

Supporting Information

Pd(II)/*N,N'*-Disulfonyl Bisimidazoline-Catalyzed Enantioselective Synthesis of Cyclic Quaternary Centers and Mechanistic Investigations

Yu-Xin Wang,^{a,1} Chen-Long Li,^{b,1} Yin-Ping Liu,^a Wen-Juan Hao,^a Zhi-Xiang Yu,^{,b} and Bo Jiang^{*,a}*

^a*School of Chemistry & Materials Science, Jiangsu Normal University, Xuzhou 221116, China.*

^b*College of Chemistry, Peking University, Beijing, 100871, China*

¹*These authors contributed equally.*

E-mail: yuzx@pku.edu.cn(ZXY), jiangchem@jsnu.edu.cn(BJ);

Contents

Computational Details.....	S2-S9
Copies of Chiral HPLC Analyses of Products 3a-3x	S10-S32
Copy of Chiral HPLC Analysis of Product 3a via Scale-Up Experiment.....	S33
References.....	S33
Copies of ¹ H and ¹³ C NMR Spectra for Products 3	S34-S65

DFT Calculations

1. The simplification of **L1**
2. Energy data
3. Cartesian coordinates of all stationary points

1. The simplification of **L1**

In our previous work¹, *para*-toluenesulfonyl groups and four phenyl groups in the original ligand **L1** were simplified as the smaller methanesulfonyl and methyl groups to accelerate calculations, respectively, which was further confirmed to have little difference in terms of the Gibbs free energy. Here, to balance the calculation cost and accuracy, we only simplified **L1**'s *para*-toluenesulfonyl groups and two phenyl groups that were close to palladium center and reactive site to smaller methanesulfonyl and methyl groups, respectively. As shown in Figure S1, the energy difference of 2.8 kcal/mol between enantioselectivity-determining transition states **TS1** and **TS2**, is more accurate to predict final product **3a** with 98% ee. Therefore, we utilized this model to perform calculations and rationalize the enantioselectivity.

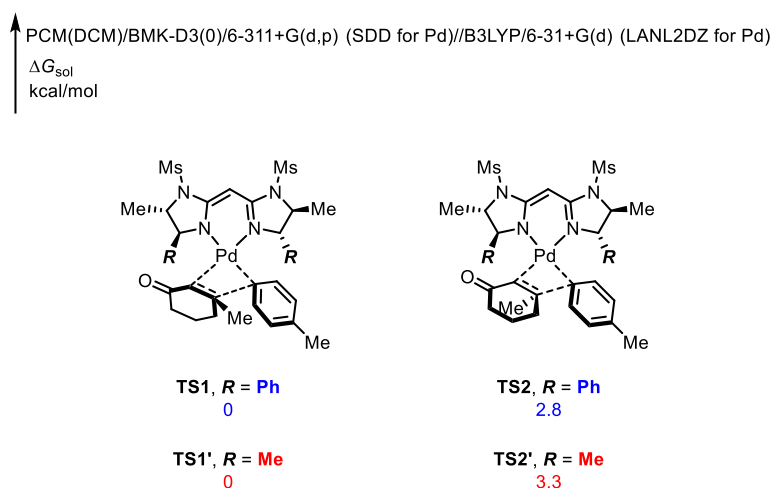


Figure S1. Energy differences between two simplifications

2. Energy data

	Gibbs Free Energy Corrections (a.u.) ^a	<i>E</i> (a.u.) ^b	Δ <i>G</i> _{solvation} (a.u.)
Int1	0.663402	-2954.319910	-0.026394
Int2	0.666420	-2954.314695	-0.024222
TS1	0.672396	-2954.308885	-0.024342
Int3	0.667834	-2954.311909	-0.024218
TS2	0.673466	-2954.305772	-0.024118
TS1'	0.576756	-2570.987609	-0.023998
TS2'	0.576747	-2570.982054	-0.024337

^a Computed at the B3LYP/6-31+G(d) level (LANL2DZ for Pd).

^b Computed at the BMK-D3(0)/6-311+G(d,p) level (SDD for Pd).

3. Cartesian coordinates of all stationary points

Int1				C	4.29723900	-2.64866800	-0.66589400
C	-1.79243800	-1.26201500	-0.39783700	H	3.00703000	-1.92395400	0.88917600
C	-2.50140500	-0.09648100	-0.08389400	C	4.59953900	-2.68754800	-2.03251900
C	-1.90694500	1.13819300	0.22030800	H	3.98342300	-1.95995400	-3.97062000
N	-0.62140800	1.44310200	0.18465300	C	5.76291600	-3.49753900	-2.56282500
C	-0.44207200	2.87954400	0.42067700	H	6.44676900	-2.87933000	-3.15905200
C	-1.76974300	3.32358200	1.10823600	H	6.34299600	-3.94304900	-1.74684300
N	-2.67866300	2.27576100	0.58044900	H	5.42224500	-4.31577800	-3.21148500
N	-2.46678000	-2.49039100	-0.61343700	H	4.91243600	-3.21281600	0.03450600
C	-1.50938600	-3.50526800	-1.11673000	C	3.22451100	1.90174300	0.42623700
C	-0.18134400	-2.88907400	-0.59437100	C	3.22743700	1.31059900	1.75728600
N	-0.47615900	-1.45033200	-0.50300000	C	4.13981500	1.65105900	2.70034000
S	-4.35636100	2.36600000	0.77285600	C	4.24531800	2.97338100	0.10905700
O	-4.60990300	3.72491900	1.26776100	H	3.78807300	3.94277400	0.36387500
O	-4.85041500	1.20531600	1.52375000	H	4.41563200	2.98050500	-0.97166300
S	-4.10726400	-2.82495600	-0.38824600	C	5.54093800	2.77229700	0.90545400
O	-4.92122600	-1.79217100	-1.03979500	H	6.22748600	3.60765500	0.72690200
O	-4.26176000	-4.23397400	-0.76802500	H	6.04409500	1.86318000	0.55108500
H	-3.57448400	-0.16651400	-0.04746000	C	5.25074600	2.63302900	2.40575800
H	0.38401700	3.03770100	1.12488100	H	4.96473600	3.60953600	2.83188400
H	-2.10278700	4.30091500	0.75478700	H	6.15655100	2.33073300	2.94765100
H	-1.72061700	-4.46598600	-0.64442600	C	4.08934800	1.07944600	4.08773200
H	0.60978300	-3.05286100	-1.32952800	H	4.99413800	0.48947300	4.28999000
C	-4.35553500	-2.68012100	1.39278100	H	4.06959100	1.88409400	4.83591500
H	-4.13220700	-1.65809100	1.70494900	H	3.21598700	0.43908200	4.23956200
H	-3.70906500	-3.40619300	1.88924700	H	2.43774200	0.59166200	1.96518200
H	-5.40924300	-2.90969900	1.57170200	O	2.38978400	1.59447300	-0.44305900
C	-4.98884400	2.25054800	-0.91203900	C	0.25059000	-3.50734000	0.73415300
H	-4.71117000	1.28711800	-1.34303900	C	0.93795700	-4.73047400	0.72520900
H	-4.57944200	3.08240100	-1.48786700	C	-0.05803500	-2.92158400	1.96807600
H	-6.07614300	2.33018800	-0.83128800	C	1.29945700	-5.36041800	1.91763400
C	-1.67986900	3.31087600	2.63719900	H	1.20490800	-5.18774000	-0.22594200
H	-0.96457800	4.07334000	2.97163700	C	0.30202500	-3.54974300	3.16583700
H	-1.33843400	2.33349500	2.99776000	H	-0.56730400	-1.96285600	1.99180100
H	-2.65081800	3.53516000	3.08740800	C	0.97994700	-4.77151600	3.14608700
C	-1.56262800	-3.64035100	-2.64019300	H	1.83624400	-6.30560600	1.88835800
H	-2.55055500	-3.98437700	-2.96058800	H	0.05210200	-3.08102900	4.11515200
H	-0.81774400	-4.37307200	-2.97504000	H	1.26053700	-5.25871100	4.07663200
H	-1.34544200	-2.68155400	-3.12425400	C	-0.14398800	3.68096700	-0.84549100
Pd	0.91228100	0.05232100	-0.40855100	C	0.44568800	4.94905800	-0.73044300
C	2.39257000	-1.16751000	-1.04458500	C	-0.47835200	3.21006700	-2.12041900
C	2.69645600	-1.20554200	-2.41670900	C	0.68854000	5.73419300	-1.85991800
C	3.21147900	-1.90476200	-0.17886700	H	0.71693100	5.32797500	0.25464100
C	3.77626800	-1.95243500	-2.90062100	C	-0.23673600	3.99268600	-3.25413400
H	2.08967500	-0.64327700	-3.12422500	H	-0.91112000	2.21993200	-2.22599900

C	0.34520100	5.25696900	-3.12932600	C	2.49532500	-1.12468600	2.26552800
H	1.14578300	6.71483200	-1.75022500	C	3.84171000	-0.38461600	0.42358100
H	-0.49964700	3.60932600	-4.23717200	C	3.61808000	-1.10067800	3.10059400
H	0.53418200	5.86333000	-4.01158700	H	1.53620500	-1.41393600	2.69188100
Int2				C	4.96658700	-0.36446300	1.26213800
C	-0.53864200	1.84757900	0.42903200	H	3.96337100	-0.06159200	-0.60614400
C	-1.83587800	1.38164700	0.22443200	C	4.87965300	-0.72545200	2.61257000
C	-2.17304200	0.08402500	-0.19391900	H	3.50607500	-1.37098600	4.14992800
N	-1.36689300	-0.93359100	-0.45231400	H	5.92593400	-0.05140800	0.85167000
C	-2.18238800	-2.14192500	-0.68993600	C	6.09564900	-0.72106100	3.51246100
C	-3.59537200	-1.59887600	-1.04666100	H	6.45833700	-1.74073500	3.70166900
N	-3.53219000	-0.29185500	-0.34787400	H	6.92171500	-0.15721300	3.06538500
N	-0.29711700	3.21069100	0.72927700	H	5.87199300	-0.27296000	4.48812800
C	1.11859000	3.39228700	1.12203600	C	0.73299100	-2.73490300	-2.66453200
C	1.73784100	2.15344800	0.41746300	C	0.95000900	-3.02194000	-1.21606000
N	0.62316300	1.19270000	0.34775900	C	2.21015500	-3.27542100	-0.72913800
S	-4.90720300	0.67313400	-0.13349700	C	1.94543800	-2.39926200	-3.51888500
O	-6.03533700	-0.18163700	-0.52054600	H	2.16131600	-3.30528800	-4.10641000
O	-4.72149400	1.98174000	-0.77328600	H	1.65132900	-1.62995800	-4.24102400
S	-1.43125400	4.46313600	0.85509000	C	3.16813600	-1.98533100	-2.69959700
O	-2.56381900	4.03814900	1.68603100	H	4.05195300	-1.90827500	-3.34353200
O	-0.64322600	5.64228300	1.23224500	H	2.99241200	-0.99151000	-2.27382400
H	-2.63815400	2.08103500	0.37668300	C	3.43113600	-2.97923000	-1.56334500
H	-1.79653700	-2.67475000	-1.56067400	H	3.77001600	-3.94532300	-1.97677700
H	-4.38684900	-2.20566400	-0.60298500	H	4.24093700	-2.63225100	-0.91248300
H	1.49360000	4.32516200	0.69801500	C	2.42322800	-4.05209500	0.53726500
H	2.53066100	1.75390200	1.05051900	H	3.16337300	-3.57010900	1.18320400
C	-2.02912000	4.69004700	-0.83108000	H	2.81845900	-5.04448200	0.27351400
H	-2.52447800	3.77789300	-1.16839600	H	1.49516000	-4.19008600	1.09827900
H	-1.17763900	4.94827600	-1.46319000	H	0.09662700	-3.42842800	-0.68115100
H	-2.74533500	5.51475700	-0.78586600	O	-0.36963500	-2.88722900	-3.17808100
C	-4.98279200	0.93047300	1.65030100	C	2.33210200	2.49854500	-0.94668700
H	-4.09153400	1.46501500	1.98316000	C	3.61738200	3.06006200	-1.00667000
H	-5.07278100	-0.04525000	2.13100700	C	1.62502000	2.31616300	-2.14205700
H	-5.87571300	1.53562400	1.82803900	C	4.18010400	3.43950000	-2.22720700
C	-3.81455400	-1.45519400	-2.55489300	H	4.18574800	3.19601300	-0.08791600
H	-3.79956400	-2.44568000	-3.02524900	C	2.18535700	2.69553800	-3.36725300
H	-3.01905500	-0.85487000	-3.00948100	H	0.63690700	1.86683200	-2.11651200
H	-4.78157900	-0.98909400	-2.76407400	C	3.46305100	3.25895200	-3.41514600
C	1.31183700	3.38248500	2.64070900	H	5.17785800	3.87110100	-2.25187800
H	0.77636000	4.21704300	3.10257300	H	1.61987600	2.54877300	-4.28458300
H	2.37778900	3.48411500	2.87999800	H	3.89785900	3.55260500	-4.36722800
H	0.94985900	2.44352600	3.07444900	C	-2.20813800	-3.09488200	0.50347100
Pd	0.79858600	-0.84295100	-0.05825600	C	-1.99219200	-2.65986100	1.81835200
C	2.58815500	-0.77854200	0.90616800	C	-2.49082300	-4.45310600	0.28525900
				C	-2.06805000	-3.55724100	2.88893500

H	-1.75269500	-1.61657900	2.00215300
C	-2.56663300	-5.35262700	1.35192600
H	-2.65055100	-4.80880500	-0.73144700
C	-2.35641000	-4.90590600	2.66071400
H	-1.90056700	-3.20074200	3.90271300
H	-2.78611600	-6.40034100	1.16095000
H	-2.41388900	-5.60270300	3.49312500

TS1

C	-0.22456000	1.87297800	0.25987700
C	-1.57167500	1.65200500	-0.04488700
C	-2.11609200	0.40620300	-0.38023100
N	-1.49400300	-0.75777300	-0.53166300
C	-2.49174300	-1.84094600	-0.61584500
C	-3.79619200	-1.12058400	-1.06145200
N	-3.51233700	0.24373700	-0.55116200
N	0.24626500	3.17105700	0.59327300
C	1.61753300	3.05636800	1.14491500
C	2.04578700	1.73349200	0.45046500
N	0.78272600	1.00534400	0.25617600
S	-4.72552200	1.39938000	-0.32431000
O	-5.97365700	0.71487100	-0.67929200
O	-4.35270100	2.65166600	-0.99308600
S	-0.66884400	4.58467900	0.78187200
O	-1.88897600	4.31309800	1.55218000
O	0.28827000	5.59234800	1.25478900
H	-2.24714500	2.48650000	0.01685800
H	-2.20311100	-2.55082200	-1.39247600
H	-4.67235600	-1.52218300	-0.54895100
H	2.21302500	3.90482800	0.80415400
H	2.69643200	1.17304400	1.12562800
C	-1.15258100	5.00943700	-0.90249700
H	-1.75757600	4.20566700	-1.32556200
H	-0.24521000	5.18093100	-1.48413100
H	-1.74316700	5.92582600	-0.82192300
C	-4.73168500	1.70441400	1.45427800
H	-3.76990900	2.12460200	1.75436000
H	-4.93996200	0.76107300	1.96254500
H	-5.53261400	2.42673000	1.63303200
C	-4.01102400	-1.14191800	-2.57614700
H	-4.16739600	-2.17341900	-2.91378800
H	-3.13522900	-0.74266300	-3.09950100
H	-4.89029100	-0.55082100	-2.84838000
C	1.64071000	2.96746500	2.67355900
H	1.23725500	3.87954400	3.12234800
H	2.67484900	2.84545000	3.01950800

H	1.05691000	2.10909800	3.02452500
Pd	0.57920500	-1.07104500	-0.22985900
C	2.45965800	-1.57356700	0.67558500
C	2.20139100	-1.79681300	2.04601200
C	3.72721300	-1.07823500	0.33448600
C	3.15522400	-1.51542900	3.02180600
H	1.23669700	-2.19153600	2.35788200
C	4.69600800	-0.82529400	1.31234900
H	3.97569900	-0.85887200	-0.69847100
C	4.43161800	-1.03873600	2.67153900
H	2.91204000	-1.67972600	4.07027400
H	5.66903100	-0.44380200	1.00809300
C	5.48228000	-0.79016400	3.72804900
H	5.86953300	-1.73556900	4.13137400
H	6.33277300	-0.23062900	3.32458500
H	5.07356300	-0.22410400	4.57379300
C	0.21474700	-3.05321800	-2.37428700
C	0.56273400	-3.09568100	-0.92571800
C	1.94244100	-3.27241100	-0.54472900
C	1.25763800	-2.58650900	-3.38430200
H	1.37905000	-3.41509200	-4.09601000
H	0.82227200	-1.75822500	-3.95612000
C	2.60525700	-2.20599000	-2.76133000
H	3.38572200	-2.18506200	-3.53127100
H	2.54671100	-1.19623900	-2.33785000
C	2.97063500	-3.20820700	-1.66432500
H	2.99177400	-4.22203100	-2.10036400
H	3.97077900	-3.03566100	-1.25895700
C	2.23009700	-4.33735500	0.49813600
H	3.23592100	-4.24535300	0.91661700
H	2.15279100	-5.31311500	-0.00471600
H	1.50091100	-4.32803000	1.31073600
H	-0.17886100	-3.62175700	-0.32399000
O	-0.87929500	-3.45124800	-2.76965400
C	2.80357900	1.99829900	-0.85147200
C	4.15930100	2.35878900	-0.79245800
C	2.18137500	1.94252600	-2.10475900
C	4.87587900	2.65812000	-1.95298300
H	4.66013000	2.40265000	0.17340300
C	2.89516700	2.24413100	-3.27052400
H	1.13650500	1.65447700	-2.16783700
C	4.24381900	2.60180400	-3.20026300
H	5.92550200	2.93417100	-1.88490700
H	2.39360900	2.19845700	-4.23447300
H	4.79784600	2.83487400	-4.10606300
C	-2.66197800	-2.60298800	0.69647400

C	-2.40689100	-2.01854000	1.94510500	C	-0.09720200	3.09606700	-2.91173200
C	-3.12425000	-3.92796900	0.65819800	H	0.64698900	3.77224300	-3.34171300
C	-2.62479800	-2.73523500	3.12650900	H	-1.04931400	3.26435700	-3.43015200
H	-2.02404100	-1.00318700	1.99286200	H	0.21411900	2.06145300	-3.09301300
C	-3.34089900	-4.64771600	1.83648800	Pd	-0.90972600	-0.67444200	0.24549900
H	-3.30931700	-4.40040200	-0.30489500	C	-2.71659600	-0.38582700	-0.60669200
C	-3.09386300	-4.05132400	3.07726900	C	-2.82736100	-0.98115500	-1.87615600
H	-2.42552400	-2.26392300	4.08635700	C	-3.81988800	0.31629100	-0.11344900
H	-3.69680000	-5.67392000	1.78522900	C	-4.01425000	-0.89414200	-2.61188900
H	-3.26125800	-4.60830600	3.99578900	H	-1.98508400	-1.52276800	-2.30462500
Int3				C	-5.00892800	0.39942400	-0.85403700
C	0.90509400	1.73449300	-0.17604200	H	-3.76911200	0.82591100	0.84475000
C	2.04548300	1.11472800	0.34173700	C	-5.13039500	-0.20330900	-2.11214200
C	2.14499400	-0.25541100	0.63143300	H	-4.06911700	-1.36907800	-3.59068500
N	1.17325700	-1.15488100	0.63682100	C	-6.40905100	-0.10768100	-2.91517400
C	1.77787200	-2.49931800	0.53978400	H	-6.81947100	-1.10106100	-3.13819000
C	3.19753600	-2.31237200	1.14672000	H	-7.17746700	0.45608300	-2.37518600
N	3.39853100	-0.86531300	0.87924400	H	-6.24238900	0.39416300	-3.87720900
N	0.94584400	3.08588400	-0.61689600	H	-5.85129500	0.95341900	-0.44176600
C	-0.27706800	3.36209400	-1.41419600	C	-1.65638000	-3.94758300	1.13808600
C	-1.23236500	2.35330000	-0.72643300	C	-1.42231600	-2.62008000	1.76498400
N	-0.33551000	1.25681900	-0.32158700	C	-2.44814300	-1.85730400	2.26726500
S	4.93593000	-0.17423500	0.72848000	C	-3.09615000	-4.38994100	0.92788000
O	5.86973800	-1.23631600	1.11865400	H	-3.33072500	-5.05386200	1.77539700
O	4.94645800	1.11663400	1.42663000	H	-3.13685900	-5.01465700	0.02921000
S	2.32404300	4.06583100	-0.78890000	C	-4.09226100	-3.22695200	0.86928300
O	3.43875400	3.30806200	-1.37193600	H	-5.11920900	-3.61014700	0.89002300
O	1.83824200	5.28053300	-1.45336400	H	-3.97260500	-2.68808300	-0.07460600
H	2.95243500	1.68985100	0.39922800	C	-3.88622800	-2.24559500	2.02839000
H	1.22088200	-3.22211200	1.13983400	H	-4.23632500	-2.69350900	2.97528000
H	3.94427000	-2.89147200	0.60026000	H	-4.49540600	-1.34651000	1.88404600
H	-0.58767100	4.39380600	-1.24409200	C	-2.20908100	-0.76612300	3.27473800
H	-1.96303500	1.98657400	-1.45037100	H	-2.72631800	0.15884600	2.99722900
C	2.75165100	4.48754300	0.91063000	H	-2.62244500	-1.08181100	4.24468500
H	2.99361200	3.58164700	1.46847700	H	-1.14563500	-0.55002200	3.40387100
H	1.90540400	5.01764600	1.35072900	H	-0.41435300	-2.44973400	2.12850800
H	3.62835900	5.13724900	0.84485000	O	-0.71775500	-4.70337700	0.91039100
C	5.14128900	0.15028200	-1.03452500	C	-1.97411600	3.00451700	0.44167500
H	4.40621600	0.89299200	-1.35099700	C	-3.09777700	3.80159700	0.17394900
H	5.03003300	-0.79184000	-1.57489700	C	-1.54440800	2.87708100	1.76778600
H	6.15334200	0.54711100	-1.15136000	C	-3.77385000	4.45967800	1.20300500
C	3.27627800	-2.63210300	2.64087200	H	-3.45383000	3.89907200	-0.85027400
H	3.08453200	-3.69988500	2.80406400	C	-2.21917600	3.53510900	2.80289300
H	2.53253400	-2.05525500	3.20296500	H	-0.68519500	2.25257700	1.99245700
H	4.27087100	-2.39655500	3.03044600	C	-3.33517500	4.32860900	2.52553500
				H	-4.64425500	5.06992600	0.97445000

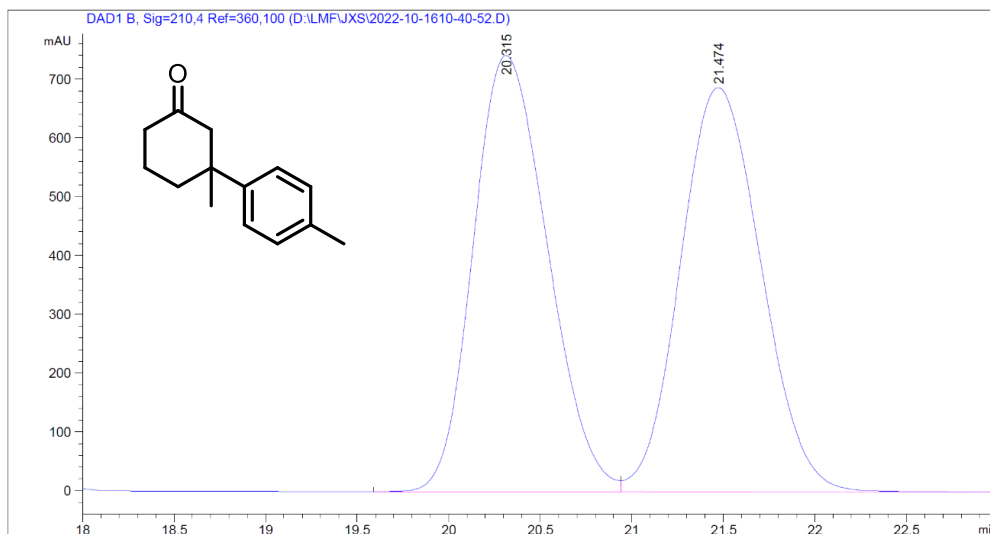
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C	1.82238500	-3.03062900	-0.89355600	H	3.96473300	1.33429800	3.45964200
C	1.89763600	-4.41625900	-1.10353500	C	-2.57378000	1.80993800	-2.95232400
C	1.83818100	-2.18159300	-2.00865500	H	-2.44152800	2.69673800	-3.57911600
C	2.00379600	-4.94052400	-2.39352400	H	-3.54548500	1.36069300	-3.19327800
H	1.84847100	-5.08945300	-0.25127400	H	-1.78815000	1.08532700	-3.19312800
C	1.94396000	-2.70419200	-3.30242100	Pd	-0.30748200	-1.26246500	0.28522300
H	1.75215300	-1.10821500	-1.86990900	C	-2.19056900	-2.19952900	-0.09817100
C	2.03082600	-4.08467800	-3.49975300	C	-2.52990000	-2.39485400	-1.45351600
H	2.05305600	-6.01742900	-2.53507900	C	-3.24966000	-1.94534100	0.79333400
H	1.95407600	-2.02945000	-4.15541700	C	-3.85557900	-2.35779400	-1.88680800
H	2.10974600	-4.49073400	-4.50517300	H	-1.75214400	-2.57141300	-2.19020500
TS2				C	-4.57701000	-1.91575400	0.36315900
C	-0.41551300	1.73271300	-0.52712300	H	-3.04302000	-1.75945000	1.84317800
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C	1.76975800	1.03376400	0.39295400	H	-4.07674800	-2.50534600	-2.94259600
N	1.56968600	-0.26715500	0.59697200	C	-6.34738900	-2.15826900	-1.44007900
C	2.86799100	-0.87702900	0.94729100	H	-6.74712100	-3.18178600	-1.42975500
C	3.66961100	0.28911000	1.57888500	H	-6.98592000	-1.55353800	-0.78700000
N	3.07607100	1.40440600	0.80346900	H	-6.45025200	-1.78205700	-2.46424800
N	-1.22159600	2.76205300	-1.07577300	H	-5.36471100	-1.70734000	1.08390400
C	-2.52997700	2.19212000	-1.47084400	C	1.52552000	-3.81346900	0.73080000
C	-2.55703900	0.97899300	-0.50423500	C	0.24160200	-3.17279000	1.13807500
N	-1.13403500	0.62678900	-0.34241600	C	-0.97045800	-3.79448600	0.66334500
S	3.81179200	2.92340000	0.70055400	C	1.64245000	-4.43032800	-0.65460200
O	5.09439200	2.77070000	1.39659200	H	1.94367800	-5.47660600	-0.50644000
O	2.87307900	3.97584600	1.10952200	H	2.47458300	-3.94156600	-1.17284100
S	-0.80265600	4.37119300	-1.37855600	C	0.33900600	-4.34585600	-1.45354300
O	0.51055600	4.43325900	-2.03107100	H	0.37634300	-5.01772000	-2.31908400
O	-1.98099400	4.94930600	-2.03602700	H	0.21091100	-3.32777700	-1.84119400
H	1.30055100	2.96382000	-0.35789400	C	-0.83613500	-4.71461600	-0.54529400
H	2.73603300	-1.66910900	1.68536900	H	-0.65401600	-5.72077900	-0.12982800
H	4.73417000	0.21584900	1.35187200	H	-1.78316900	-4.78109200	-1.08640900
H	-3.32022700	2.90868400	-1.24232600	C	-1.91820300	-4.32237000	1.72613100
H	-3.10142200	0.15761800	-0.97208900	H	-2.89846800	-4.58427200	1.31975800
C	-0.64168200	5.10994700	0.25911200	H	-1.45776600	-5.23460700	2.13423700
H	0.16516000	4.61547100	0.80360000	H	-2.04480700	-3.62557500	2.55689800
H	-1.59814000	5.01110800	0.77567100	H	0.25255000	-2.91393800	2.19979400
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C	4.13991600	3.12805300	-1.06127100	C	-3.24405100	1.34725800	0.81664600
H	3.19614100	3.12740400	-1.61003000	C	-4.62839500	1.58396200	0.82139300
H	4.79282300	2.31508200	-1.38388200	C	-2.54047600	1.49068900	2.01780900
H	4.63913700	4.09492900	-1.16636800	C	-5.29341200	1.95167800	1.99204800
C	3.45654200	0.44009500	3.08696100	H	-5.19436500	1.47496700	-0.10252500
				C	-3.20324900	1.85824000	3.19560800

