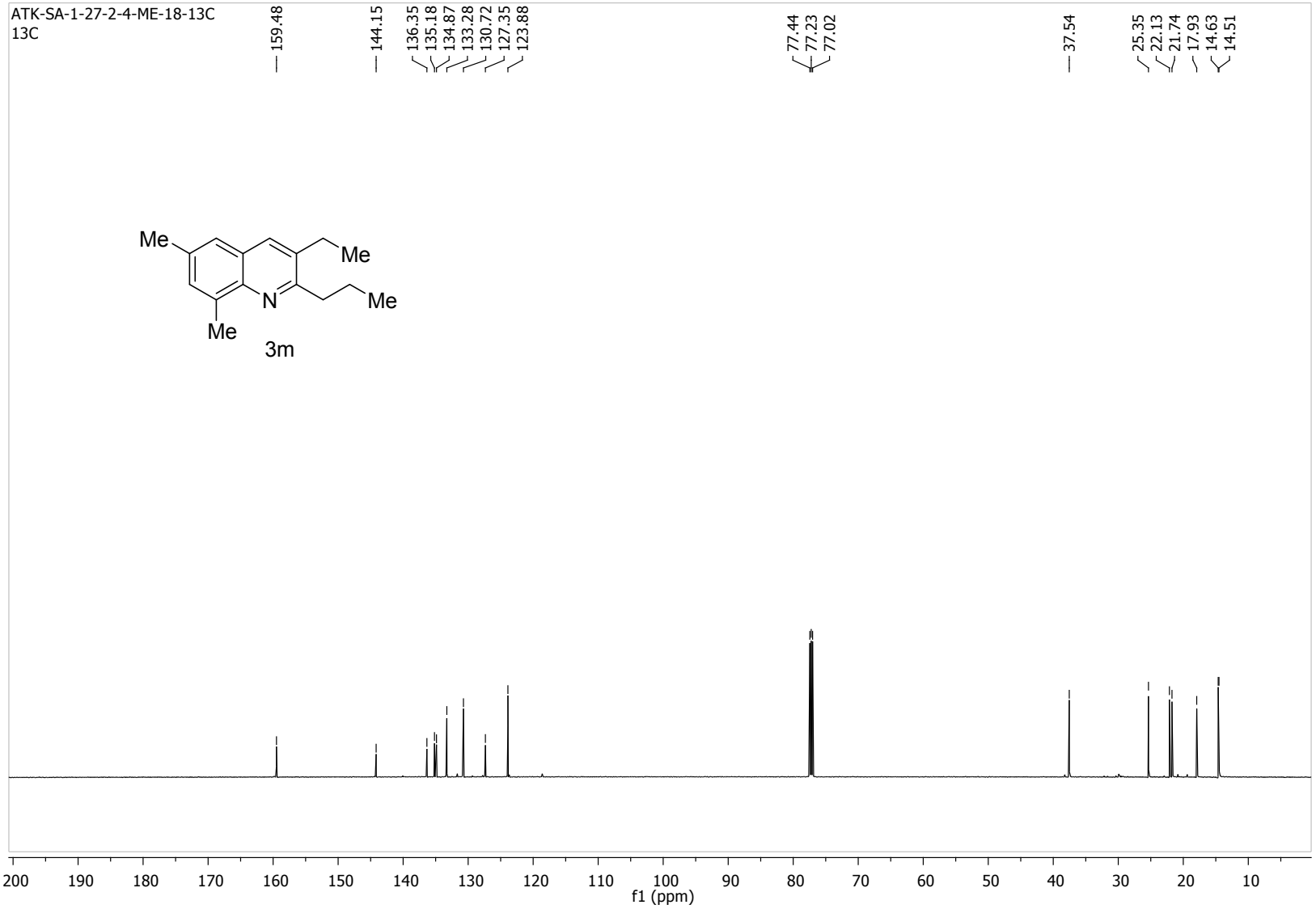
Sample Name	SA-2,4-OME-A	**Position**	Vial 1	**Instrument Name**	QTOF	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	SA-2,4-OME-A.d	**ACQ Method**		**Comment**		**Acquired Time**	6/7/2018 3:55:32 PM



^{1}H NMR spectra of compound: 3m

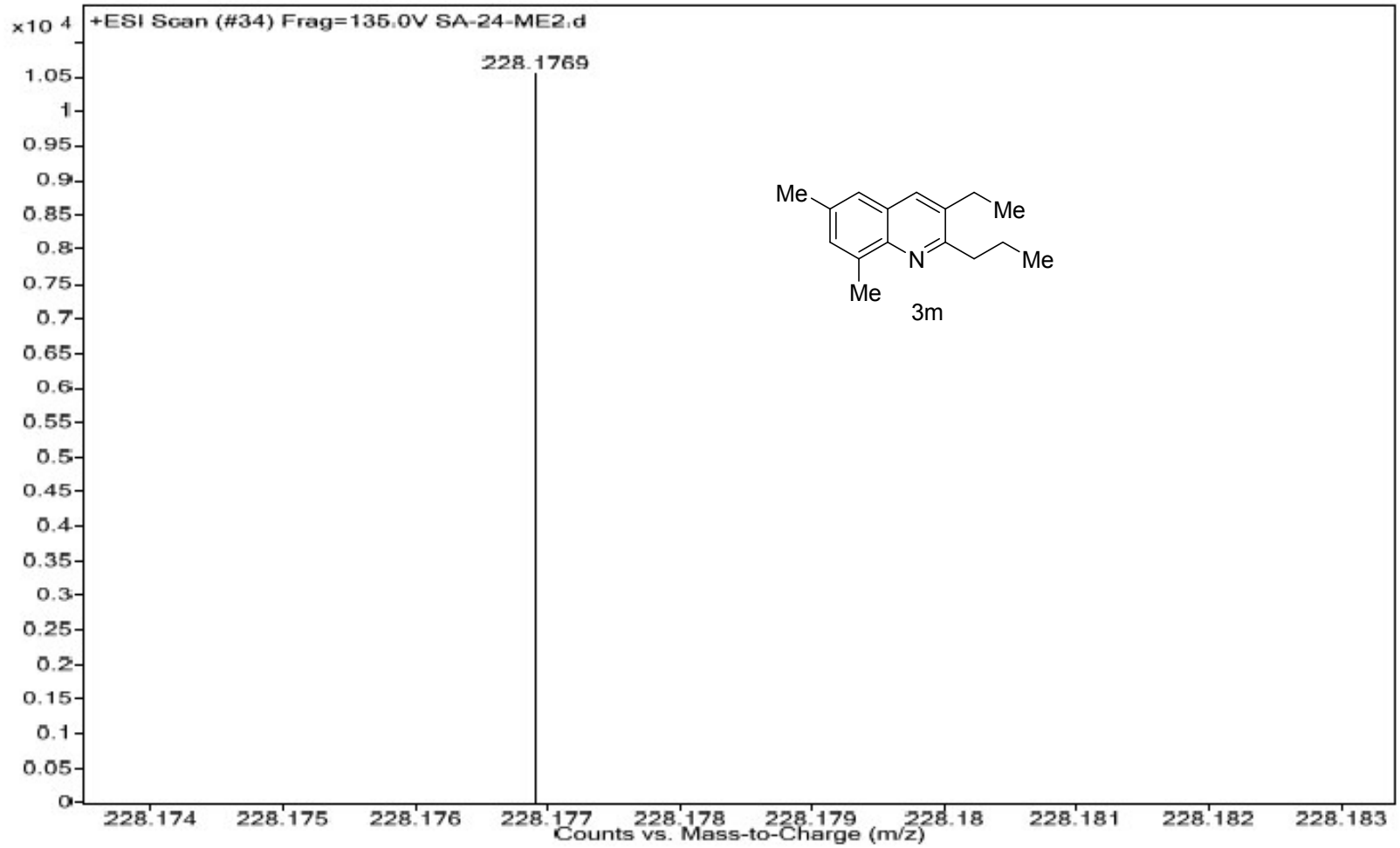


^{13}C NMR spectra of compound: 3m

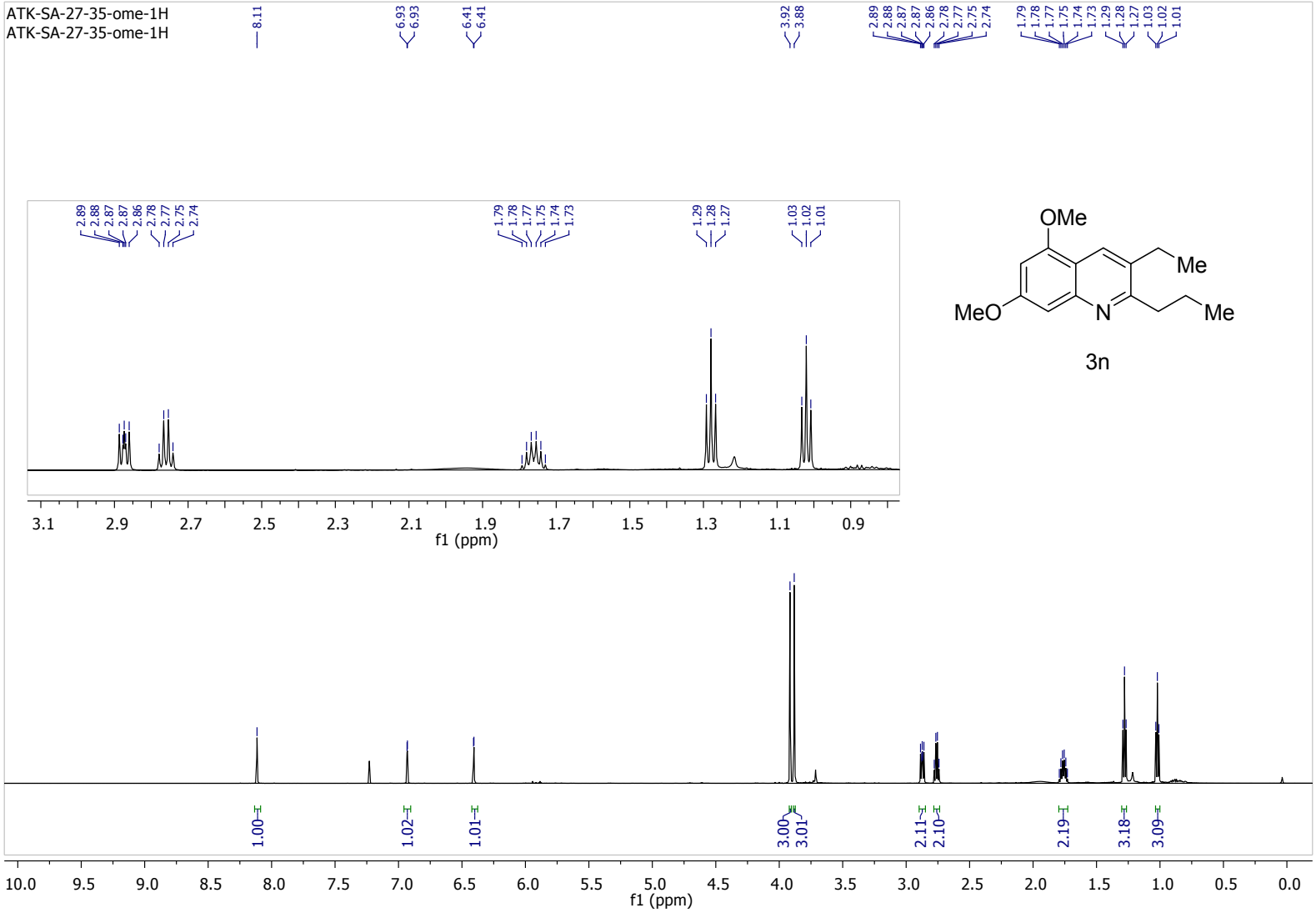


HRMS spectra of compound: 3m

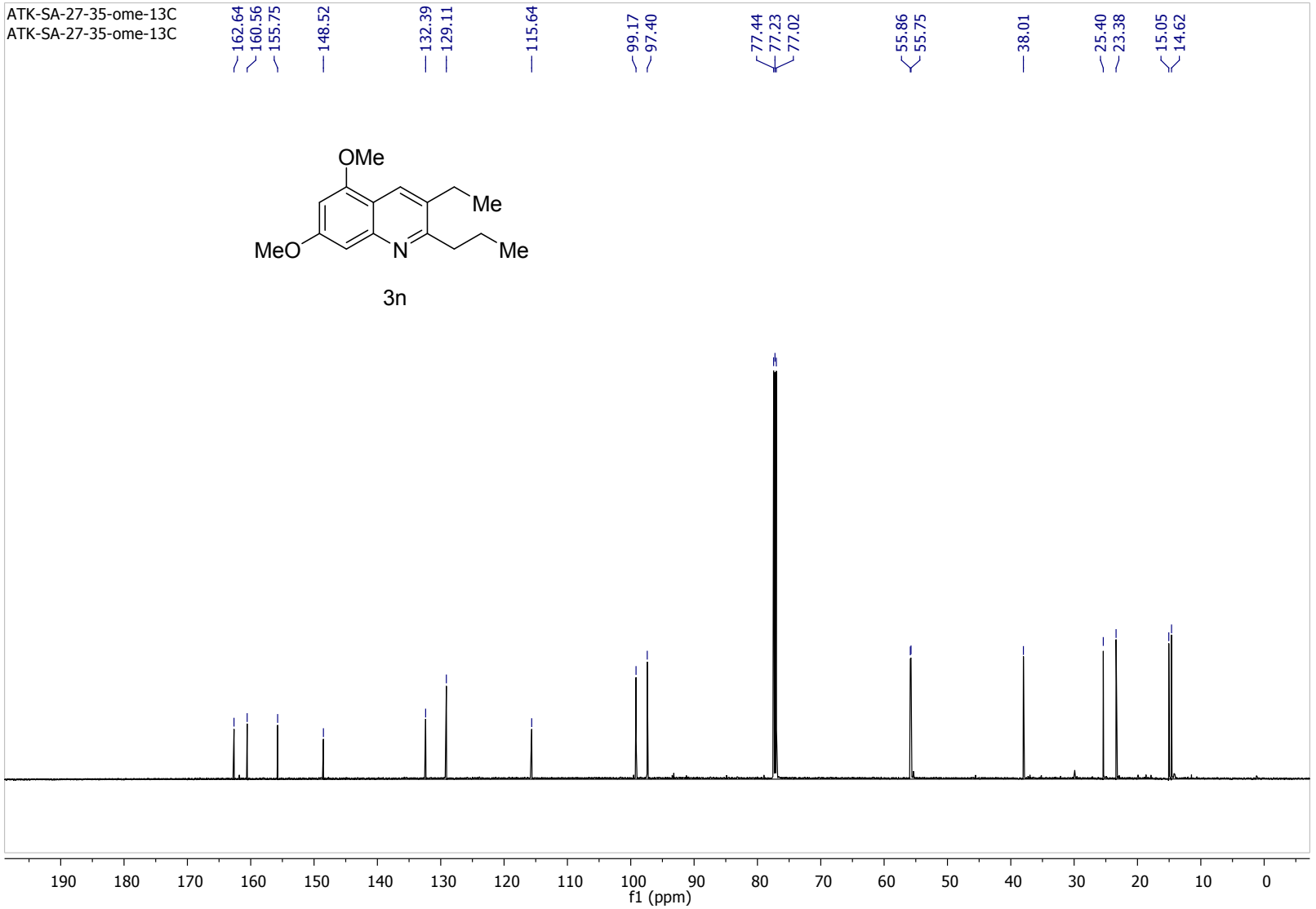
Sample Name	**Position**	**Instrument Name**	**User Name**
Inj Vol	**InjPosition**	**SampleType**	**IRM Calibration Status**
Data Filename	**ACQ Method**	**Comment**	**Acquired Time**



^{1}H NMR spectra of compound: 3n

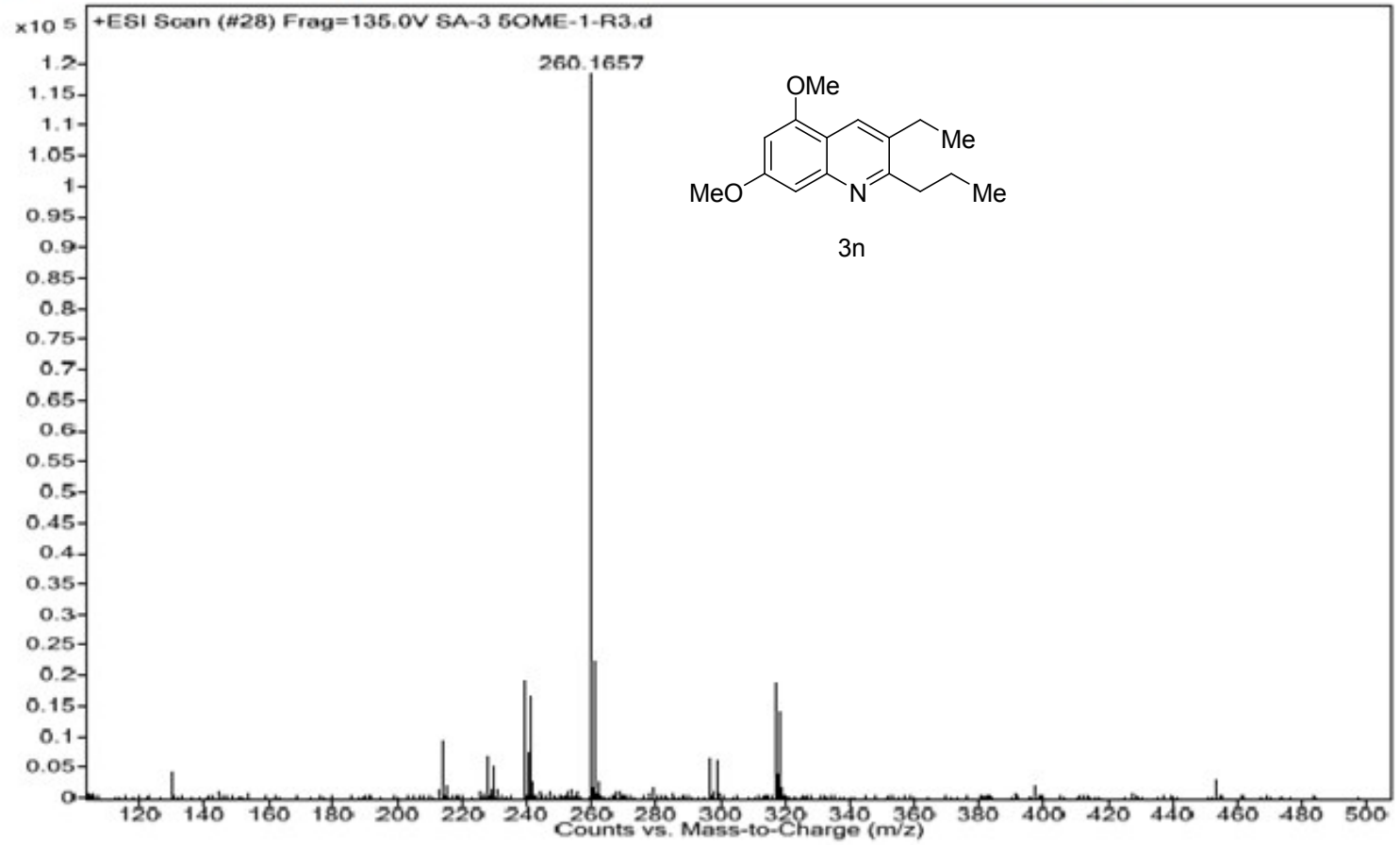


^{13}C NMR spectra of compound: 3n

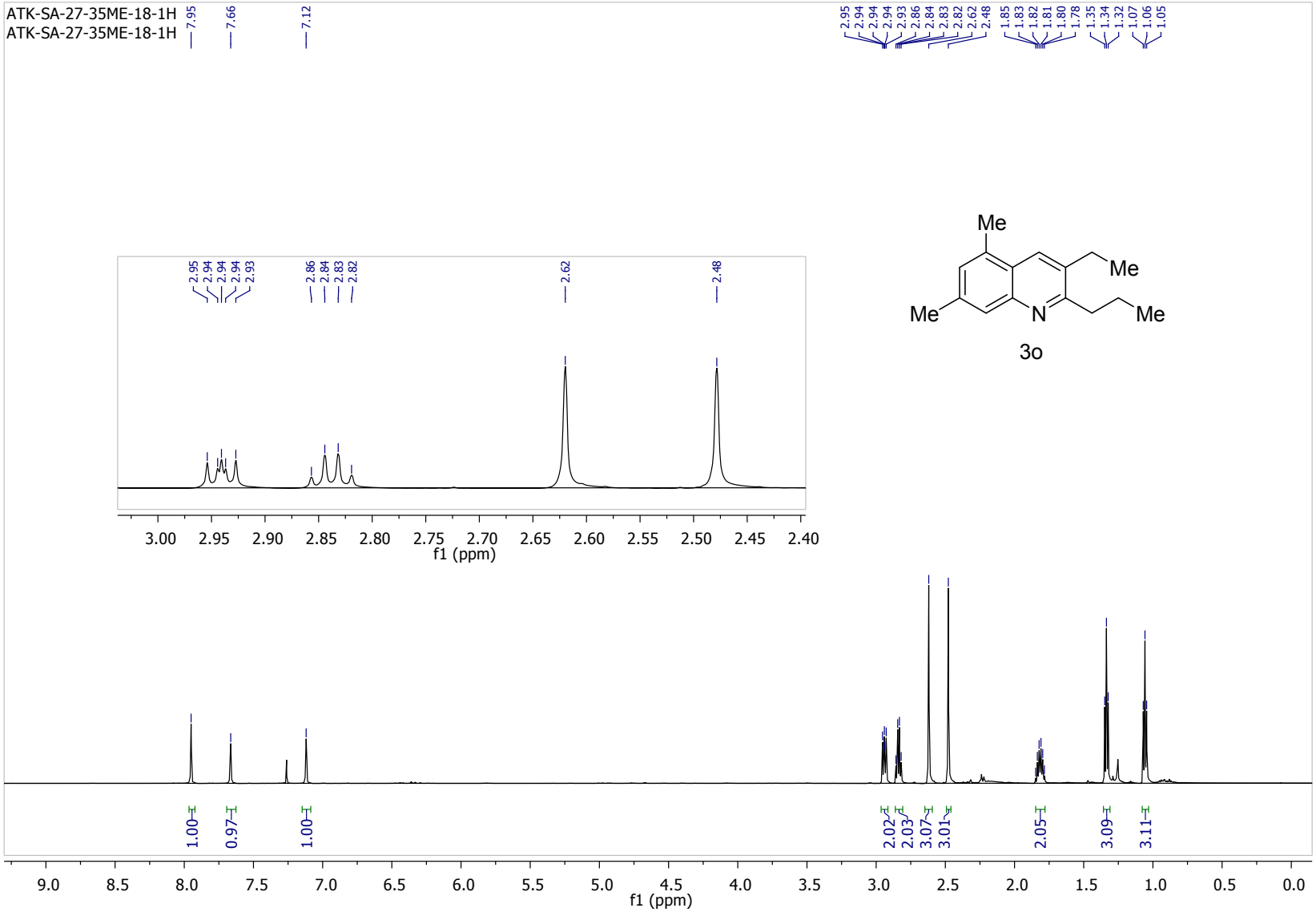


HRMS spectra of compound: 3n

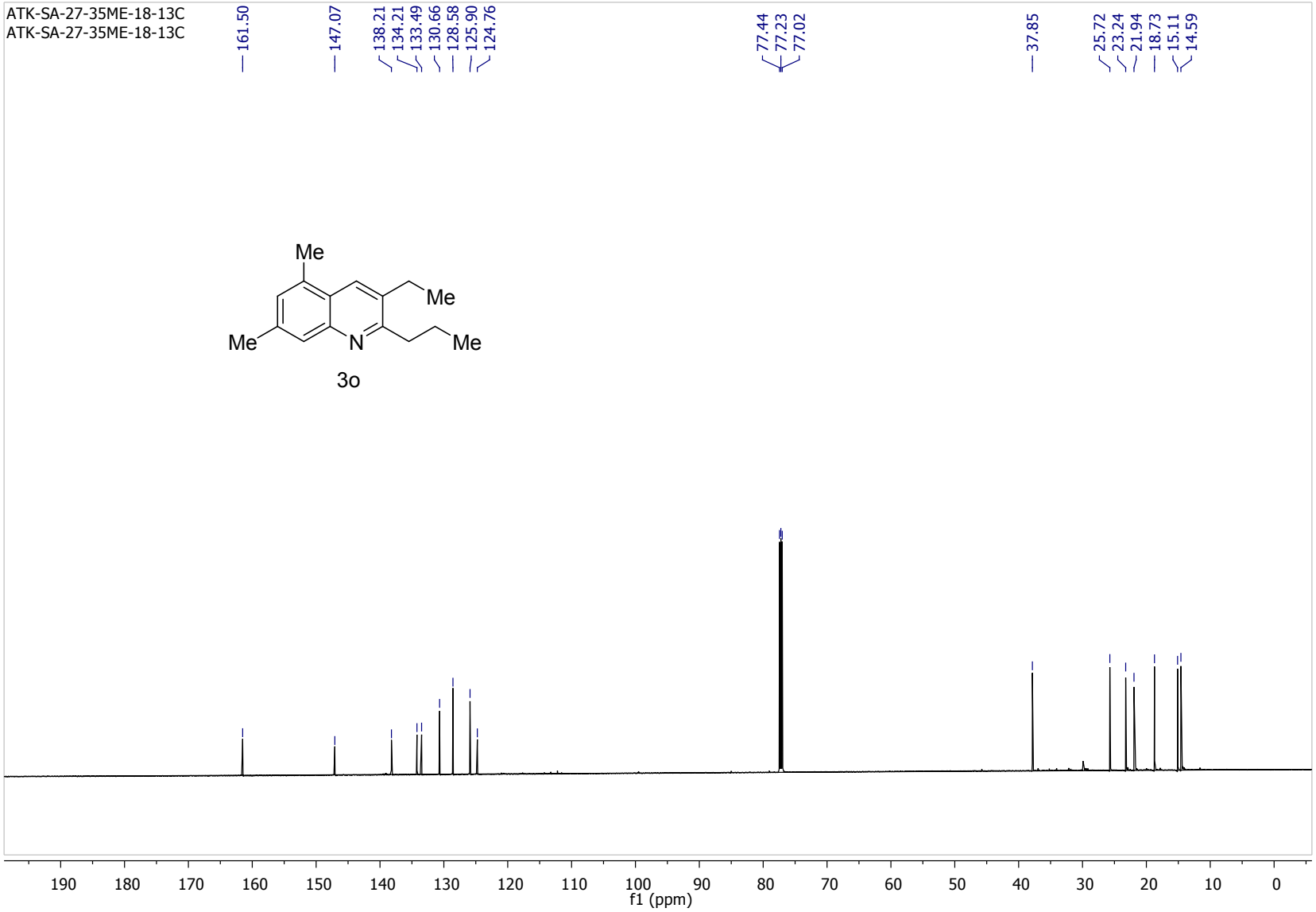
Sample Name	**Position**	**Instrument Name**	**User Name**
Inj Vol	**InjPosition**	**SampleType**	**IRM Calibration Status**
Data Filename	**ACQ Method**	**Comment**	**Acquired Time**



^{1}H NMR spectra of compound: 3o

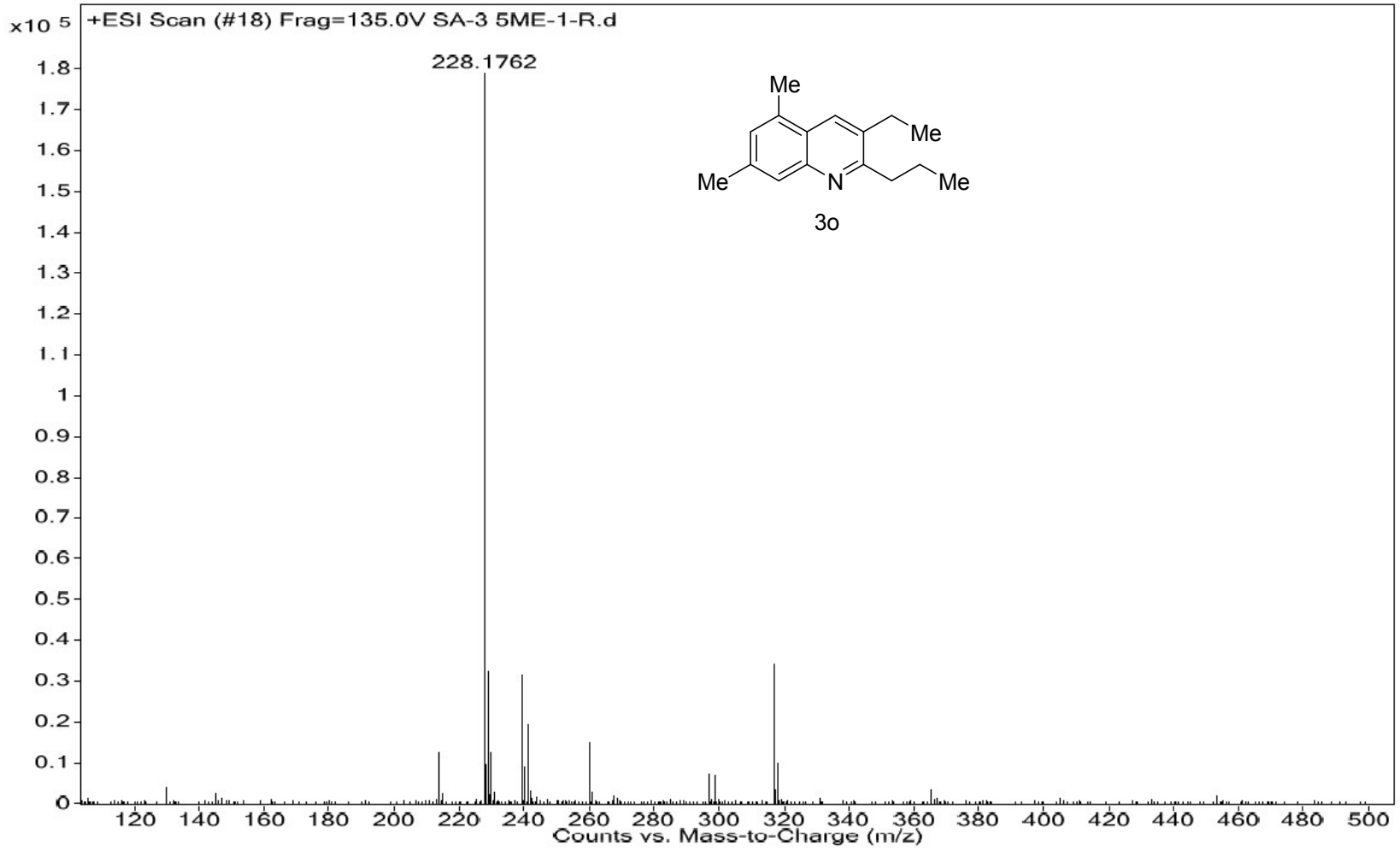


^{13}C NMR spectra of compound: 3o

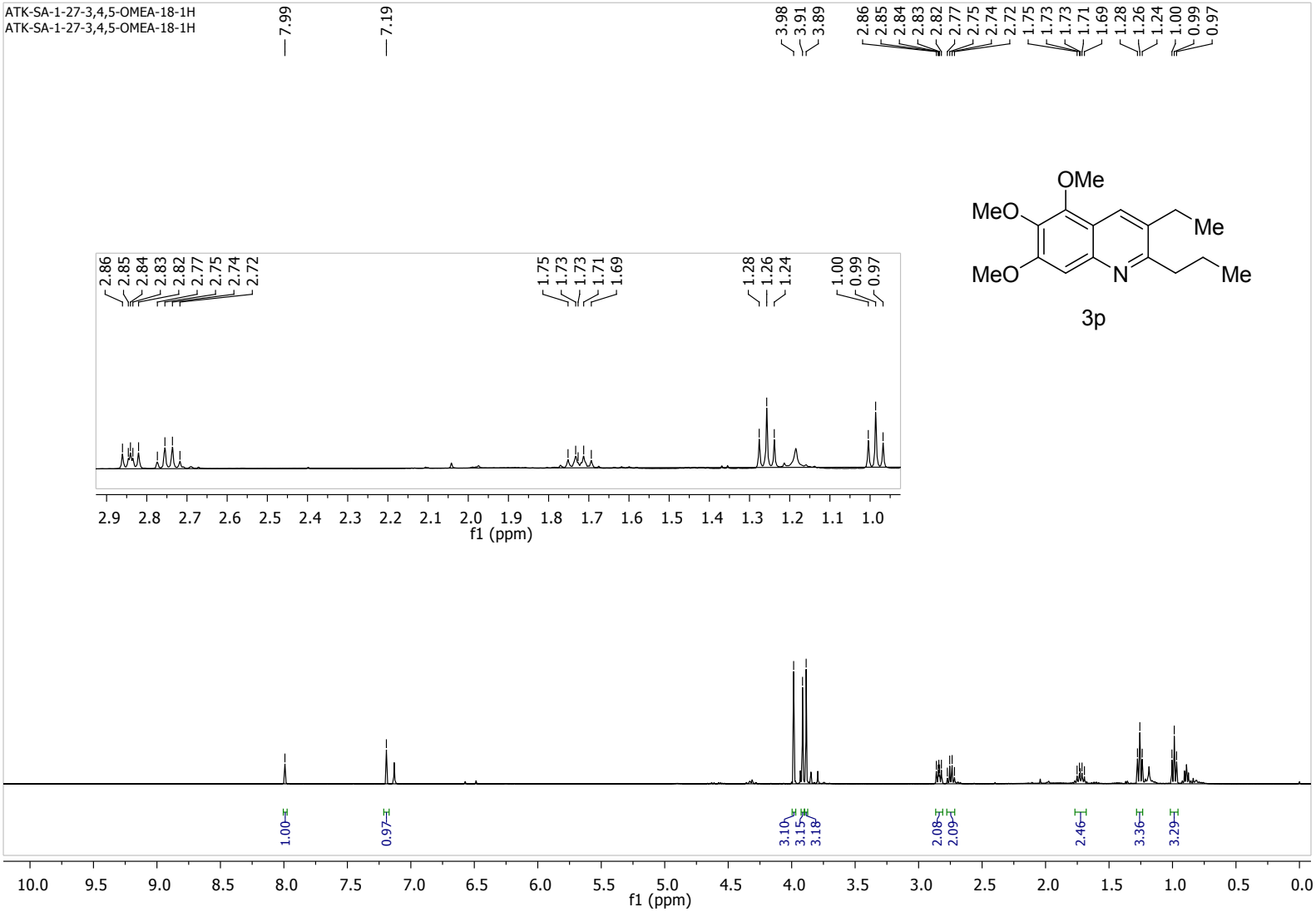


HRMS spectra of compound: 3o

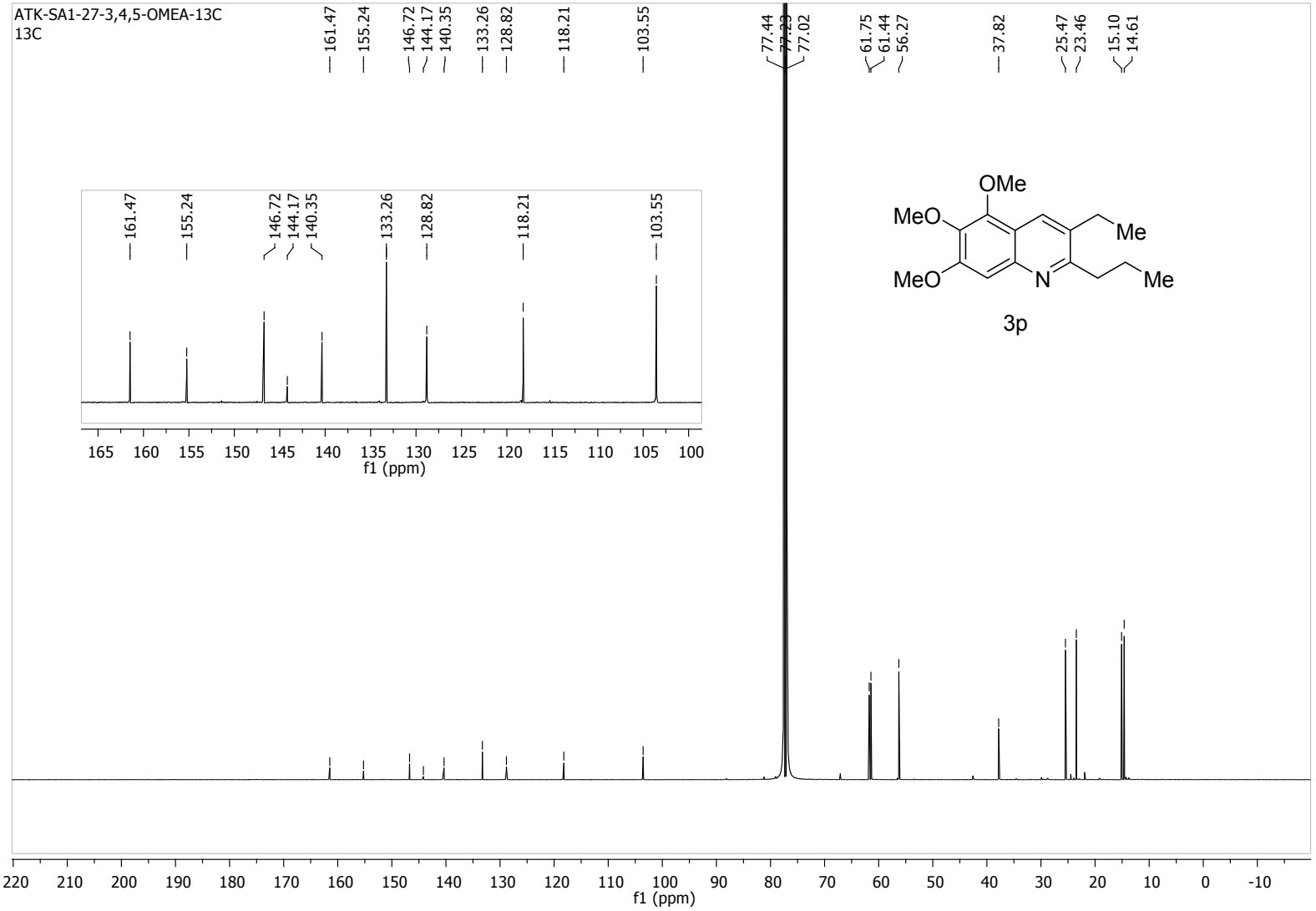
Sample Name	**Position**	**Instrument Name**	**User Name**
Inj Vol	**InjPosition**	**SampleType**	**IRM Calibration Status**
Data Filename	**ACQ Method**	**Comment**	**Acquired Time**



^{1}H NMR spectra of compound: 3p

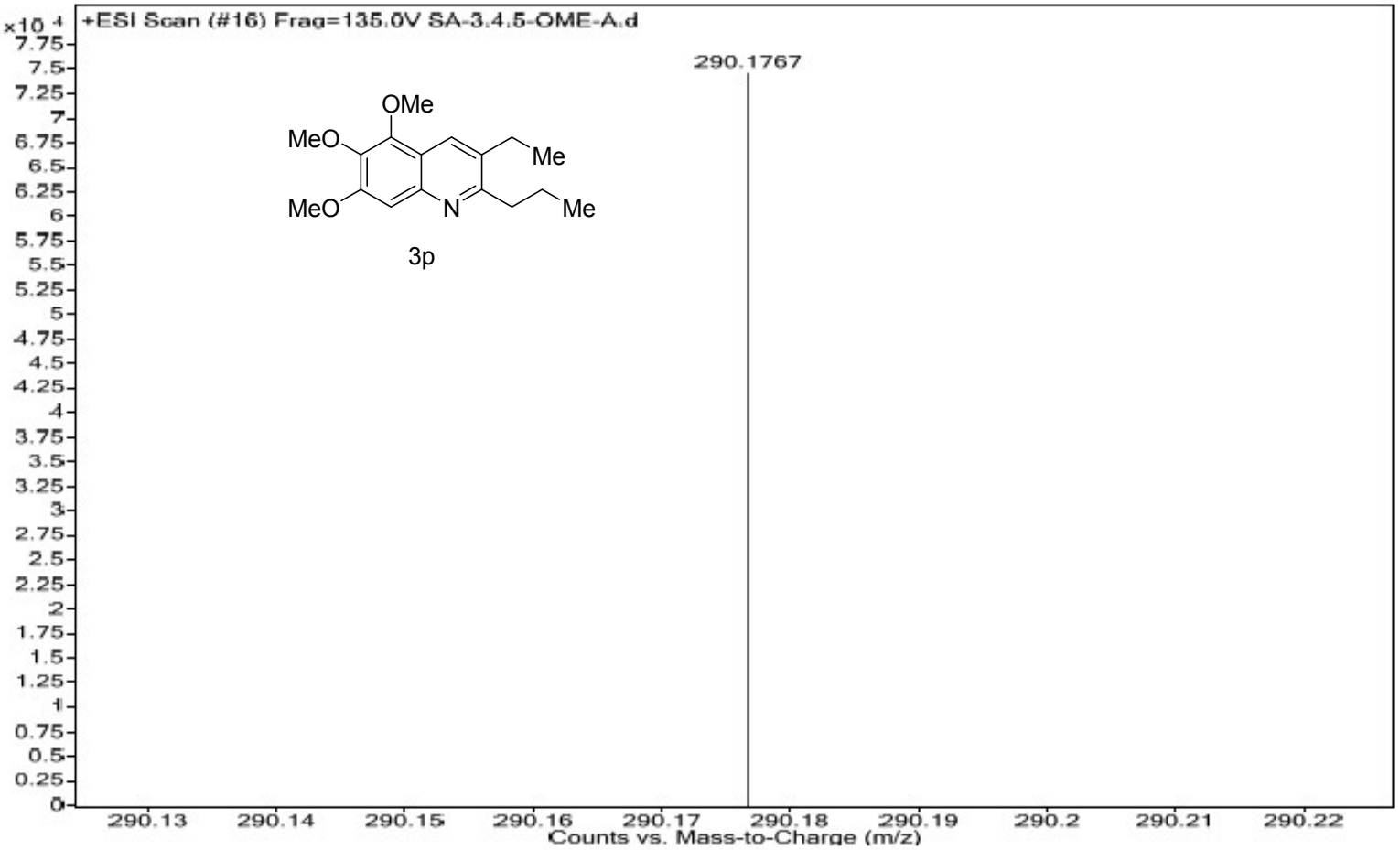


^{13}C NMR spectra of compound: 3p

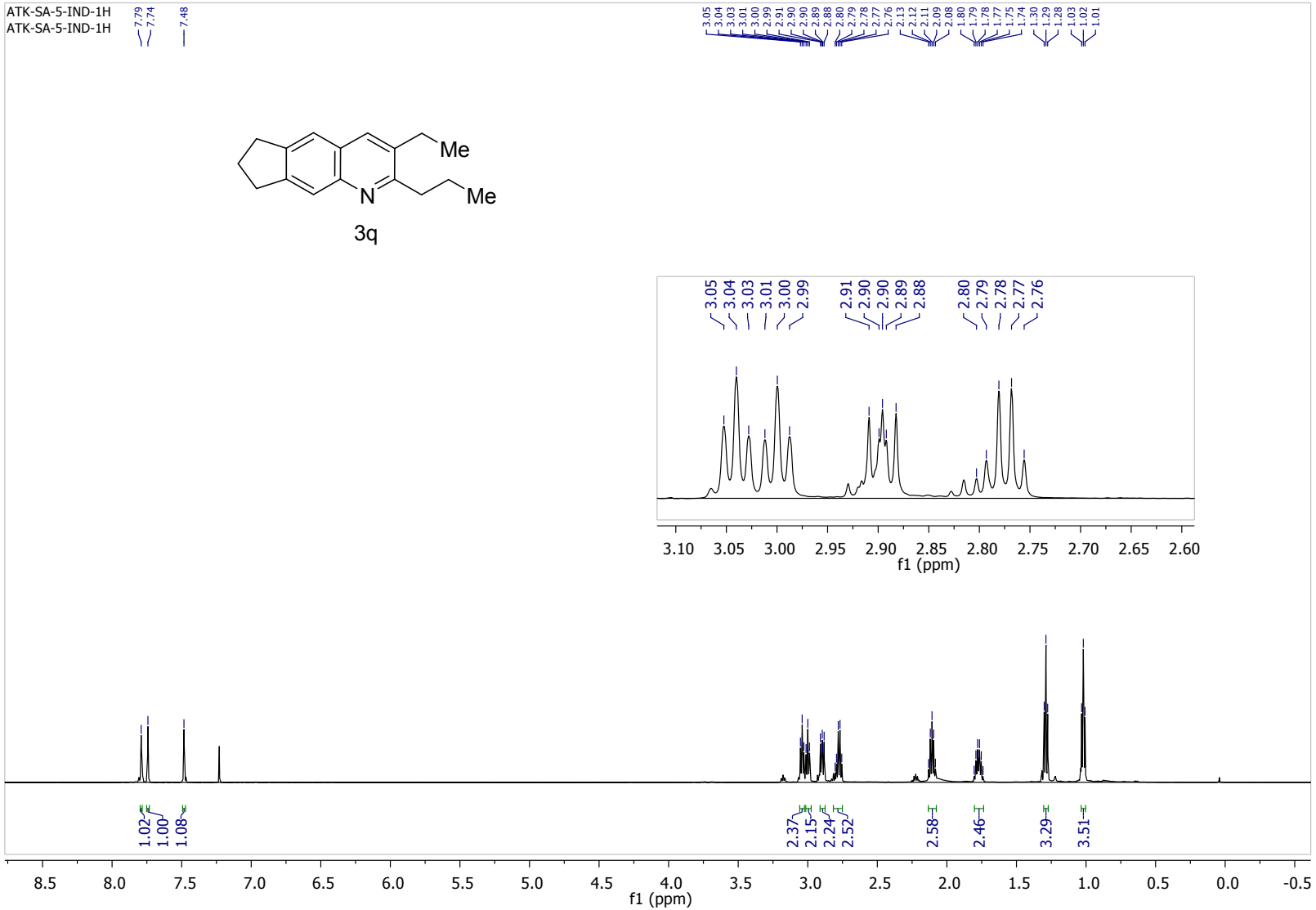


HRMS spectra of compound: 3p

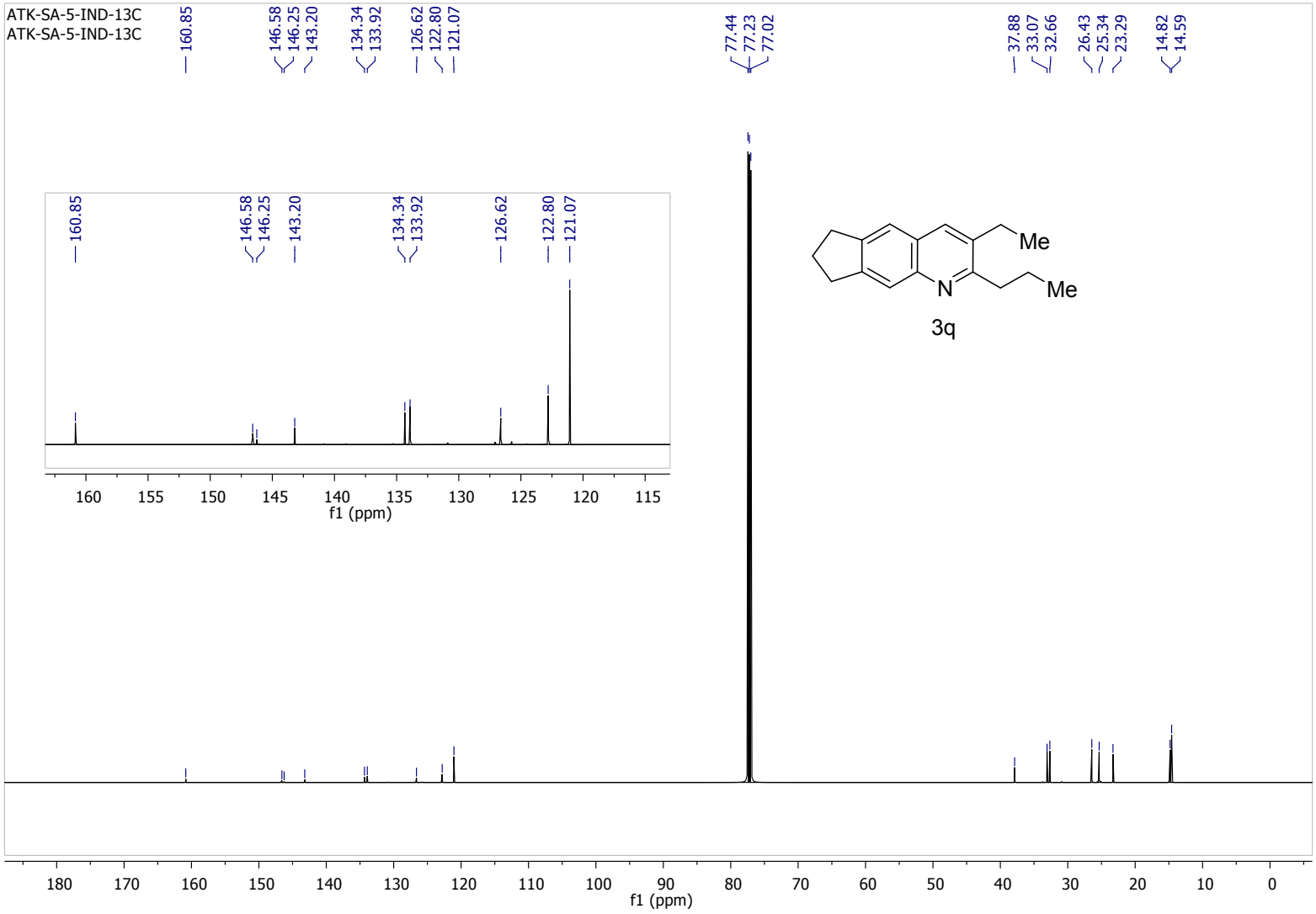
Sample Name	SA-3,4,5-OME-A	**Position**	Vial 1	**Instrument Name**	QTOF	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	SA-3,4,5-OME-A.d	**ACQ Method**		**Comment**		**Acquired Time**	6/7/2018 3:58:15 PM