H	-1.47127100	1.30520300	2.03382400	H	0.94869400	-3.80282200	-2.86443800
C	-4.58032400	2.08976100	3.18892400	H	1.44397700	-2.09292300	-2.89894000
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H	-2.63720200	1.96495200	4.11809100	H	4.11706900	0.62485200	-1.83468200
H	-5.09401400	2.37629100	4.10314500	H	4.40906100	-0.84505700	-2.84772600
C	3.60846500	-1.44315500	-0.26900200	H	5.78453800	0.01158100	-2.07144600
C	4.70027300	-2.30164300	-0.06227100	C	2.71063000	-3.95675800	0.71684900
C	3.26944500	-1.09692800	-1.58324400	H	2.29290600	-4.96179100	0.58331700
C	5.43833100	-2.79599800	-1.13875600	H	2.19946500	-3.48834500	1.56490100
H	4.95785100	-2.60503300	0.94971800	H	3.77550300	-4.05023800	0.94962100
C	4.00777300	-1.59055700	-2.66612100	C	-1.28254100	2.44900100	2.18537000
H	2.41861100	-0.44765200	-1.76387500	H	-0.37036500	2.43636000	2.79378200
C	5.09484400	-2.44034200	-2.44875600	H	-1.86872800	1.56363300	2.44462200
H	6.27551300	-3.46537900	-0.95650600	H	-1.86384600	3.34183000	2.45027400
H	3.72927700	-1.30872700	-3.67902700	C	-0.03744900	4.09308900	-1.07706800
H	5.66734600	-2.82546300	-3.28895300	H	0.76714900	4.79709900	-1.30735000
TS1'				H	-0.99339000	4.62201200	-1.17941900
C	1.05891100	1.39473800	0.31988000	H	-0.01639000	3.27641500	-1.80732600
C	2.08943000	0.46130900	0.17530900	Pd	-1.17166600	-0.70995100	-0.00664100
C	1.89045600	-0.88853200	-0.13397800	C	-3.10617200	0.17610900	-0.35745000
N	0.74783800	-1.55249300	-0.26944200	C	-3.13712300	0.52619800	-1.72471100
C	1.02421200	-2.86479000	-0.89993600	C	-3.87698000	0.95802300	0.51637000
C	2.50673100	-3.13916700	-0.55978800	C	-3.87180400	1.61798000	-2.18328300
N	2.98792700	-1.74023400	-0.41834900	H	-2.56692900	-0.05560500	-2.44583200
N	1.34227500	2.76998400	0.56269500	C	-4.63855800	2.03690300	0.05367500
C	0.09618100	3.55187100	0.34906800	H	-3.88749100	0.74849300	1.58097600
C	-0.93058300	2.45005400	0.69022300	C	-4.65099500	2.38917400	-1.30228900
N	-0.25415000	1.19628300	0.29938900	H	-3.84902700	1.87083400	-3.24197800
S	4.62031300	-1.32149500	-0.51991100	H	-5.22263500	2.61895700	0.76445300
O	5.31873600	-2.58018300	-0.80653800	C	-5.48790500	3.53930500	-1.81076300
O	5.00428800	-0.51154900	0.64282300	H	-5.85025100	4.16567500	-0.98889200
S	2.86087000	3.51986000	0.55428400	H	-4.91759200	4.17634900	-2.49737100
O	3.67998400	3.04177800	-0.56736500	H	-6.36559100	3.17644100	-2.36250100
O	2.57406300	4.95347300	0.69326300	C	-1.74283200	-3.38747900	1.10653300
H	3.10431400	0.80786800	0.24826600	C	-2.19892100	-2.59256900	-0.06951300
H	0.39900300	-3.63392000	-0.44580900	C	-3.47760500	-1.93207500	-0.00910500
H	3.02787600	-3.61289000	-1.39561300	C	-2.23094100	-3.00923900	2.50117500
H	0.06381700	4.37253500	1.06963600	H	-2.70849300	-3.91095800	2.90860100
H	-1.83389200	2.58481800	0.09235900	H	-1.34960000	-2.82351400	3.12671800
C	3.62550500	2.94883100	2.08499300	C	-3.20549300	-1.82563500	2.51997500
H	3.72913700	1.86265200	2.06613000	H	-3.75697700	-1.80337900	3.46754100
H	3.00508000	3.27919000	2.91976000	H	-2.64543400	-0.88496100	2.44880100
H	4.60996300	3.42264000	2.12191600	C	-4.17647600	-1.93304000	1.34222000
C	0.77623900	-2.81640300	-2.41478000	H	-4.69940100	-2.90333000	1.39939400
H	-0.25408100	-2.51555200	-2.63355400	H	-4.95803300	-1.17006800	1.37346300
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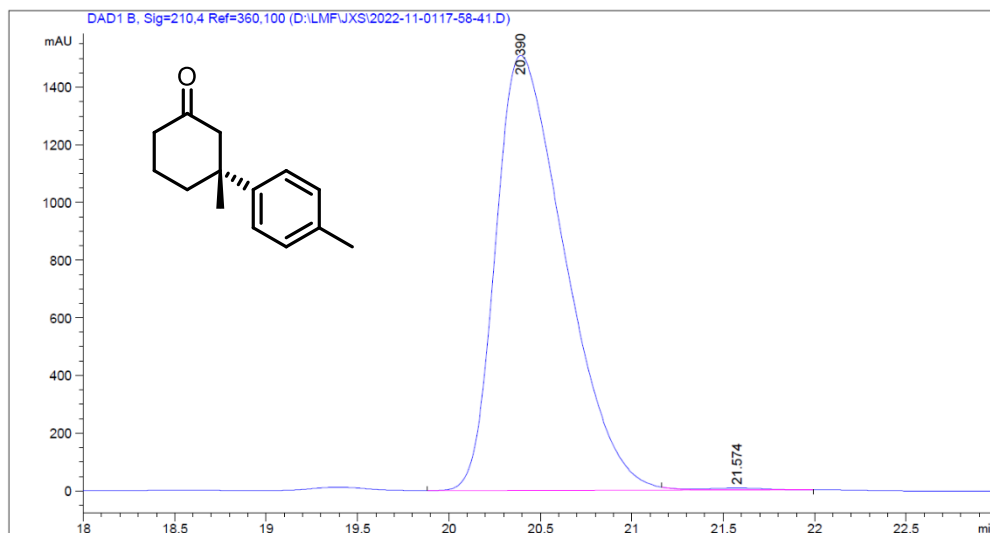
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H	-1.94367300	-3.06295200	-1.01904200	C	-0.23080700	3.92600300	-1.65057600
O	-1.03482000	-4.37987400	0.95658600	H	0.51912400	4.56574700	-2.12523100
TS2'				H	-1.18579900	4.46642000	-1.63951800
C	1.12942000	1.41439600	-0.06946600	H	-0.35403300	3.01803400	-2.25139900
C	2.13445500	0.45045500	-0.14129700	Pd	-1.15222100	-0.65891500	0.21789600
C	1.91691900	-0.91968300	0.02116800	C	-3.06248000	0.33190300	0.22317700
N	0.76636900	-1.57946300	0.10939300	C	-3.40956100	0.86269000	-1.03925700
C	1.05774900	-3.02788100	-0.00833000	C	-3.51646100	1.04316900	1.34864800
C	2.50696000	-3.15686600	0.50042100	C	-4.17092200	2.02435300	-1.16237200
N	3.01019700	-1.82953200	0.05790500	H	-3.06794100	0.37829700	-1.94810700
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C	0.18377800	3.57868000	-0.21919200	H	-3.27243100	0.69256400	2.34668100
C	-0.74806200	2.57169300	0.48962900	C	-4.64193000	2.70955000	-0.02876700
N	-0.17088000	1.24952900	0.15525700	H	-4.40243800	2.40672200	-2.15511300
S	4.65899000	-1.45593900	0.04750800	C	-5.51386300	3.93478200	-0.16633000
O	5.34064800	-2.73498700	0.28002900	H	-6.55136500	3.65604700	-0.39625300
O	4.94195400	-0.30427300	0.91467300	H	-5.52908800	4.52291100	0.75736400
S	2.96587700	3.50823400	-0.31884000	H	-5.16793500	4.58456800	-0.97865900
O	3.74910000	2.81502600	-1.34901900	H	-4.61766300	2.71794300	2.12896400
O	2.70080500	4.94761600	-0.43728200	C	-2.15389000	-3.66641600	-0.32616000
H	3.14283700	0.79166400	-0.28609500	C	-2.29777900	-2.47479400	0.55842300
H	0.38124500	-3.60533100	0.62131300	C	-3.54150000	-1.74406900	0.49559700
H	3.05066800	-3.94106600	-0.03155500	C	-2.86496600	-3.69065500	-1.67406800
H	0.30405800	4.49261200	0.36777400	H	-3.54543300	-4.55330900	-1.64547500
H	-1.75805900	2.65373900	0.08947200	H	-2.12471600	-3.91823700	-2.44999700
C	3.76659500	3.20530800	1.27040600	C	-3.63404500	-2.40286300	-1.96957600
H	3.86722200	2.12993800	1.43101100	H	-4.31322500	-2.54612500	-2.81823400
H	3.16912300	3.67812500	2.05212700	H	-2.92929000	-1.61386600	-2.25279000
H	4.75313500	3.67175800	1.20437400	C	-4.42371500	-1.98500600	-0.72654000
C	0.94301500	-3.49074600	-1.46853500	H	-5.09622700	-2.81410100	-0.44649700
H	-0.01032600	-3.18071600	-1.90285400	H	-5.06812500	-1.12240100	-0.91278600
H	1.01290500	-4.58286000	-1.53484400	C	-4.31755900	-1.67154800	1.79939800
H	1.74152300	-3.04632200	-2.07506200	H	-5.15389000	-0.96950600	1.75481700
C	4.97411900	-0.95247000	-1.65649300	H	-4.72116400	-2.67849200	1.98032900
H	4.36863200	-0.07807300	-1.90207200	H	-3.67875200	-1.42470600	2.65062600
H	4.74441300	-1.79638100	-2.30933600	H	-1.93509900	-2.69524200	1.56544400
H	6.03731500	-0.70303500	-1.70559900	O	-1.55461800	-4.66193300	0.06918200
C	2.61865600	-3.36647100	2.01237700				
H	2.18206100	-4.33682700	2.27932600				
H	2.07748600	-2.58371400	2.55572200				
H	3.66465300	-3.36229600	2.33214400				
C	-0.75485000	2.80419300	2.00898800				

Chiral HPLC analyses of products 3

(R)-3-methyl-3-(p-tolyl)cyclohexan-1-one (3a)

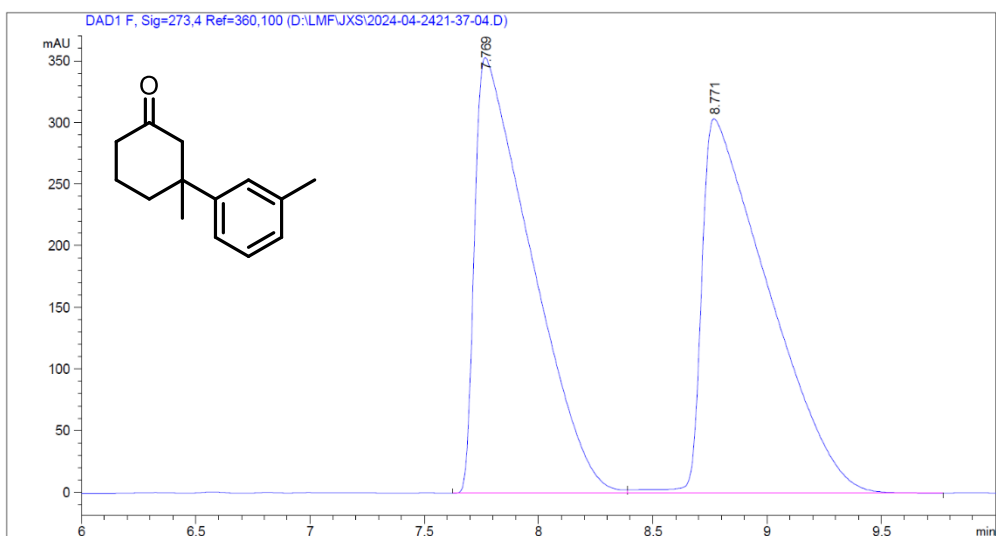


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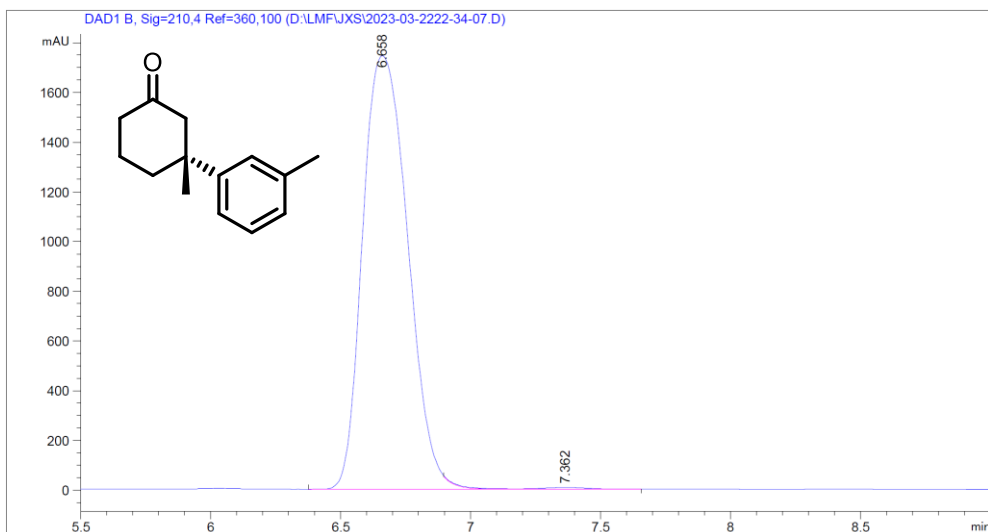


Peak	Retention time	type	width	Area	Height	Area
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1	20.390	BV R	0.4035	3.97515e4	1508.16321	99.6566
2	21.574	VB E	0.3496	136.99348	6.10905	0.3434

(R)-3-methyl-3-(*p*-tolyl)cyclohexan-1-one (**3b**)

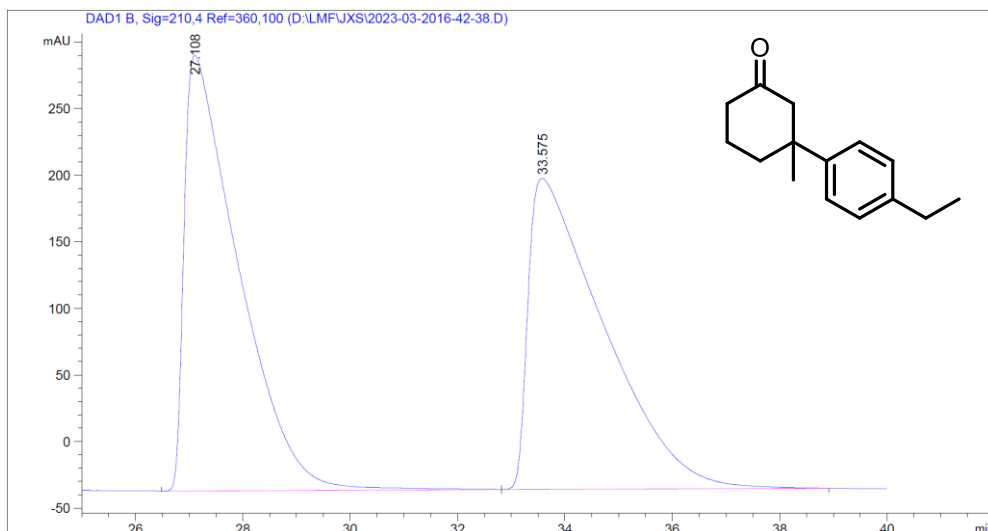


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	7.769	BV	0.2602	6063.99121	353.38046	49.5057
2	8.771	VB	0.3035	6185.08350	303.78165	50.4943

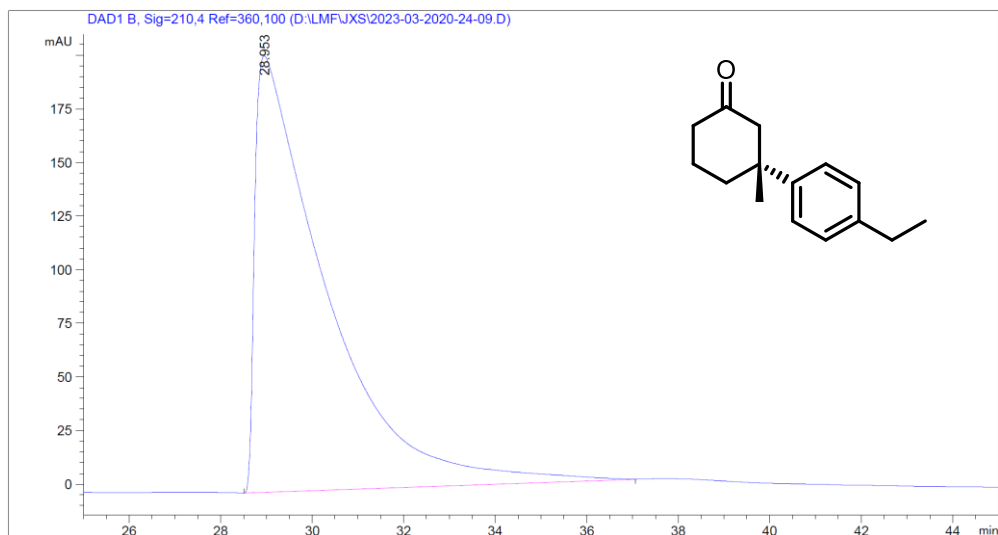


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	6.658	BV R	0.1967	2.10437e4	1744.65356	99.4324
2	7.362	VB E	0.2486	120.11810	7.05714	0.5676

(R)-3-(4-ethylphenyl)-3-methylcyclohexan-1-one (**3c**)

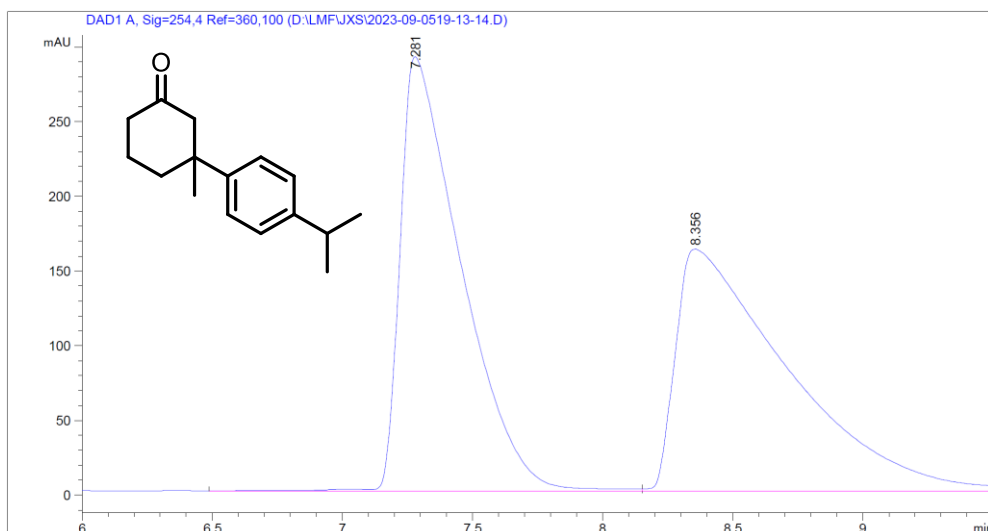


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	27.108	BB	0.9703	2.29005e4	327.28094	50.1165
2	33.575	BB	1.3167	2.27941e4	233.54535	49.8835

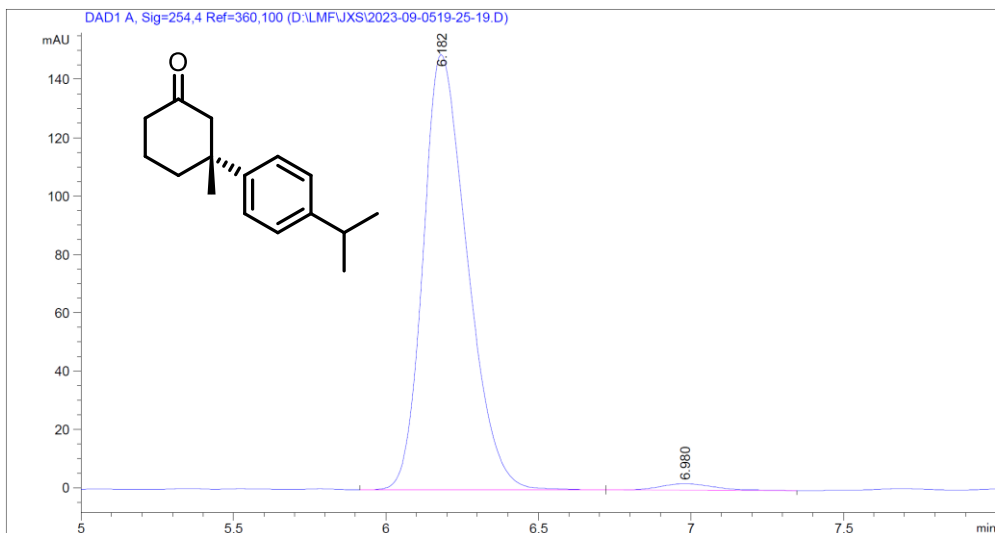


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	28.953	BB	1.4088	2.20125e4	203.37042	100.0000

(R)-3-(4-isopropylphenyl)-3-methylcyclohexan-1-one (**3d**)

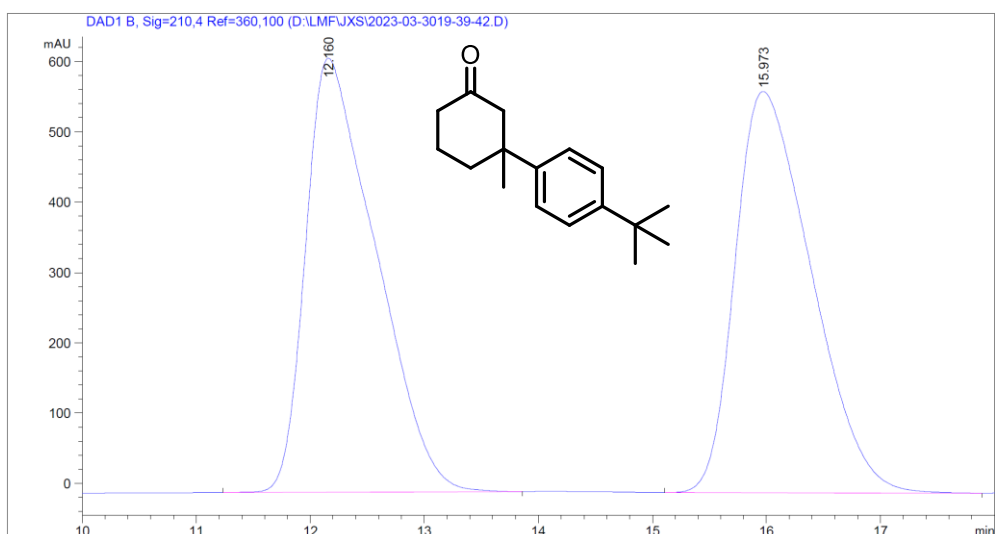


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	7.281	BV	0.2373	4716.30078	290.63715	49.1914
2	8.356	VBA	0.4229	4871.35498	161.94461	50.8086

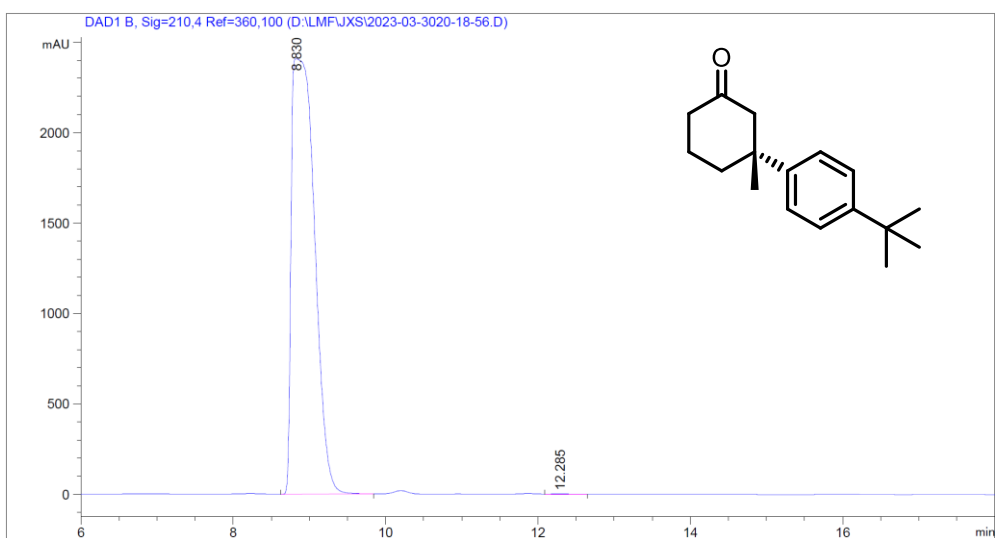


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	6.182	BB	0.1535	1503.17493	149.28059	98.2145
2	6.980	BB	0.1903	27.32707	2.24014	1.7855

(R)-3-(4-(*tert*-butyl)phenyl)-3-methylcyclohexan-1-one (**3e**)

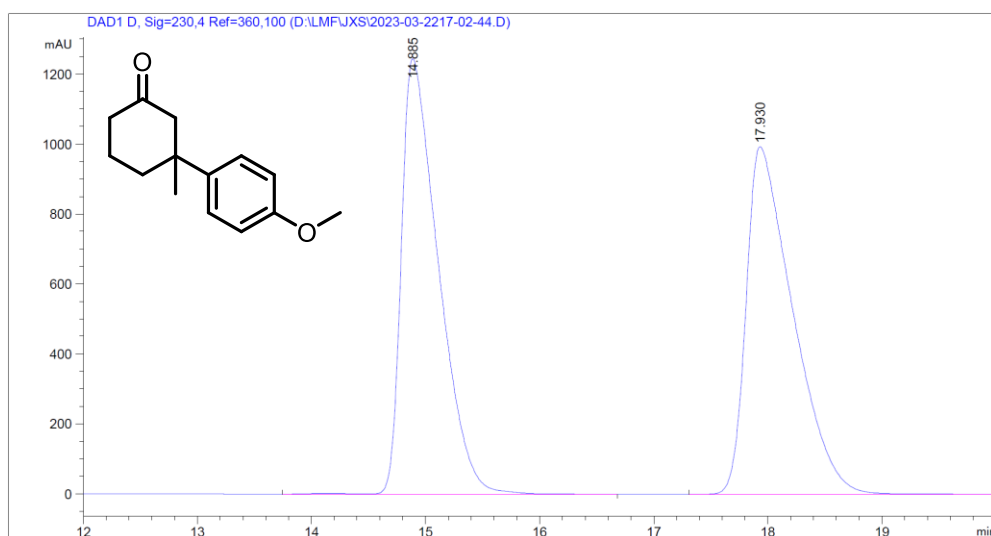


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	12.160	BB	0.6068	2.63827e4	617.11664	49.9001
2	15.973	BB	0.7374	2.64883e4	570.81543	50.0999

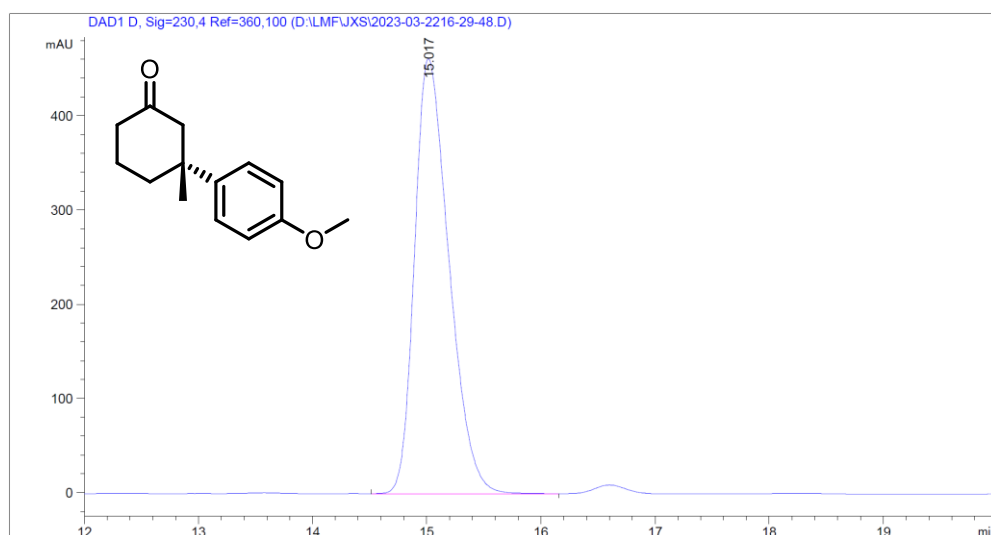


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	8.830	BB	0.2762	5.07866e4	2407.02930	99.9531
2	12.285	BB	0.2559	23.84618	1.37771	0.0469

(R)-3-(4-methoxyphenyl)-3-methylcyclohexan-1-one (**3f**)

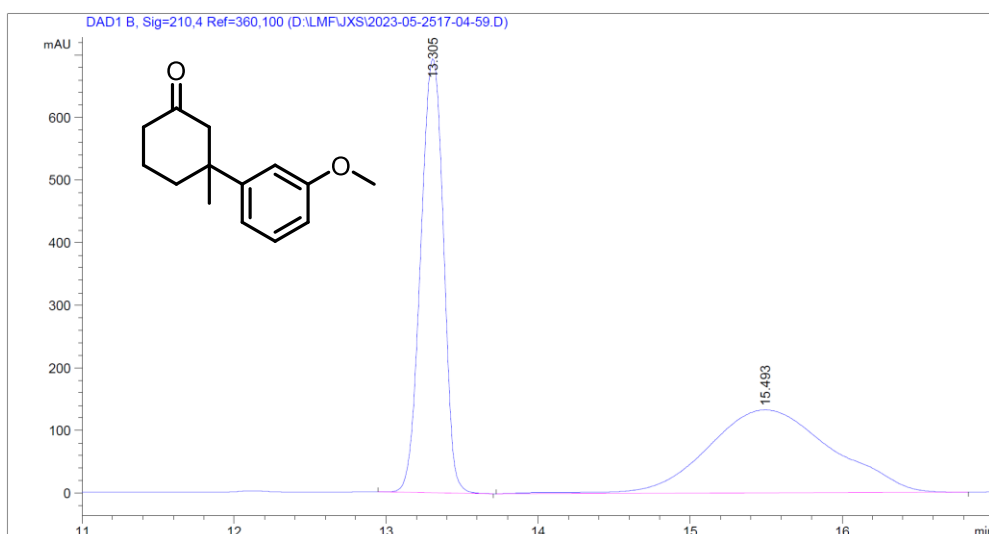


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	14.885	VB R	0.3375	2.79556e4	1244.78125	49.8103
2	17.930	BBA	0.4206	2.81685e4	993.93378	50.1897

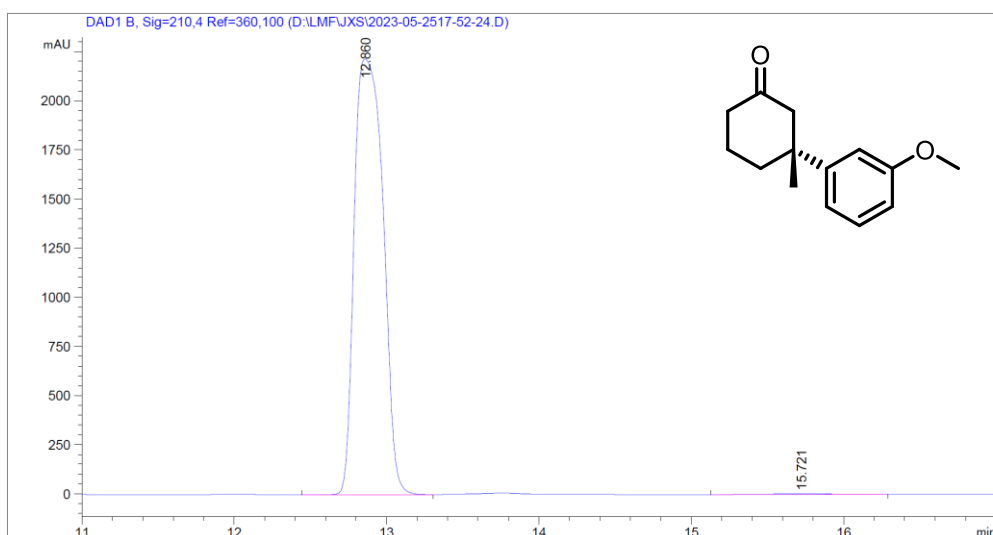


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	15.017	BB	0.3220	9655.47363	461.59216	100.0000