^{1}H NMR spectra of compound: 3q

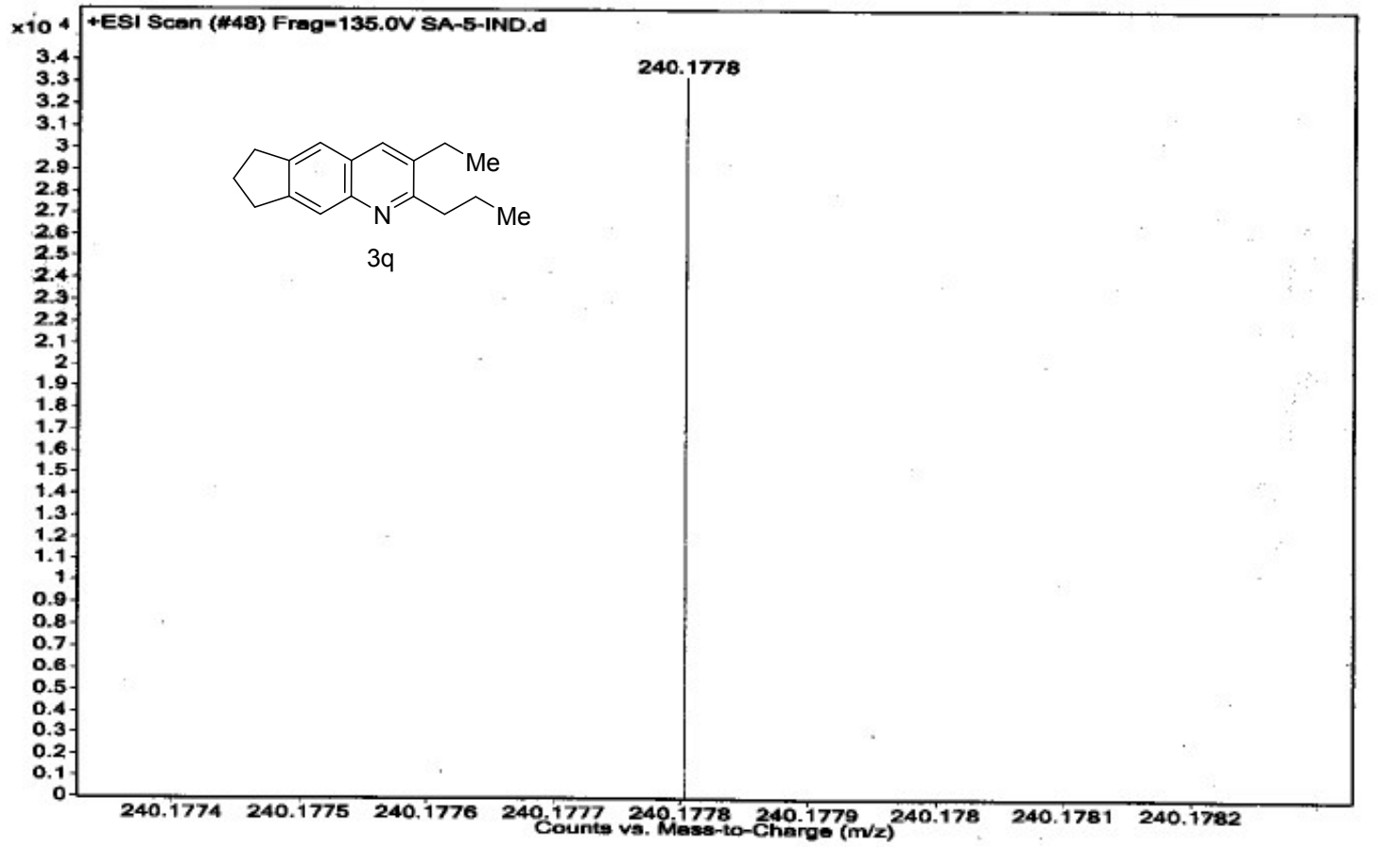


^{13}C NMR spectra of compound: 3q

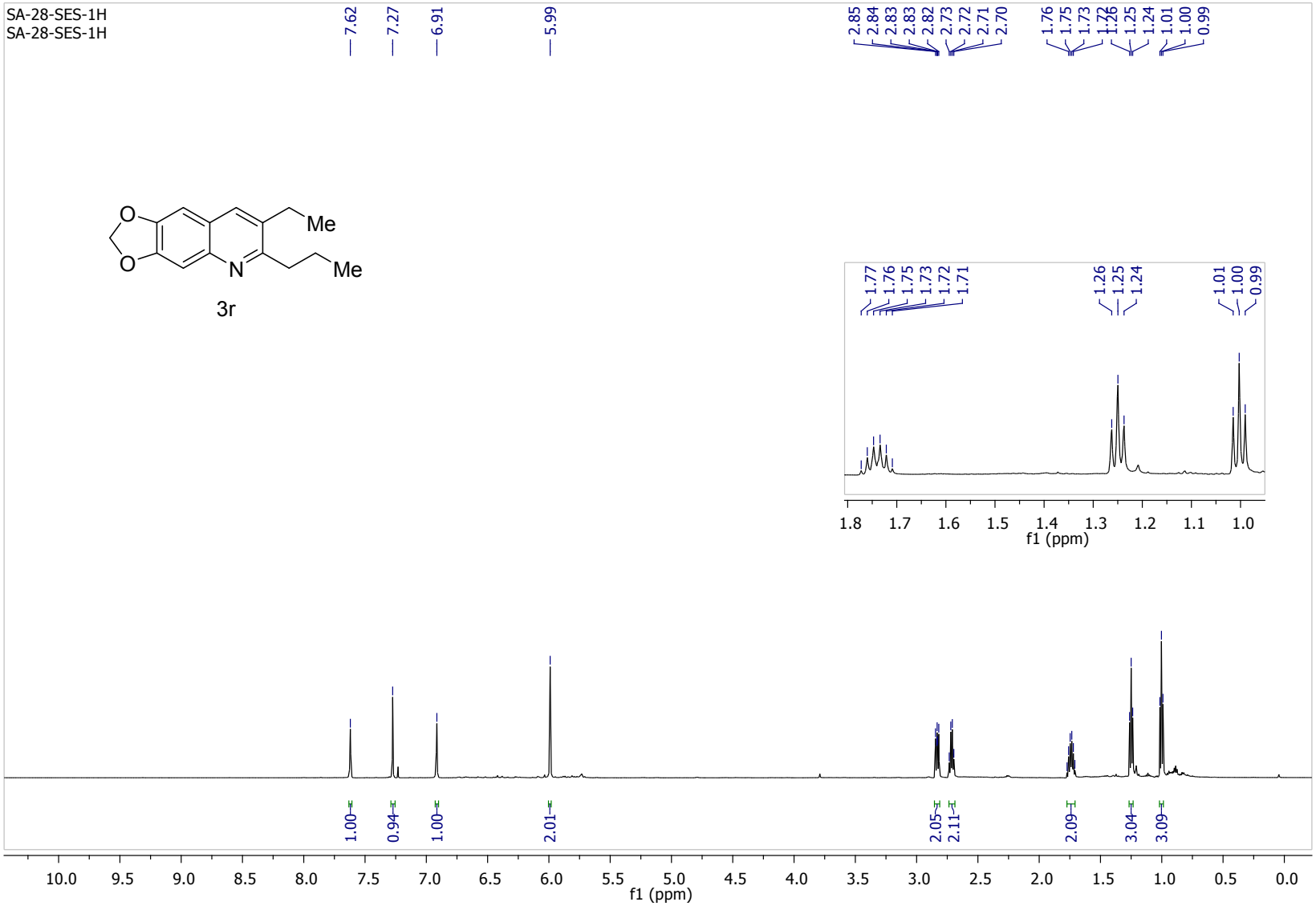


HRMS spectra of compound: 3q

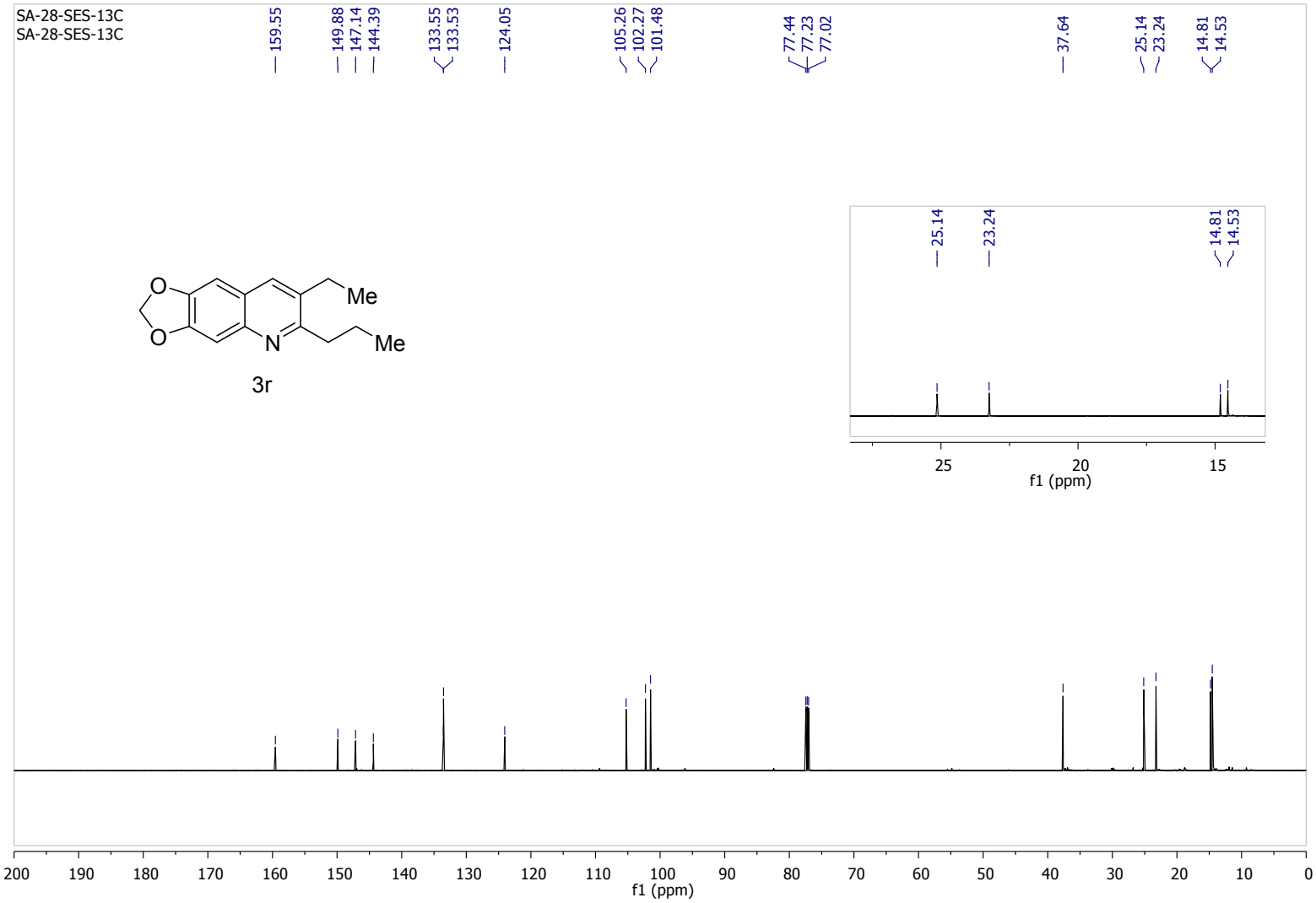
Sample Name	SA-5-IND	Position	Vial 1	Instrument Name	QTOF	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	TRM Calibration Status	Success
Data Filename	SA-5-IND.d	ACQ Method		Comment		Acquired Time	7/26/2018 10:13:33 AM



^{1}H NMR spectra of compound: 3r

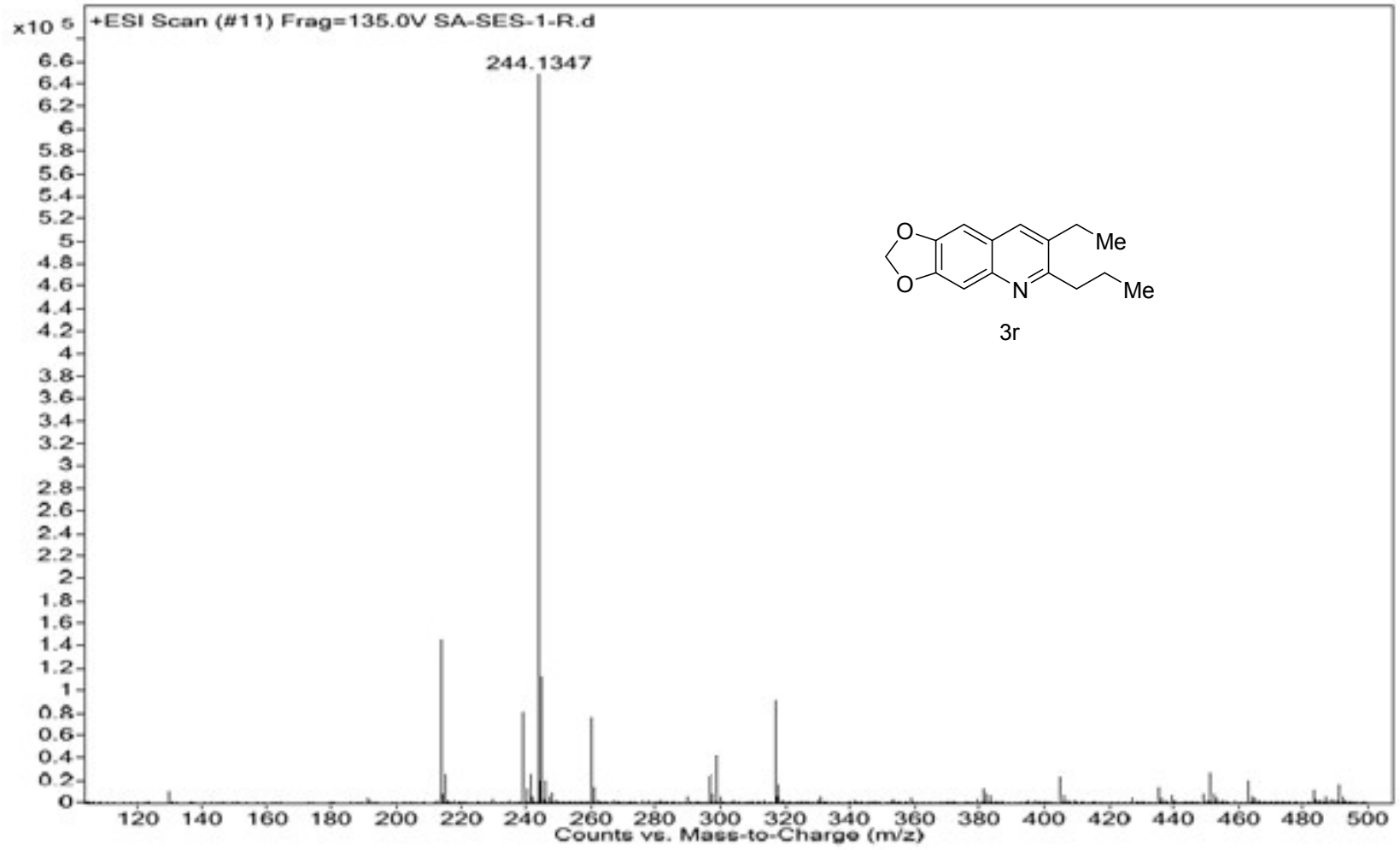


^{13}C NMR spectra of compound: 3r



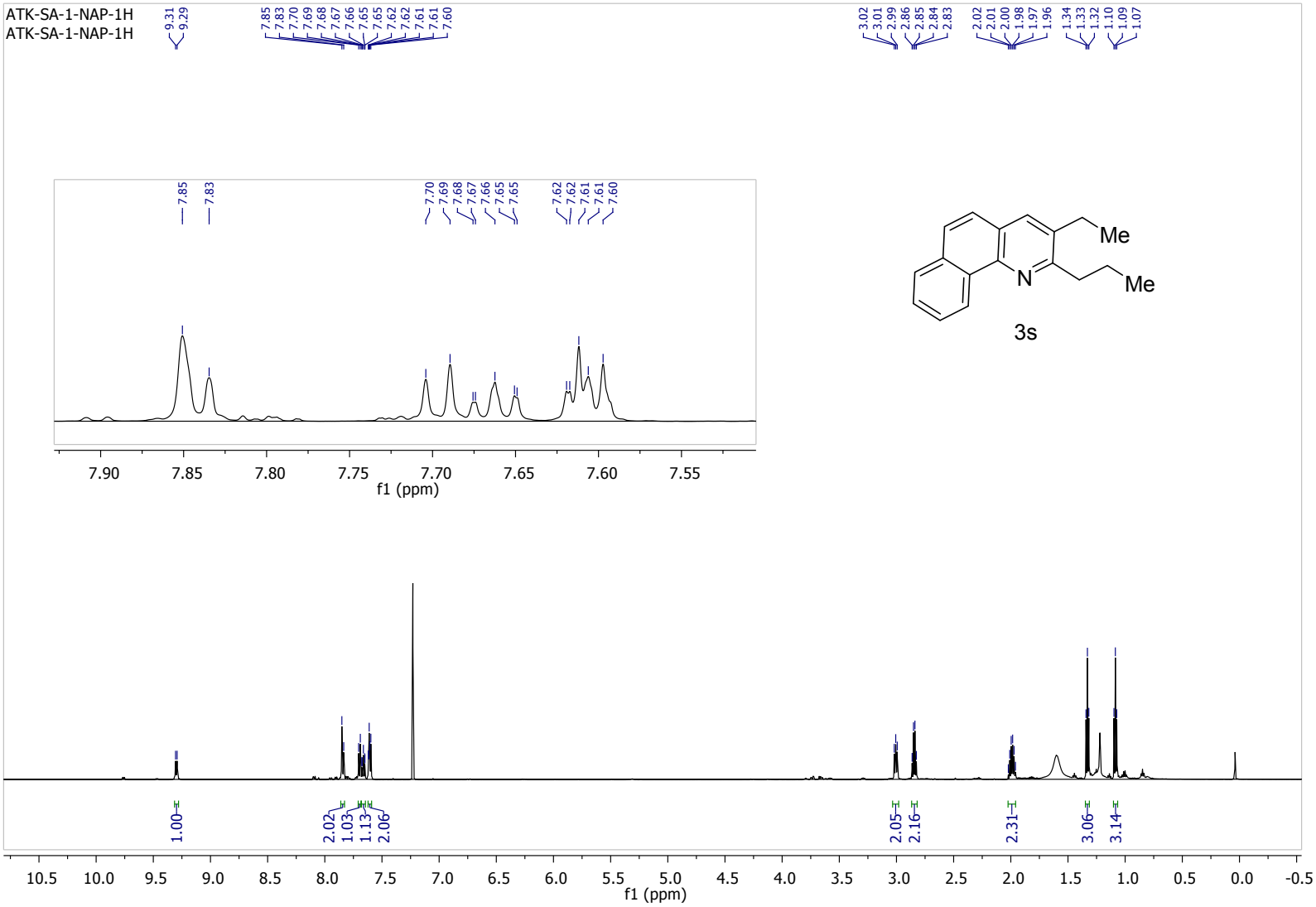
HRMS spectra of compound: 3r

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time

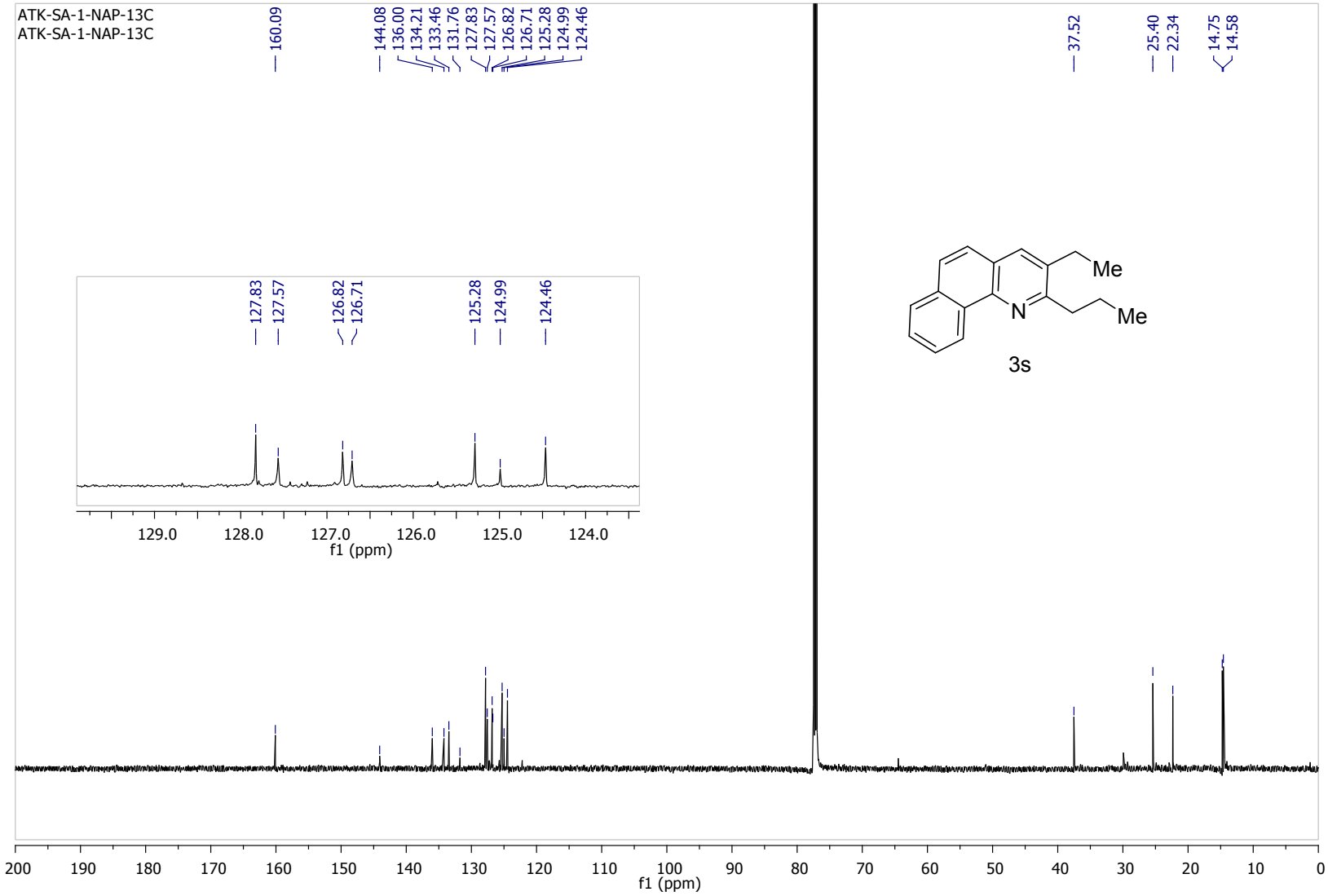


3r

^{1}H NMR spectra of compound: 3s

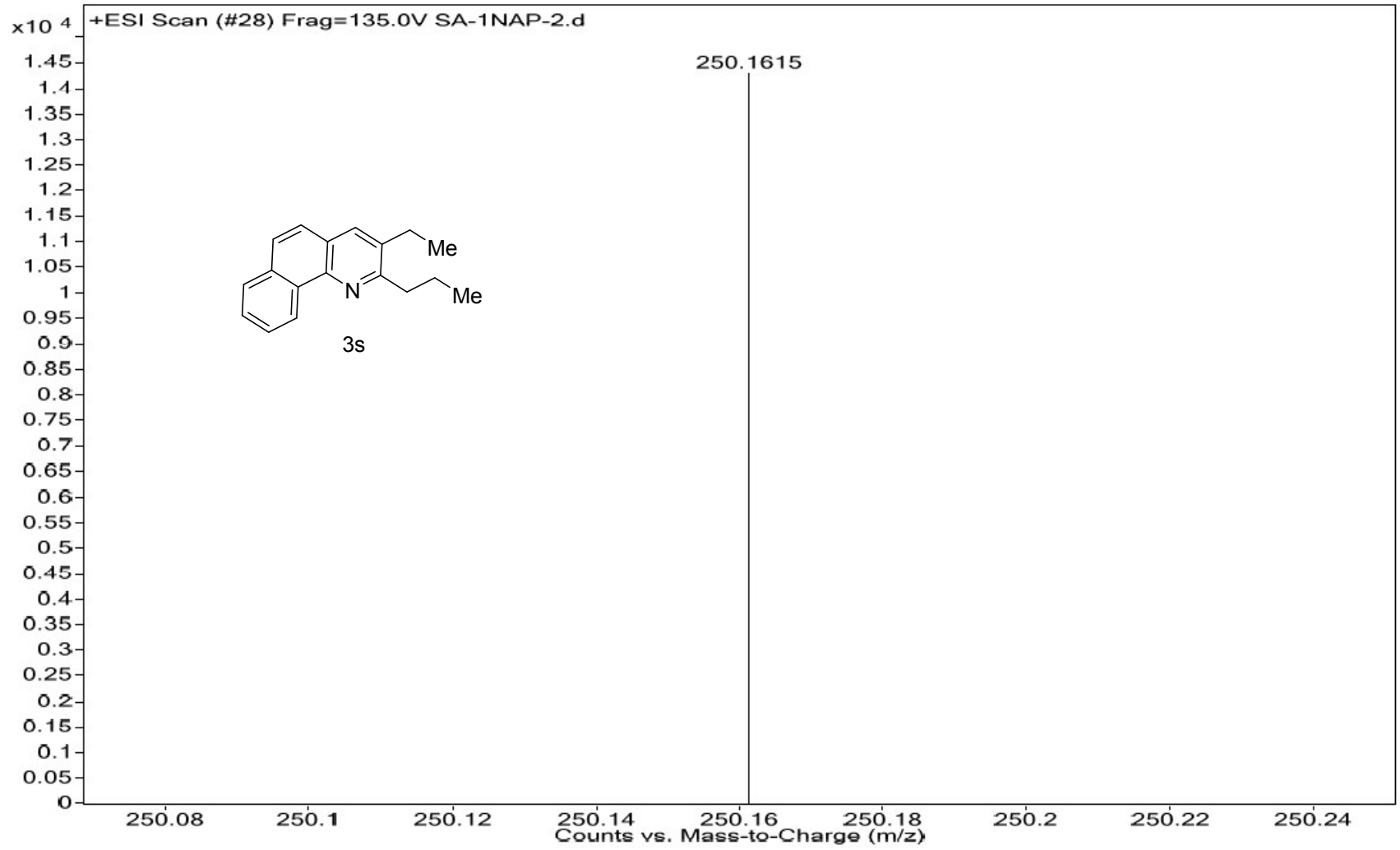


^{13}C NMR spectra of compound: 3s

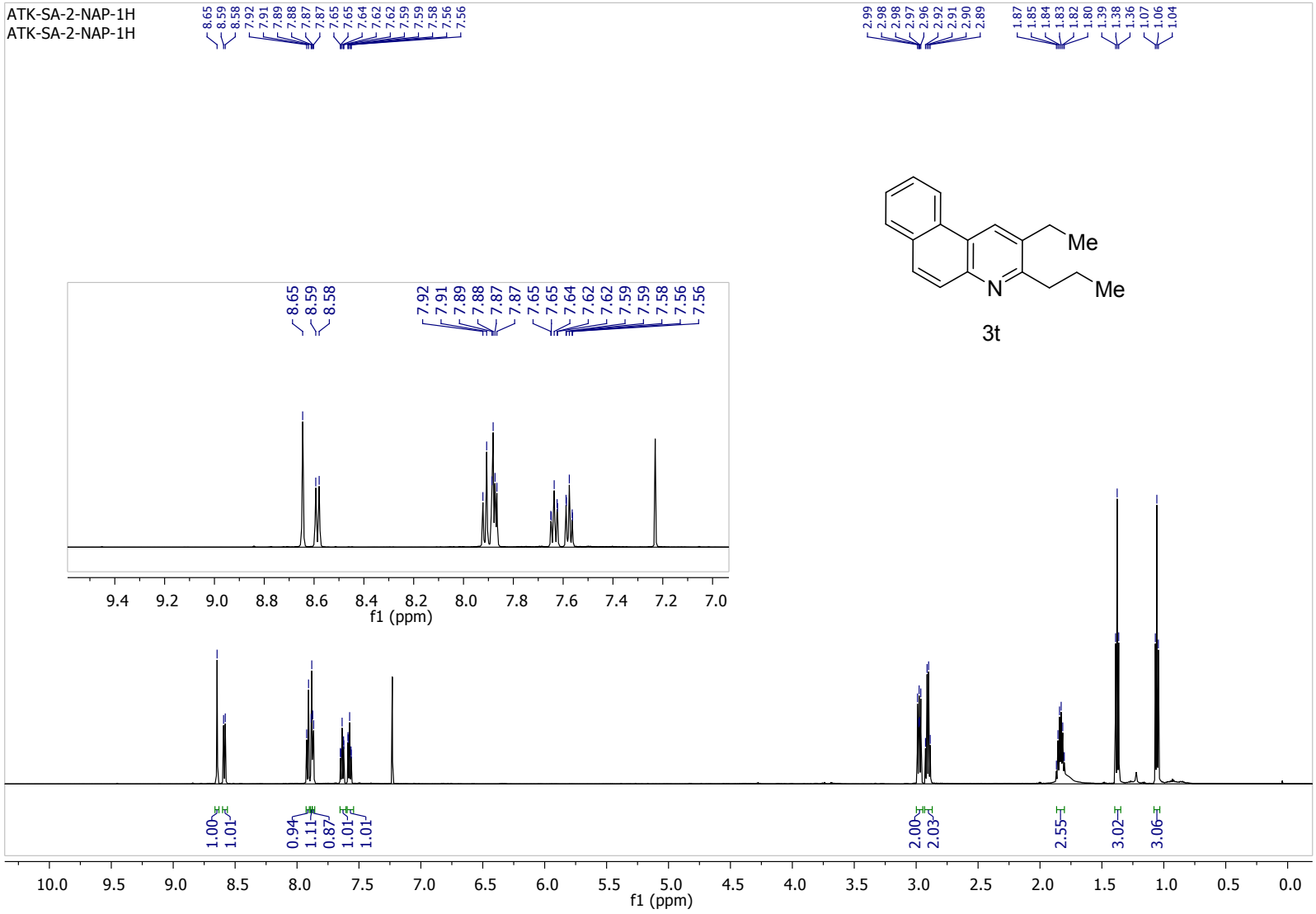


HRMS spectra of compound: 3s

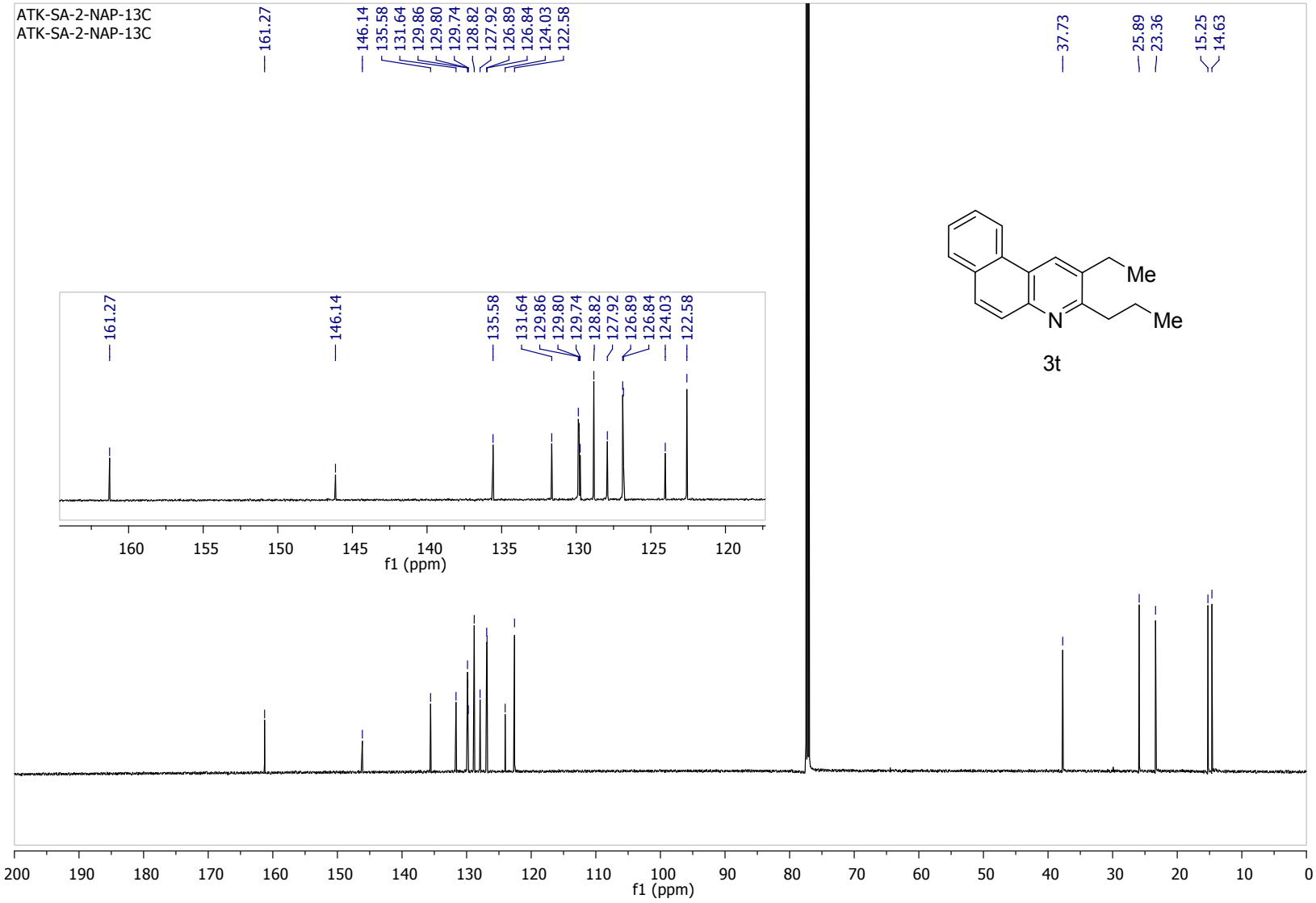
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



^{1}H NMR spectra of compound: 3t

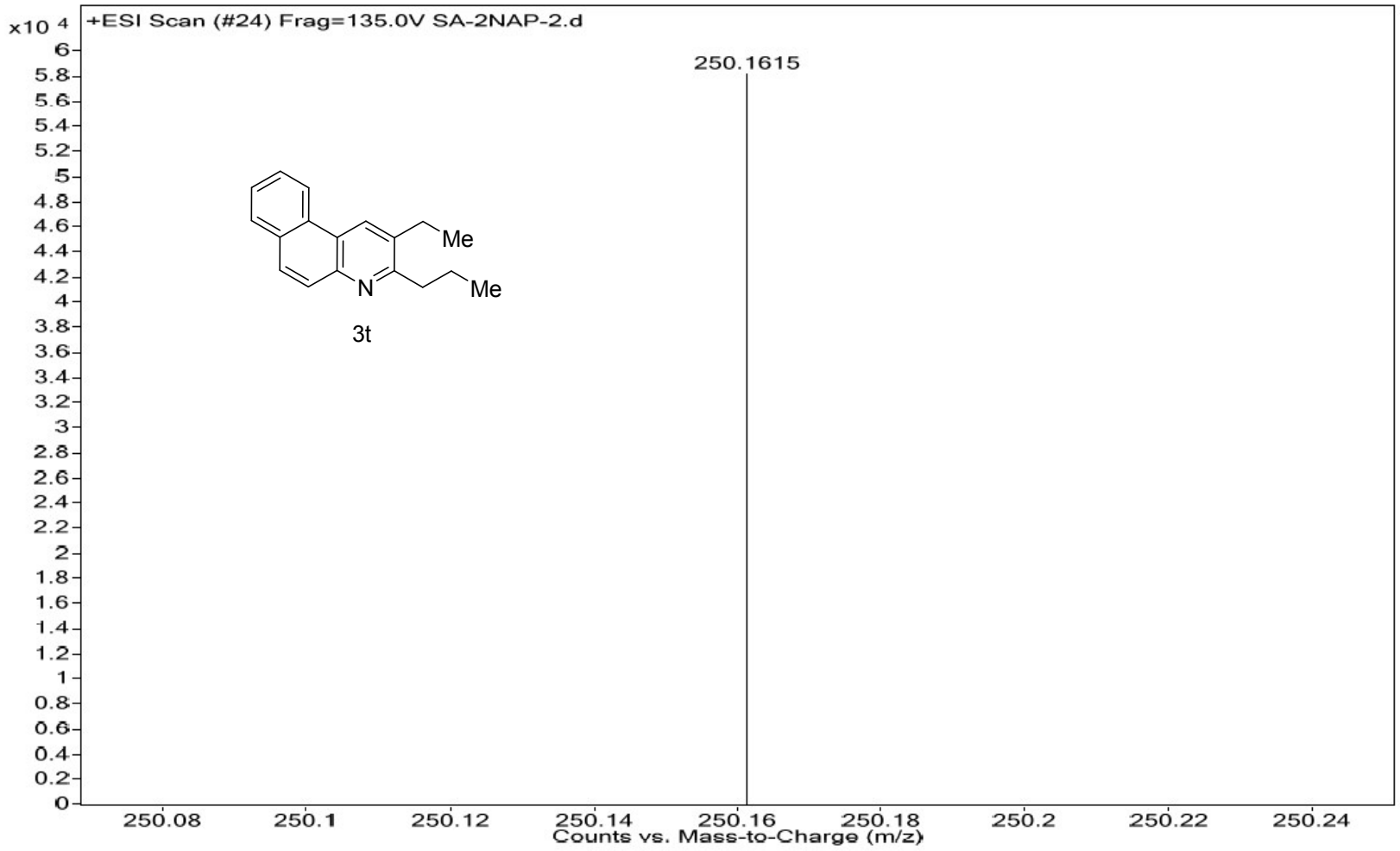


^{13}C NMR spectra of compound: 3t

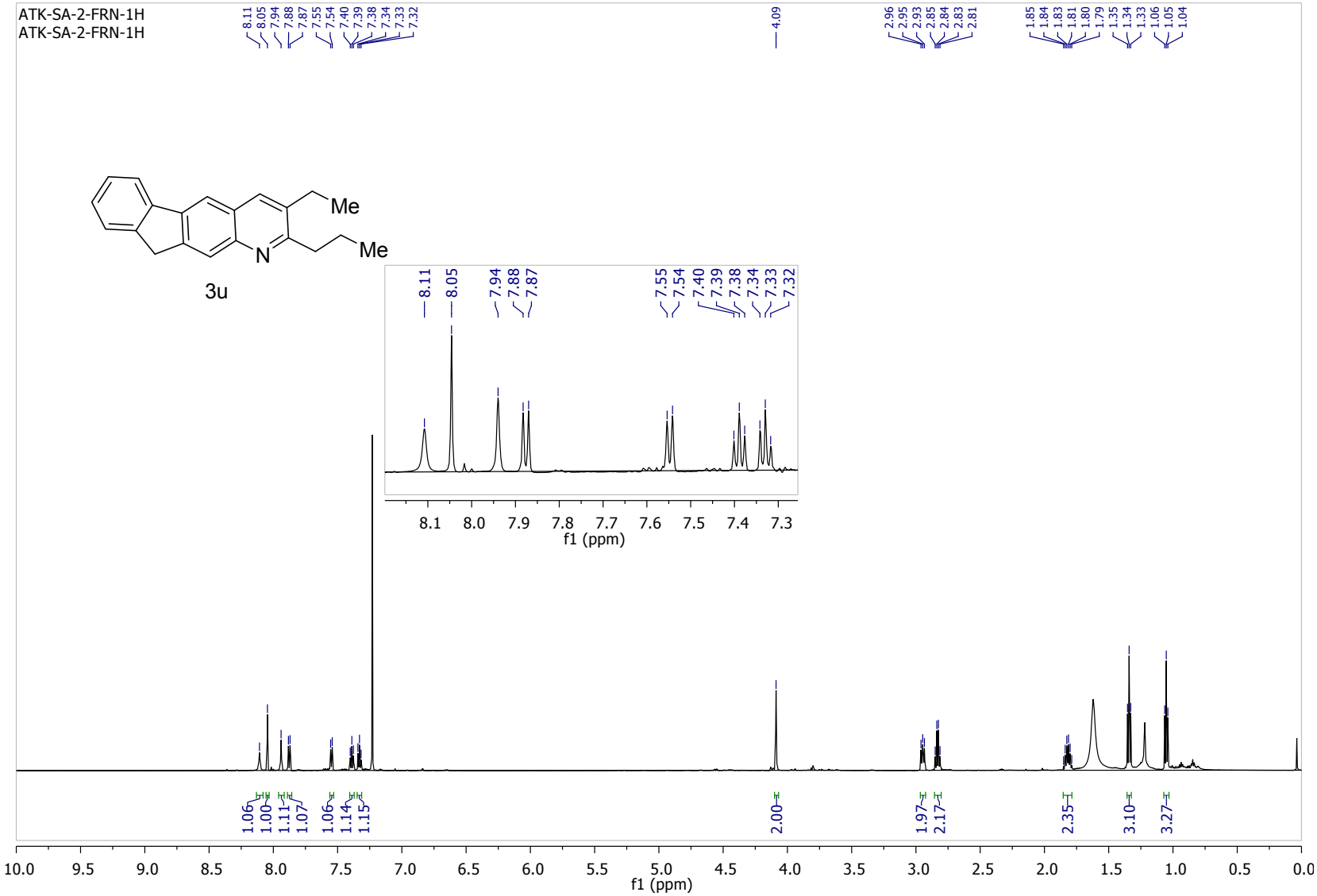


HRMS spectra of compound: 3t

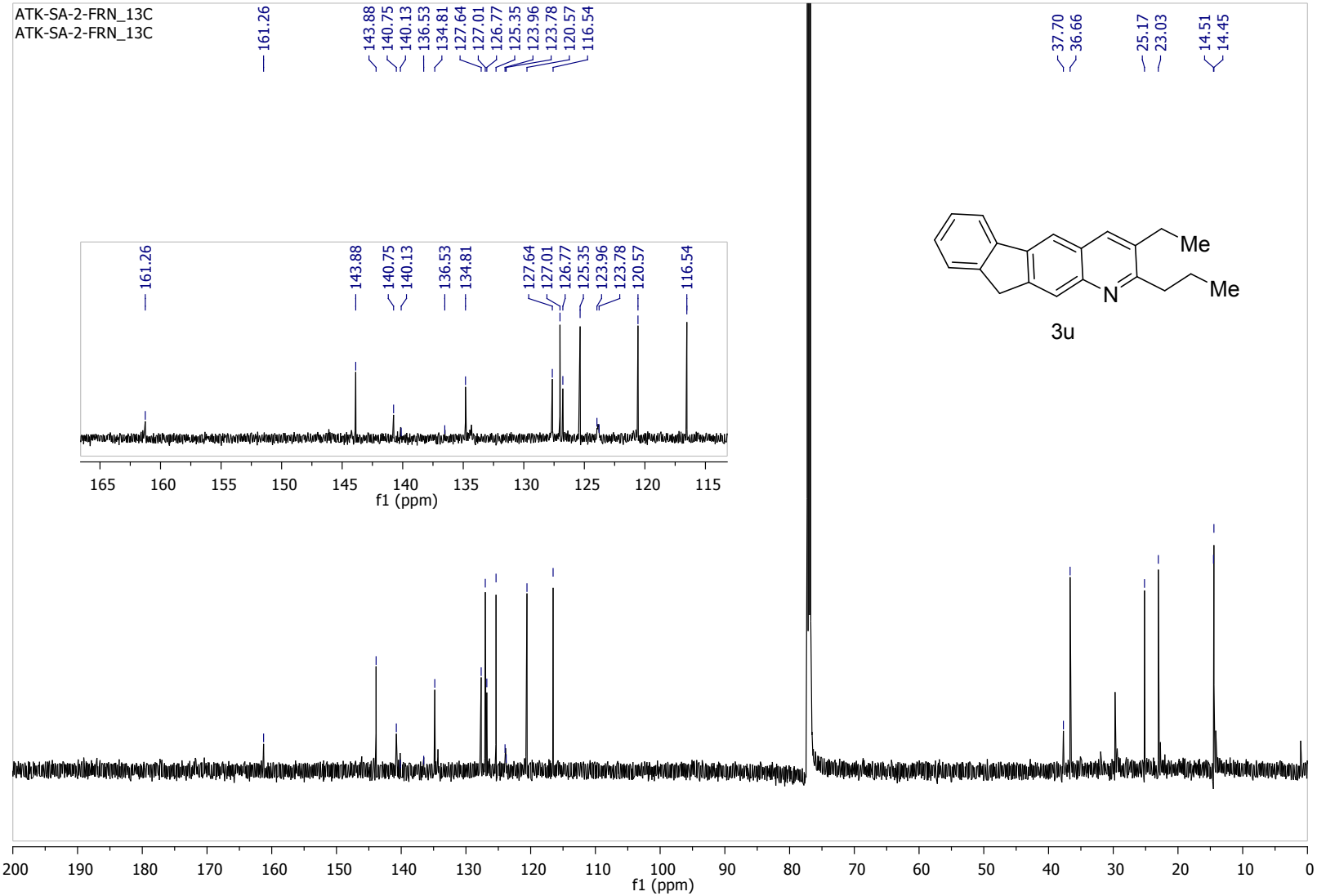
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