(R)-3-(3-methoxyphenyl)-3-methylcyclohexan-1-one (**3g**)

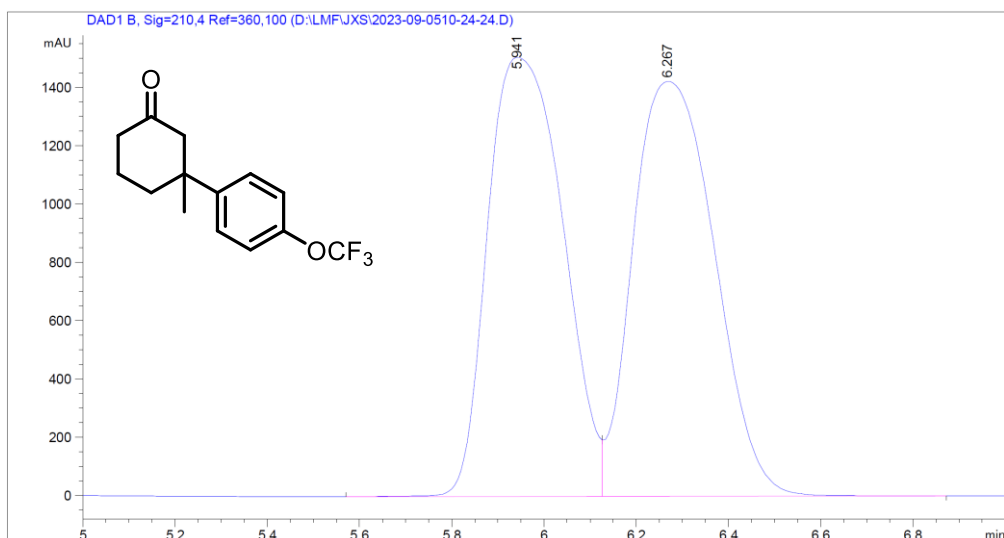


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	13.305	BB	0.1673	7211.60547	693.64056	49.0624
2	15.493	BB	0.8611	7487.25293	132.53653	50.9376

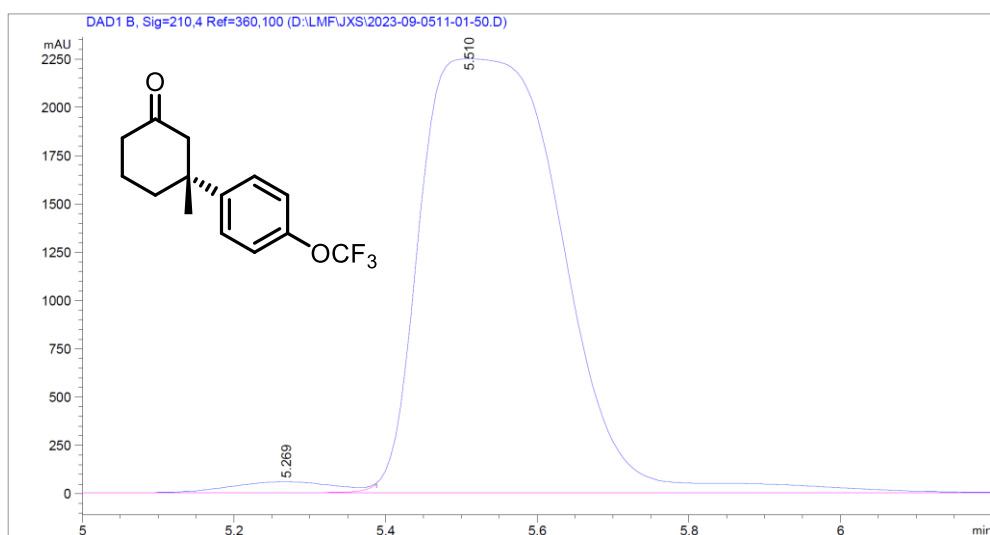


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	12.860	BB	0.2170	2.90767e4	2217.40356	99.6628
2	15.721	BB	0.4527	98.37991	3.09591	0.3372

(R)-3-methyl-3-(4-(trifluoromethyl)phenyl)cyclohexan-1-one (**3h**)

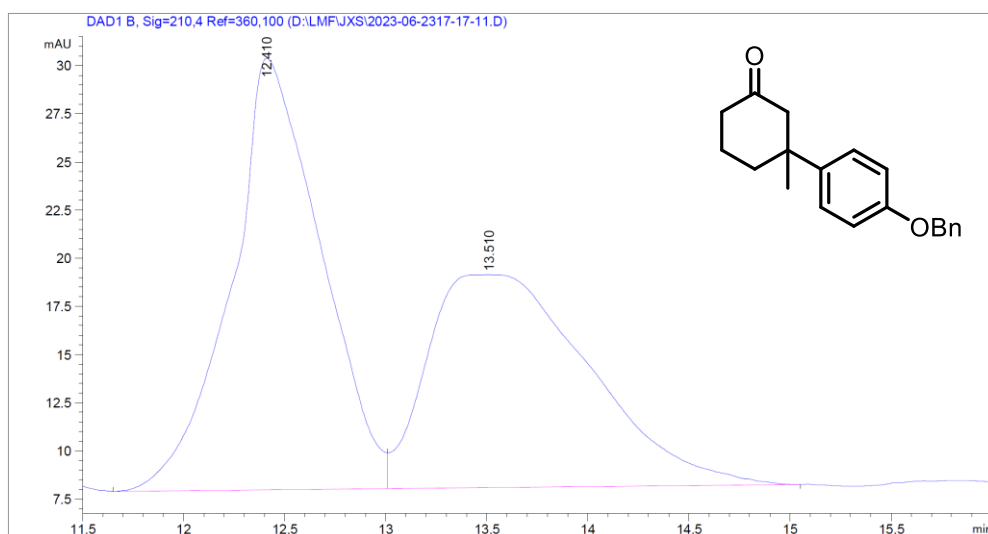


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	5.941	BV	0.1867	1.71290e4	1506.13196	49.4394
2	6.267	VB	0.2016	1.75174e4	1423.06970	50.5606

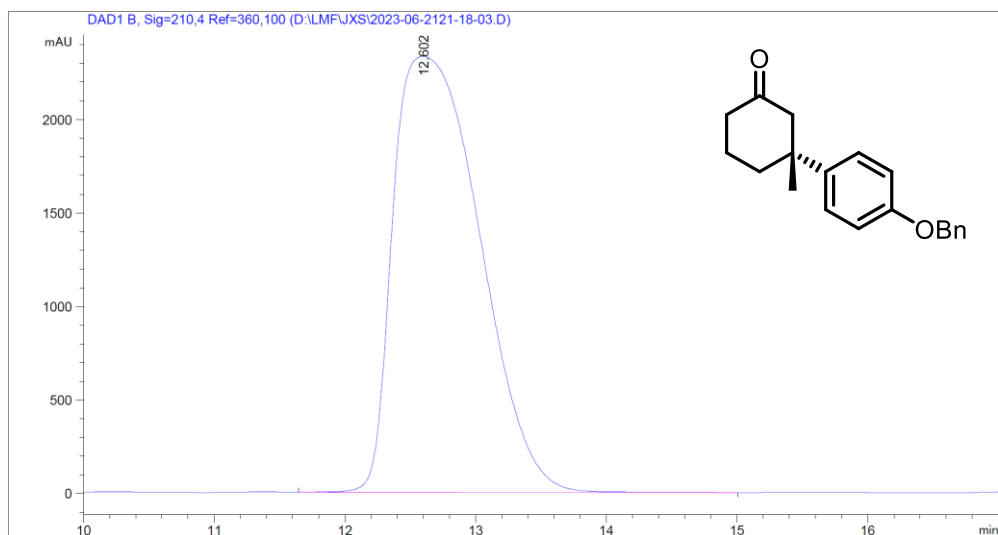


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	5.269	BV E	0.1508	526.39252	56.45766	1.7859
2	5.510	VB R	0.2103	2.89487e4	2246.39502	98.2141

(R)-3-(4-(benzyloxy)phenyl)-3-methylcyclohexan-1-one (**3i**)

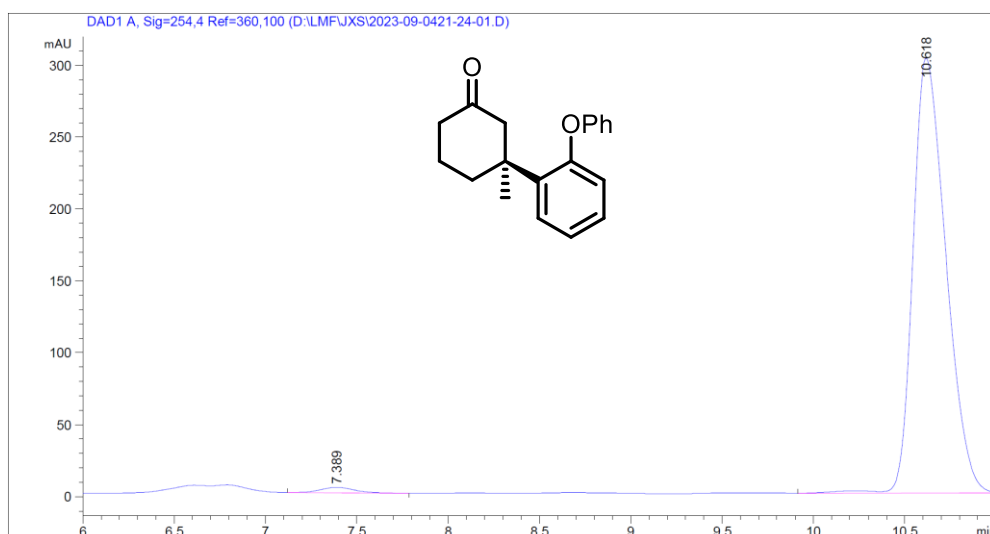


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	12.410	BV	0.4111	693.42755	22.40424	53.0272
2	13.510	VB	0.6601	614.25415	11.05786	46.9728



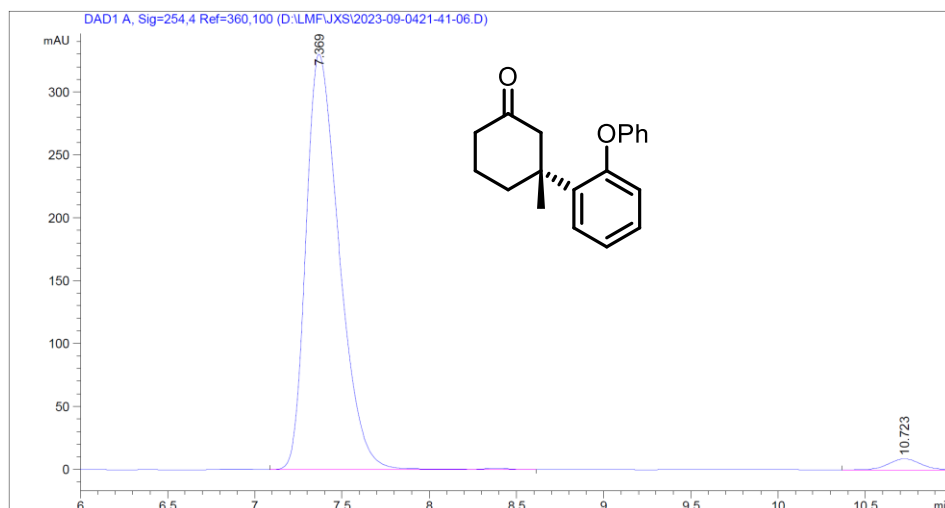
Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	12.602	BB	0.7447	1.07155e5	2329.28784	100.0000

(S)-3-methyl-3-(2-phenoxyphenyl)cyclohexan-1-one (**3j**, from Pd(II)/(*S,S,S,S*)-Bim catalysis)



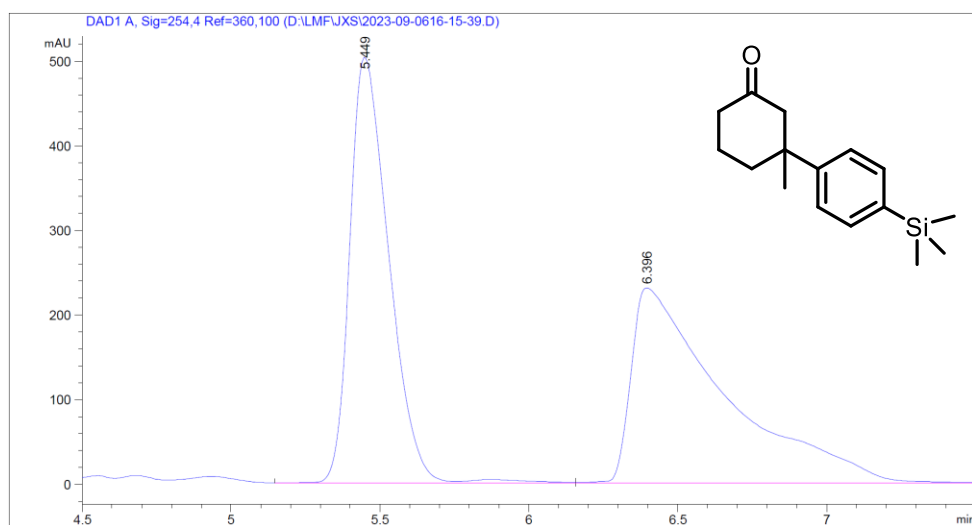
Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	7.389	BB	0.2047	50.50433	3.80995	1.3167
2	10.618	VB R	0.1930	3785.26074	302.44971	98.6833

(R)-3-methyl-3-(2-phenoxyphenyl)cyclohexan-1-one (**3j**)

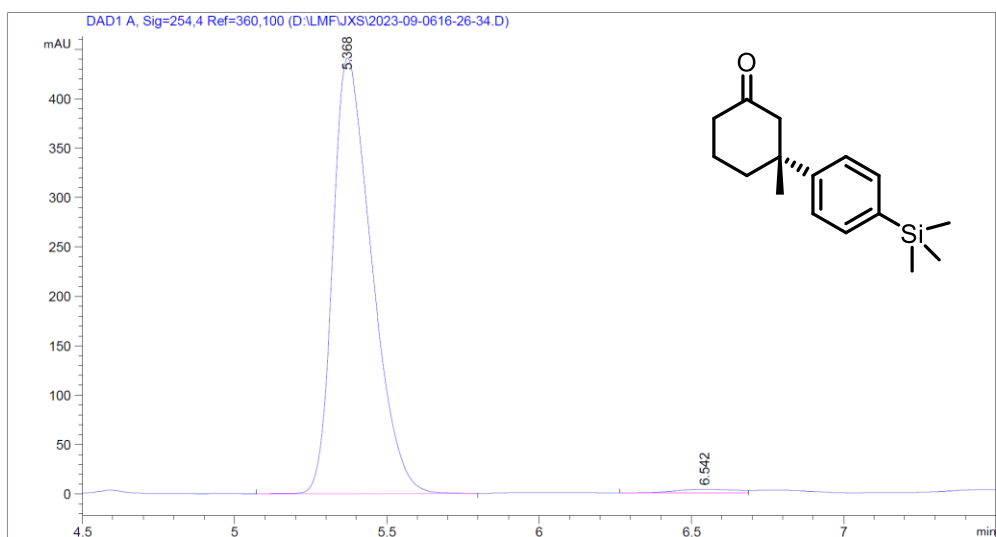


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	7.369	BV R	0.2045	4375.46240	330.31302	97.5671
2	10.723	BB	0.1944	109.10343	8.69239	2.4329

(R)-3-methyl-3-(4-(trimethylsilyl)phenyl)cyclohexan-1-one (**3k**)

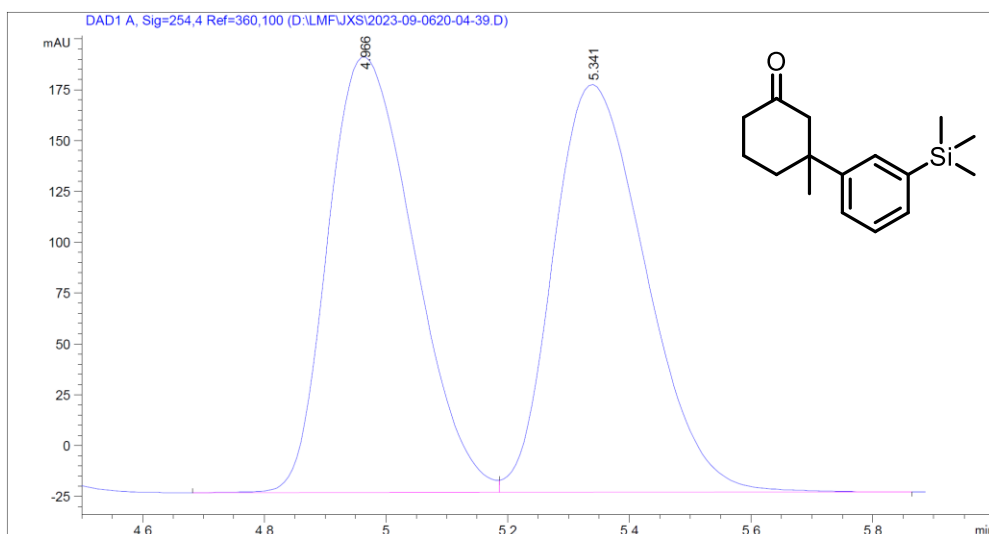


Peak	Retention time	type		width	Area	Height	Area
#	[min]			[min]	[mAU*s]	[mAU]	%
1	5.449	BV	R	0.1392	4590.65918	502.88458	47.6580
2	6.396	VB		0.3009	5041.83838	230.73708	52.3420

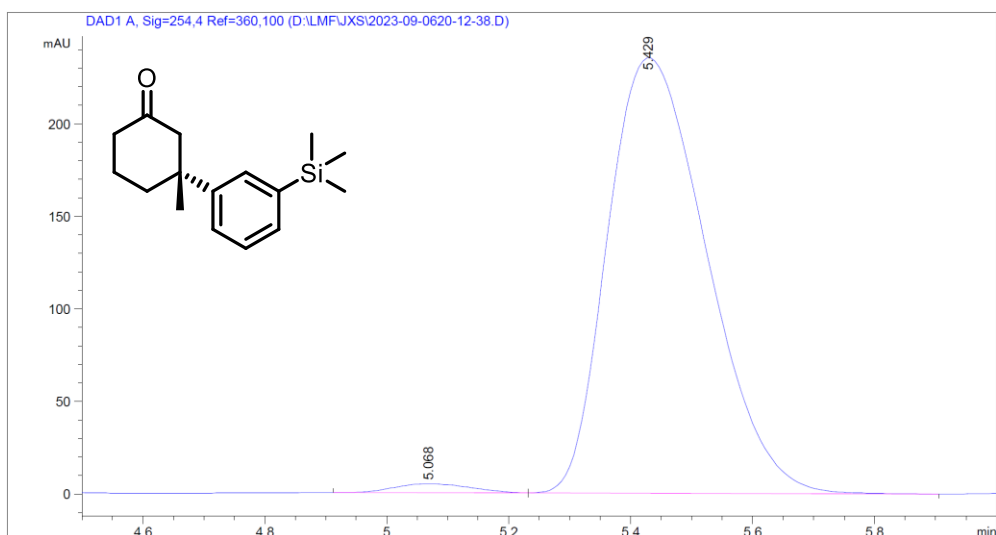


Peak	Retention time	type		width	Area	Height	Area
#	[min]			[min]	[mAU*s]	[mAU]	%
1	5.368	BB		0.1352	3901.88745	441.26447	98.6748
2	6.542	BV		0.2137	52.40126	3.78019	1.3252

(R)-3-methyl-3-(3-(trimethylsilyl)phenyl)cyclohexan-1-one (**3I**)

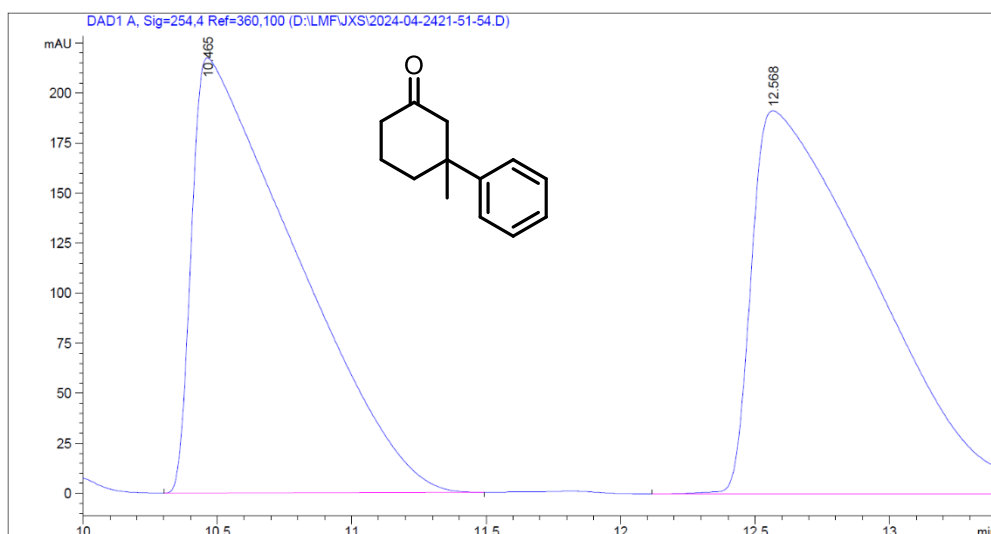


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	4.966	BV	0.1584	2100.23901	214.19560	49.7683
2	5.341	VBA	0.1673	2119.79565	200.52562	50.2317

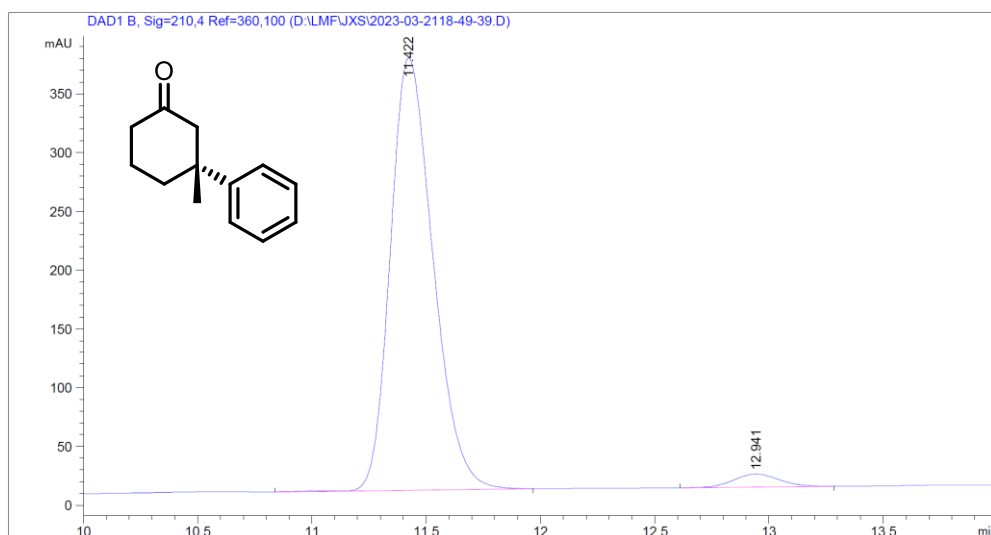


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	5.068	BV	0.1417	42.76854	4.90406	1.5869
2	5.429	VB	0.1794	2652.28613	235.50656	98.4131

(R)-3-methyl-3-phenylcyclohexan-1-one (**3m**)

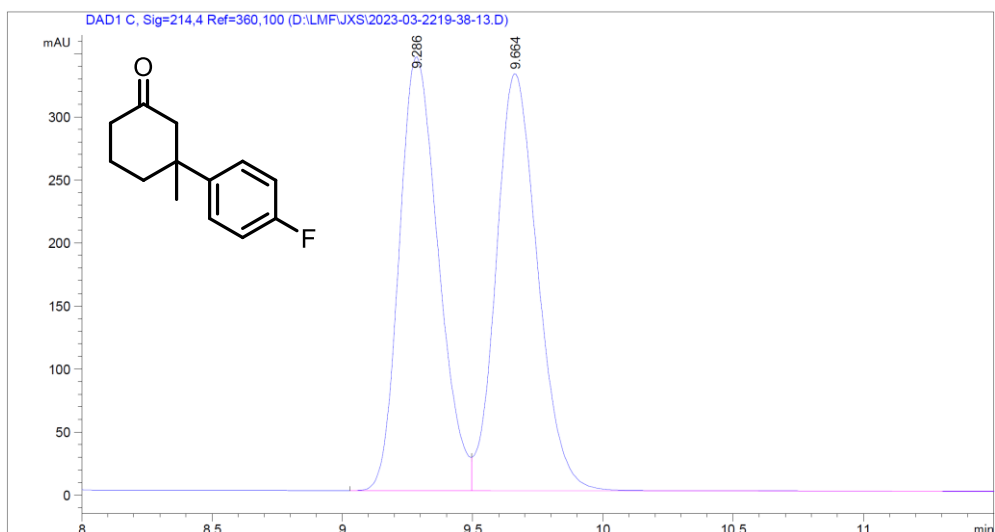


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	10.465	BB	0.3898	5847.30518	217.39720	49.4442
2	12.568	MF R	0.5209	5978.77441	191.30225	50.5558

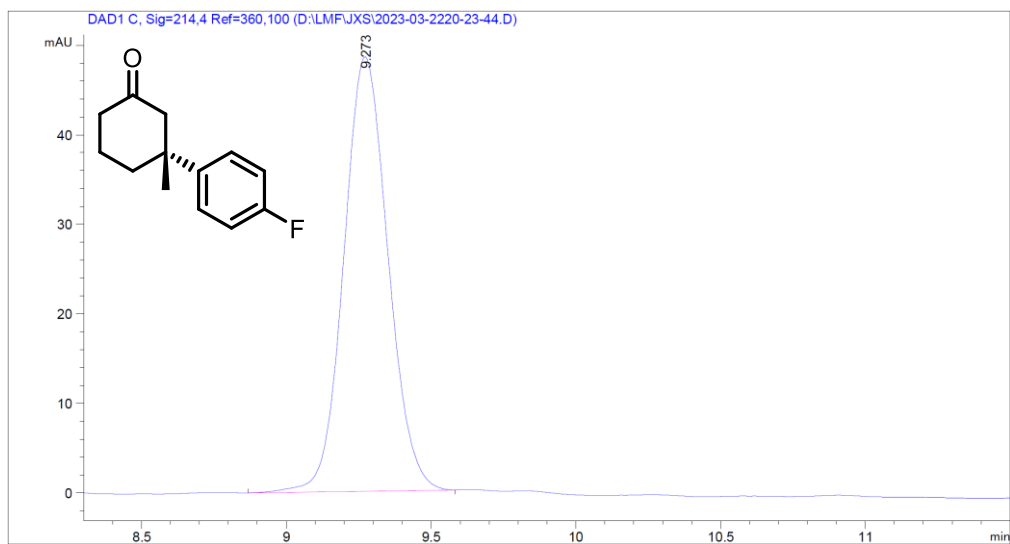


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.422	BB	0.2015	4778.05420	368.00504	96.8922
2	12.941	BB	0.2155	153.25690	11.06999	3.1078

(R)-3-(4-fluorophenyl)-3-methylcyclohexan-1-one (**3n**)

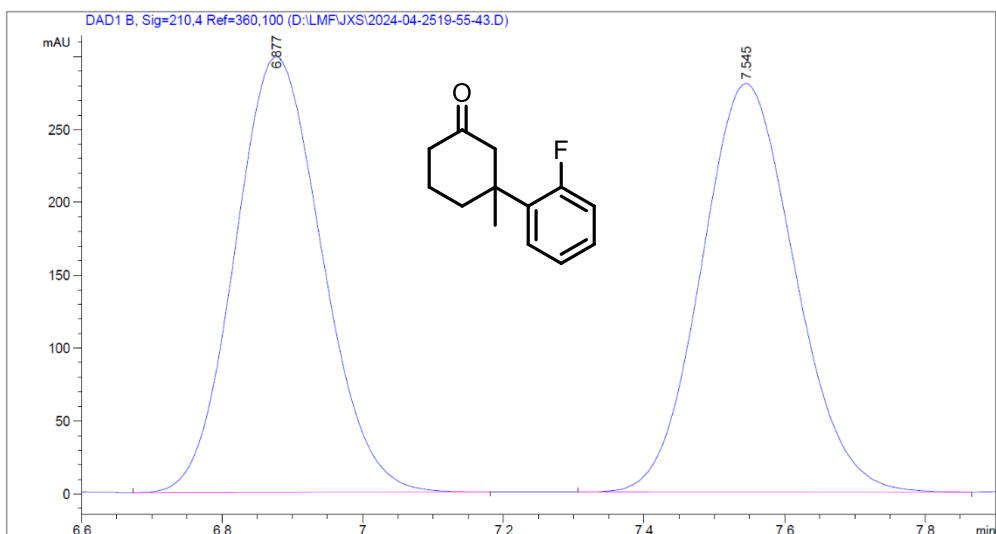


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	9.286	BV	0.1598	3592.74609	344.26984	49.3574
2	9.664	VB	0.1719	3686.29346	331.11444	50.6426