^{1}H NMR spectra of compound: 3u

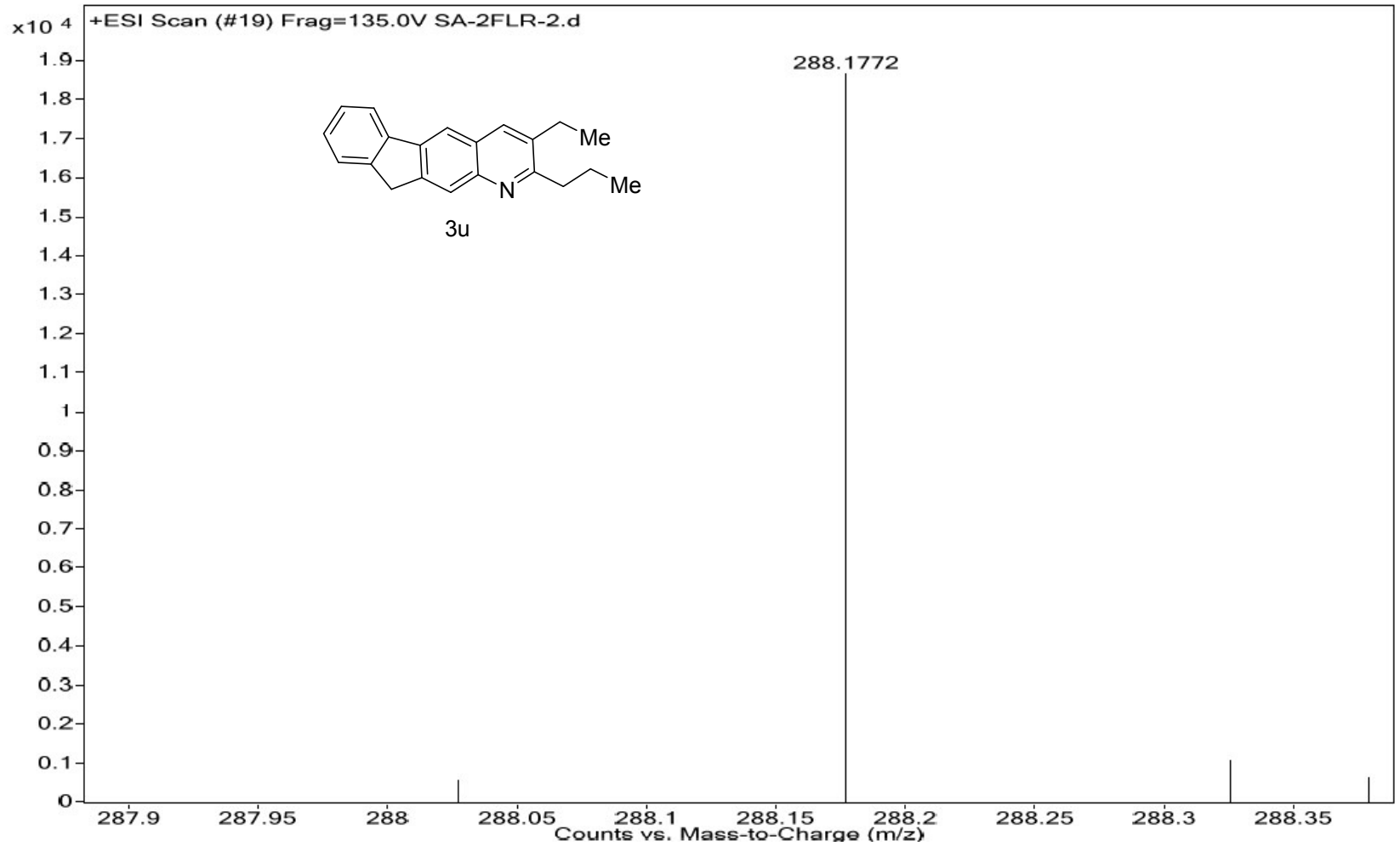


^{13}C NMR spectra of compound: 3u

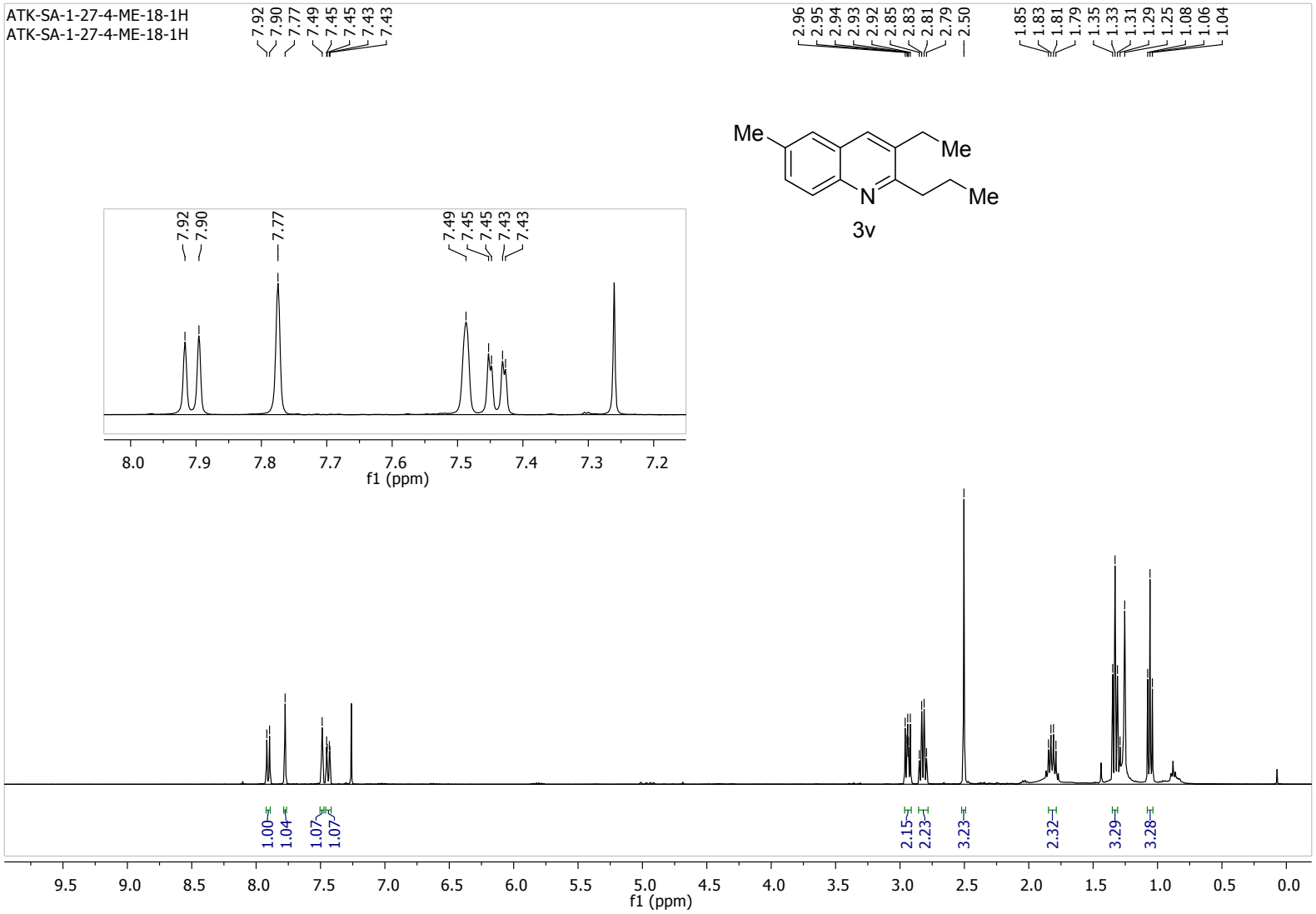


HRMS spectra of compound: 3u

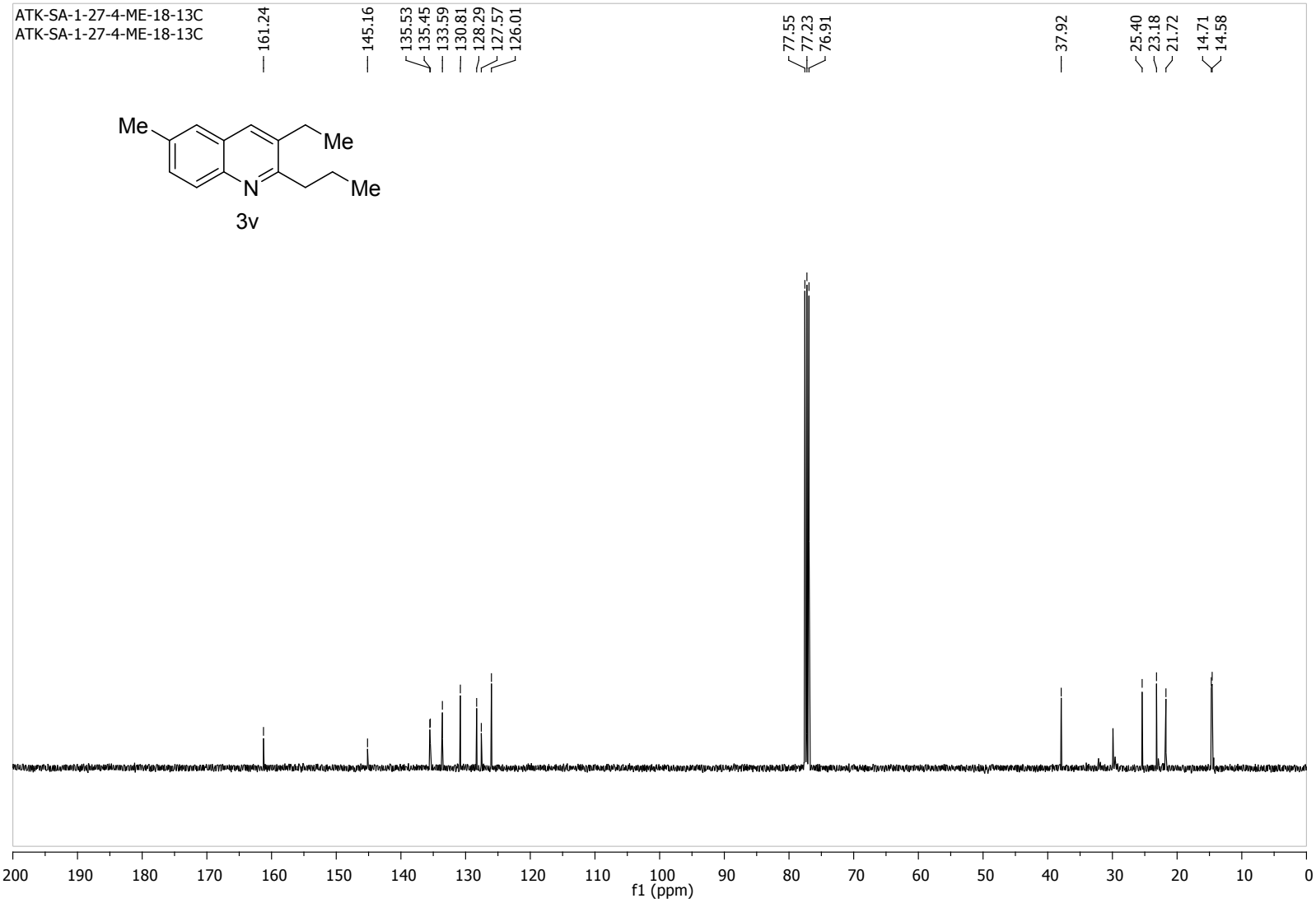
Sample Name	SA-2FLR-2	**Position**	Vial 1	**Instrument Name**	QTOF	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	SA-2FLR-2.d	**ACQ Method**		**Comment**		**Acquired Time**	6/6/2018 4:03:22 PM



^{1}H NMR spectra of compound: 3v

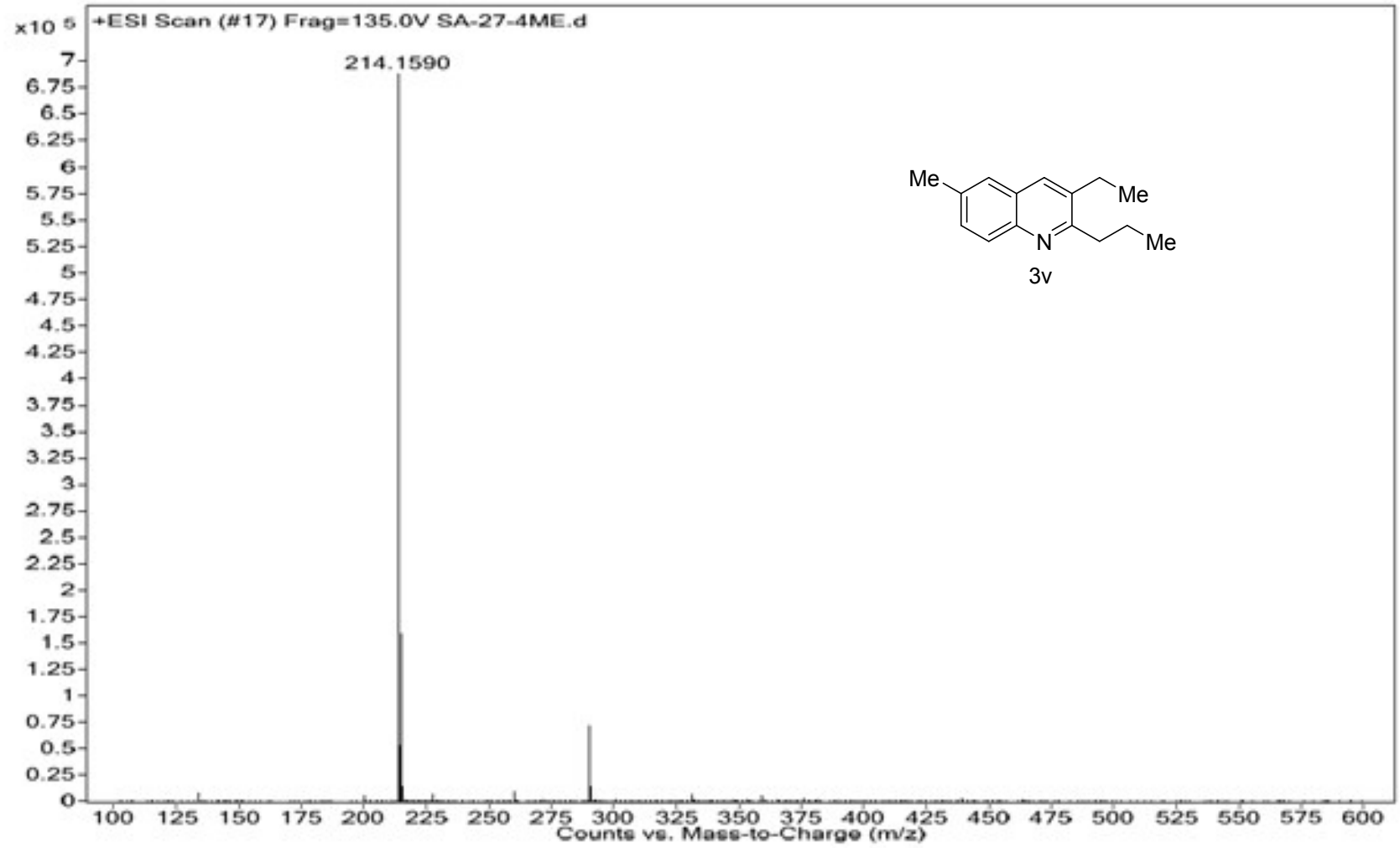


^{13}C NMR spectra of compound: 3v

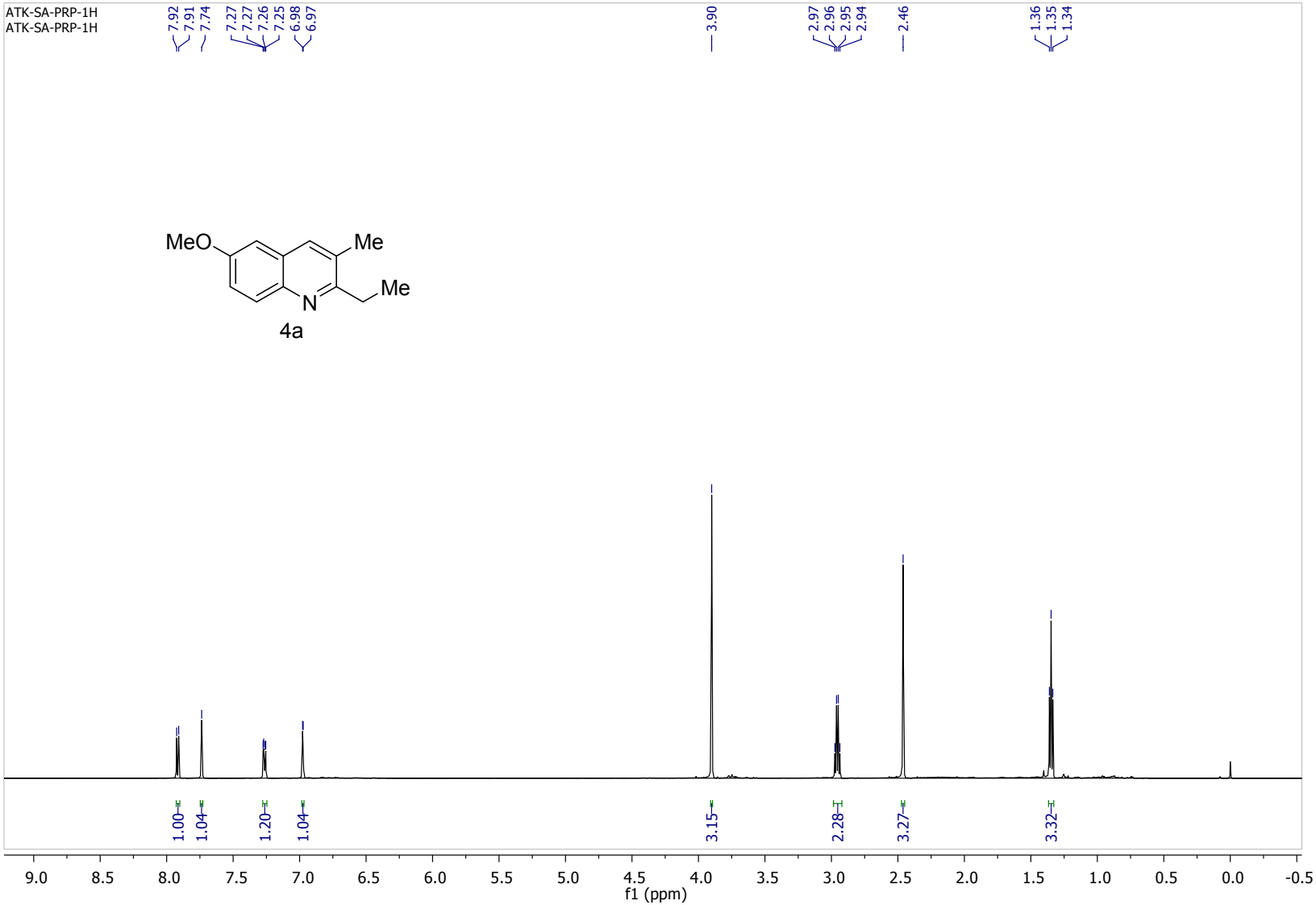


HRMS spectra of compound: 3v

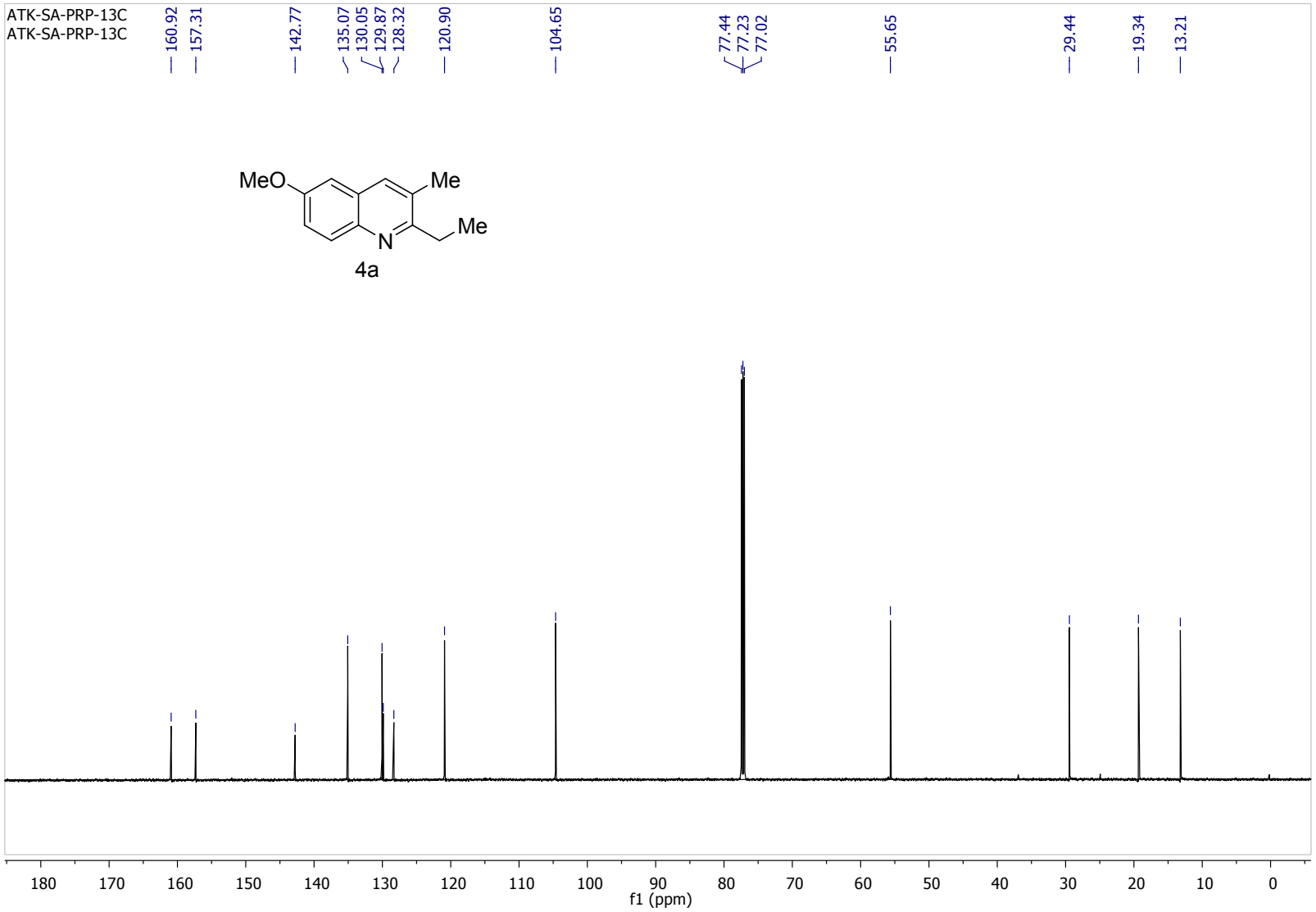
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



^{1}H NMR spectra of compound: 4a

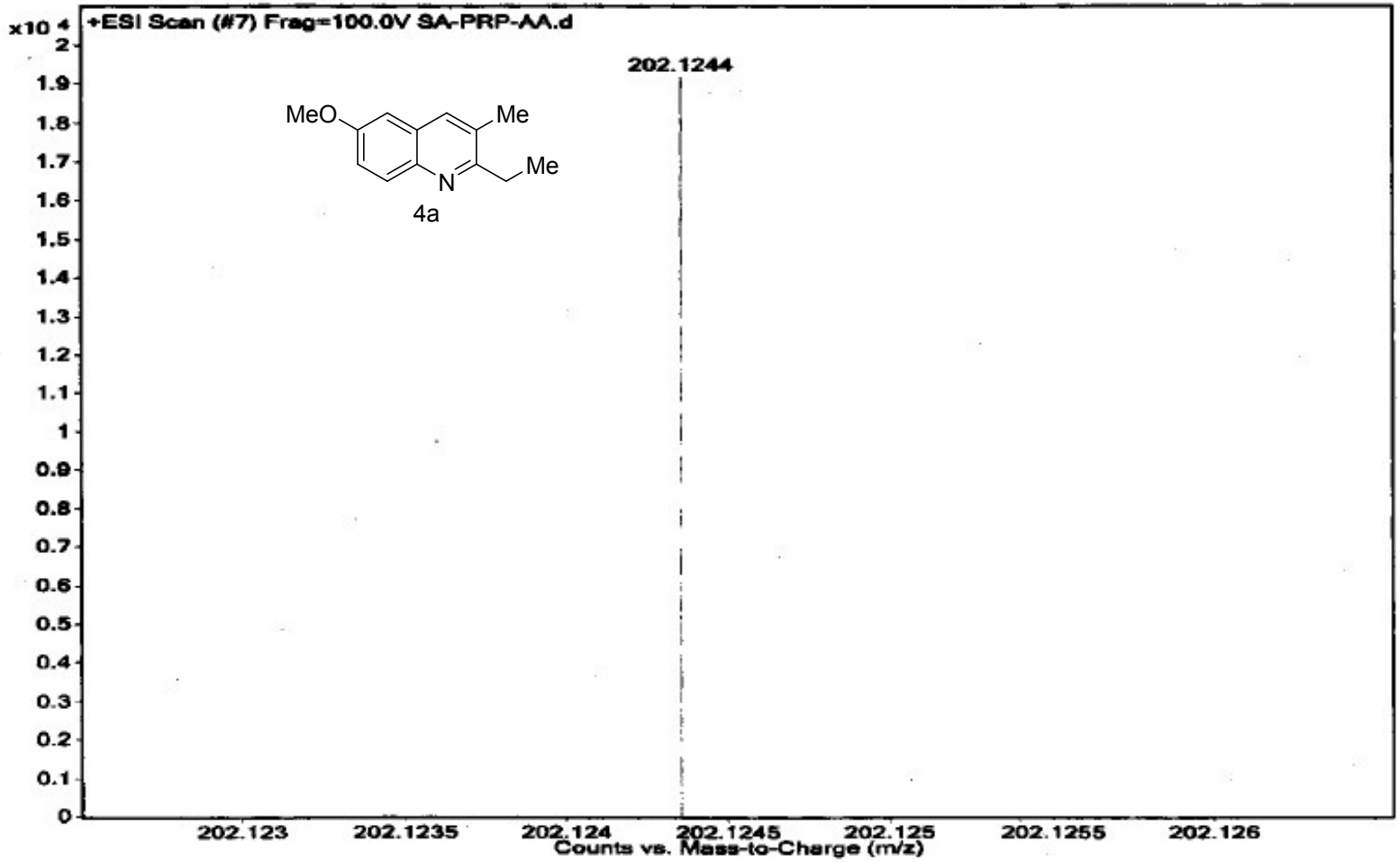


^{13}C NMR spectra of compound: 4a

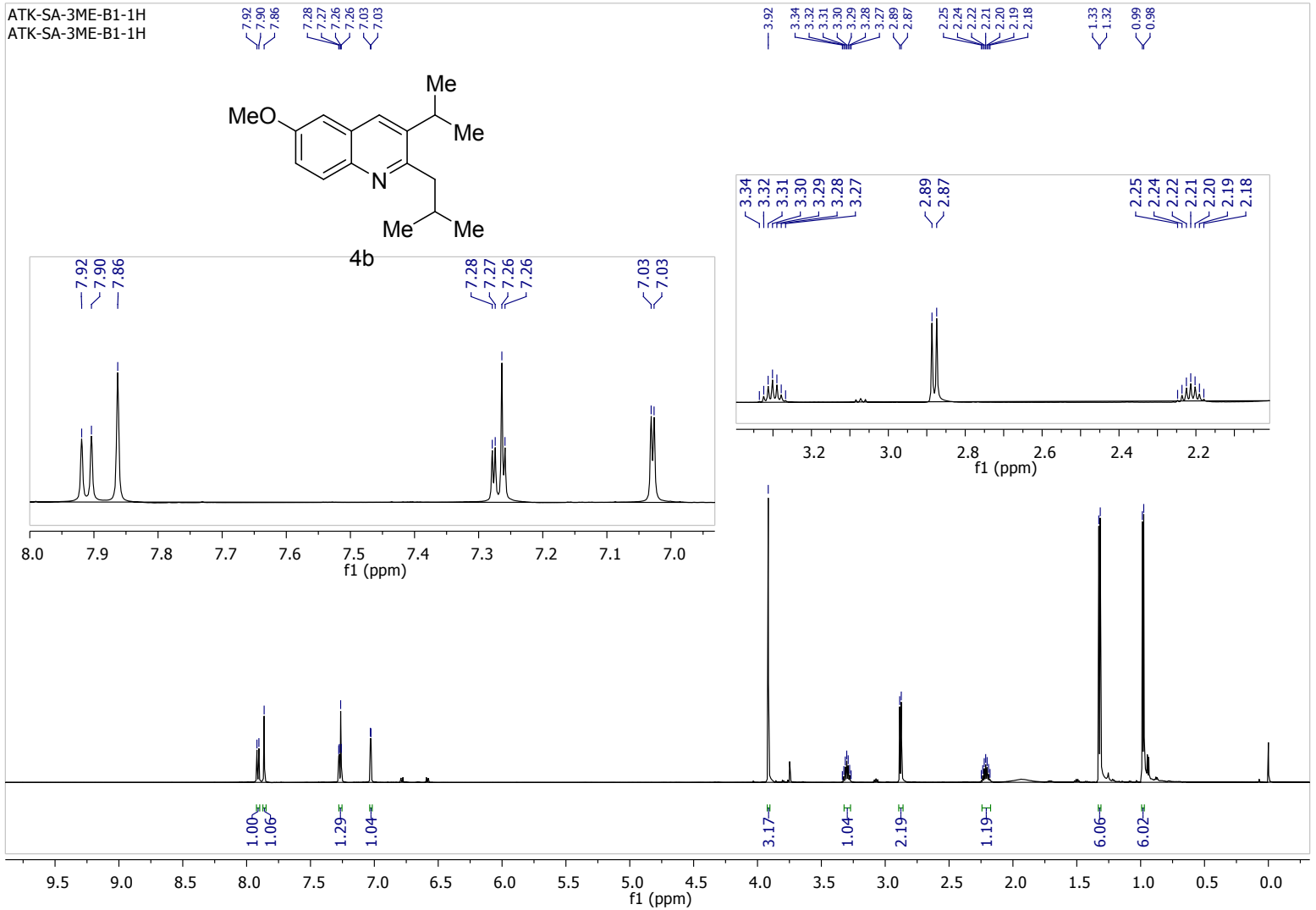


HRMS spectra of compound: 4a

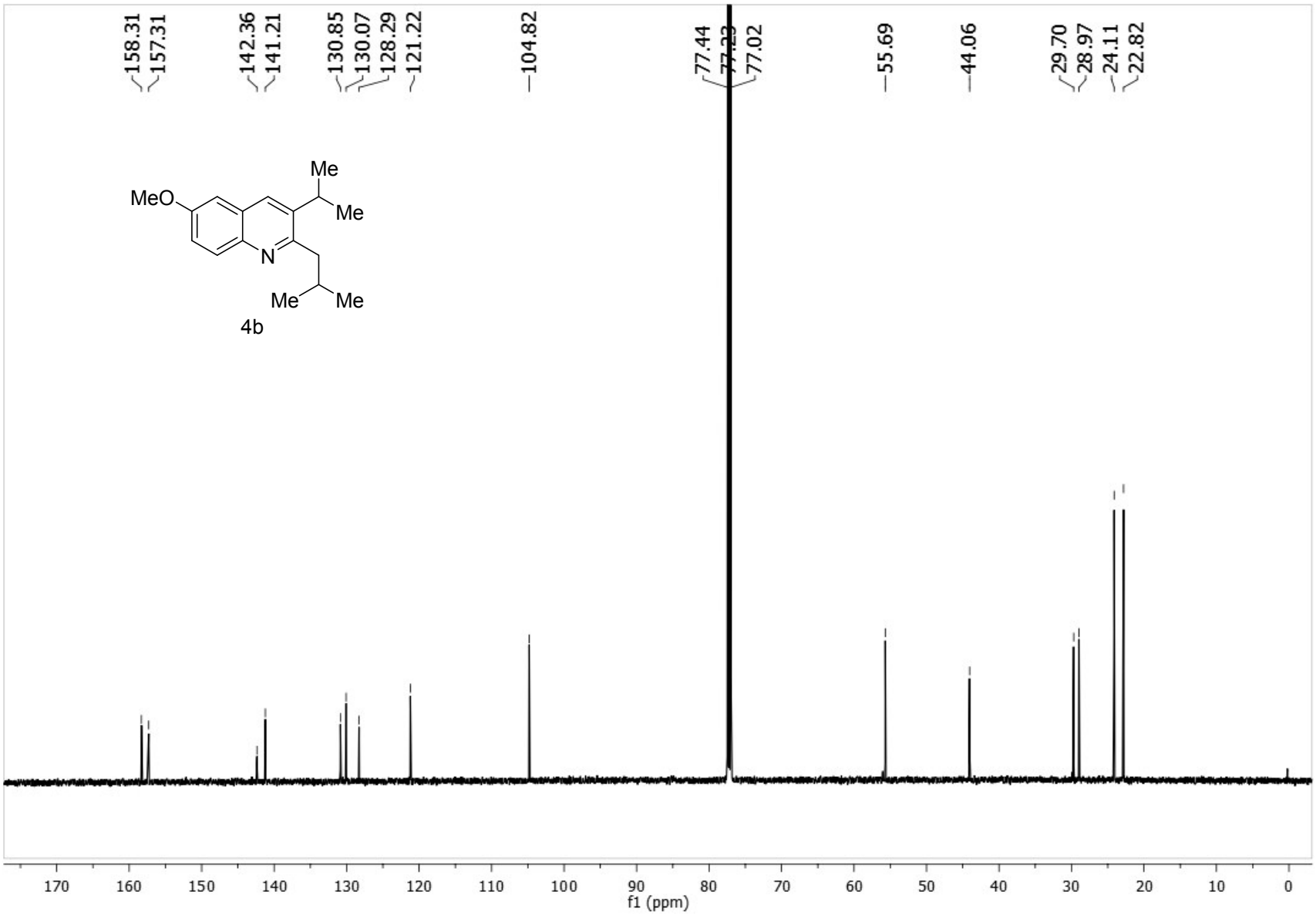
Sample Name	SA-PRP-AA	Position	Vial 1	Instrument Name	QTOF	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SA-PRP-AA.d	ACQ Method		Comment		Acquired Time	7/31/2018 11:16:18 AM



^{1}H NMR spectra of compound: 4b

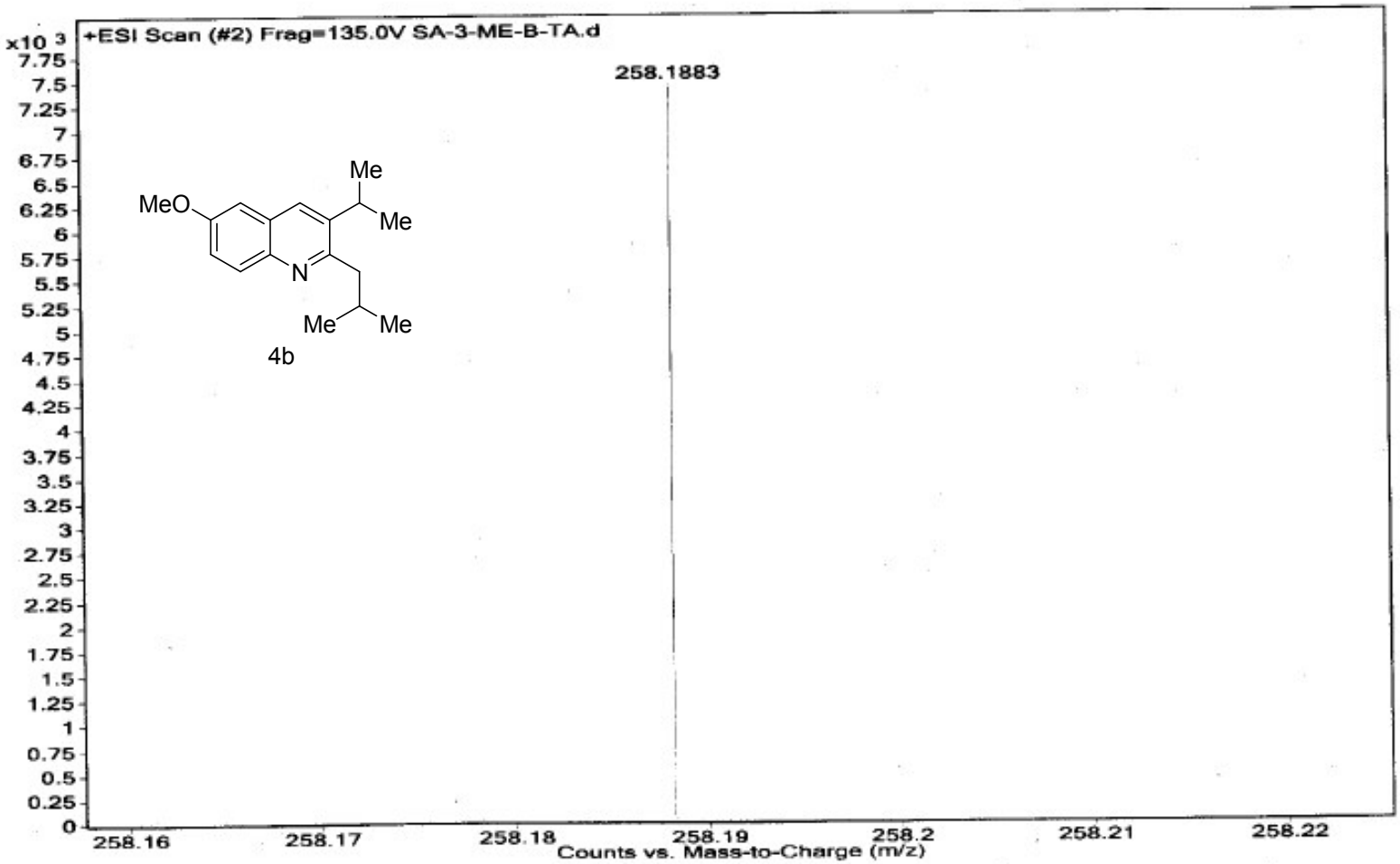


^{13}C NMR spectra of compound: 4b

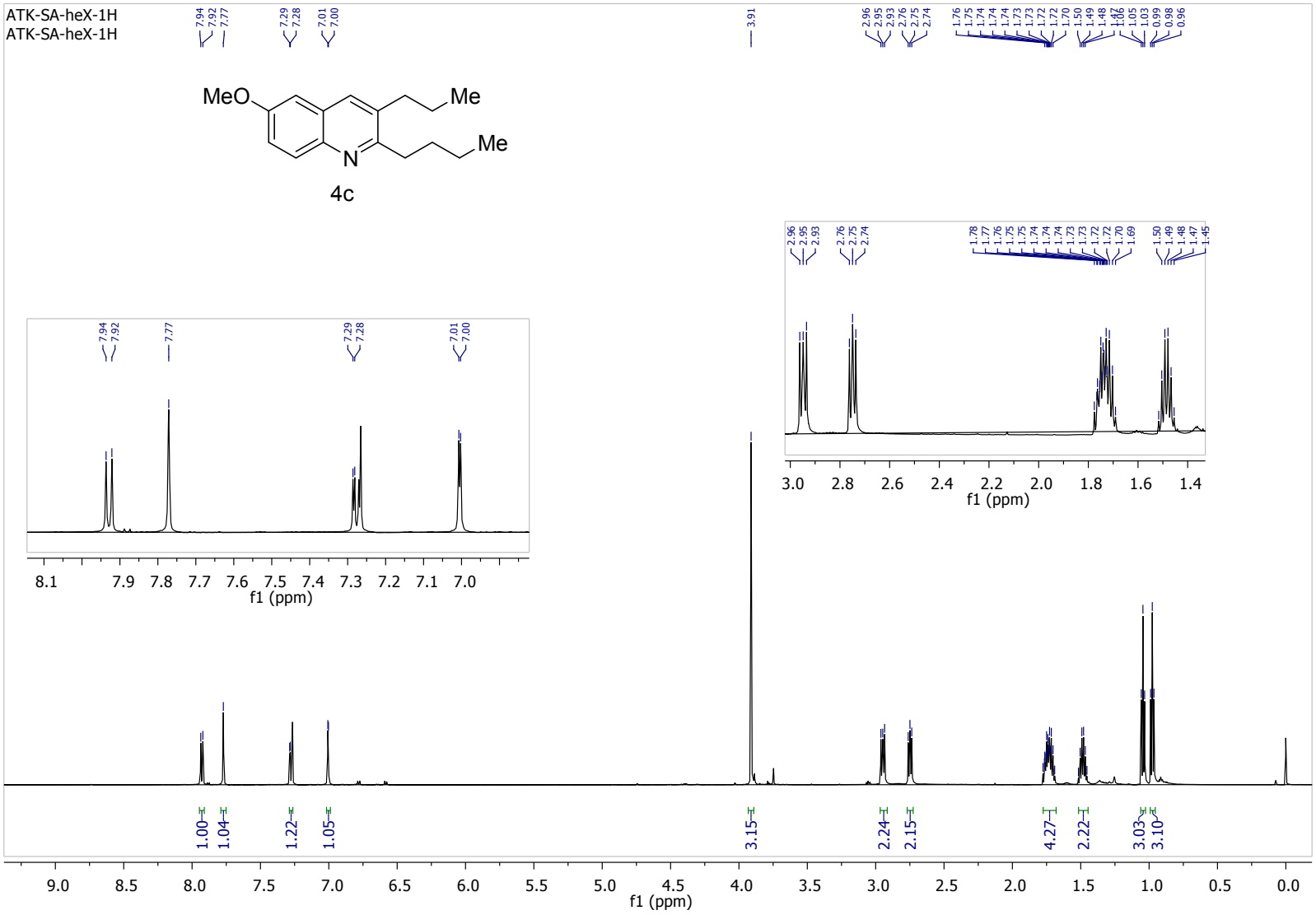


HRMS spectra of compound: 4b

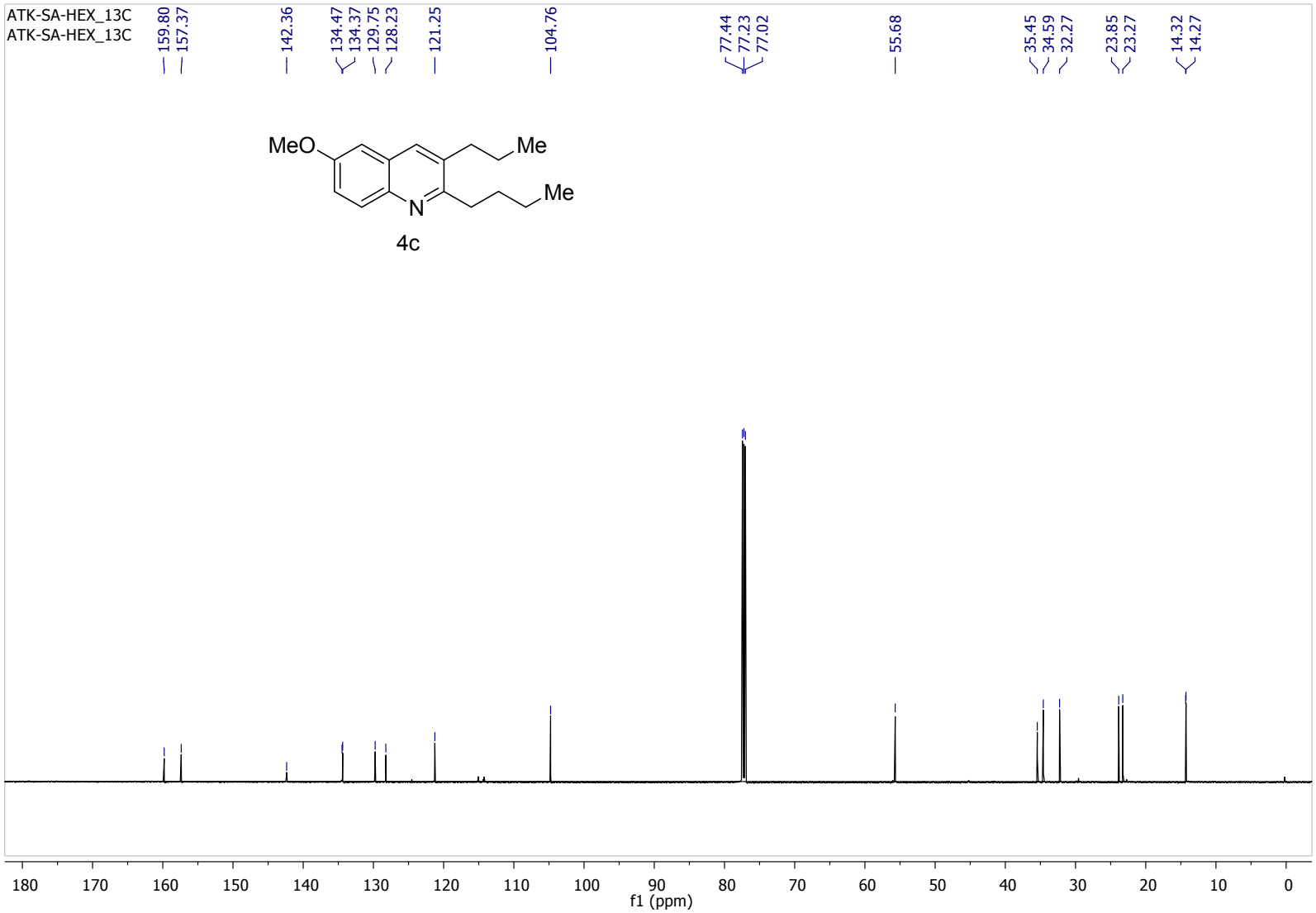
Sample Name	SA-3-ME-B-TA	**Position**	Vial 1	**Instrument Name**	QTOF	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	SA-3-ME-B-TA.d	**ACQ Method**		**Comment**		**Acquired Time**	7/27/2018 12:22:35 PM



^{1}H NMR spectra of compound: 4c

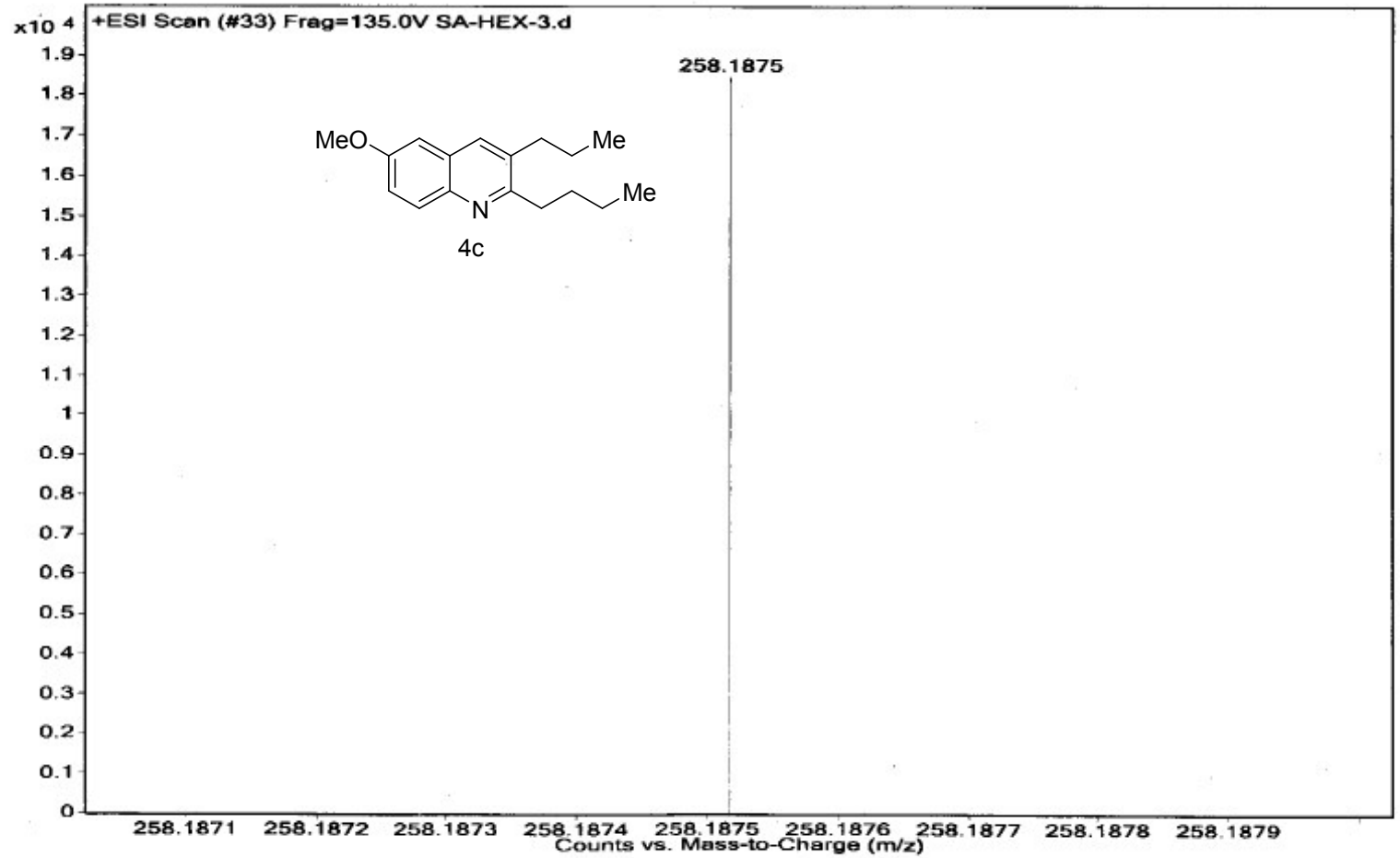


^{13}C NMR spectra of compound: 4c

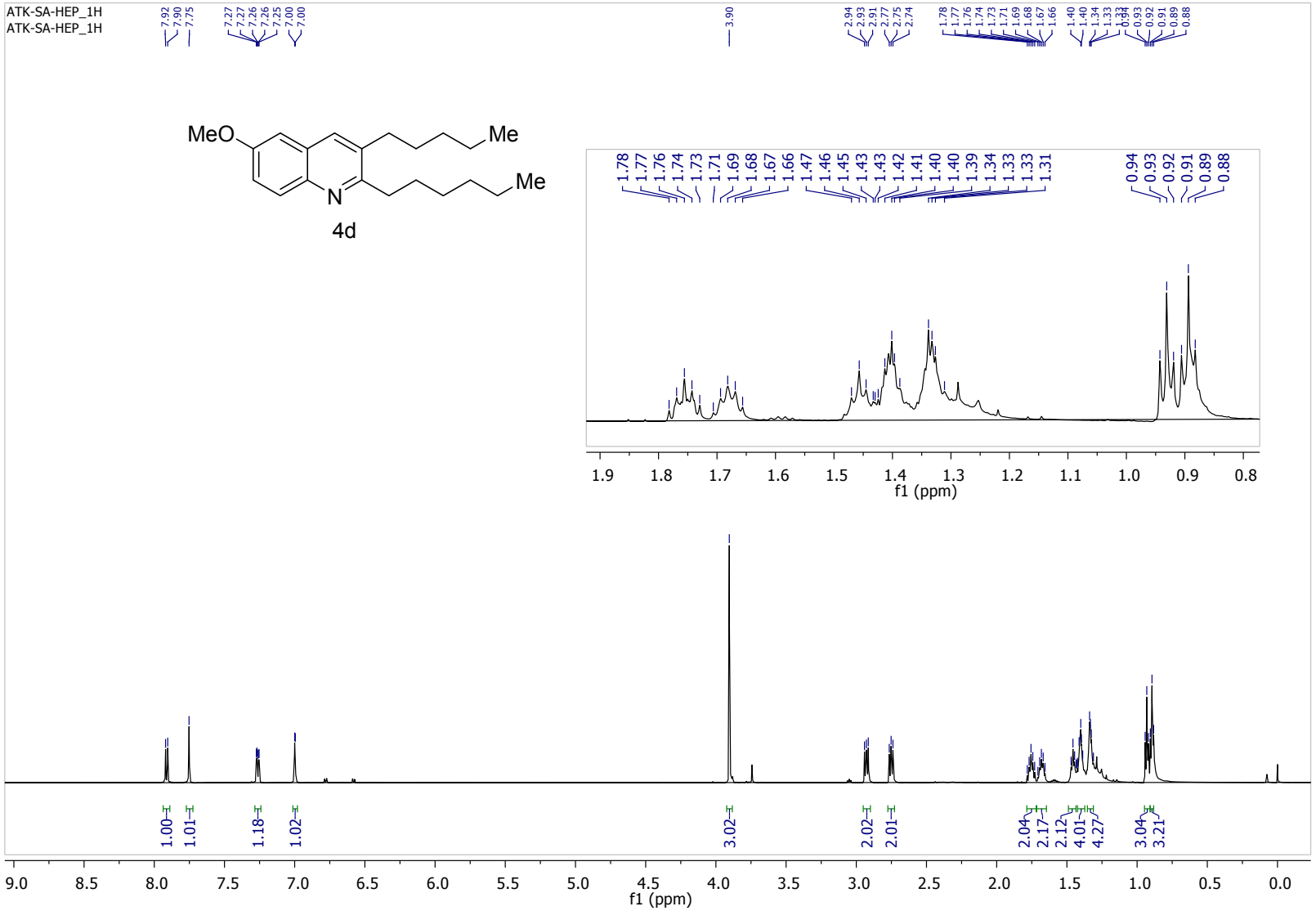


HRMS spectra of compound: 4c

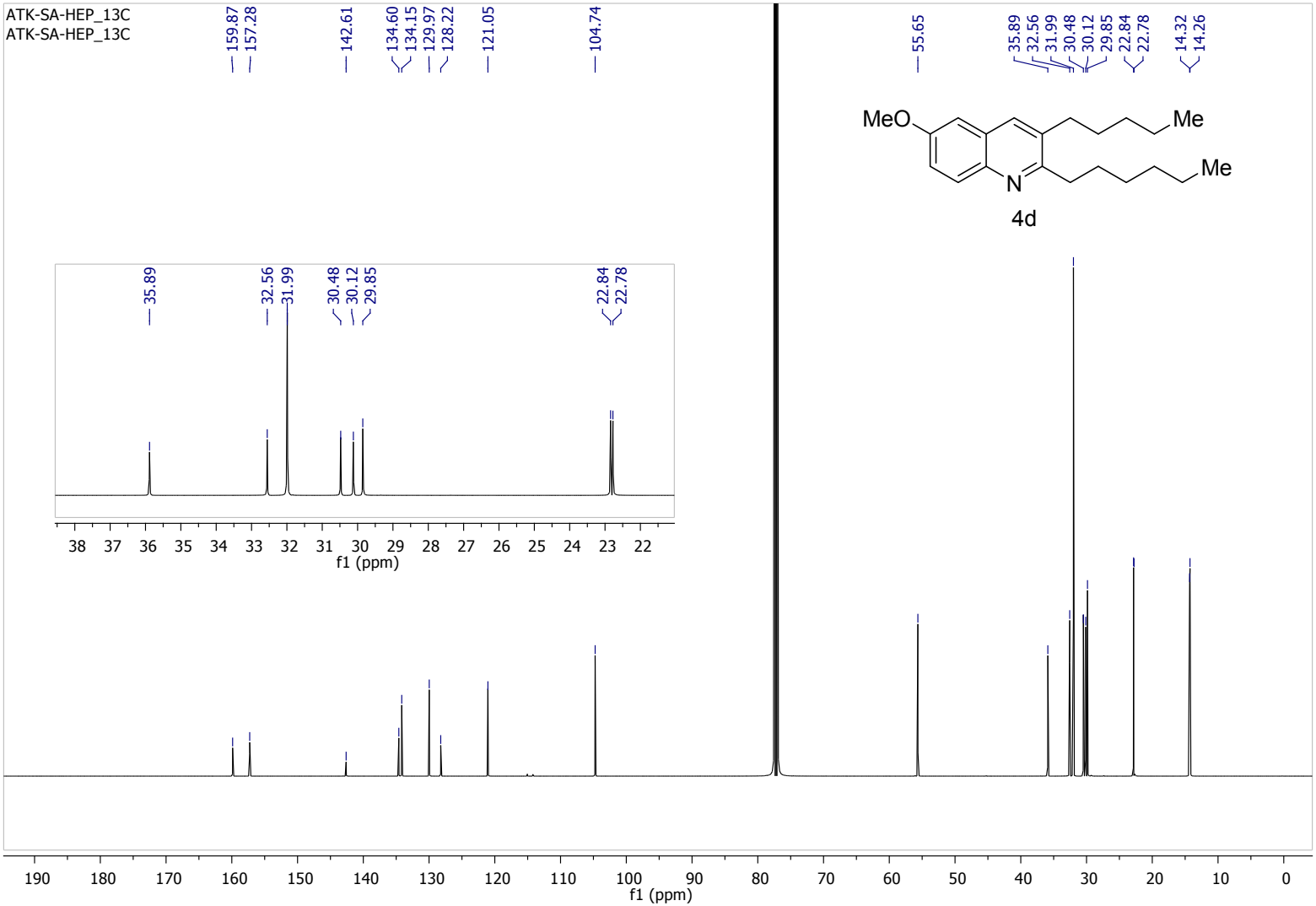
Sample Name	SA-HEX-3	**Position**	Vial 1	**Instrument Name**	QTOF	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	SA-HEX-3.d	**ACQ Method**		**Comment**		**Acquired Time**	7/27/2018 12:17:48 PM