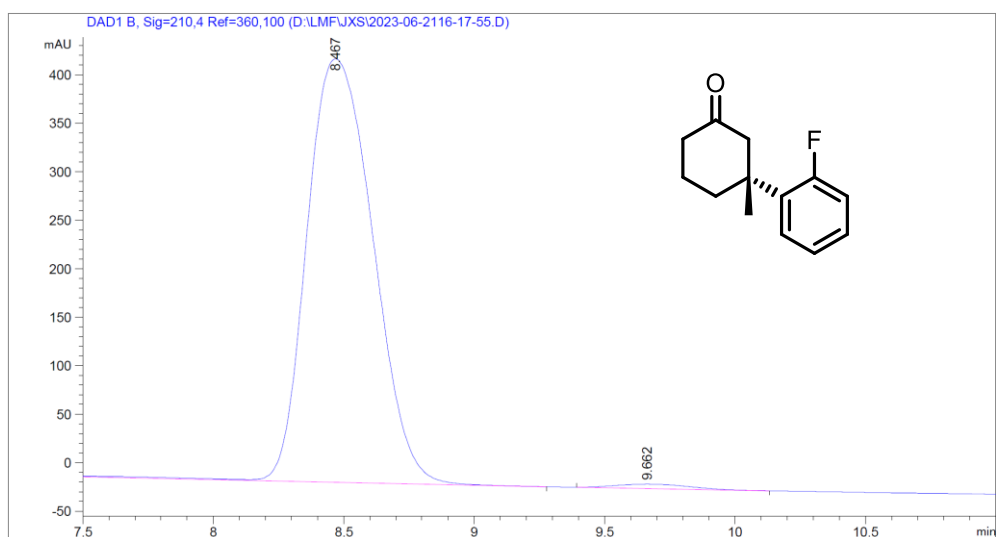


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	9.273	BB	0.1638	514.99512	48.53409	100.0000

(R)-3-(2-fluorophenyl)-3-methylcyclohexan-1-one (**3o**)

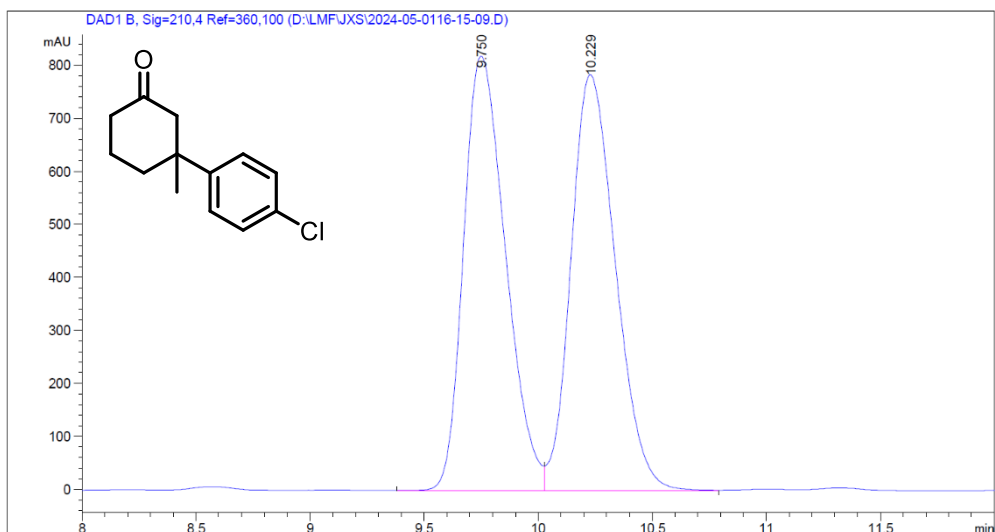


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	6.877	BB	0.1343	2570.87280	299.14127	49.8657
2	7.545	BB	0.1435	2584.72070	280.42950	50.1343

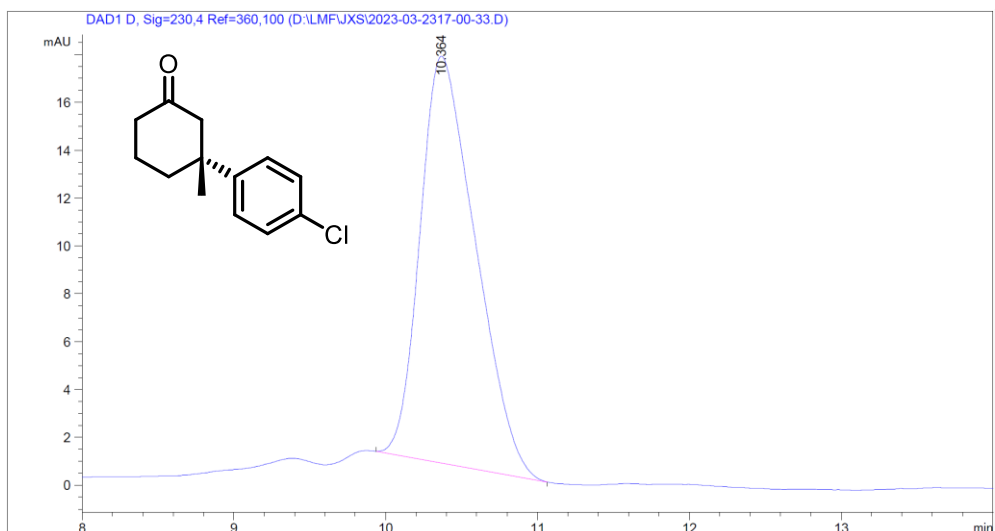


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	8.467	VB R	0.2846	7771.77295	436.76169	98.9011
2	9.662	BB	0.3105	86.35088	4.48724	1.0989

(R)-3-(4-chlorophenyl)-3-methylcyclohexan-1-one (3p)

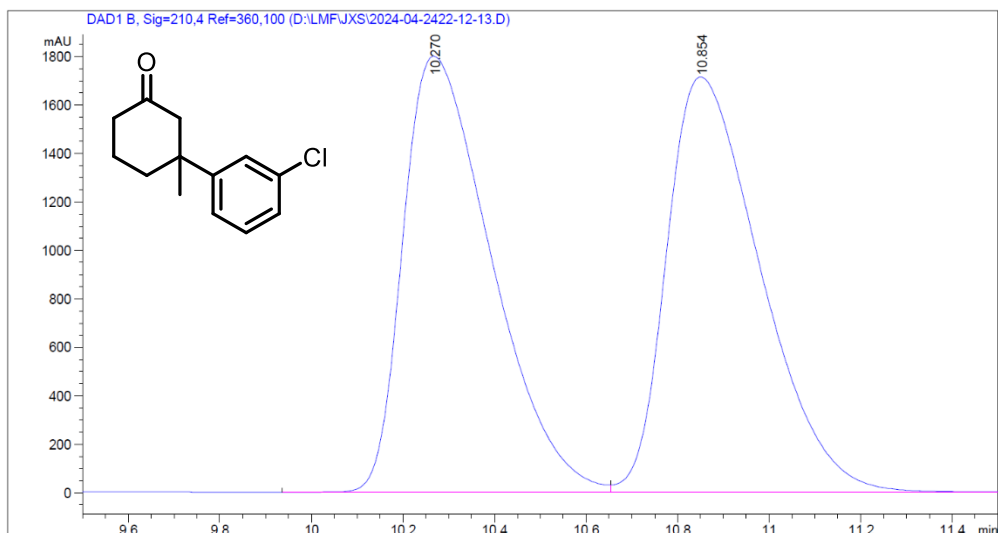


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	9.750	BV	0.1990	1.04720e4	819.69171	49.6400
2	10.229	VB	0.2120	1.06239e4	784.69159	50.3600

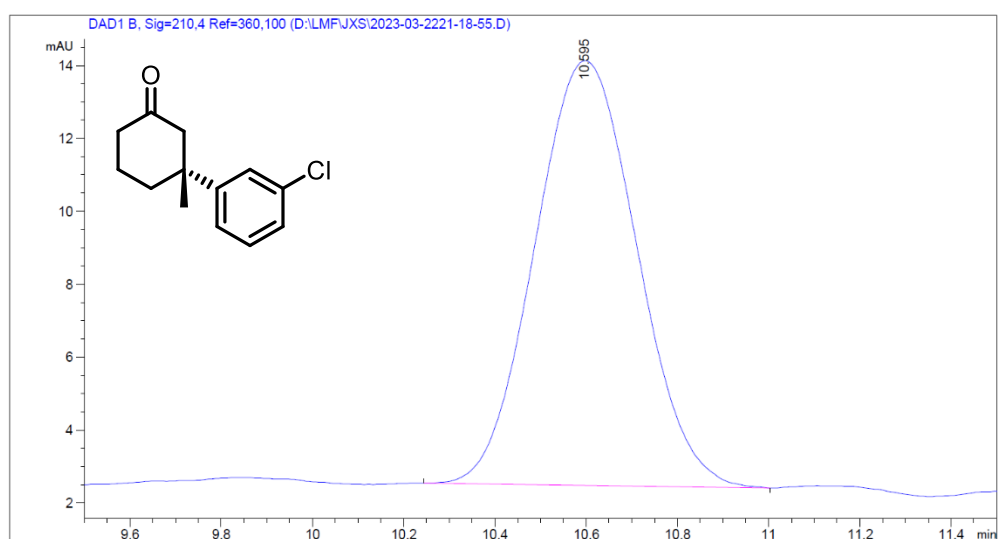


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	10.364	BB	0.3763	431.70779	16.99851	100.0000

(R)-3-(3-chlorophenyl)-3-methylcyclohexan-1-one (**3q**)

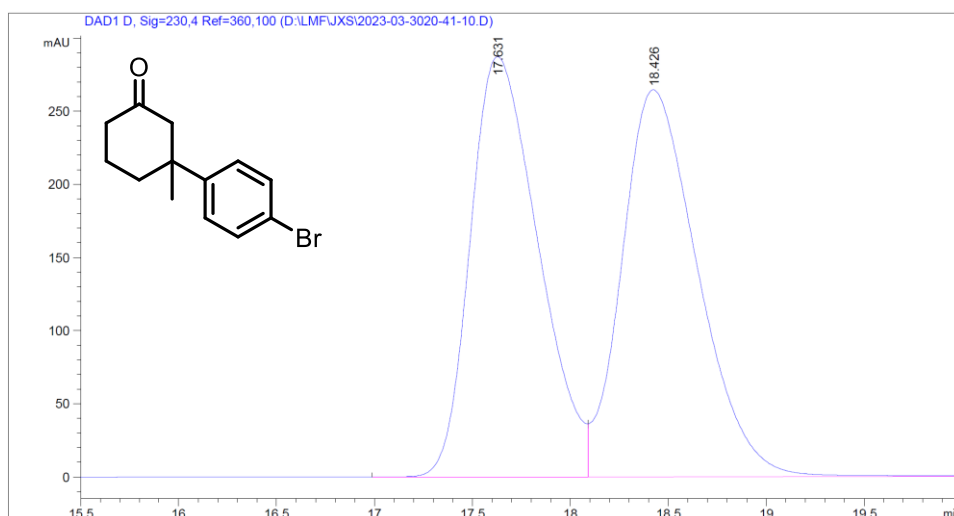


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	10.270	BV	0.2082	2.41030e4	1800.02795	49.3870
2	10.854	VV R	0.2220	2.47014e4	1715.01672	50.6130

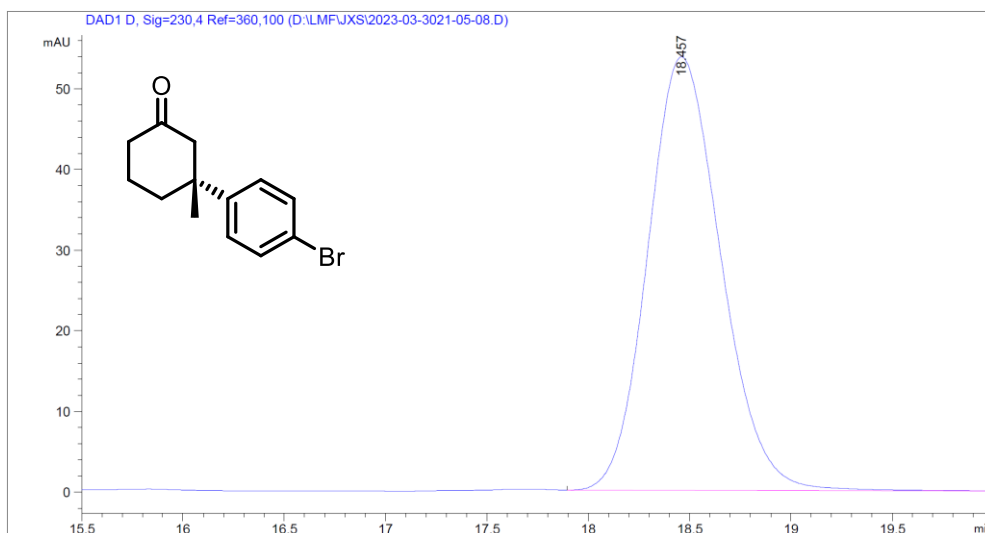


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	10.595	BB	0.2452	180.95967	11.65116	100.0000

(R)-3-(4-bromophenyl)-3-methylcyclohexan-1-one (**3r**)

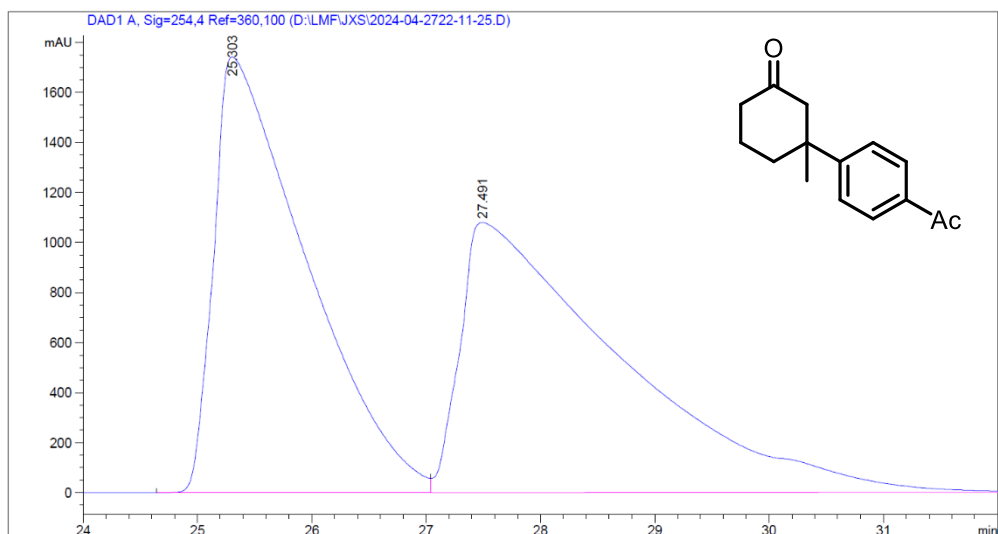


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	17.631	BV	0.3745	6910.68994	287.43448	49.0650
2	18.426	VB	0.4162	7174.08203	264.70789	50.9350

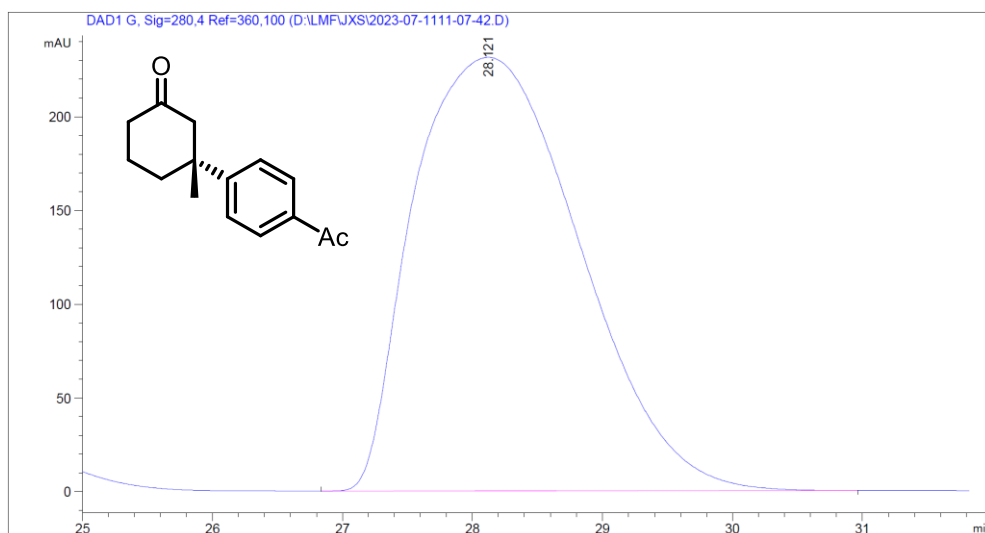


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	18.457	BB	0.3882	1346.72754	53.76304	100.0000

(R)-3-(4-acetylphenyl)-3-methylcyclohexan-1-one (**3s**)

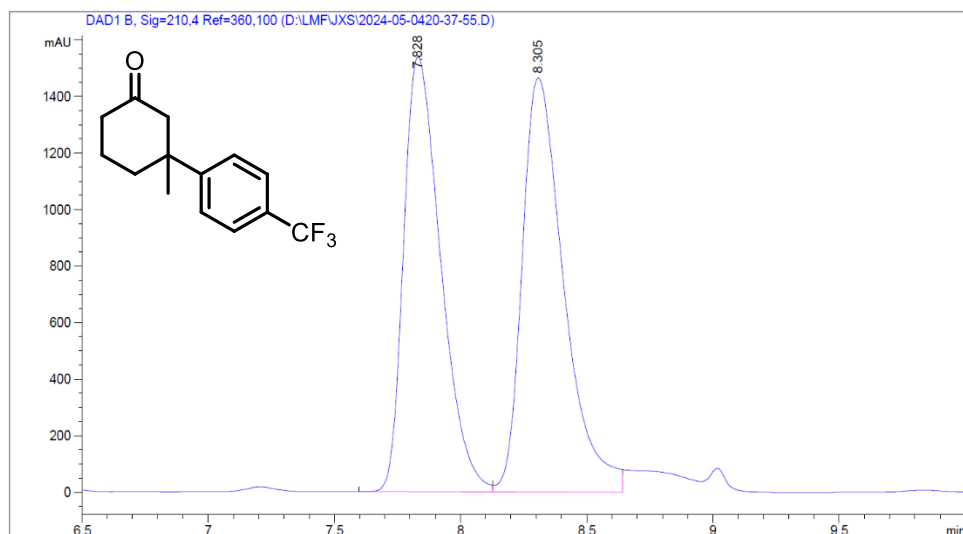


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	25.303	BV	0.7767	9.80792e4	1742.55627	48.2275
2	27.491	VB	1.2752	1.05288e5	1080.16321	51.7725

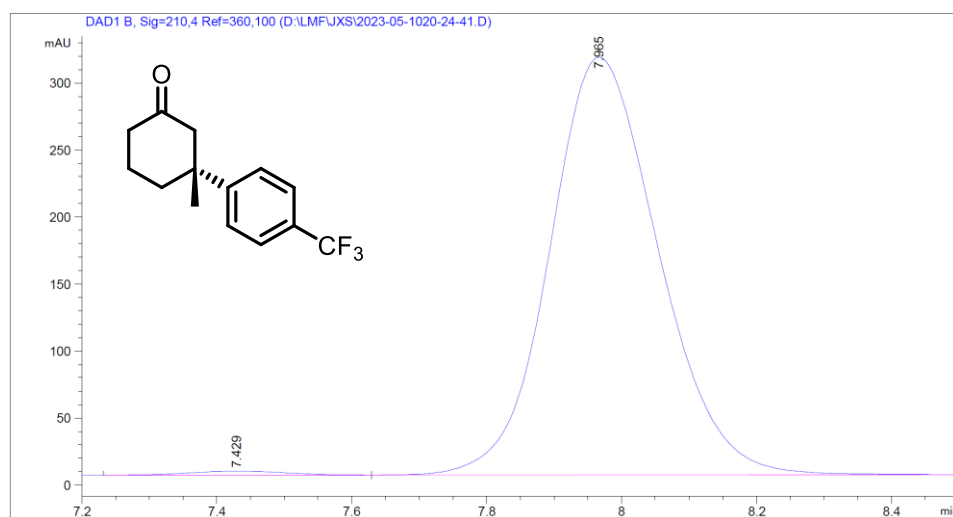


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	28.121	BB	1.4584	2.04975e4	231.19427	100.0000

(R)-3-methyl-3-(4-(trifluoromethyl)phenyl)cyclohexan-1-one (**3t**)

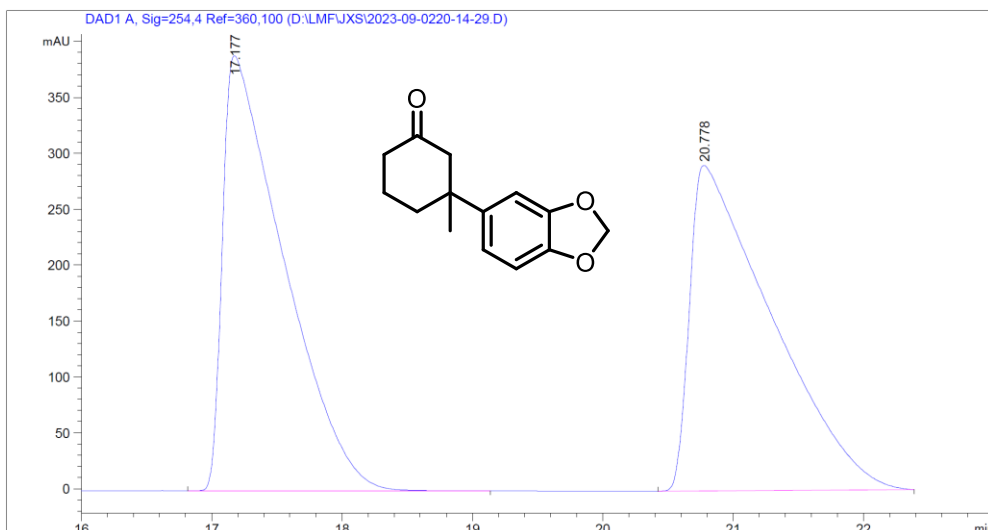


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	7.828	BV	0.1589	1.56764e4	1537.82813	48.2536
2	8.305	MF R	0.1911	1.68111e4	1466.50452	51.7464

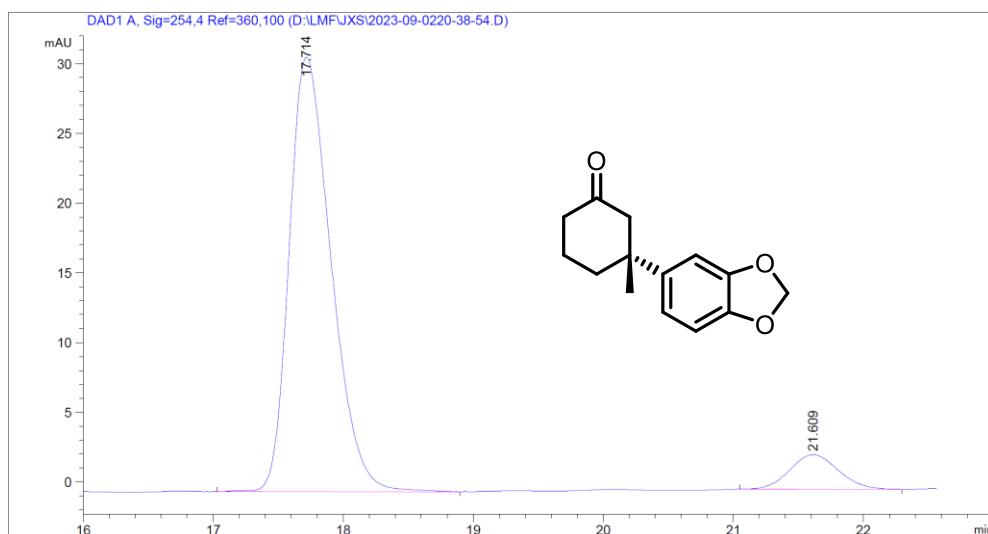


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	7.429	BV	0.1574	28.12093	2.89367	0.7990
2	7.965	VB	0.1746	3491.44189	311.93567	99.2010

(R)-3-(benzo[d][1,3]dioxol-5-yl)-3-methylcyclohexan-1-one (**3u**)

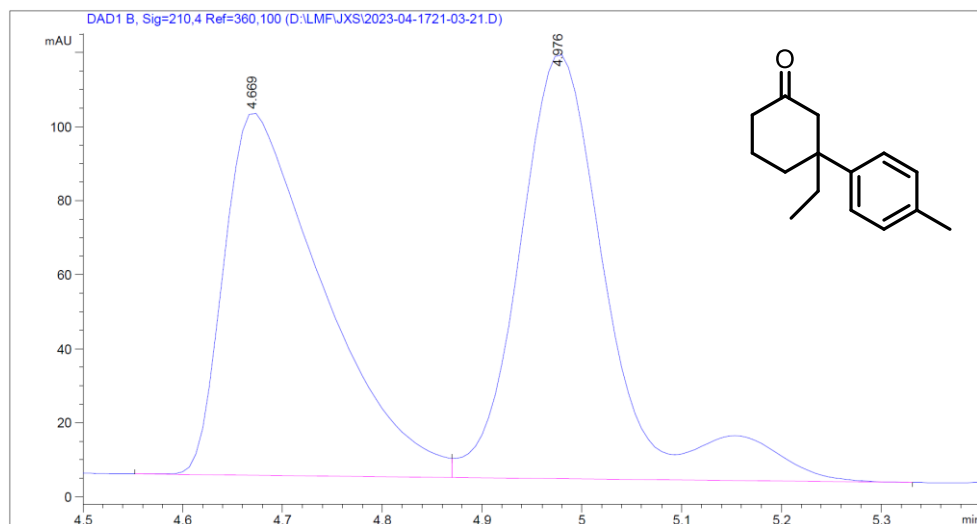


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	17.177	BB	0.4699	1.26600e4	388.78903	50.0229
2	20.778	BBA	0.6092	1.26484e4	290.91345	49.9771

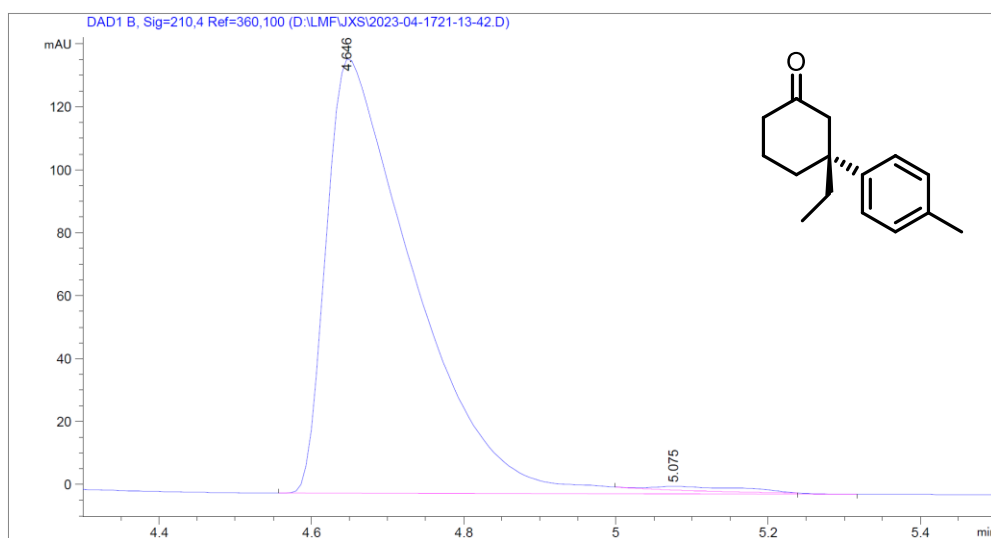


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	17.714	BB	0.3450	696.95135	31.15928	91.5366
2	21.609	BB	0.3893	64.43932	2.47844	8.4634

(R)-3-ethyl-3-(*p*-tolyl)cyclohexan-1-one (**3w**)

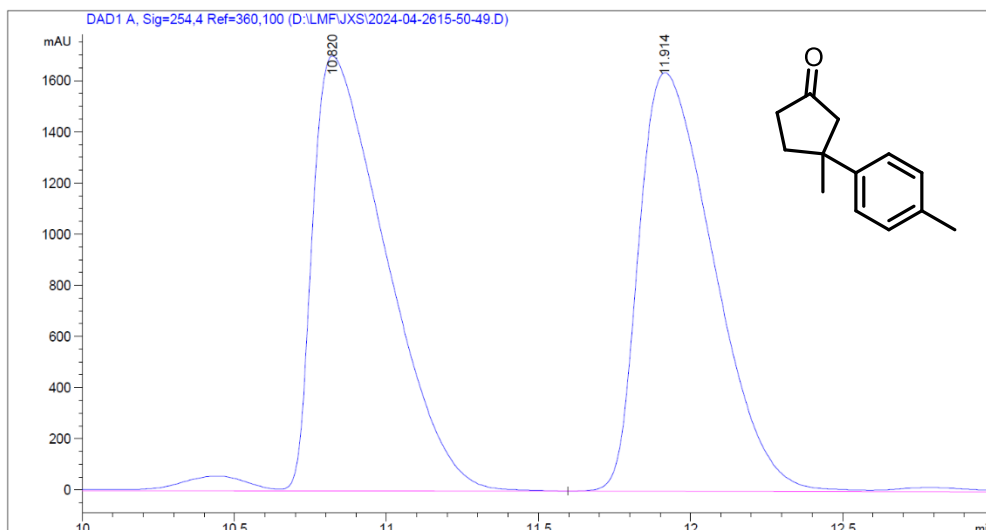


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	4.669	BV	0.1029	679.07574	97.95215	48.5656
2	4.976	VV R	0.0859	719.18774	114.70428	51.4344

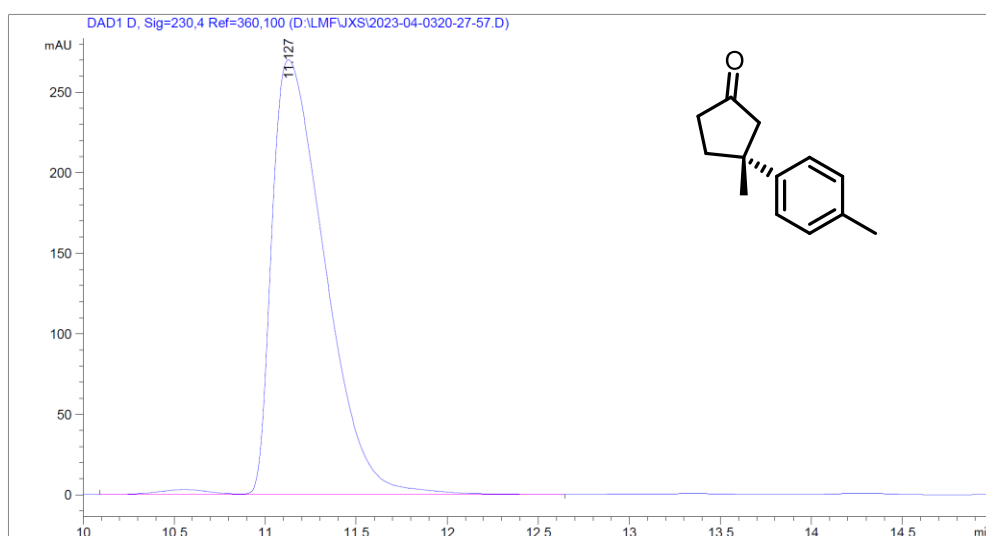


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	4.646	BV R	0.1157	1111.67126	138.39980	98.9945
2	5.075	VB E	0.1297	11.29128	1.13839	1.0055

(R)-3-methyl-3-(*p*-tolyl)cyclopentan-1-one (**3x**)

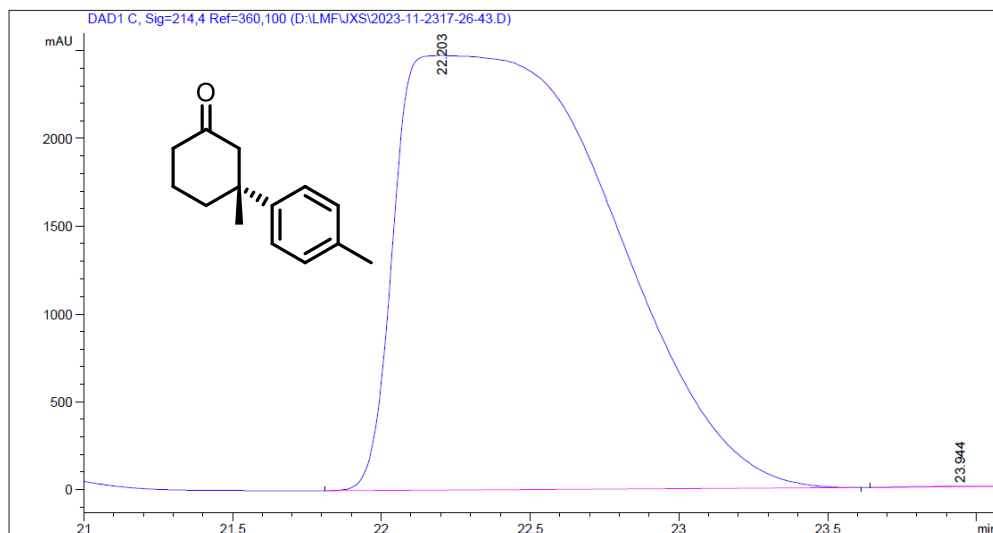


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	10.820	VB R	0.2607	2.93933e4	1701.14917	50.8610
2	11.914	BV R	0.2709	2.83981e4	1636.48816	49.1390



Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.127	VB R	0.3169	5495.48291	270.08997	100.0000

Scale-Up Experiment for the Synthesis of **3a**.

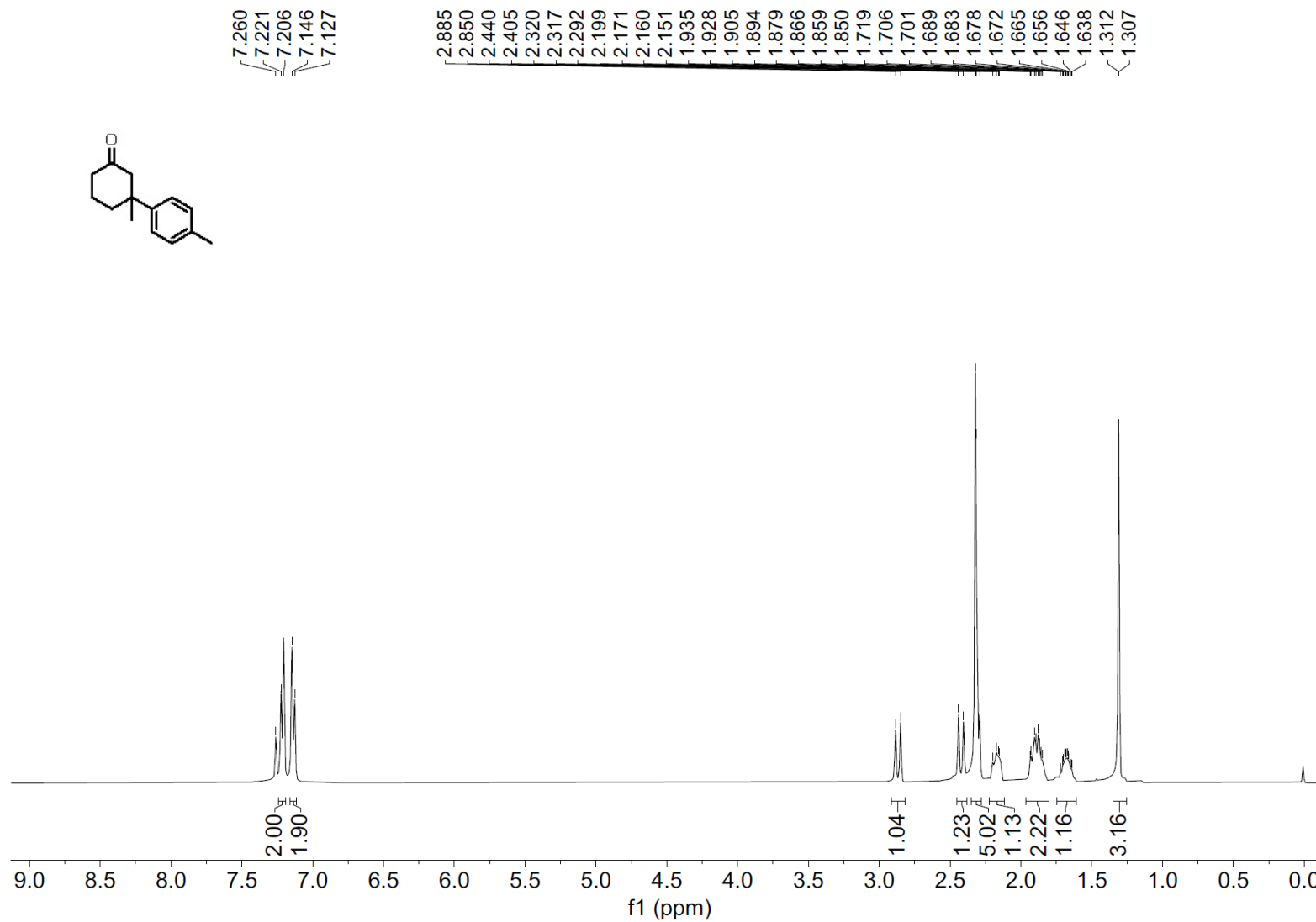


Peak	Retention time	type	width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	22.203	BB	0.5987	1.24508e5	2475.69897	99.9632
2	23.944	BBA	0.2680	45.78139	2.64376	0.0368

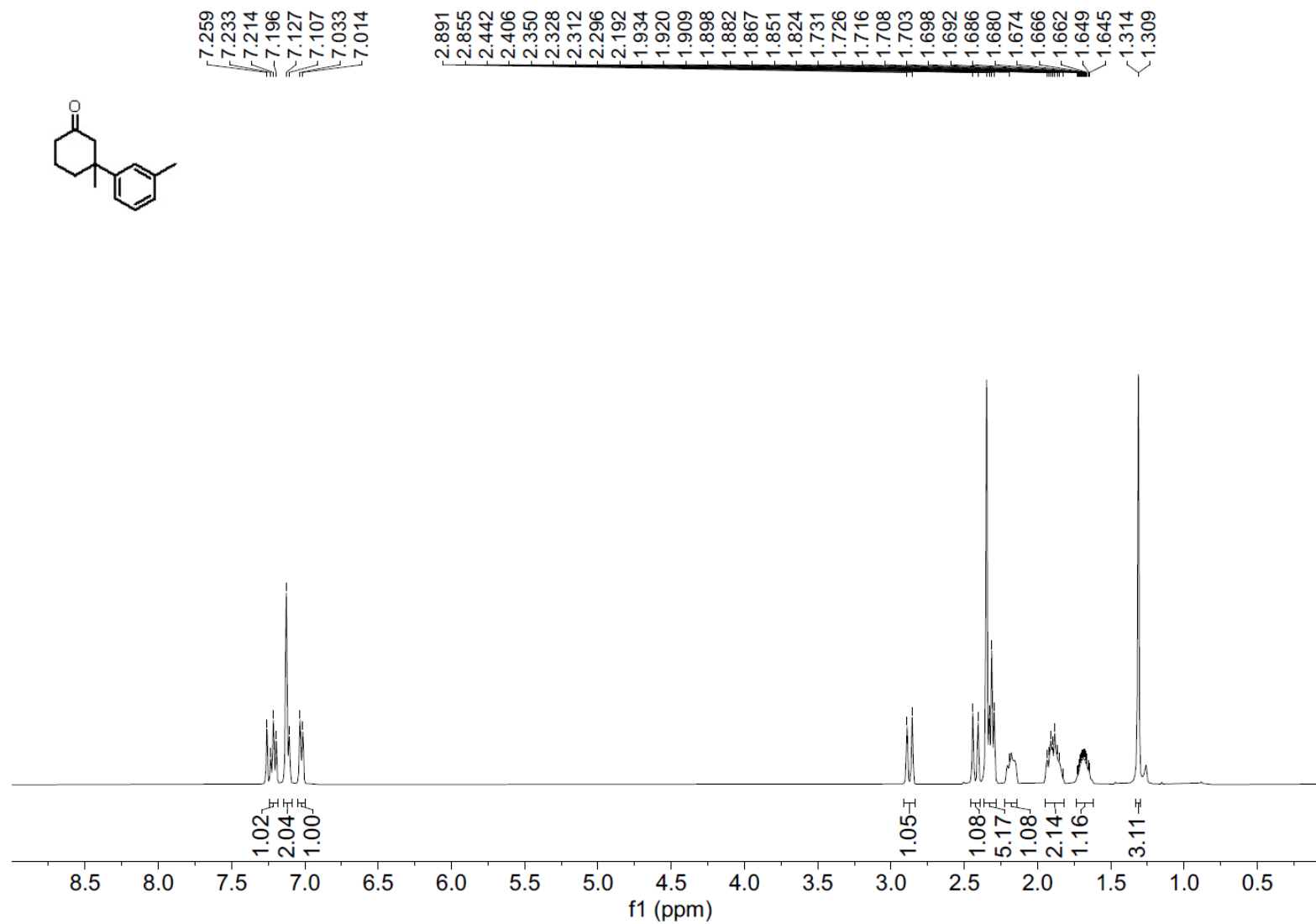
Reference

- Wang, J.-Y.; Li, C.-L.; Xu, T.; Li, M.-F.; Hao, W.-J.; Tu, S.-J.; Wang, J.; Li, G.; Yu, Z.-X.; Jiang, B. Catalytic Enantioselective Construction of 6-4 Ring-Junction All-Carbon Stereocenters and Mechanistic Insights. *Chin. J. Chem.* **2022**, *40*, 1767-1776.

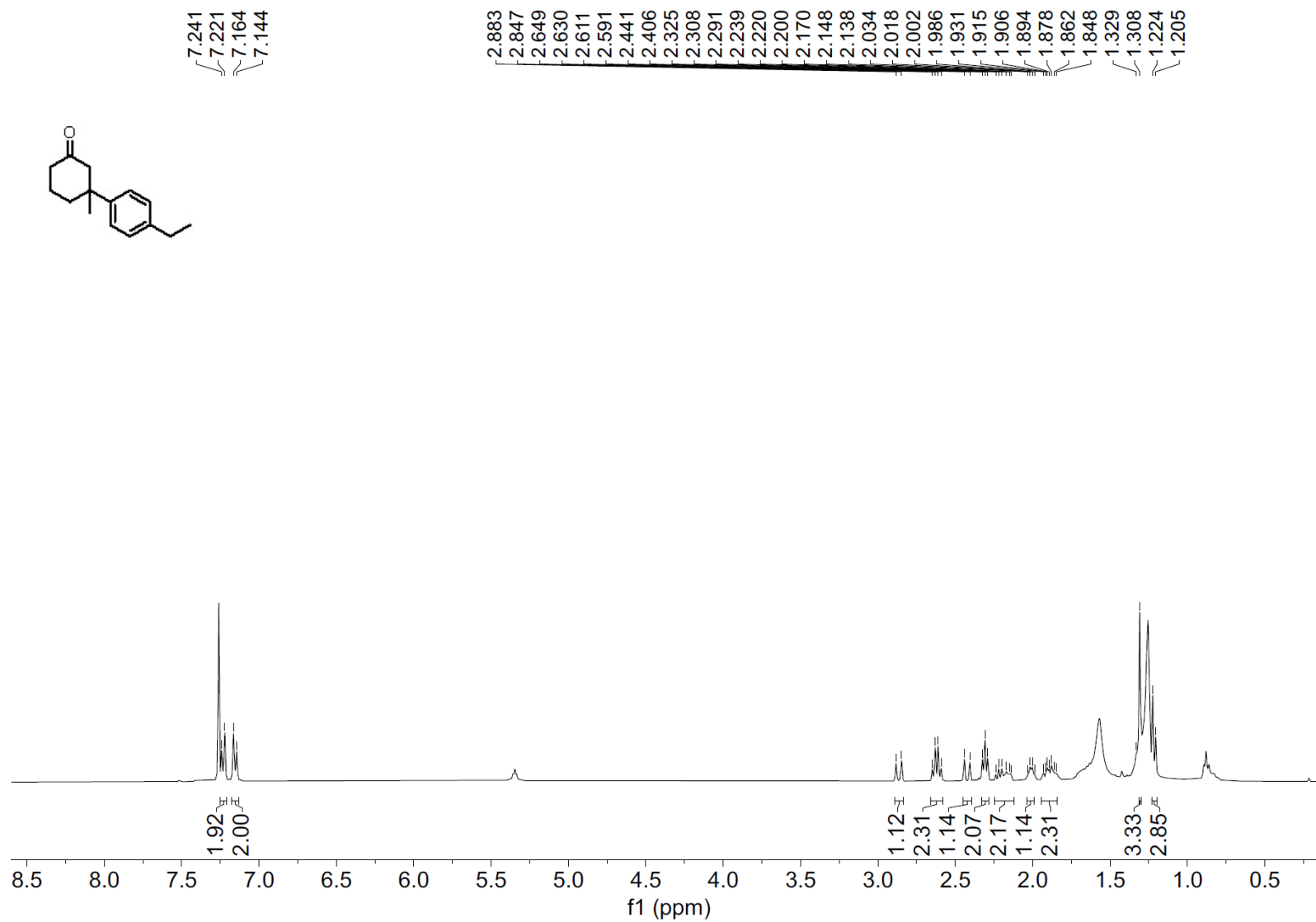
¹H and ¹³C NMR Spectra for Products 3



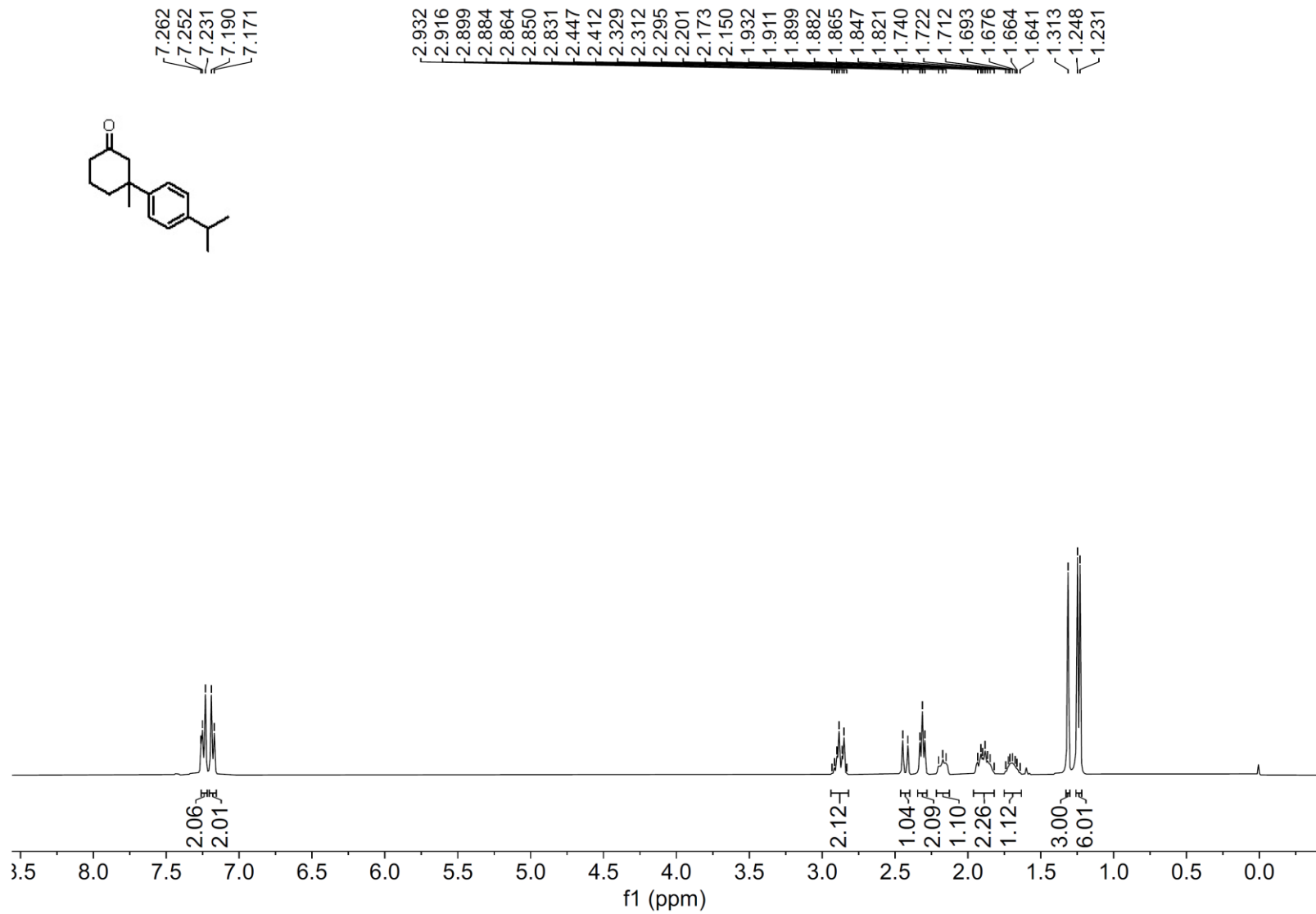
¹H NMR Spectrum of Compound 3a (CDCl₃, 400 MHz)



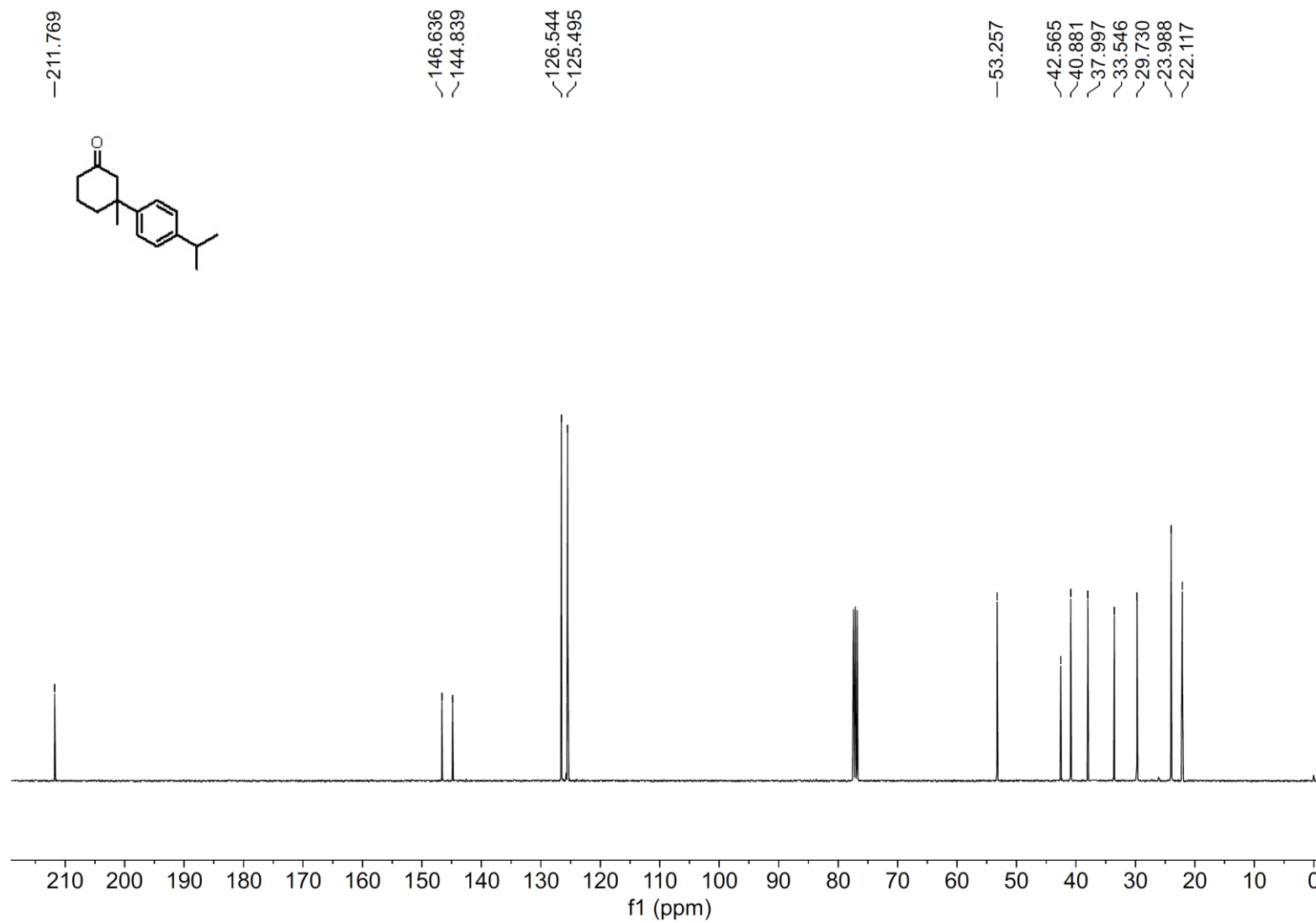
¹H NMR Spectrum of Compound 3b (CDCl₃, 400 MHz)



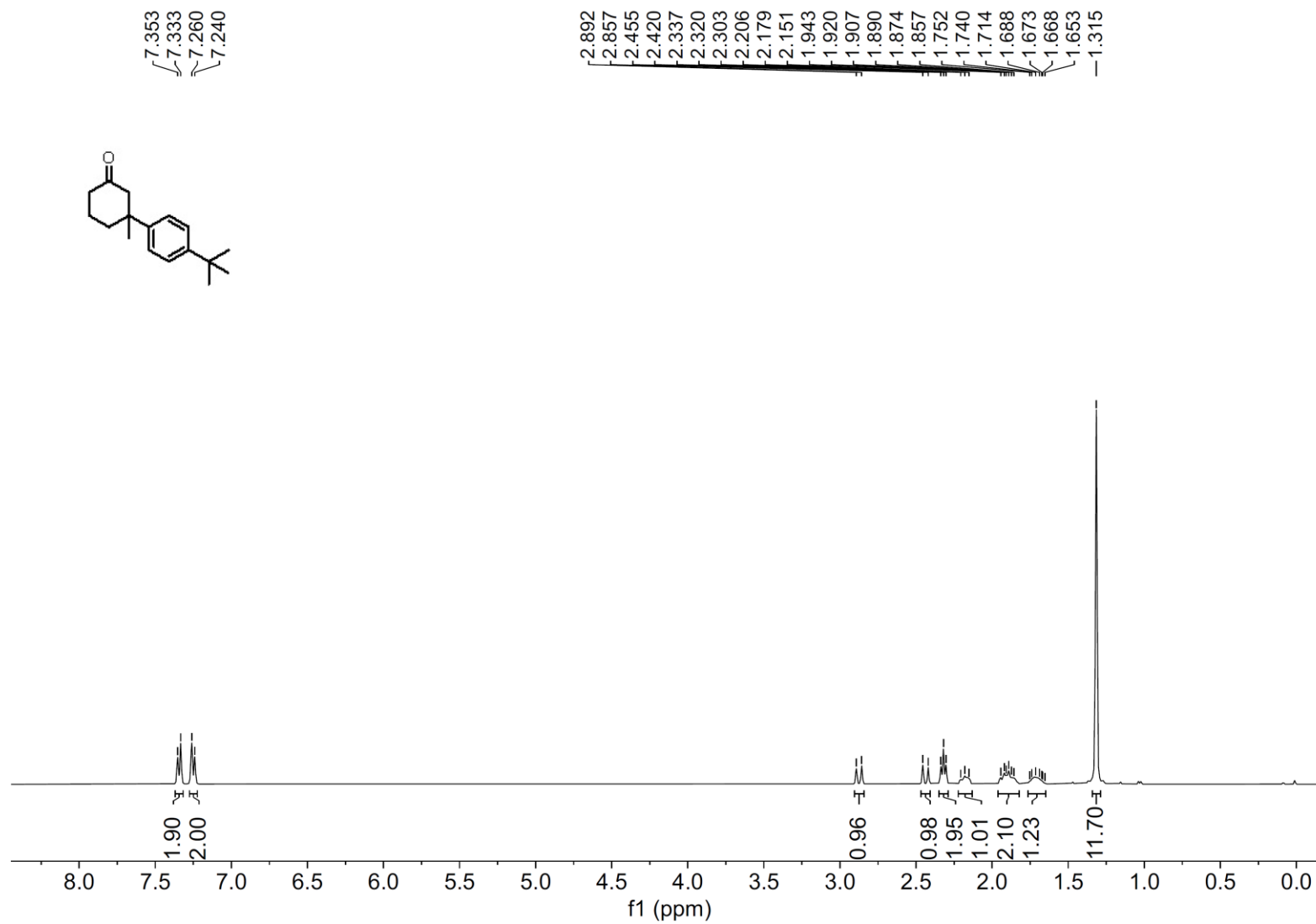
¹H NMR Spectrum of Compound 3c (CDCl₃, 400 MHz)



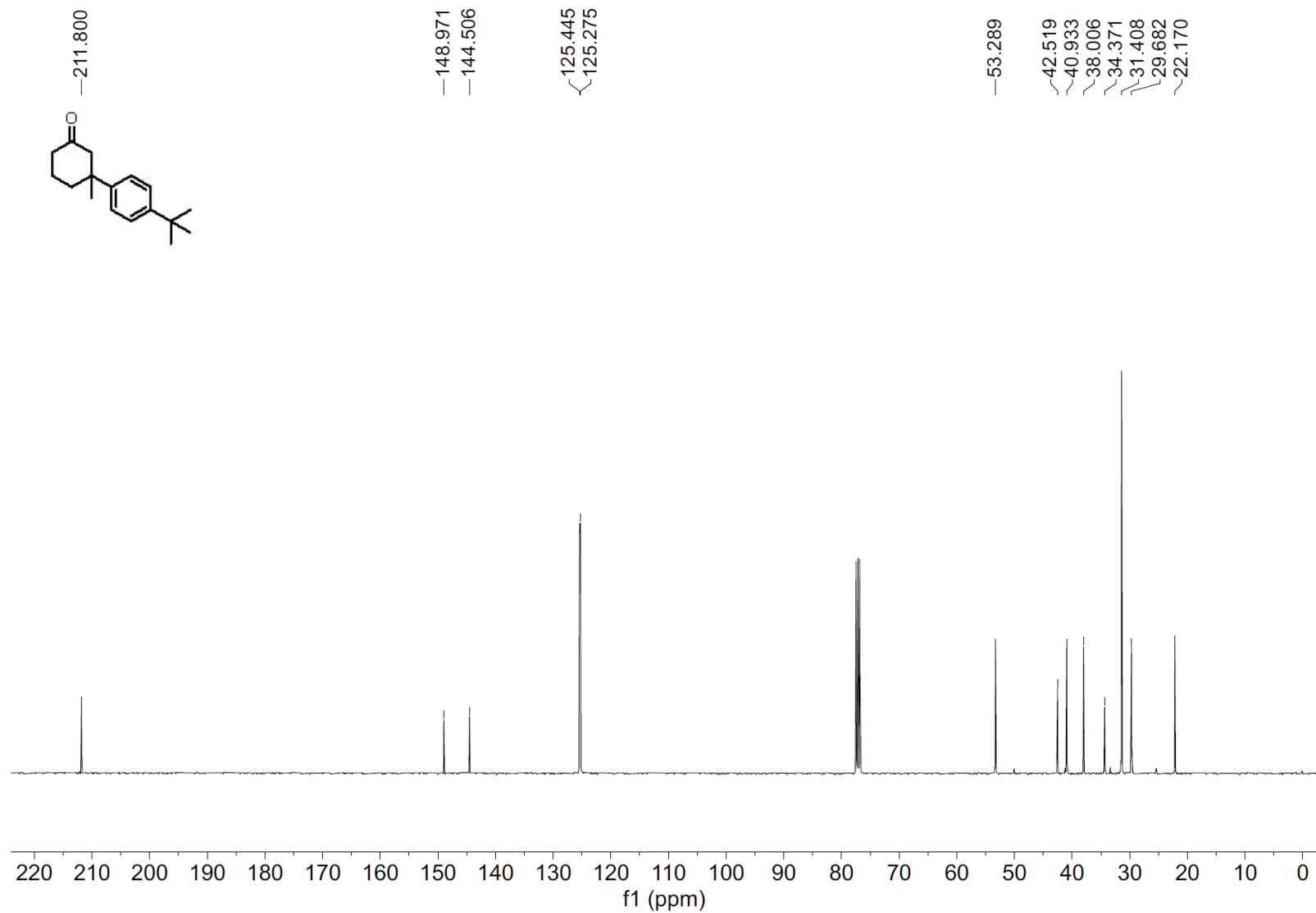
¹H NMR Spectrum of Compound 3d (CDCl₃, 400 MHz)