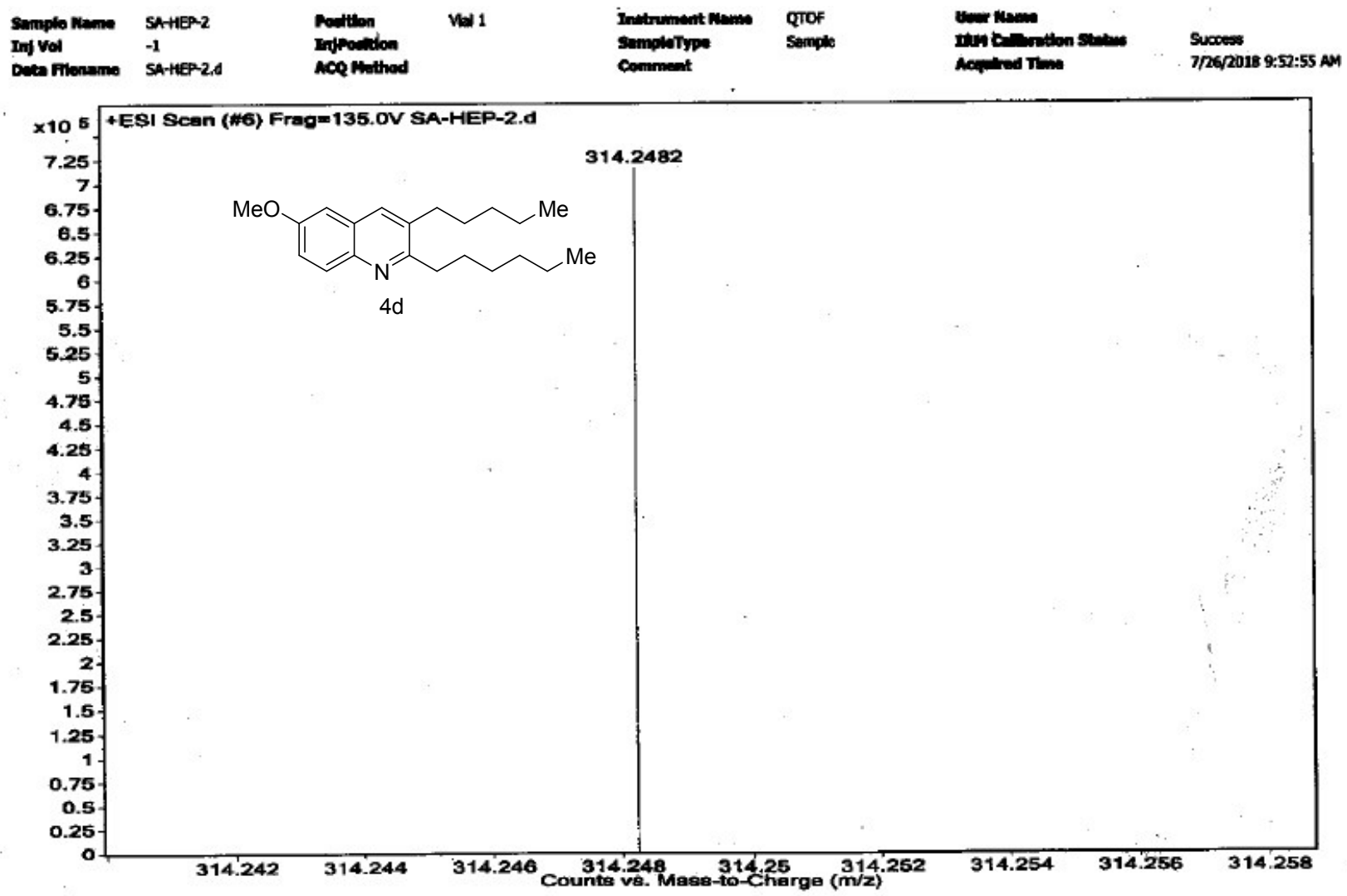
^{1}H NMR spectra of compound: 4d



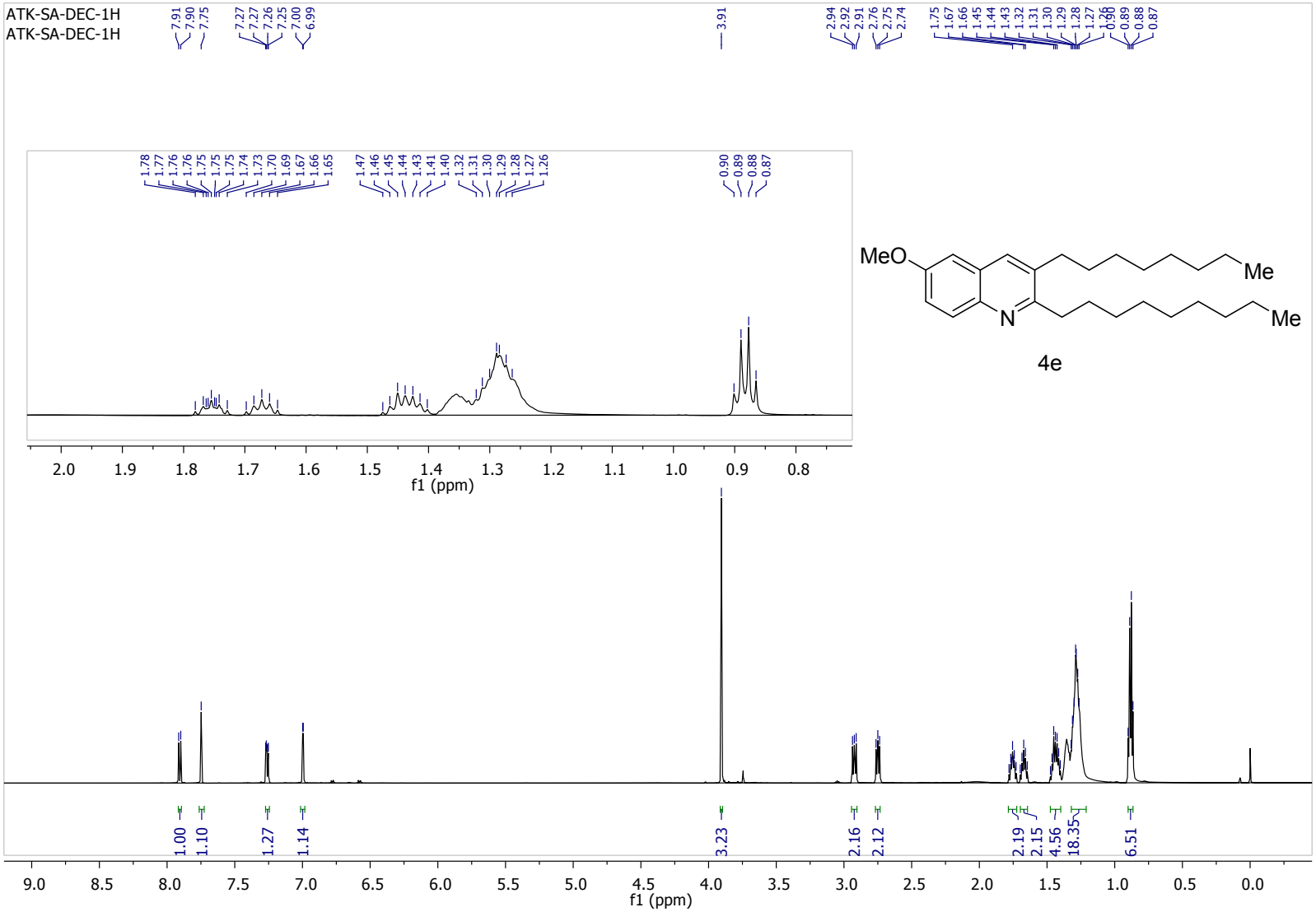
^{13}C NMR spectra of compound: 4d



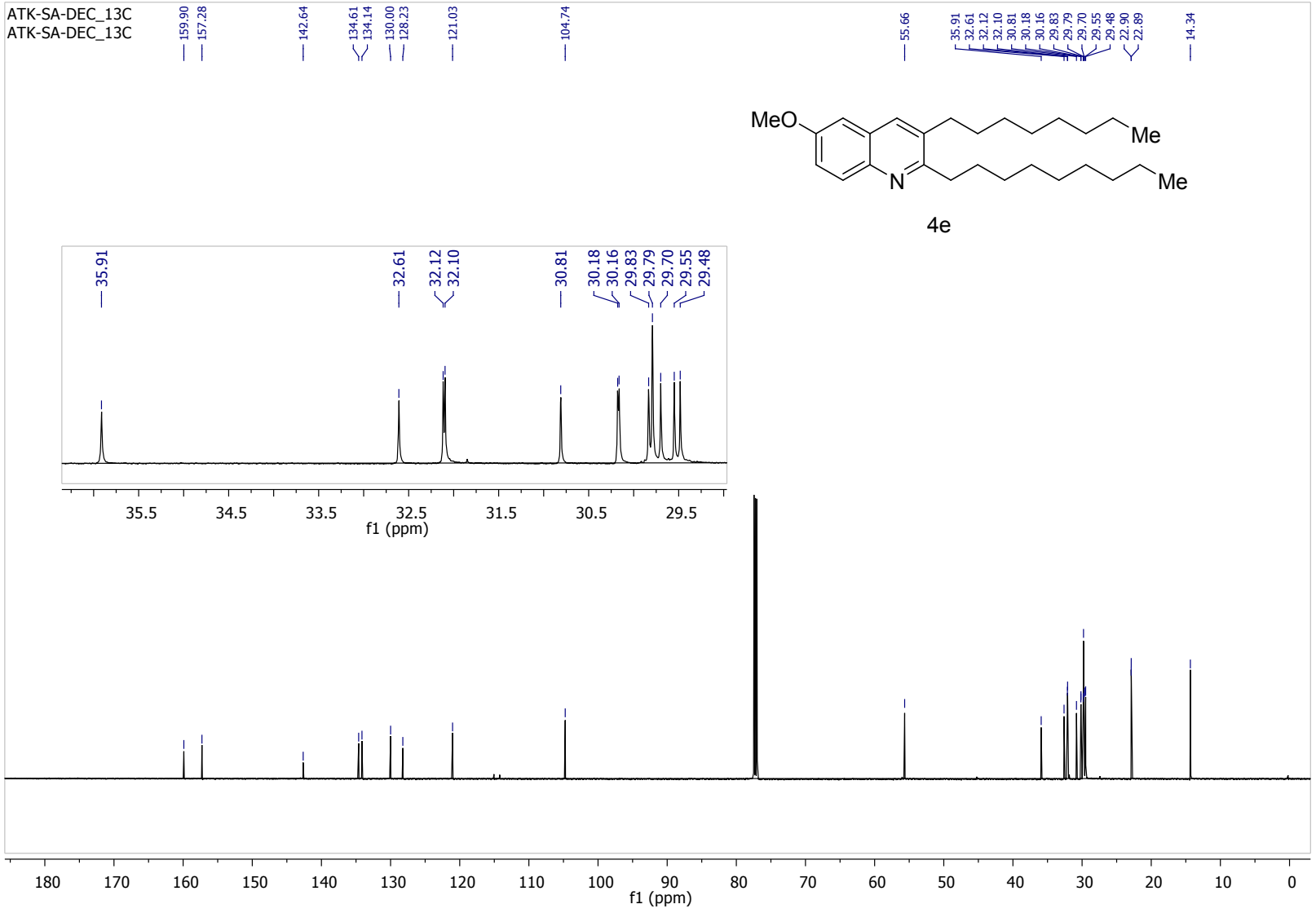
HRMS spectra of compound: 4d



^{1}H NMR spectra of compound: 4e

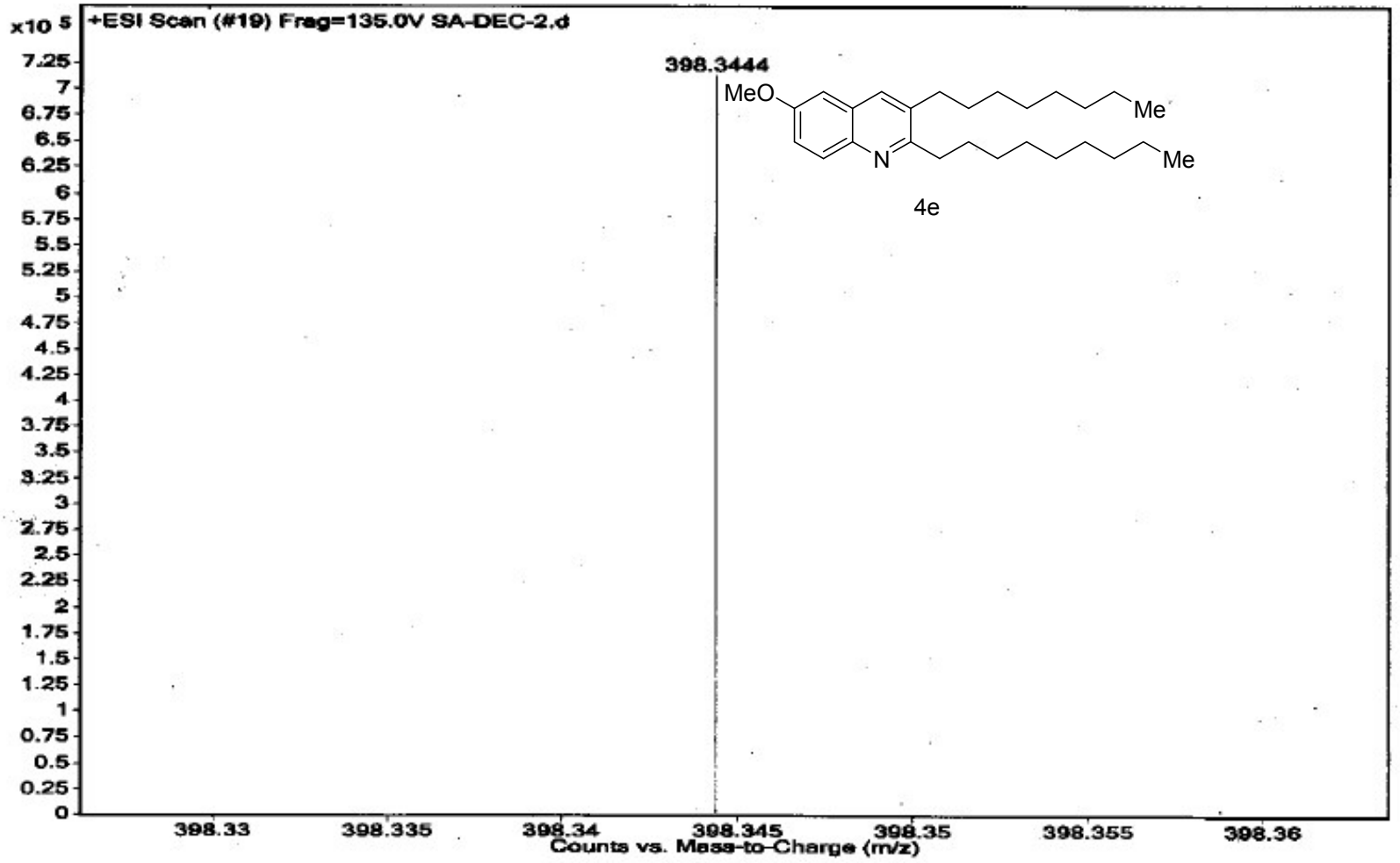


^{13}C NMR spectra of compound: 4e

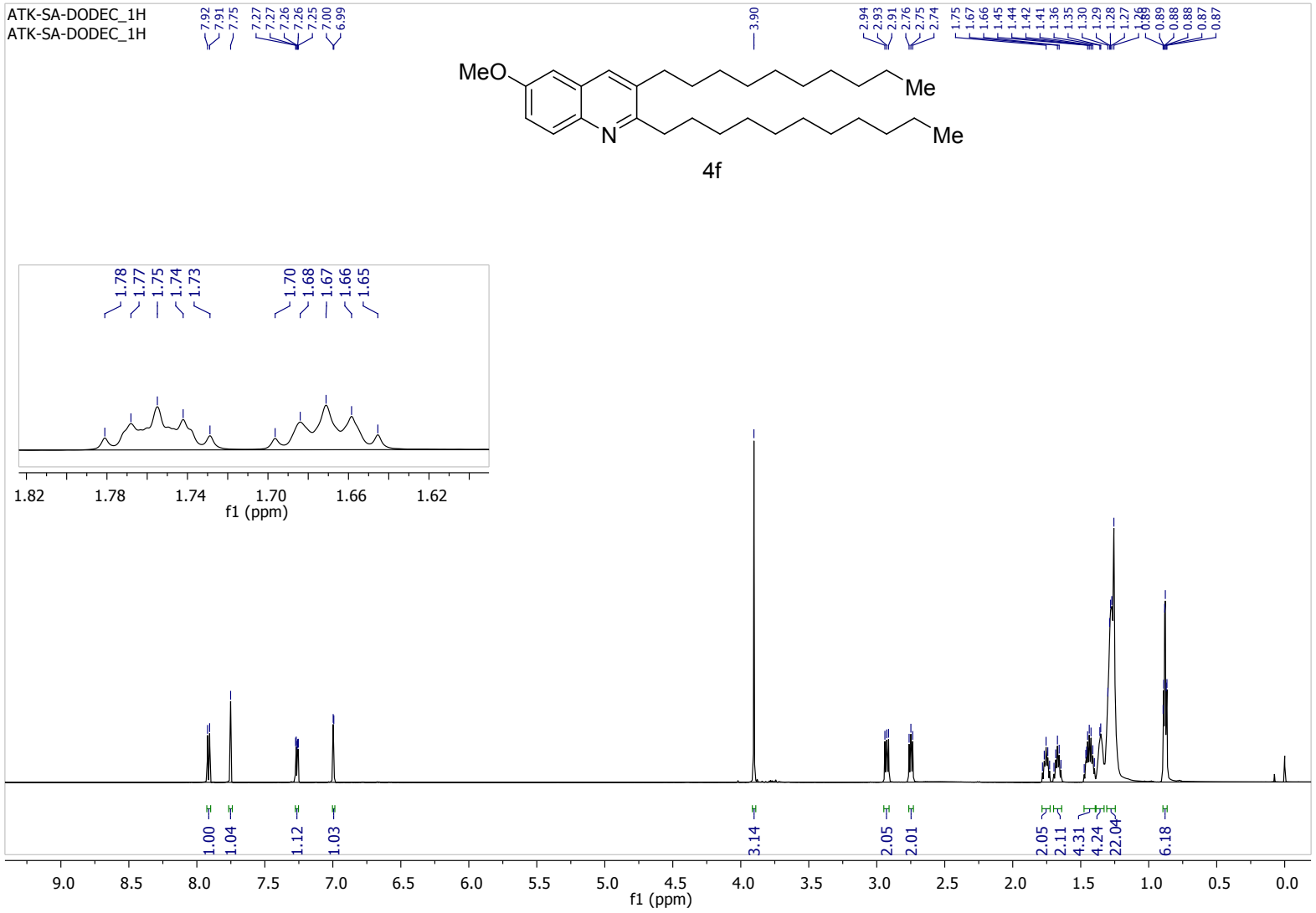


HRMS spectra of compound: 4e

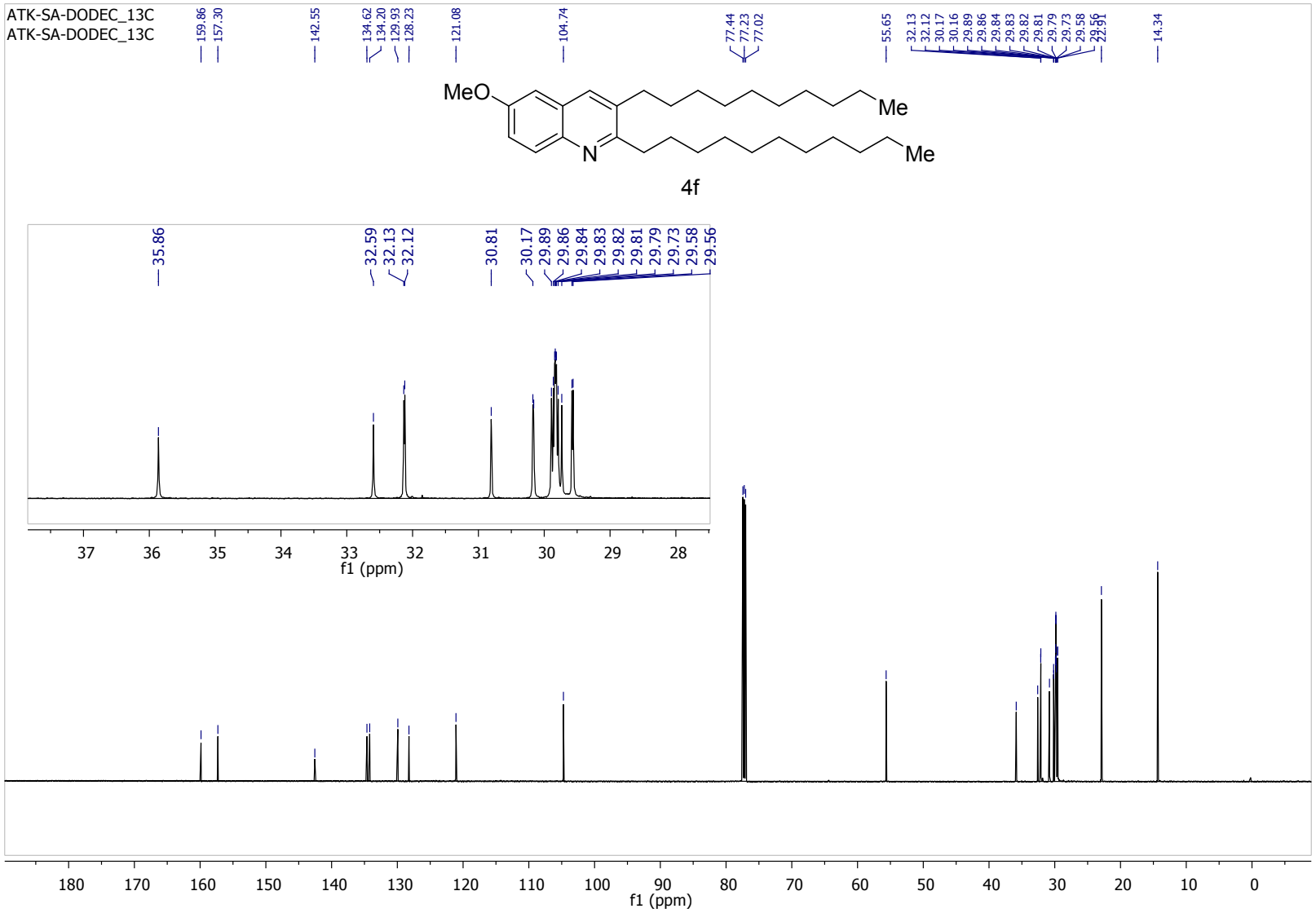
Sample Name	SA-DEC-2	Position	Vial 1	Instrument Name	QTOF	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SA-DEC-2.d	ACQ Method		Comment		Acquired Time	7/26/2018 9:43:11 AM