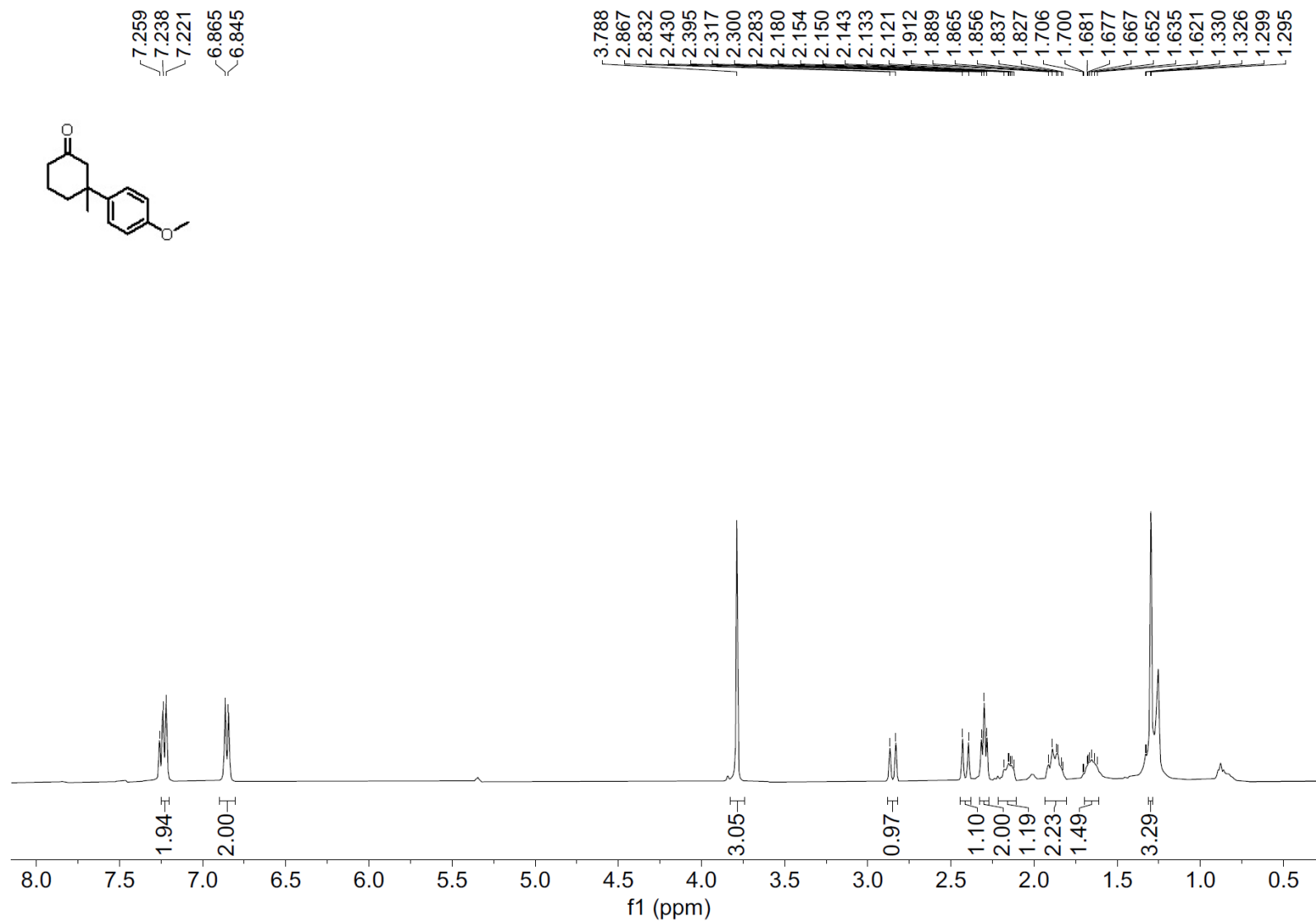
$^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of Compound 3d (CDCl_3 , 100 MHz)



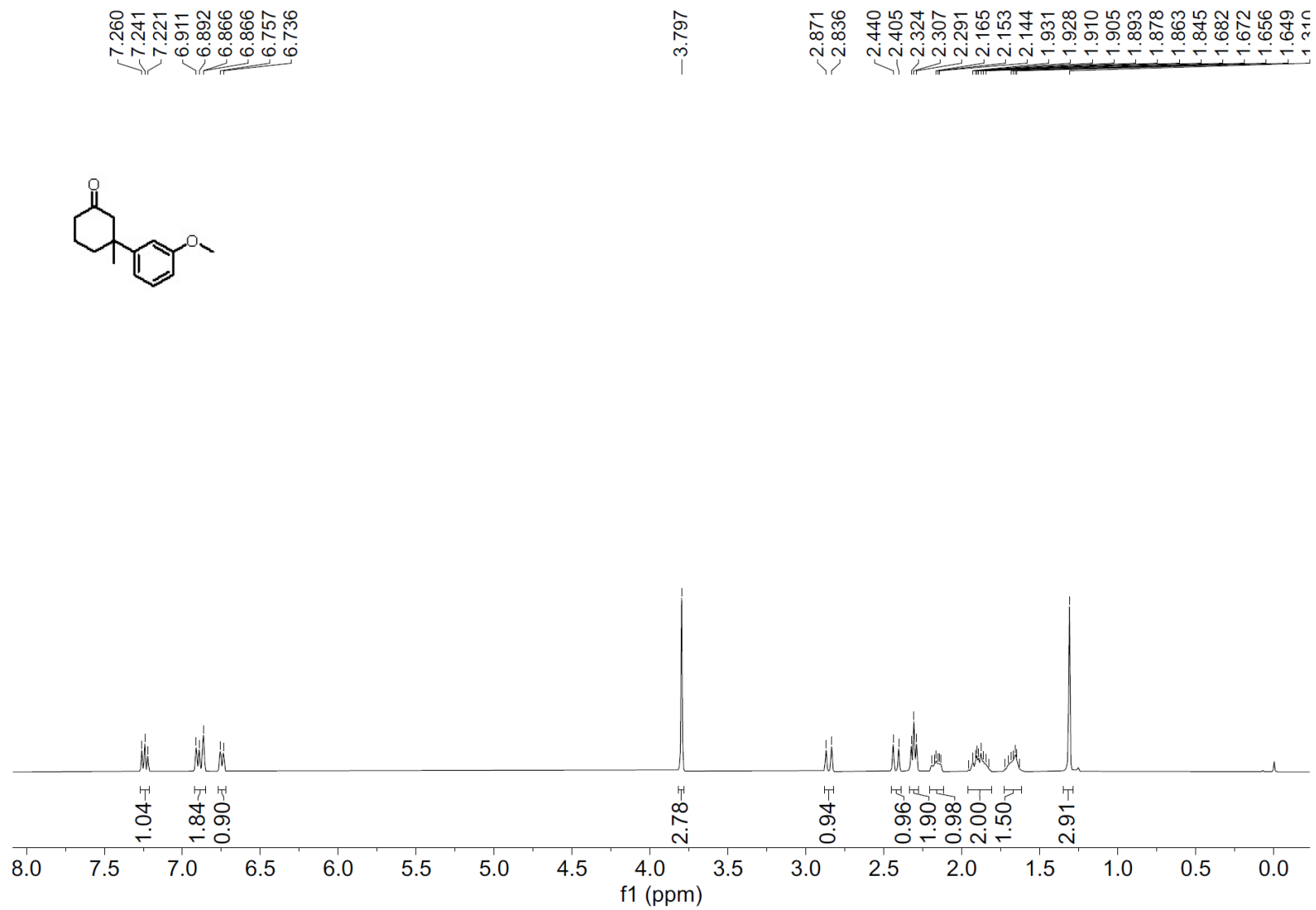
¹H NMR Spectrum of Compound 3e (CDCl₃, 400 MHz)

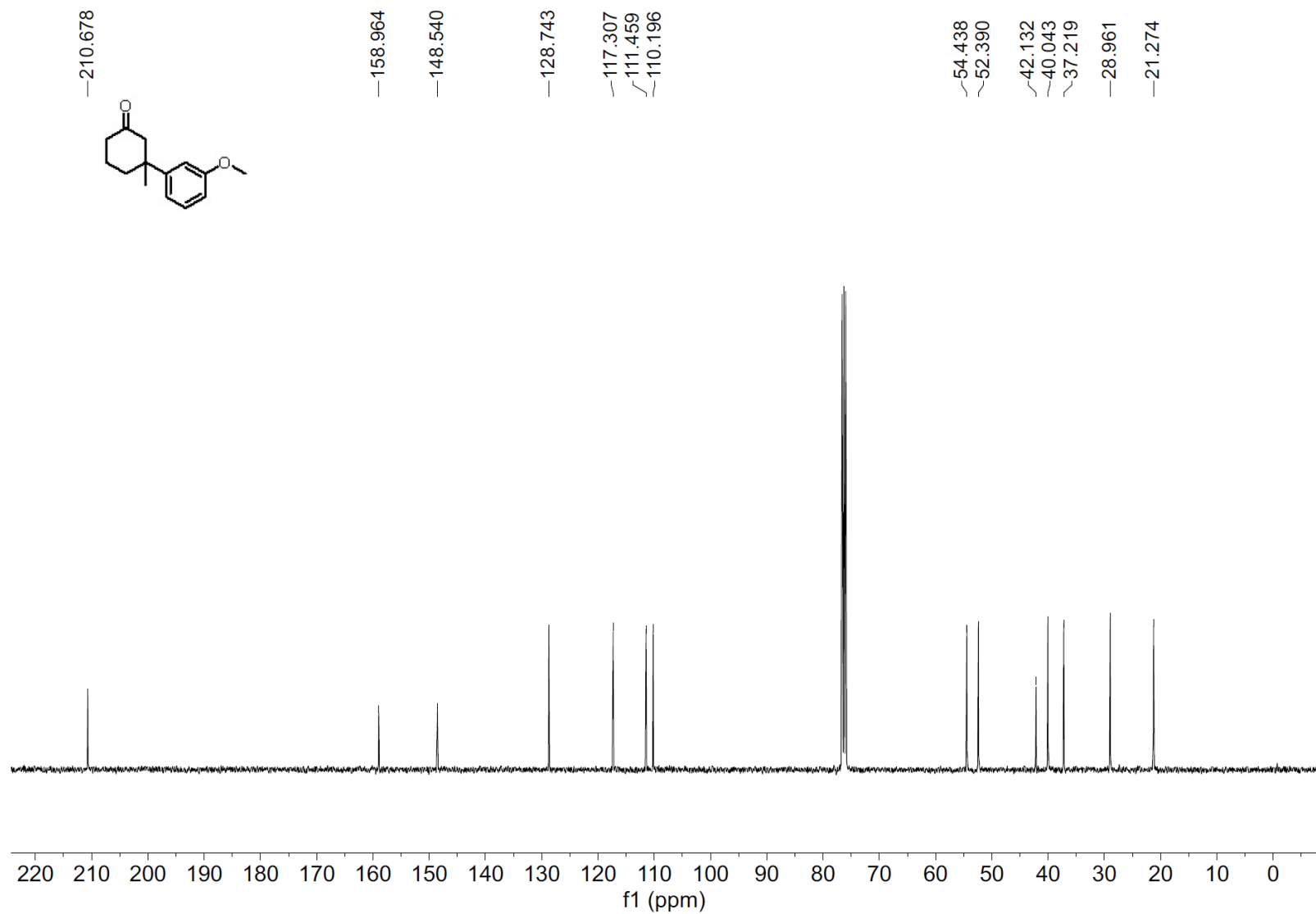


$^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of Compound 3e (CDCl_3 , 100 MHz)

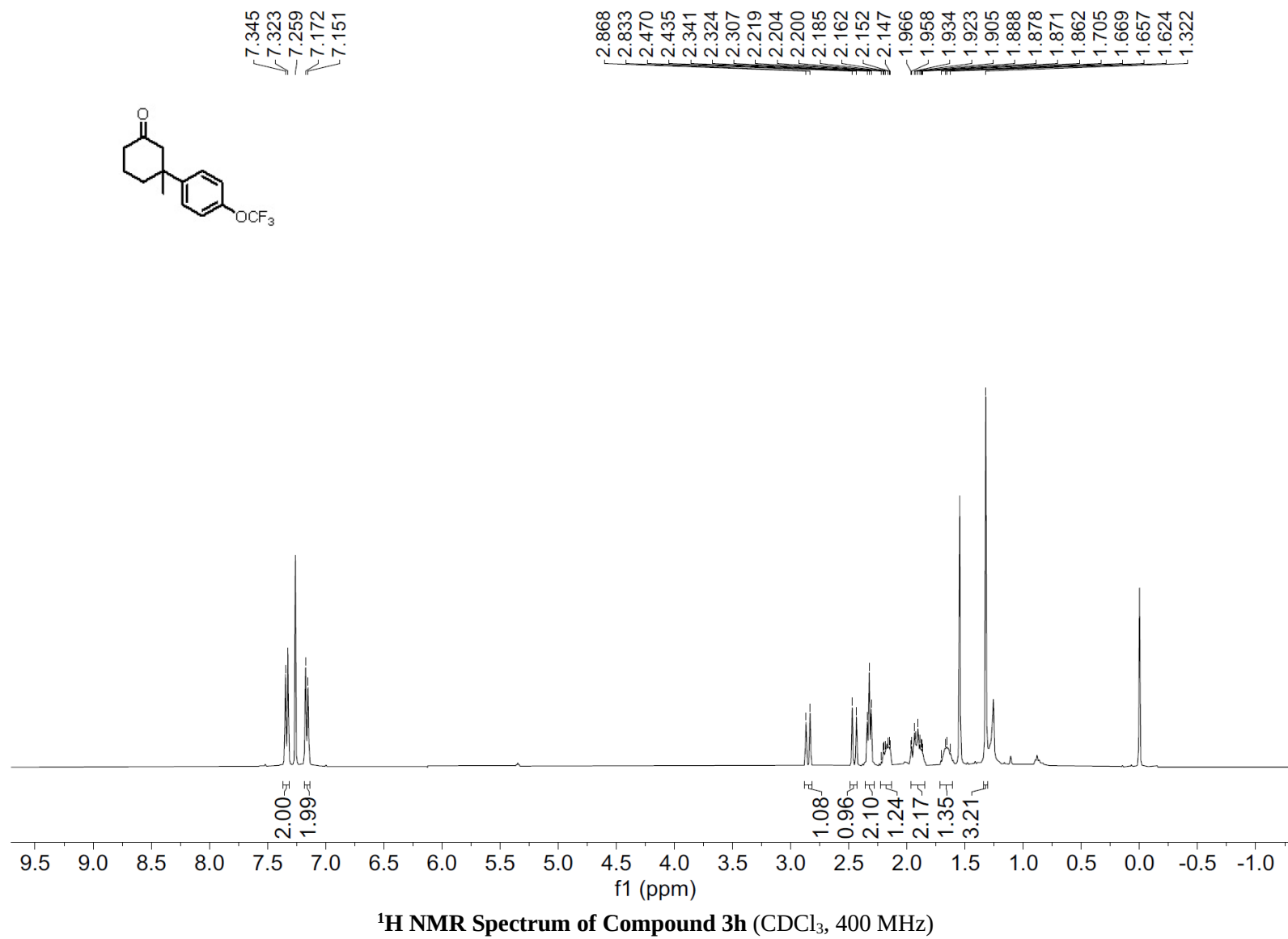


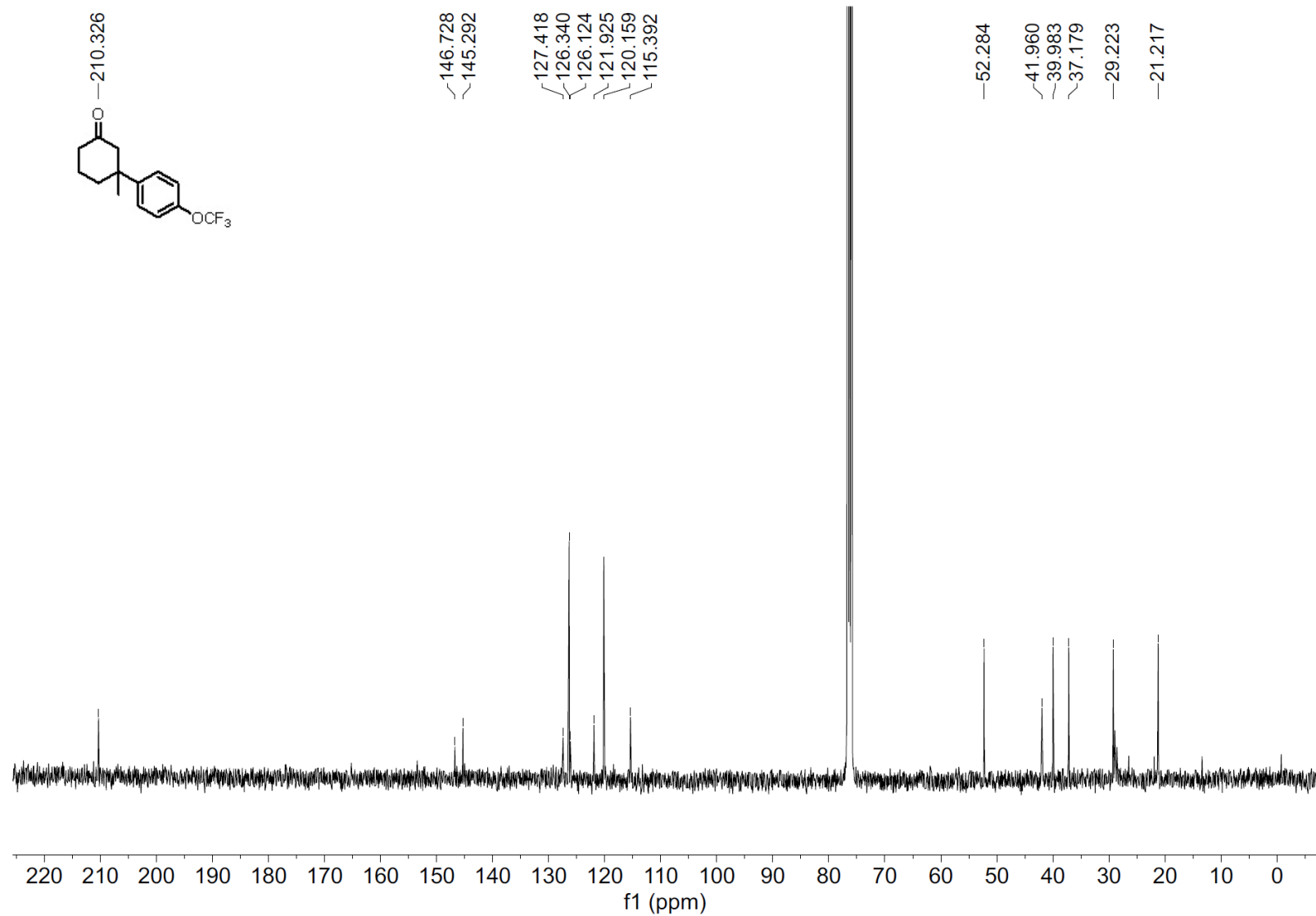
¹H NMR Spectrum of Compound 3f (CDCl₃, 400 MHz)



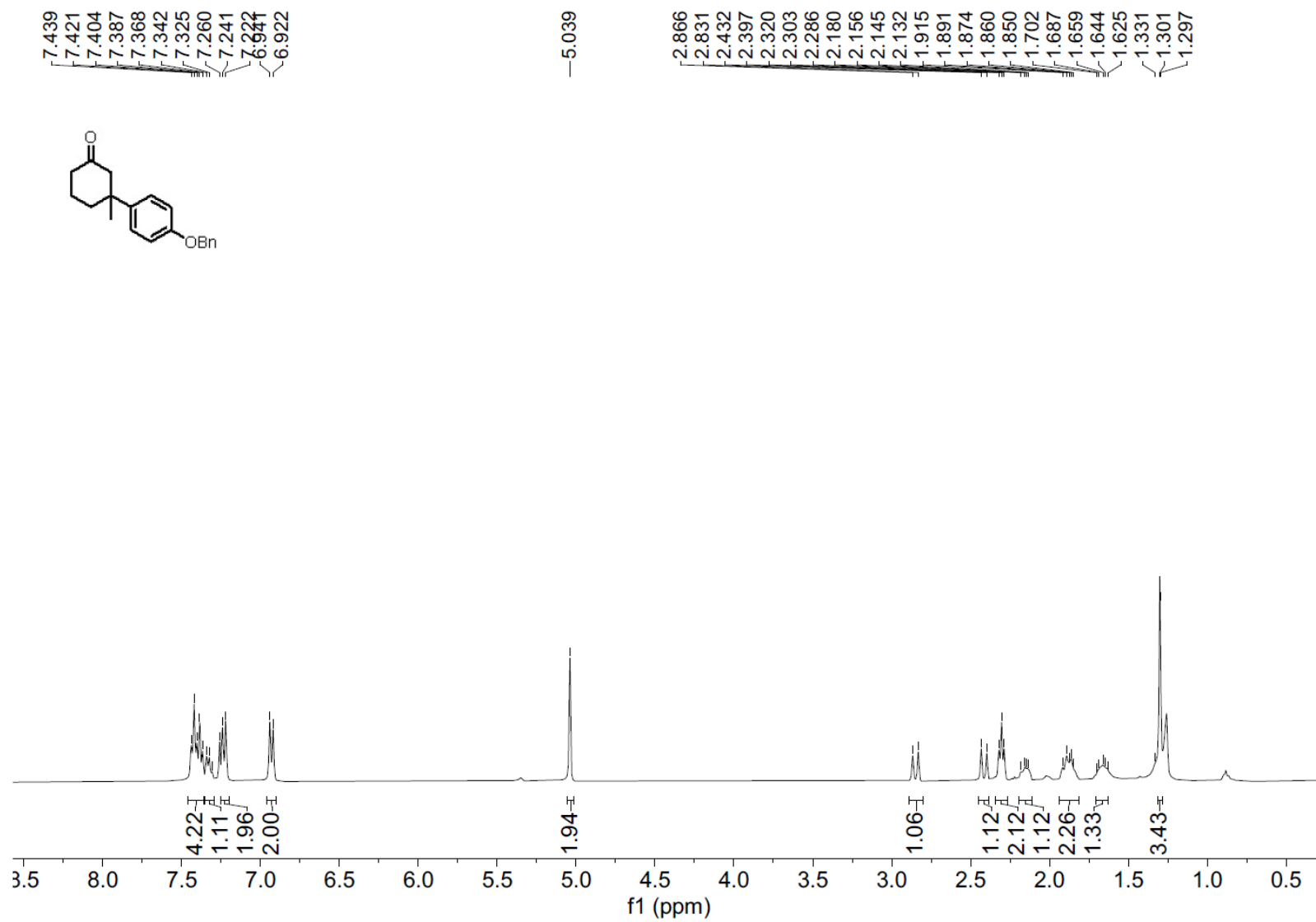


$^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of Compound 3g (CDCl_3 , 100 MHz)

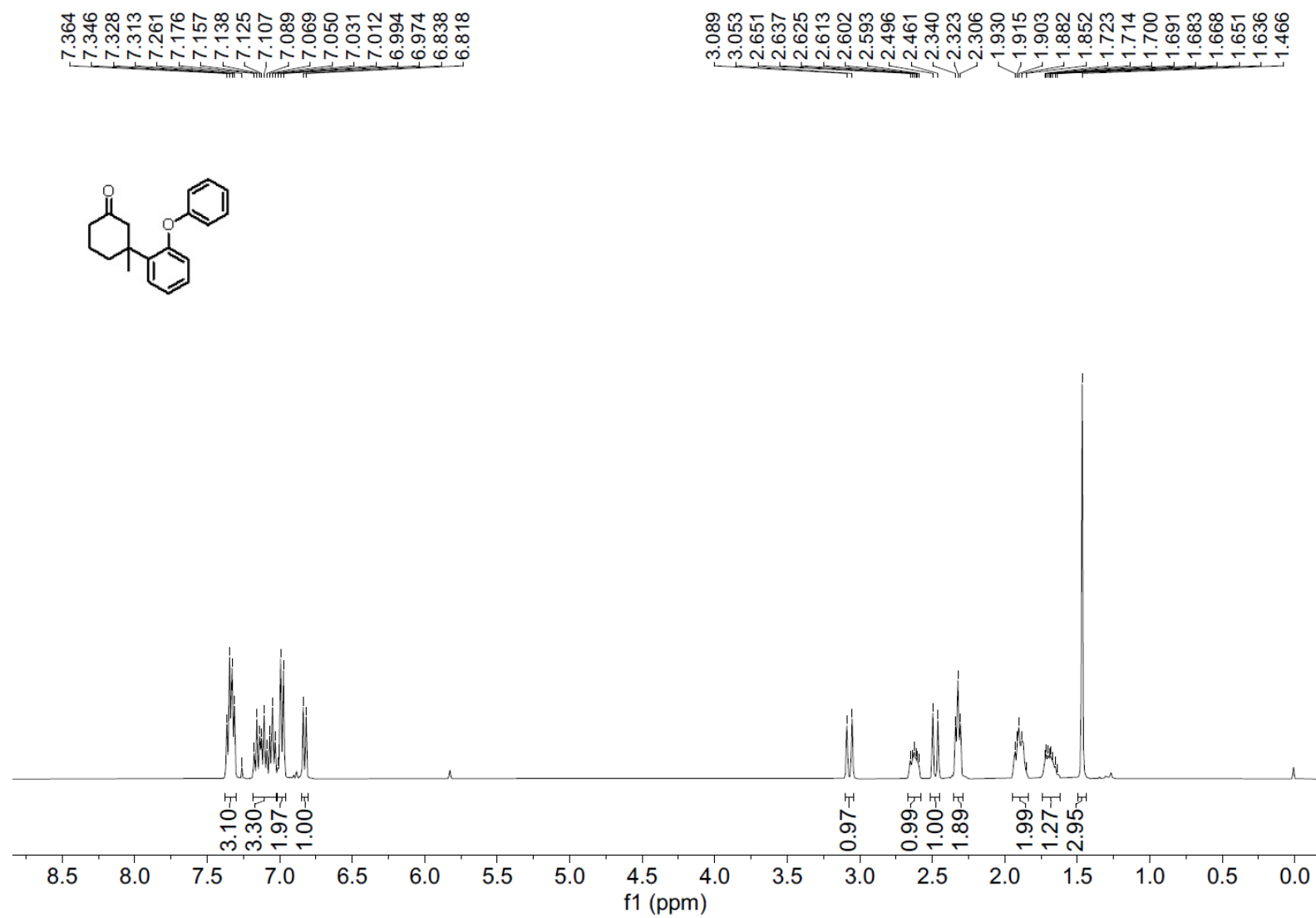


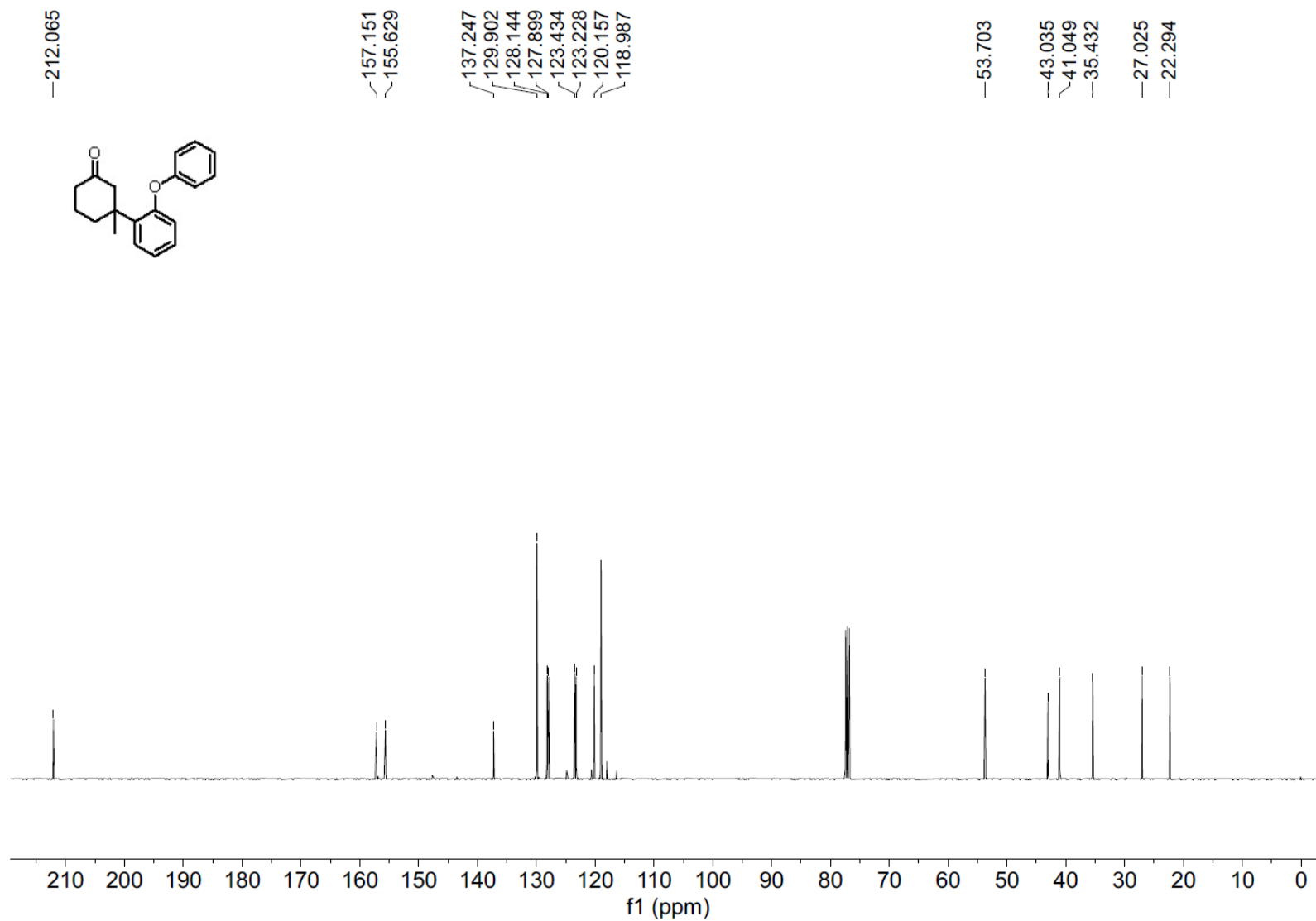


$^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of Compound 3h (CDCl_3 , 100 MHz)

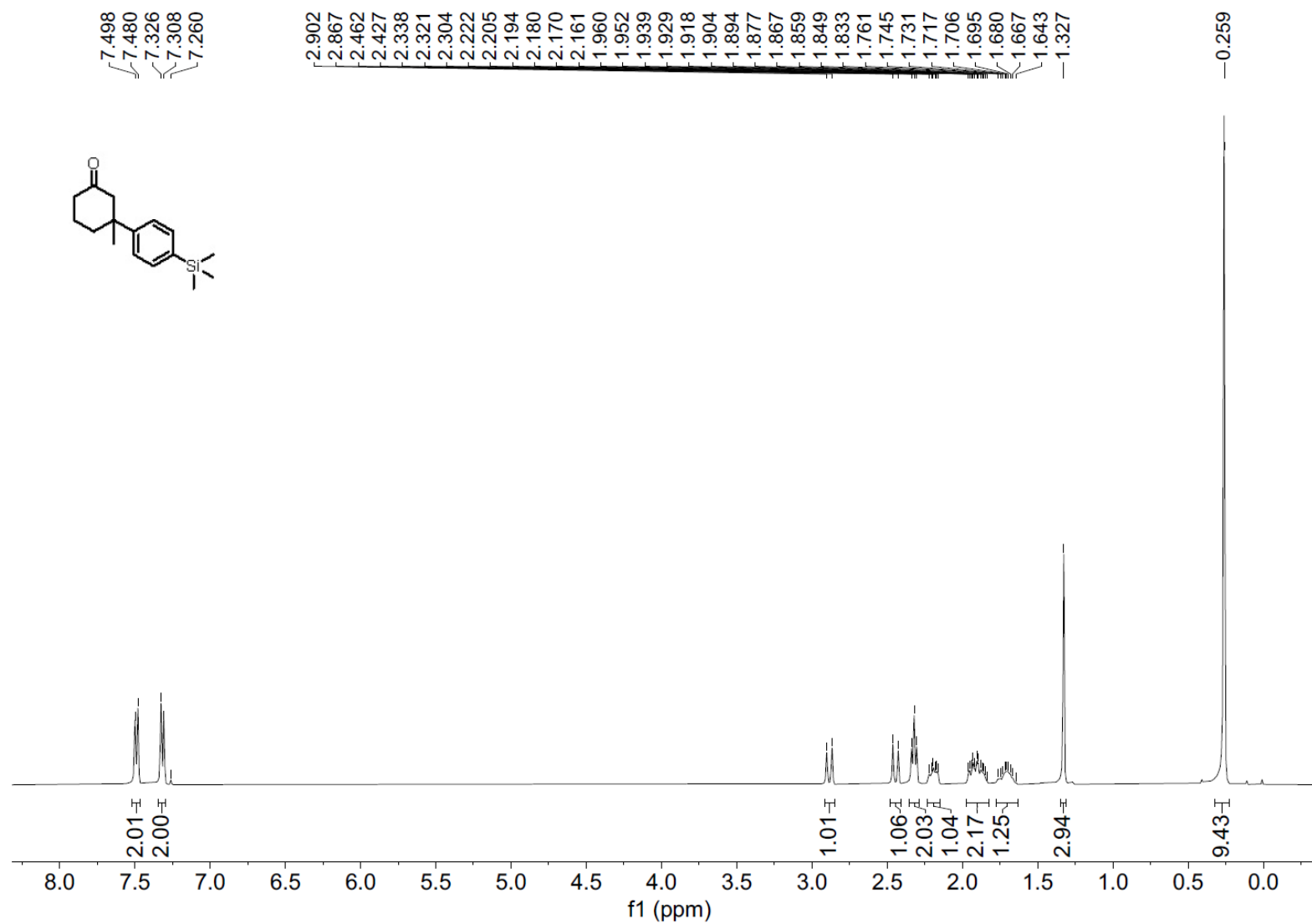


¹H NMR Spectrum of Compound 3i (CDCl₃, 400 MHz)

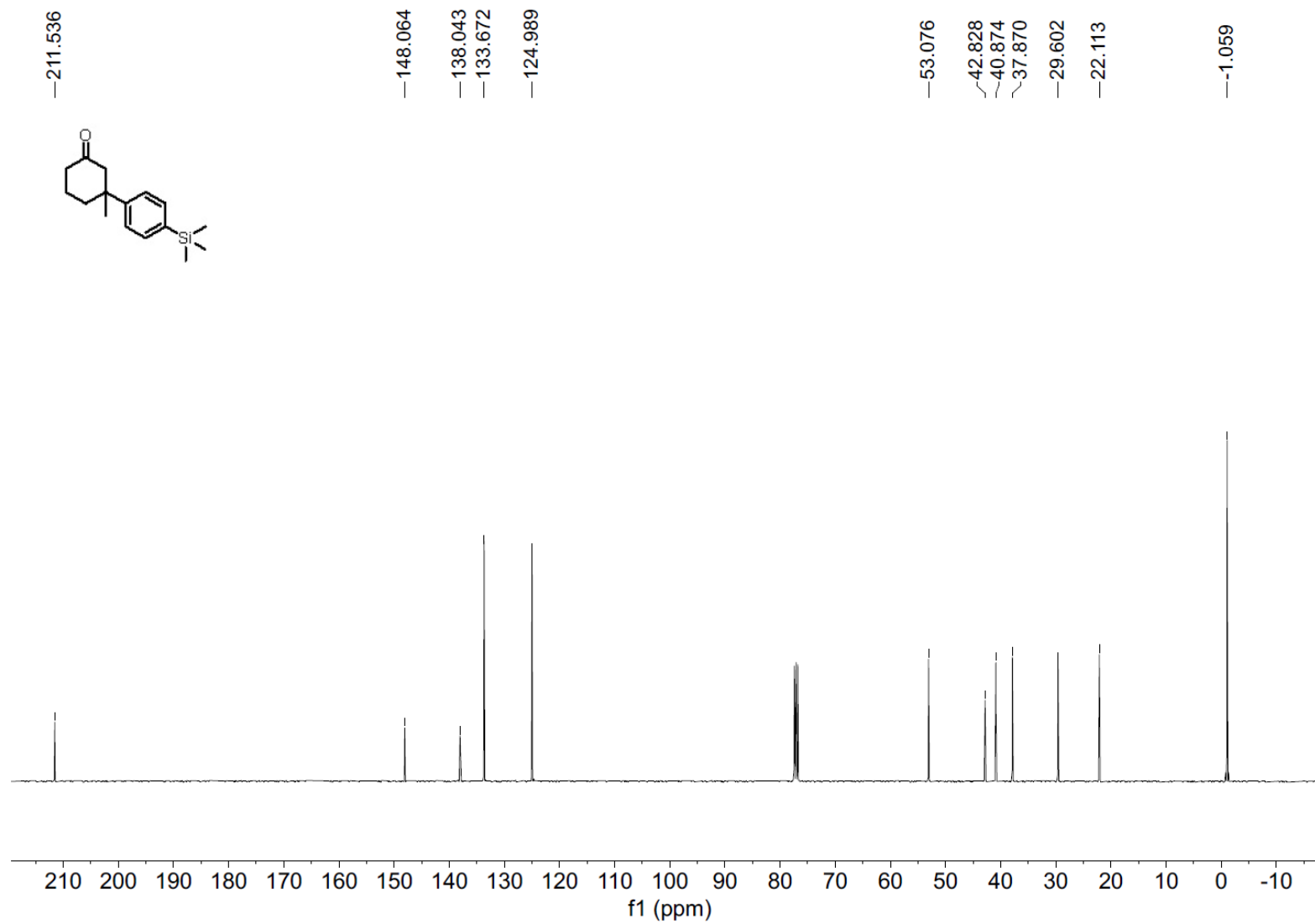




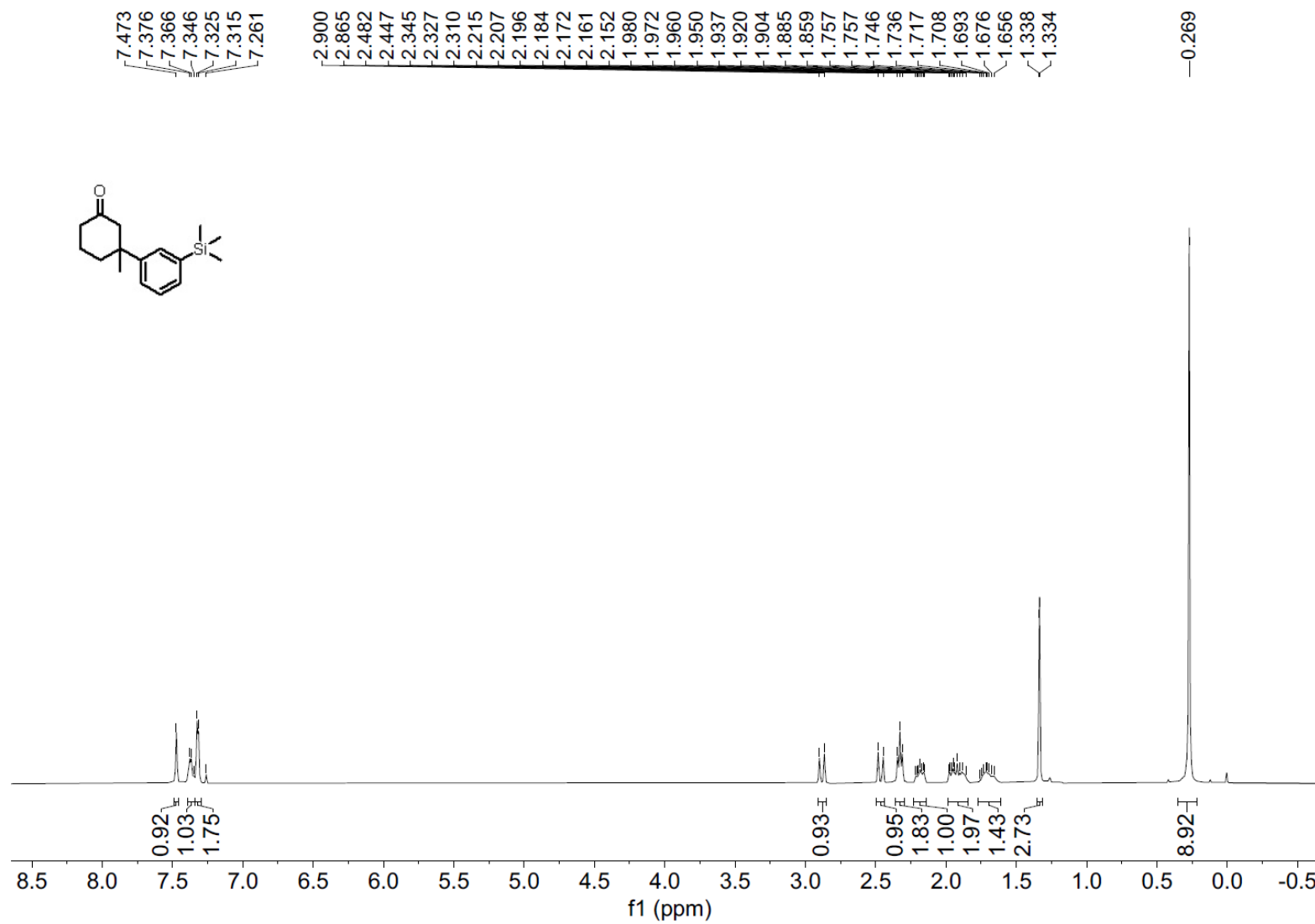
$^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of Compound 3j (CDCl₃, 100 MHz)



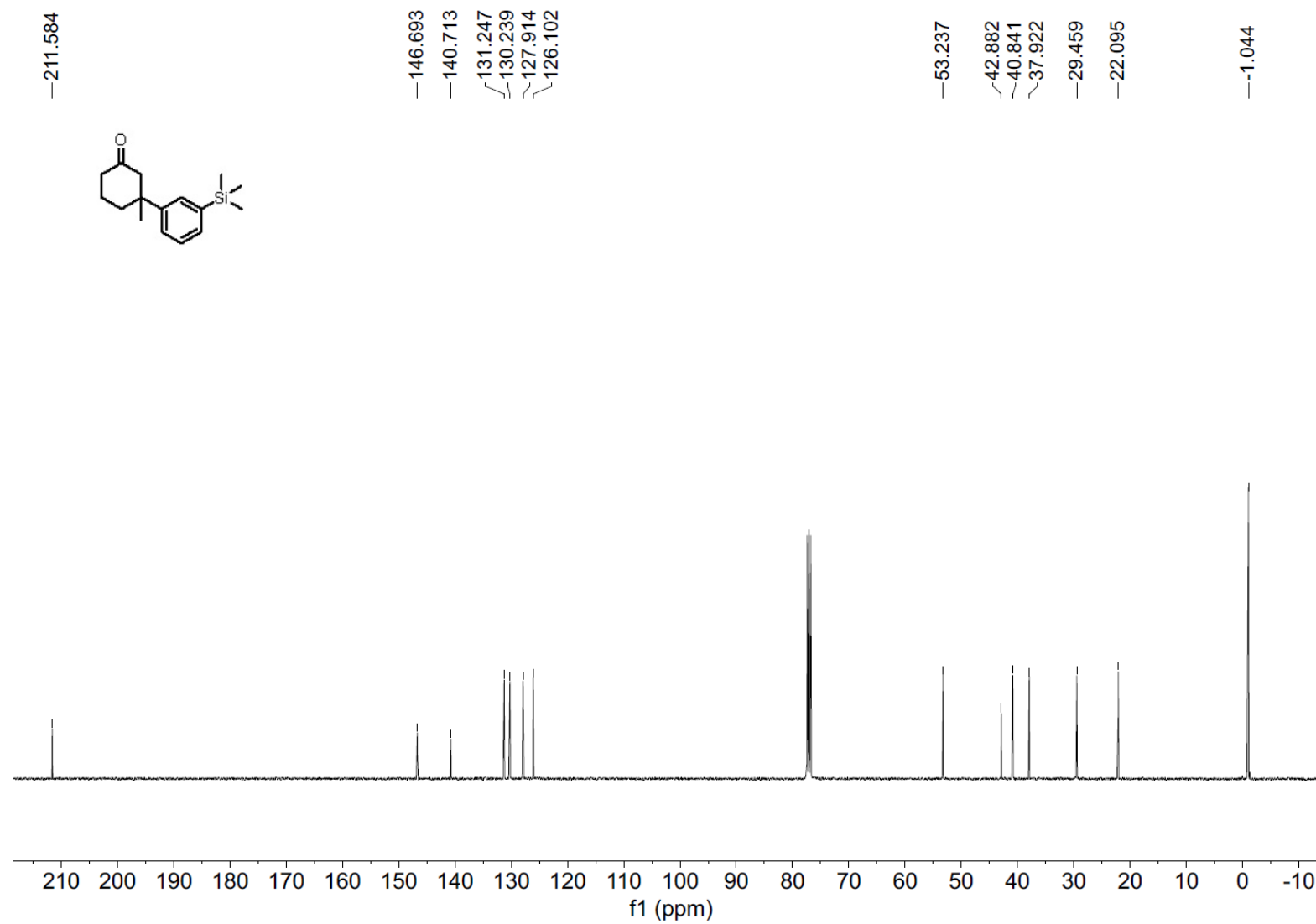
¹H NMR Spectrum of Compound 3k (CDCl₃, 400 MHz)



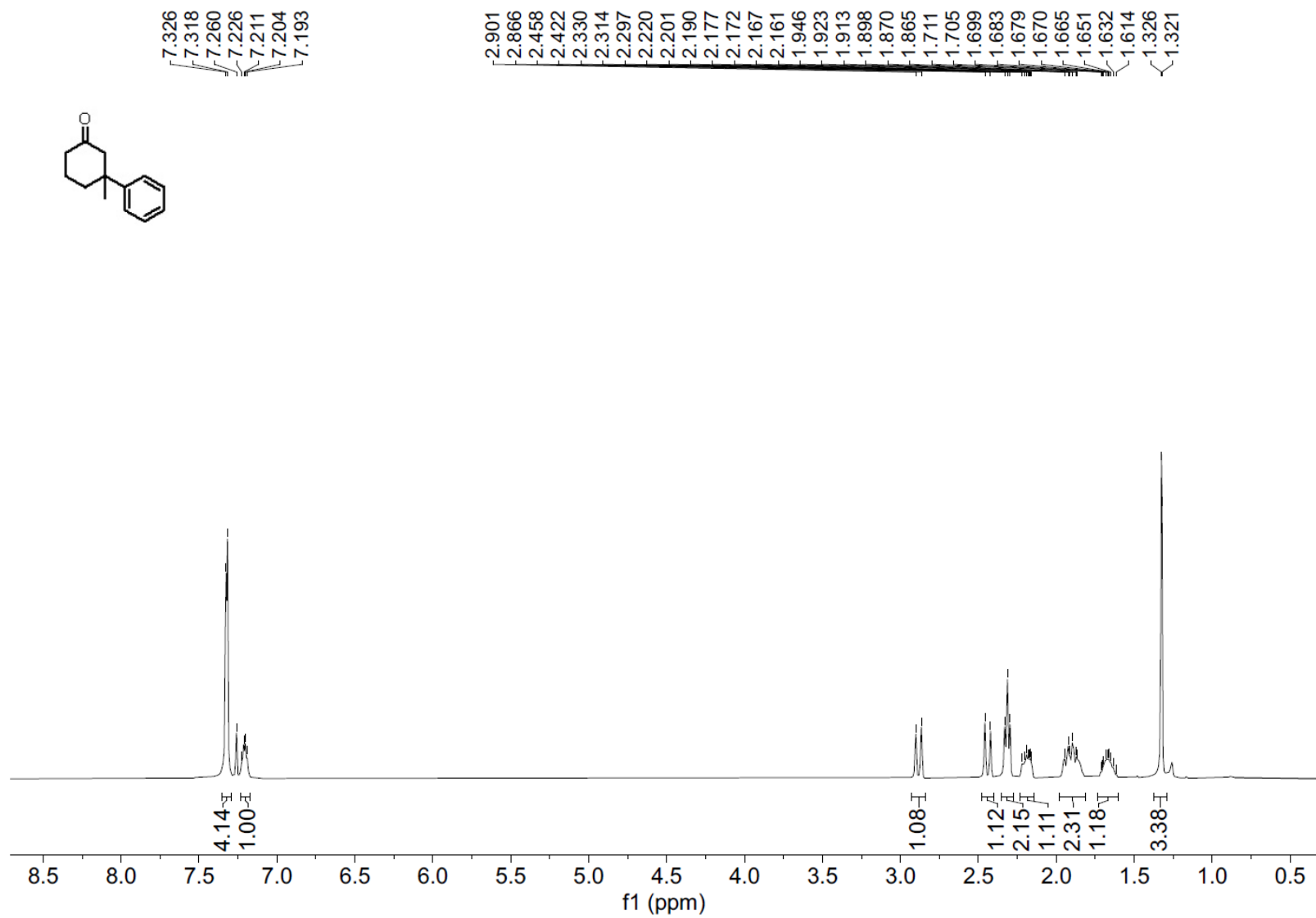
$^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of Compound 3k (CDCl_3 , 100 MHz)

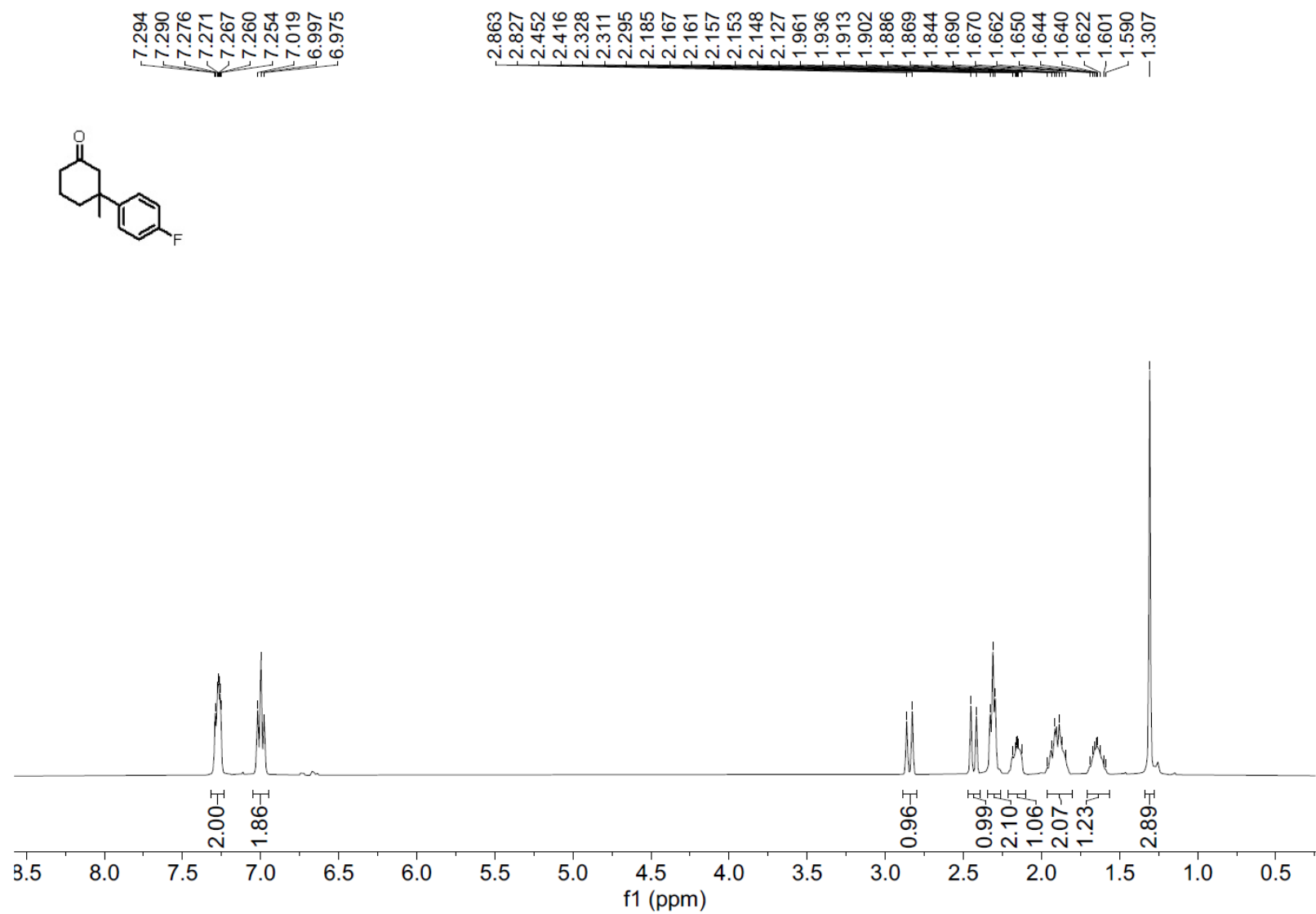


¹H NMR Spectrum of Compound 3l (CDCl₃, 400 MHz)

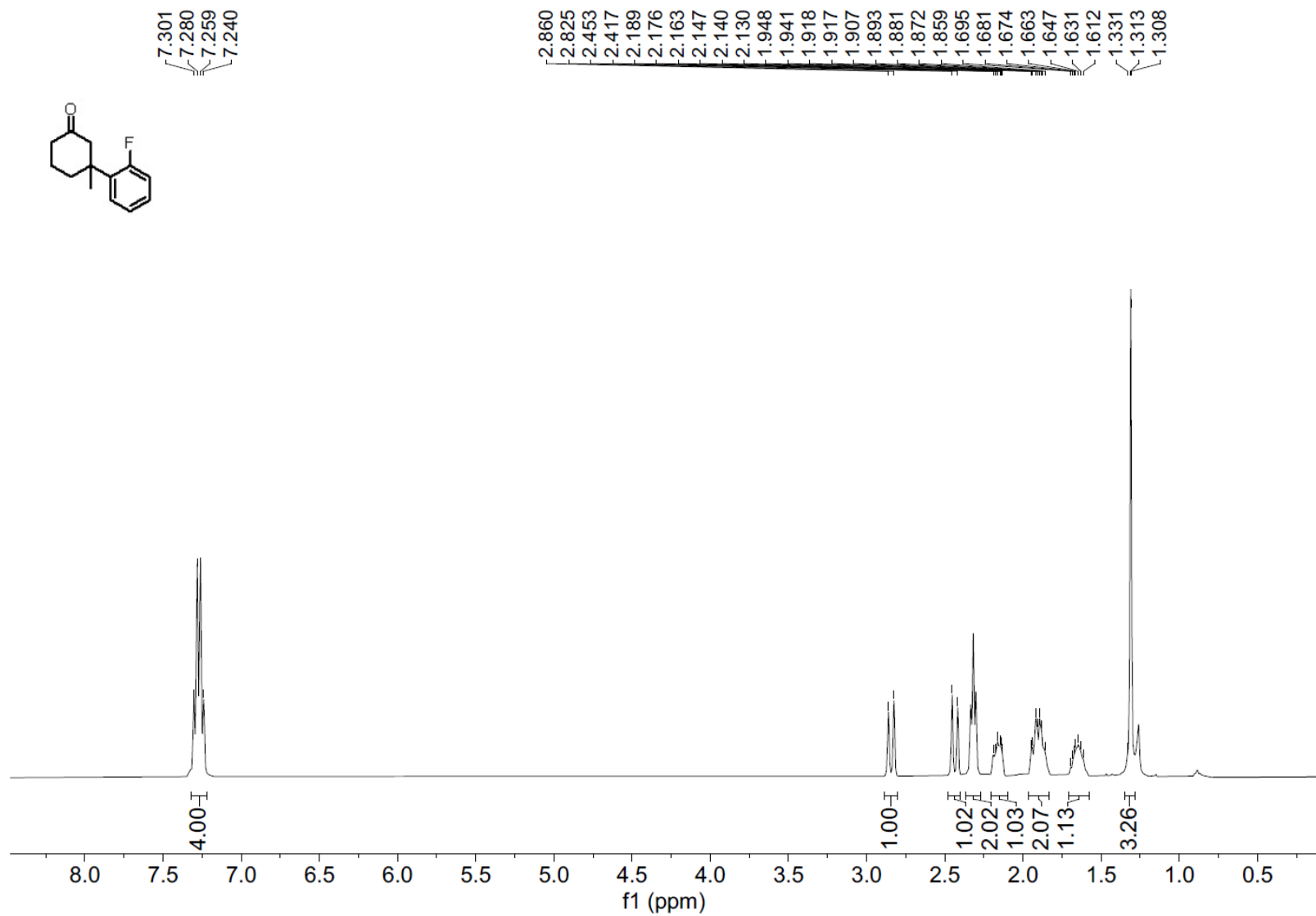


$^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of Compound 3I (CDCl_3 , 100 MHz)

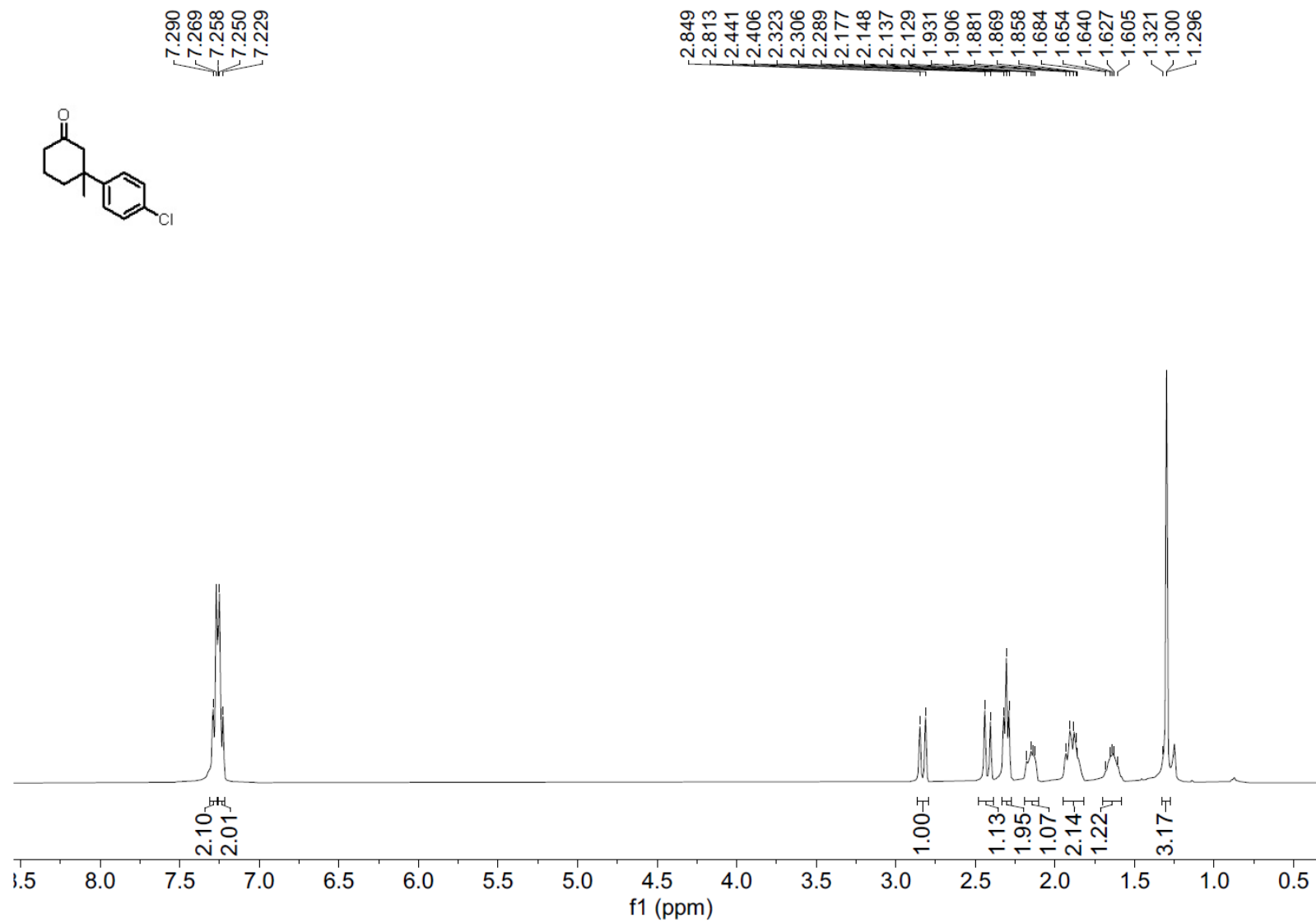




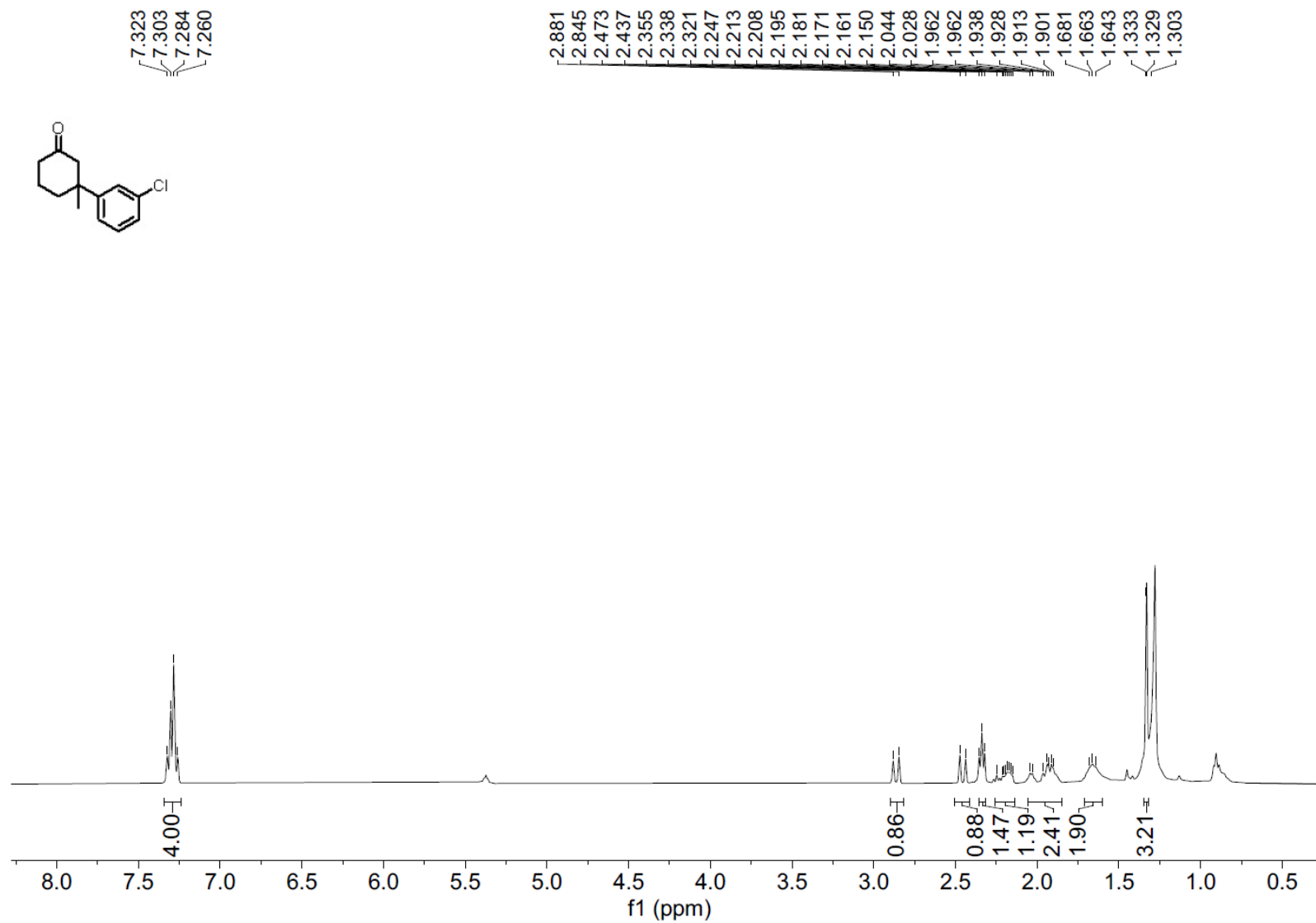
¹H NMR Spectrum of Compound 3n (CDCl₃, 400 MHz)