^{1}H NMR spectra of compound: 4f

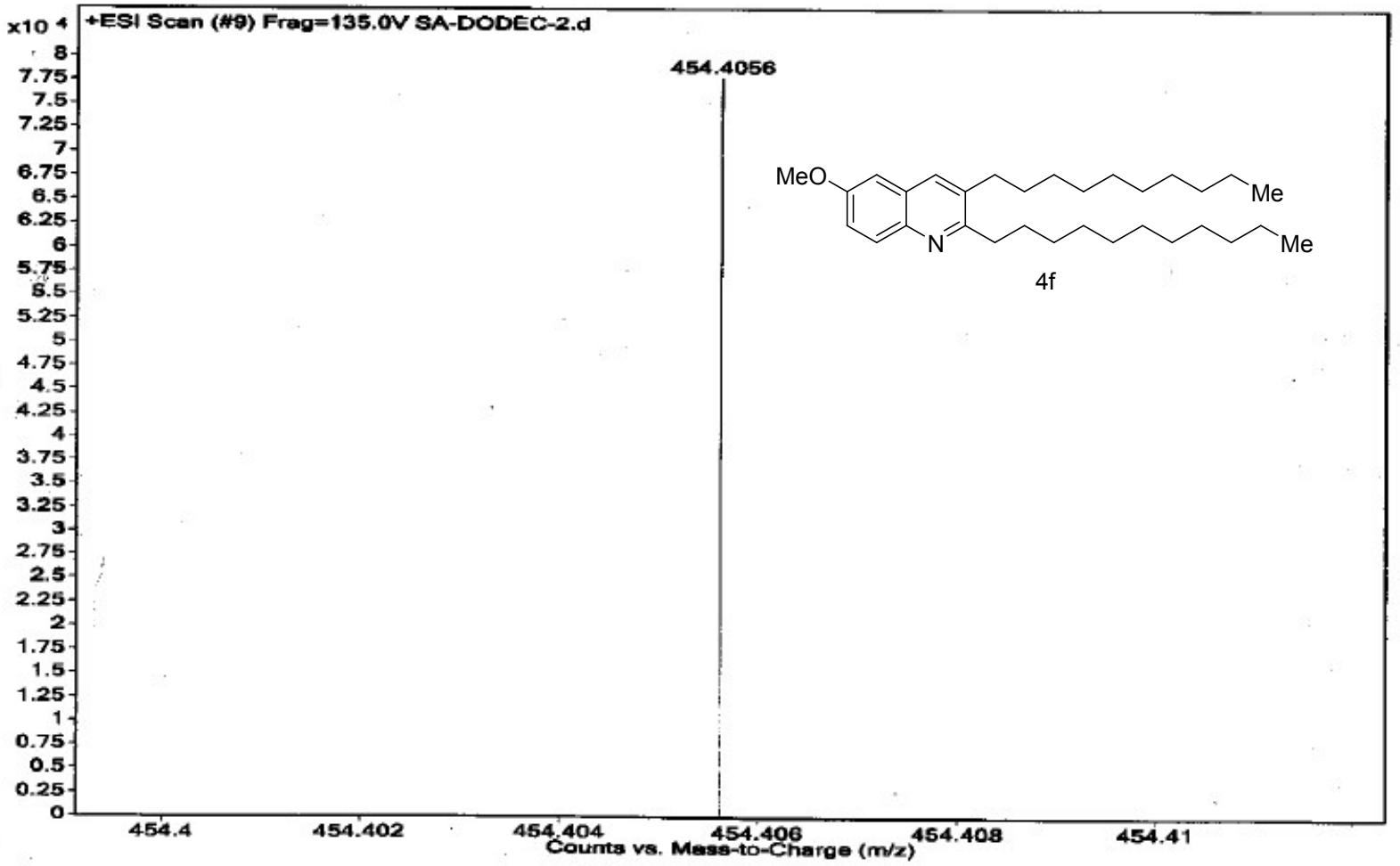


^{13}C NMR spectra of compound: 4f

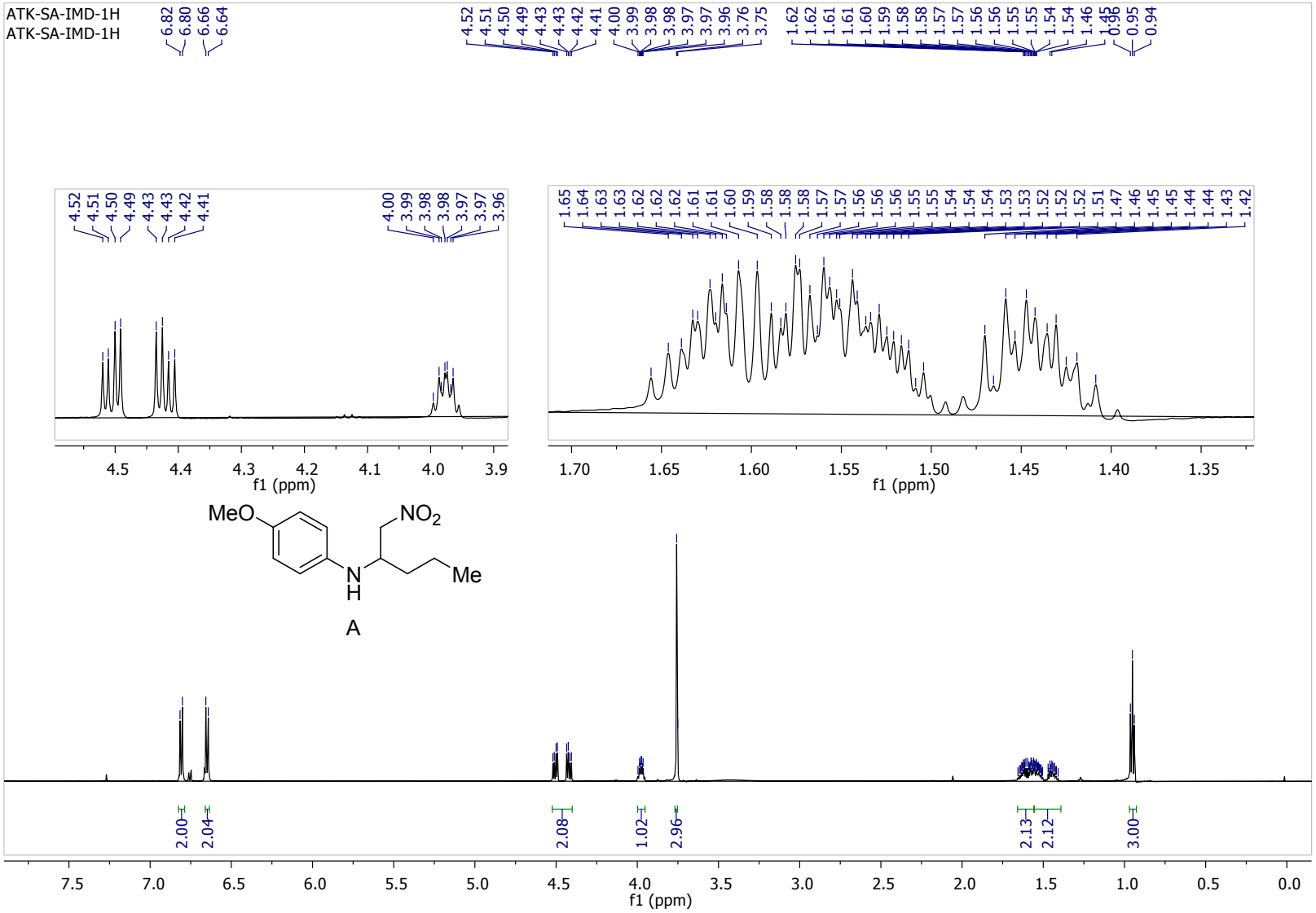


HRMS spectra of compound: 4f

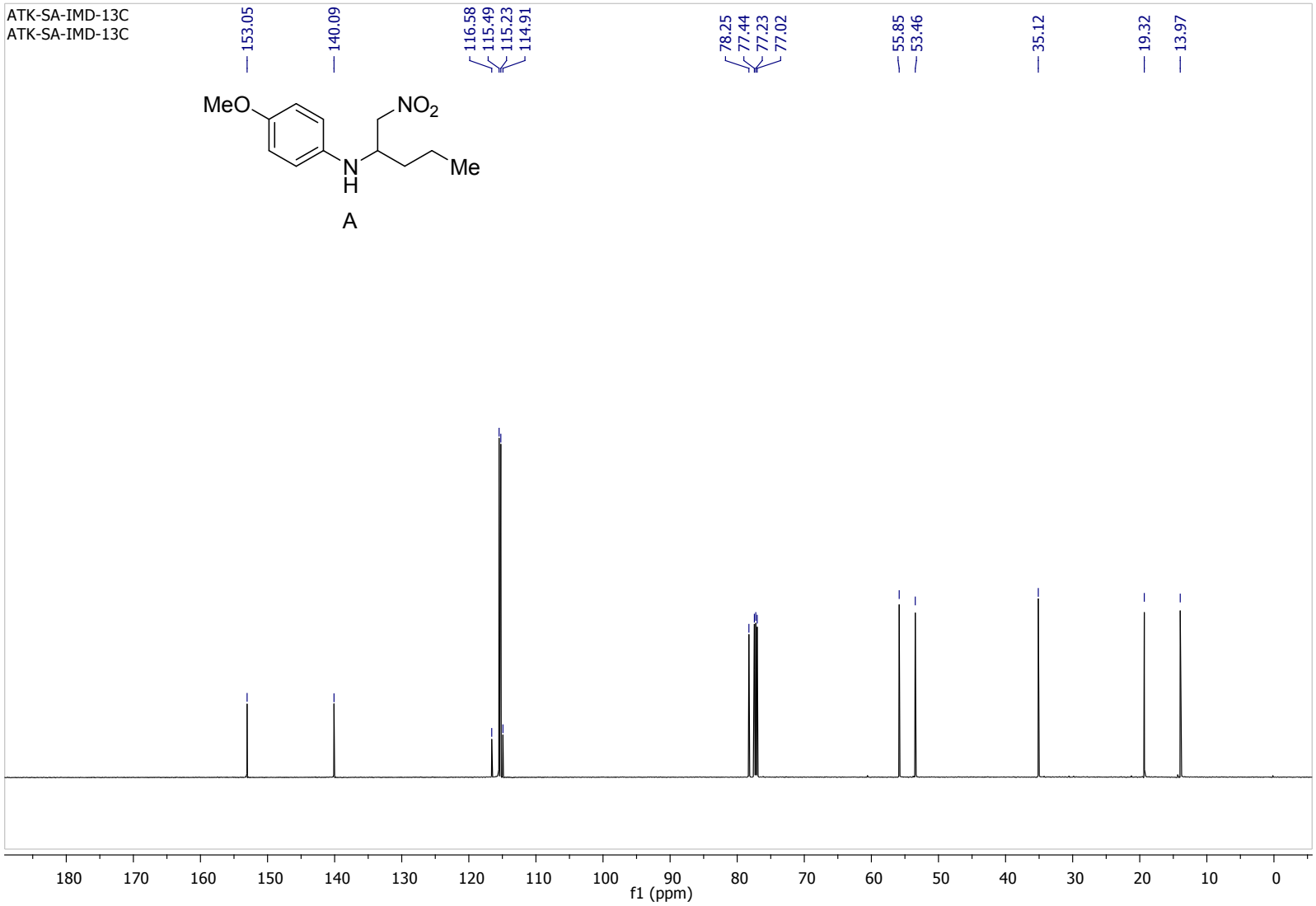
Sample Name	SA-DODEC-2	Position	Vial 1	Instrument Name	QTOF	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SA-DODEC-2.d	ACQ Method		Comment		Acquired Time	7/26/2018 9:40:00 AM



^{1}H NMR spectra of compound: A

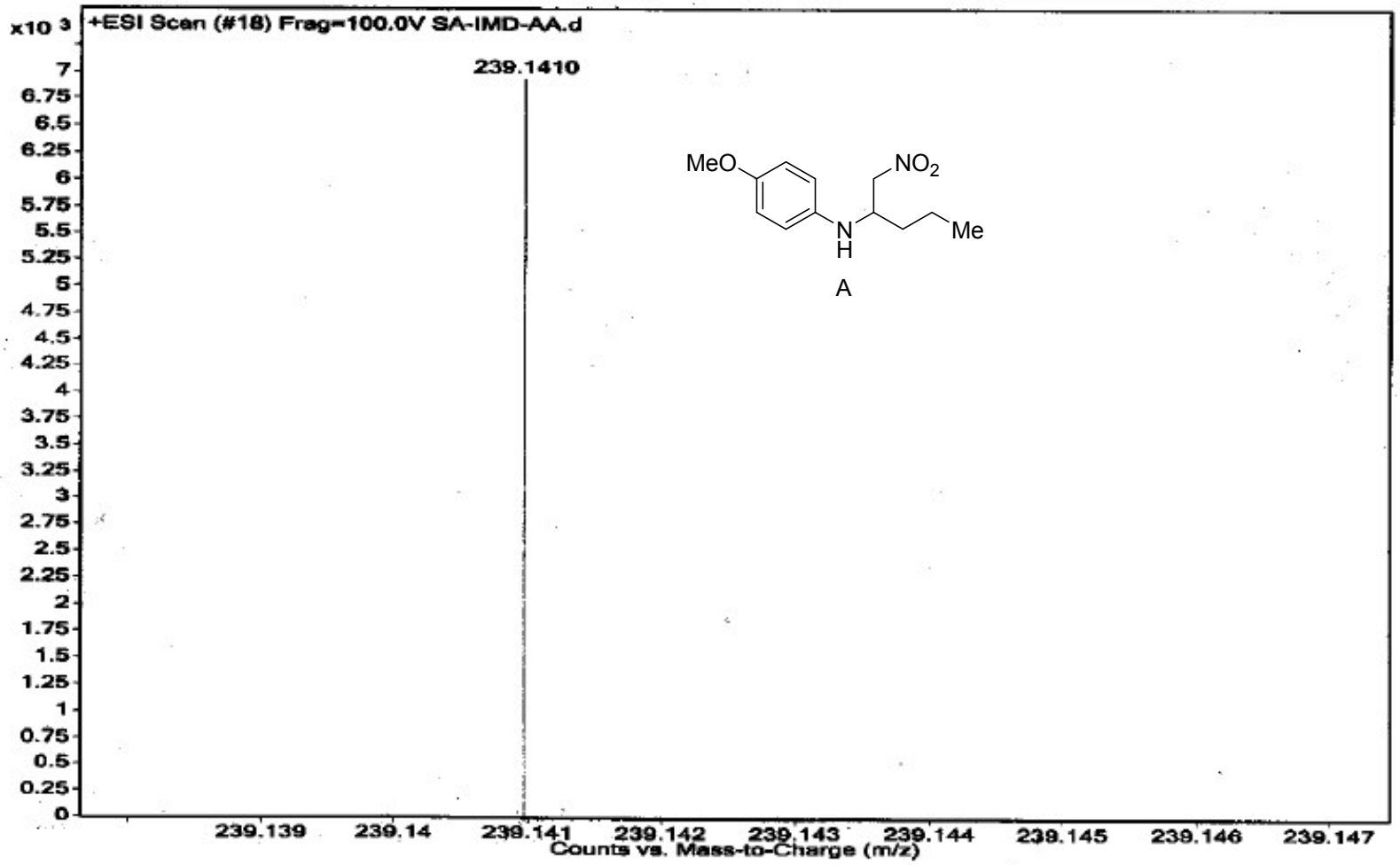


^{13}C NMR spectra of compound: A

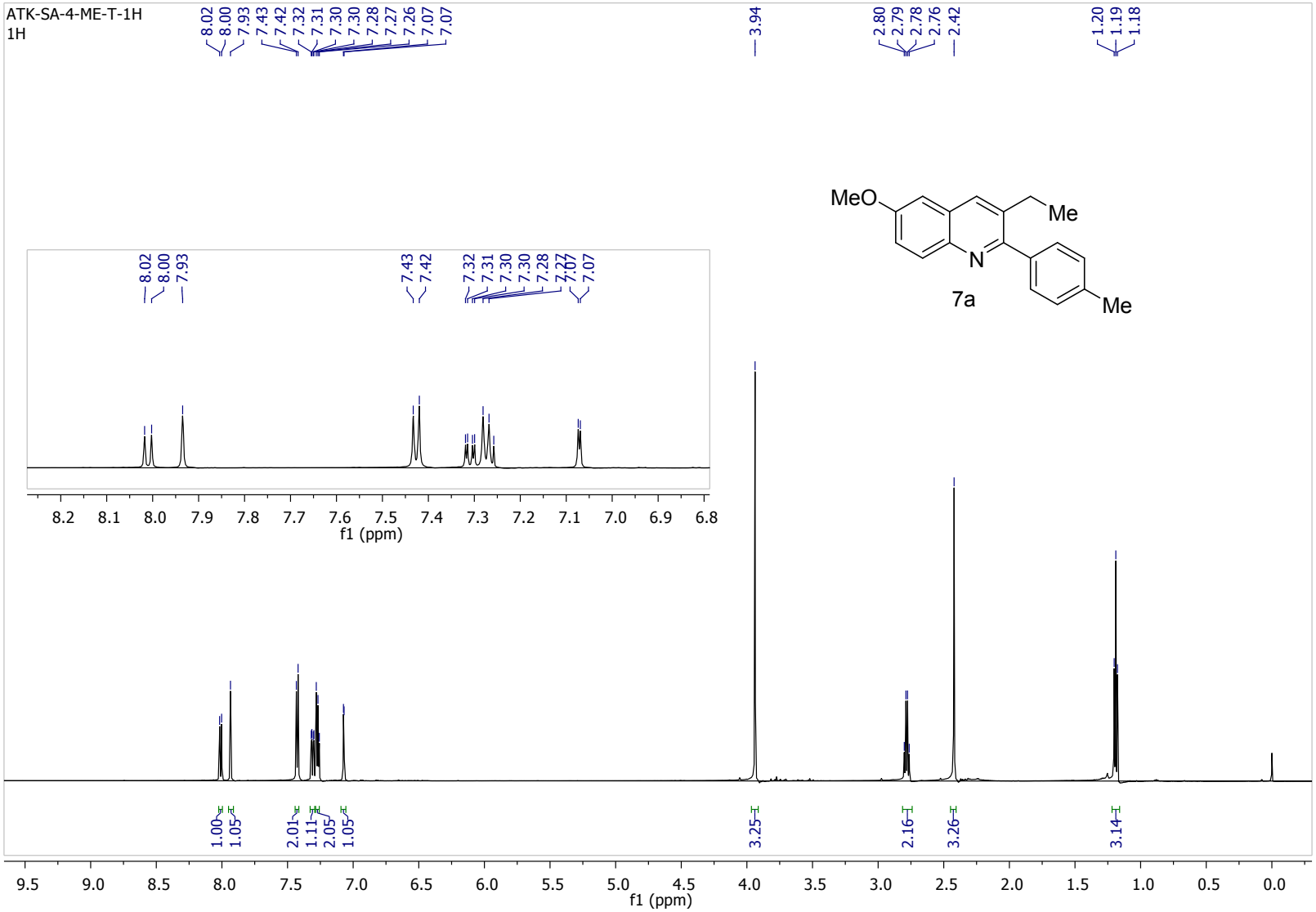


HRMS spectra of compound: A

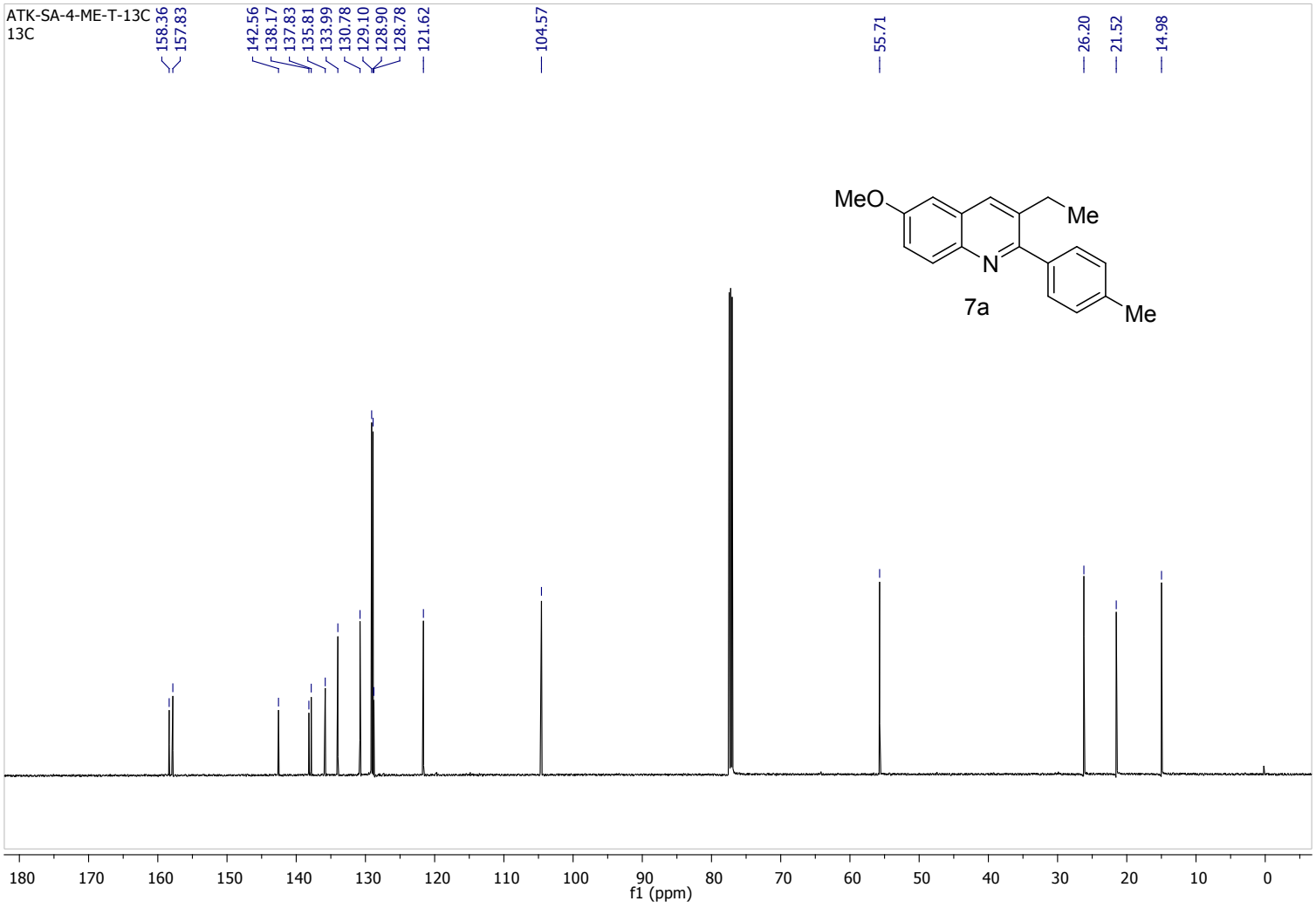
Sample Name	SA-IMD-AA	Position	Vial 1	Instrument Name	QTOF	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SA-IMD-AA.d	ACQ Method		Comment		Acquired Time	7/31/2018 11:14:37 AM



^{1}H NMR spectra of compound: 7a

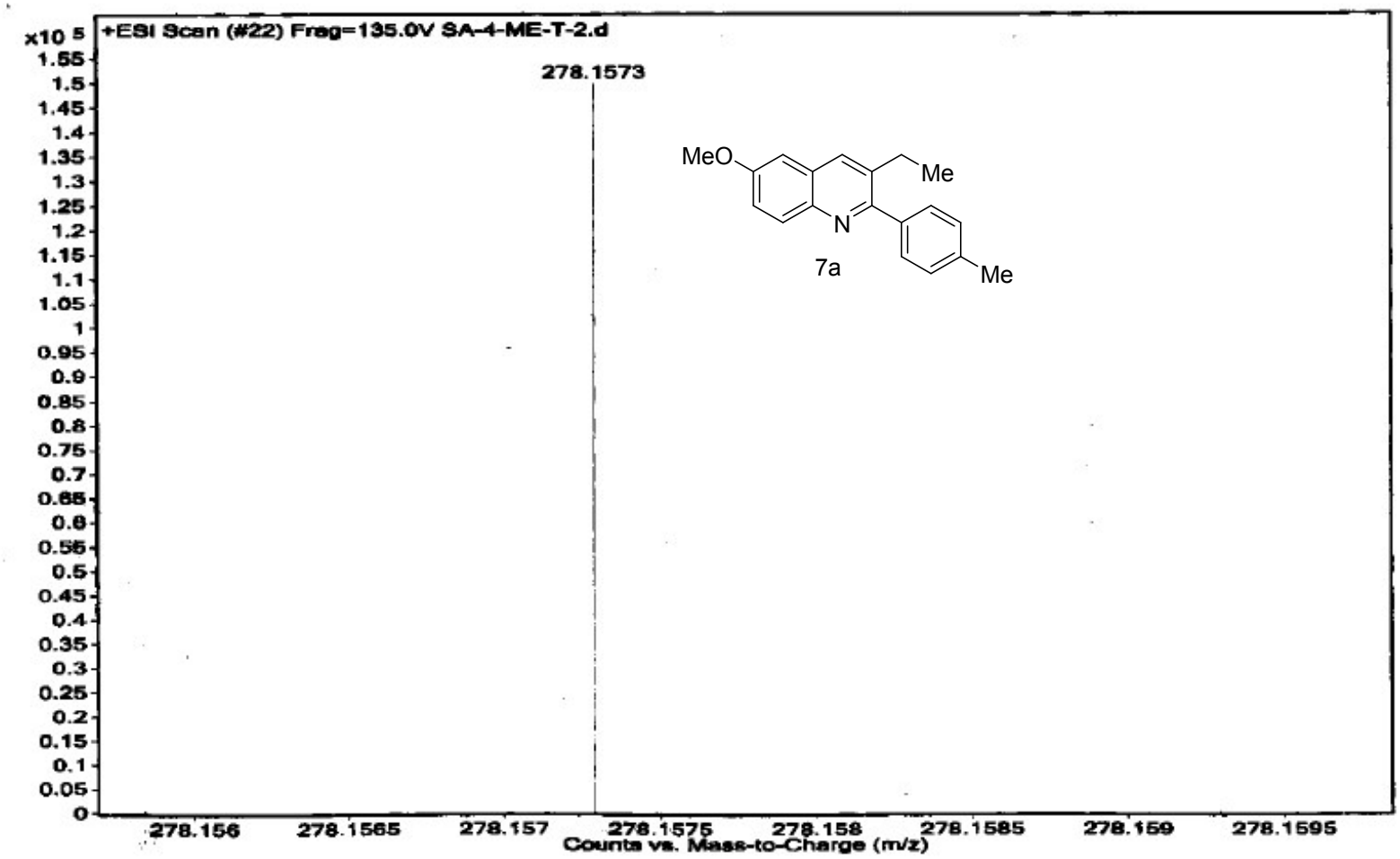


^{13}C NMR spectra of compound: 7a



HRMS spectra of compound: 7a

Sample Name	SA-4-ME-T-2	Position	Vial 1	Instrument Name	QTOF	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	ESI Calibration Status	Success
Data Filename	SA-4-ME-T-2.d	ACQ Method		Comment		Acquired Time	7/26/2018 10:04:44 AM



HRMS spectra of compound: D

Sample Name	SA-IMD-A	Position	Vial 1	Instrument Name	QTOF	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SA-IMD-A.d	ACQ Method		Comment		Acquired Time	8/17/2018 11:25:51 AM