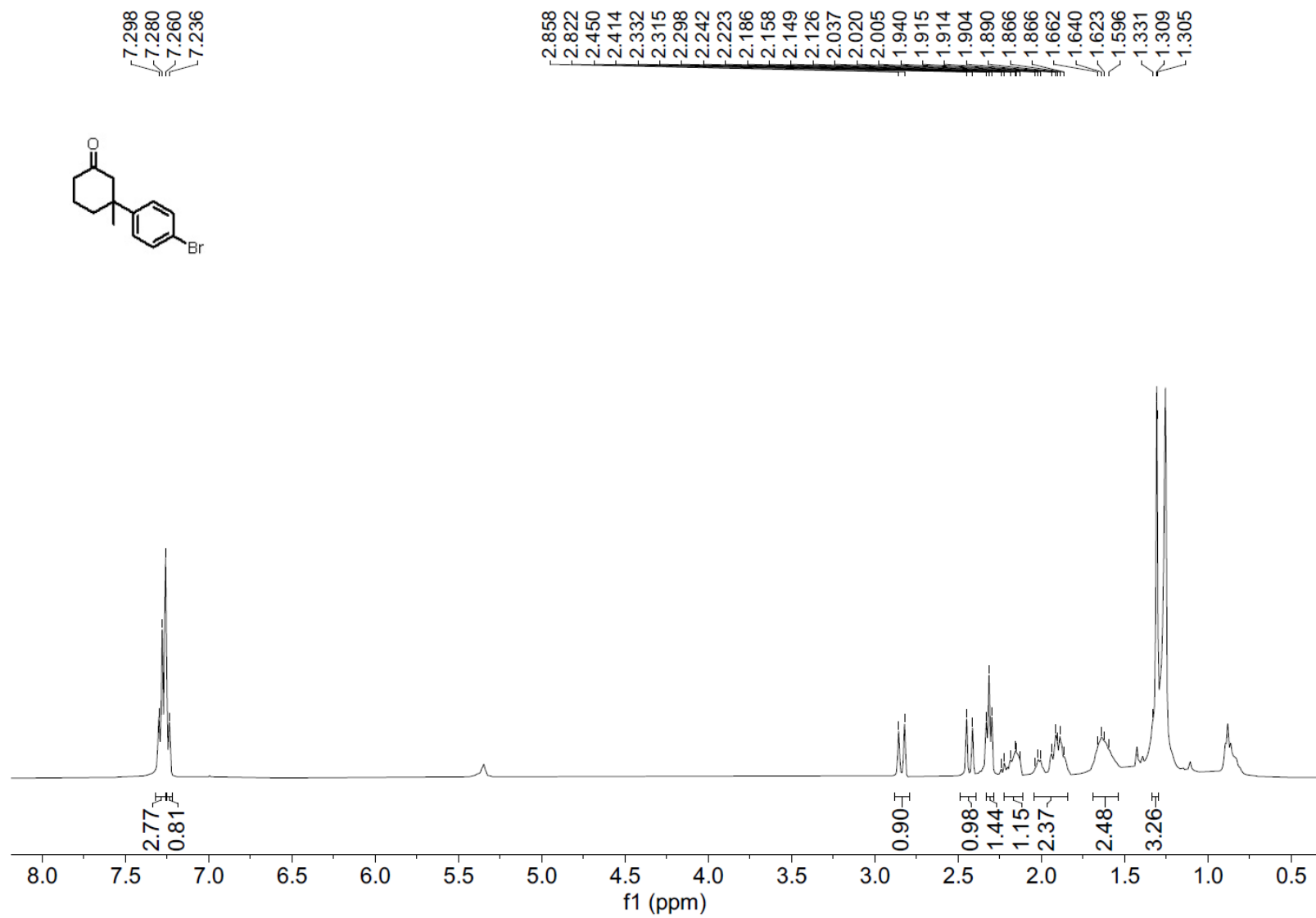
¹H NMR Spectrum of Compound 3o (CDCl₃, 400 MHz)



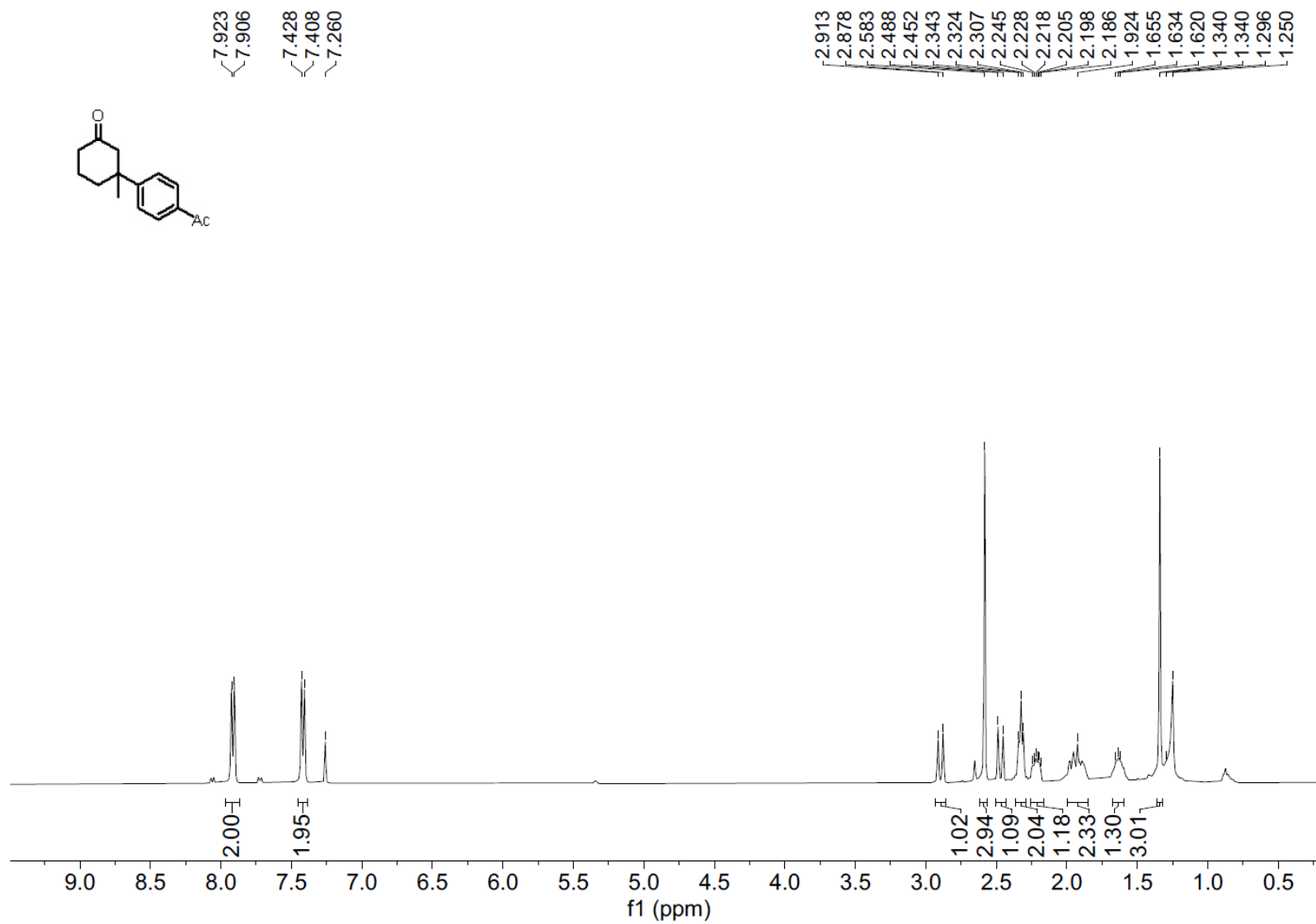
¹H NMR Spectrum of Compound 3p (CDCl₃, 400 MHz)



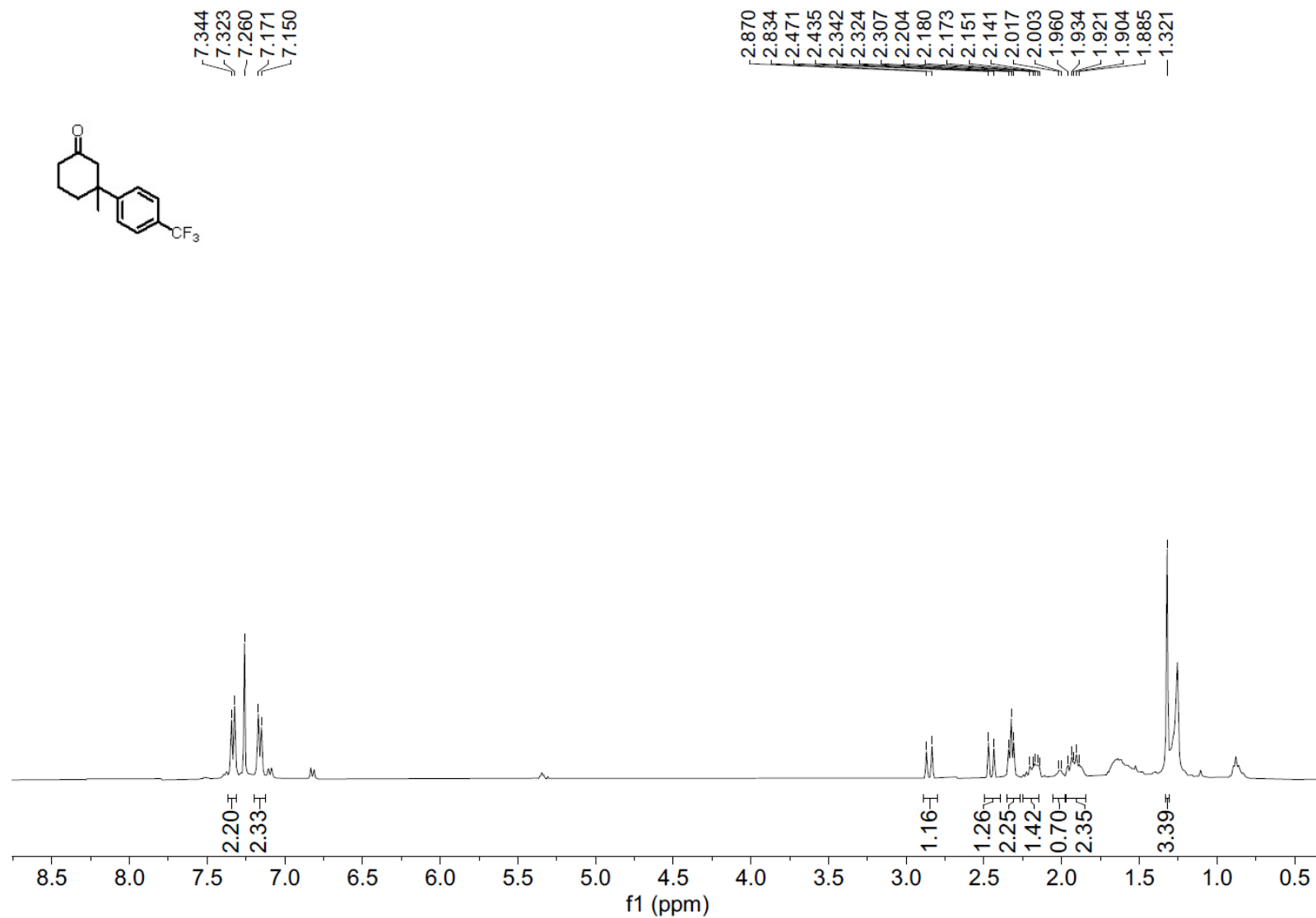
¹H NMR Spectrum of Compound 3q (CDCl₃, 400 MHz)



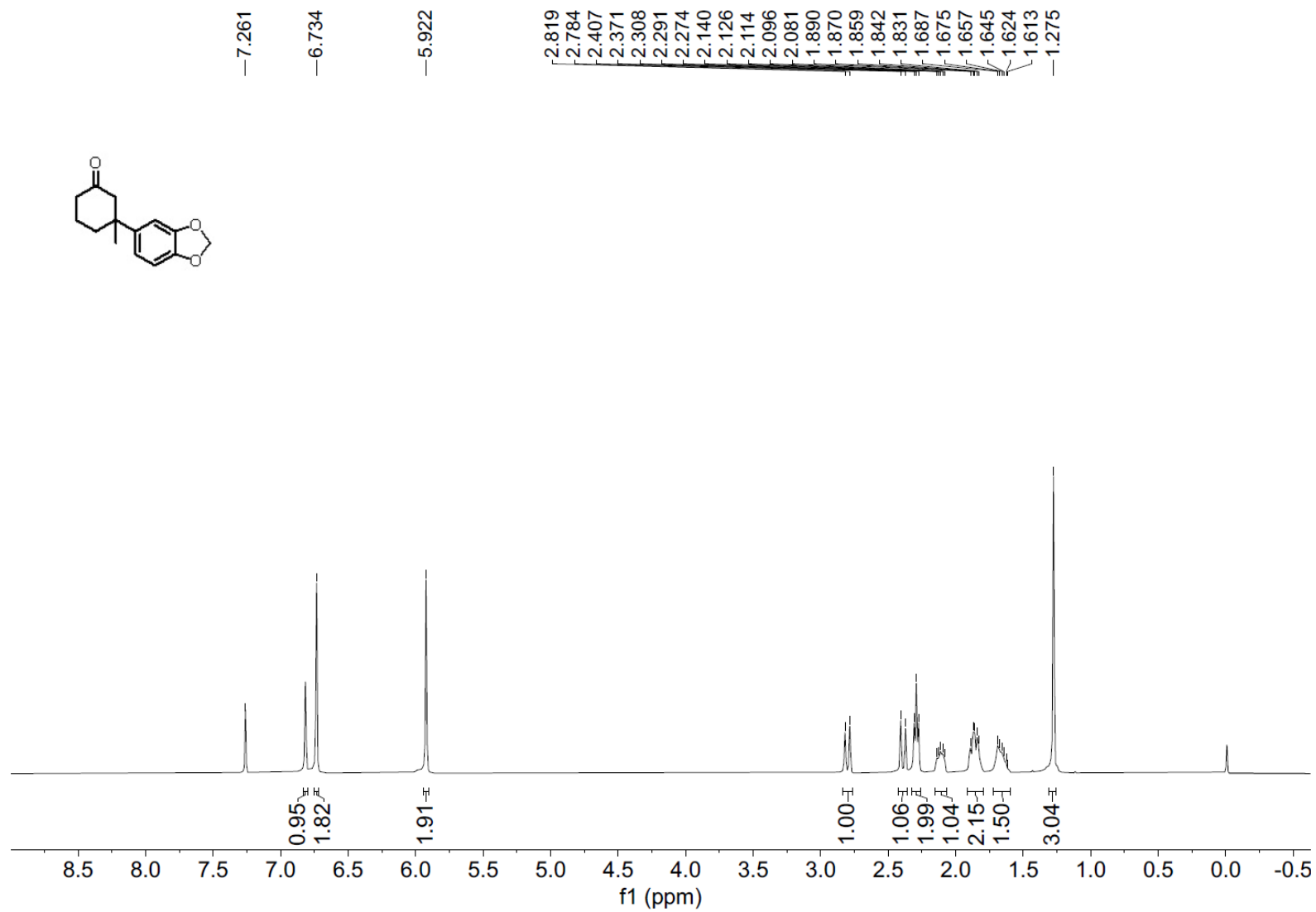
¹H NMR Spectrum of Compound 3r (CDCl₃, 400 MHz)



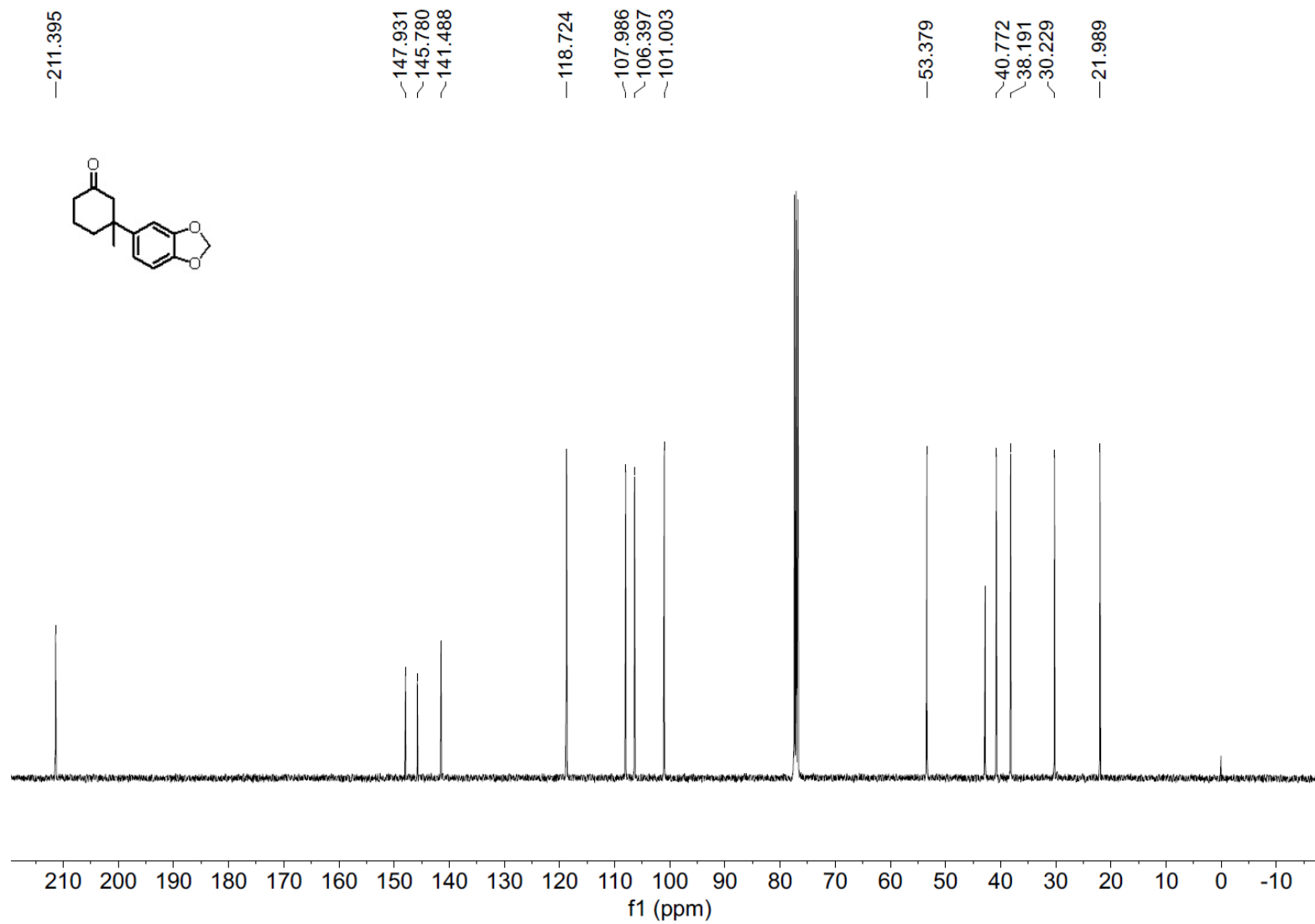
¹H NMR Spectrum of Compound 3s (CDCl₃, 400 MHz)



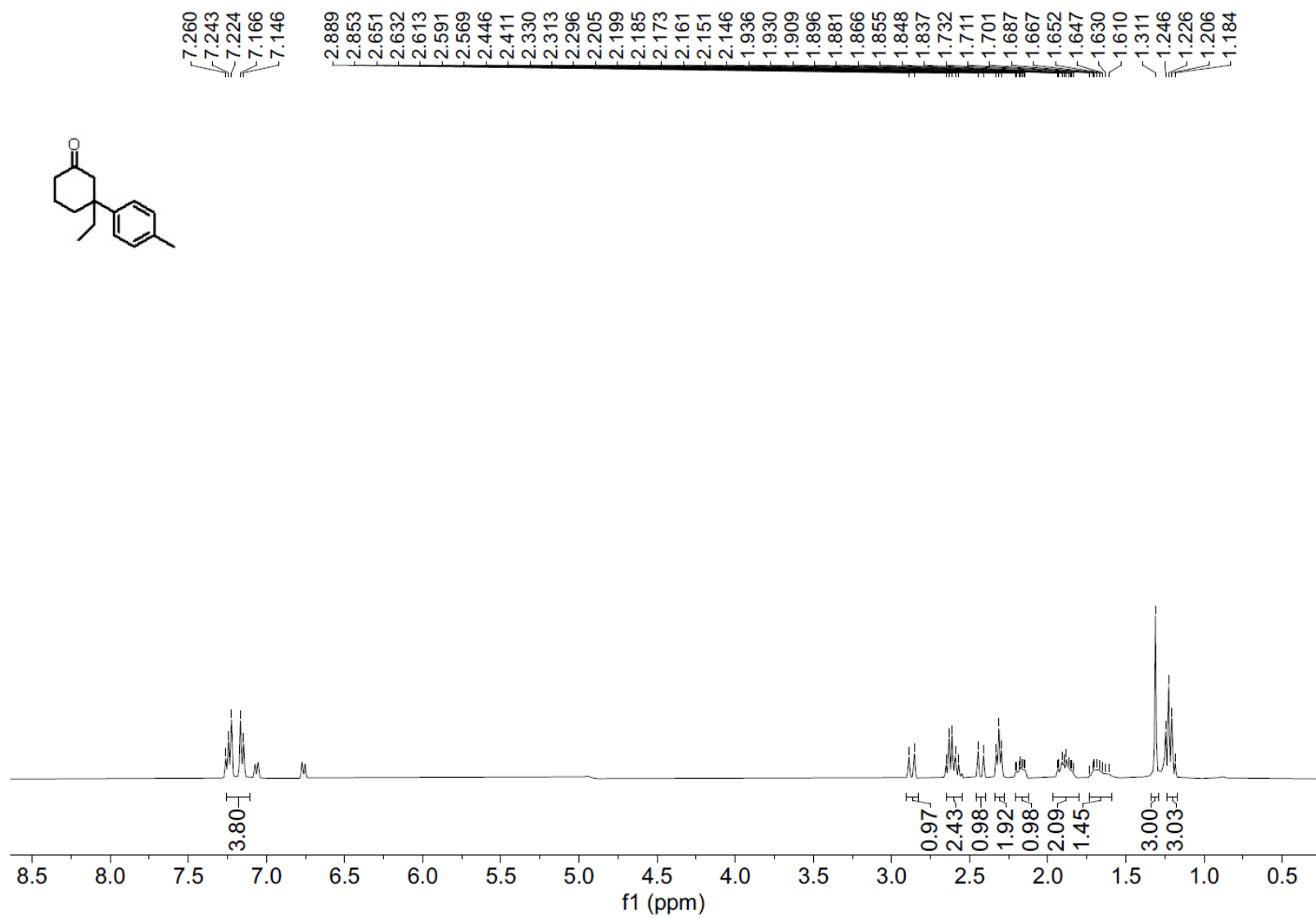
¹H NMR Spectrum of Compound 3t (CDCl₃, 400 MHz)



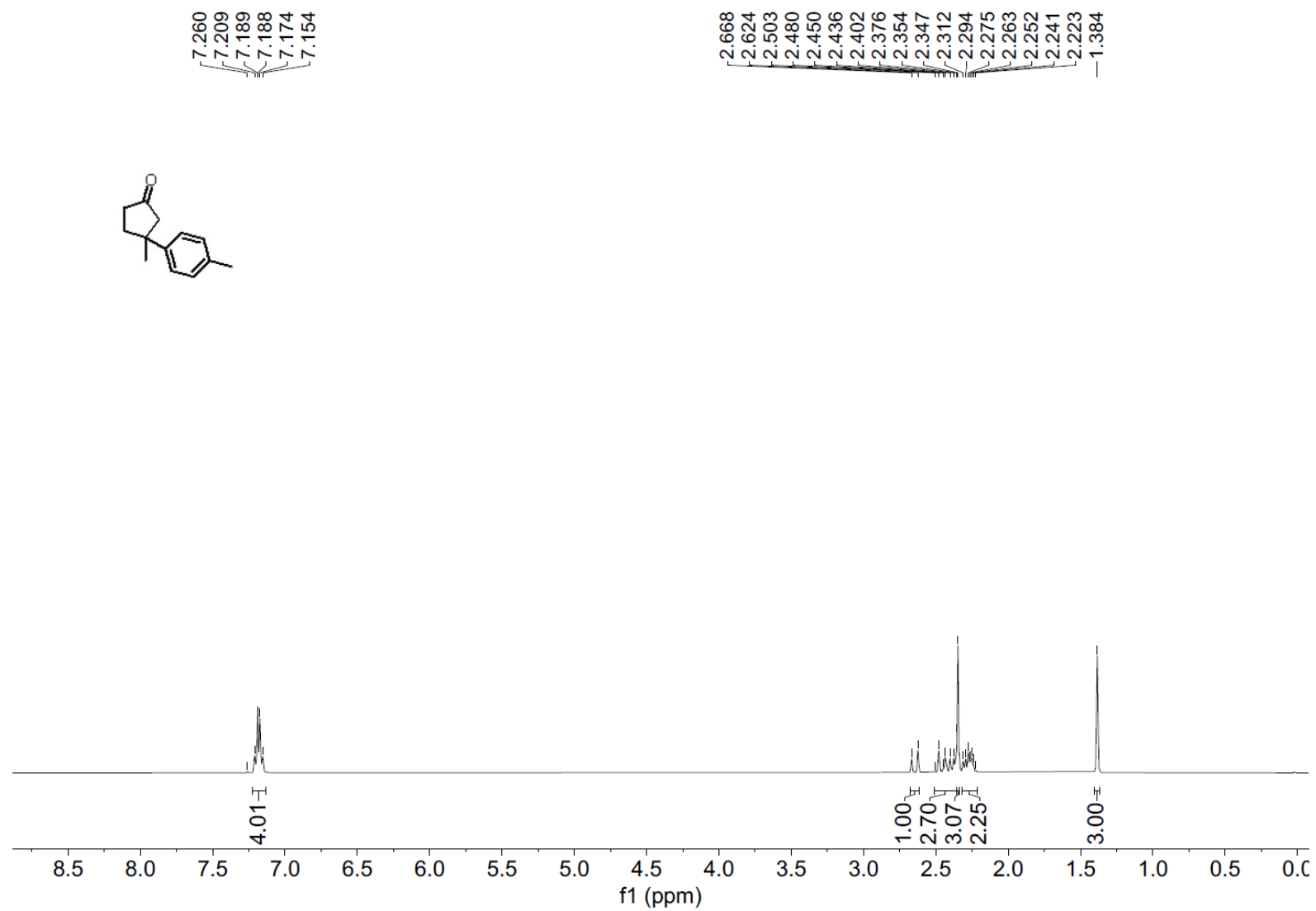
¹H NMR Spectrum of Compound 3v (CDCl₃, 400 MHz)



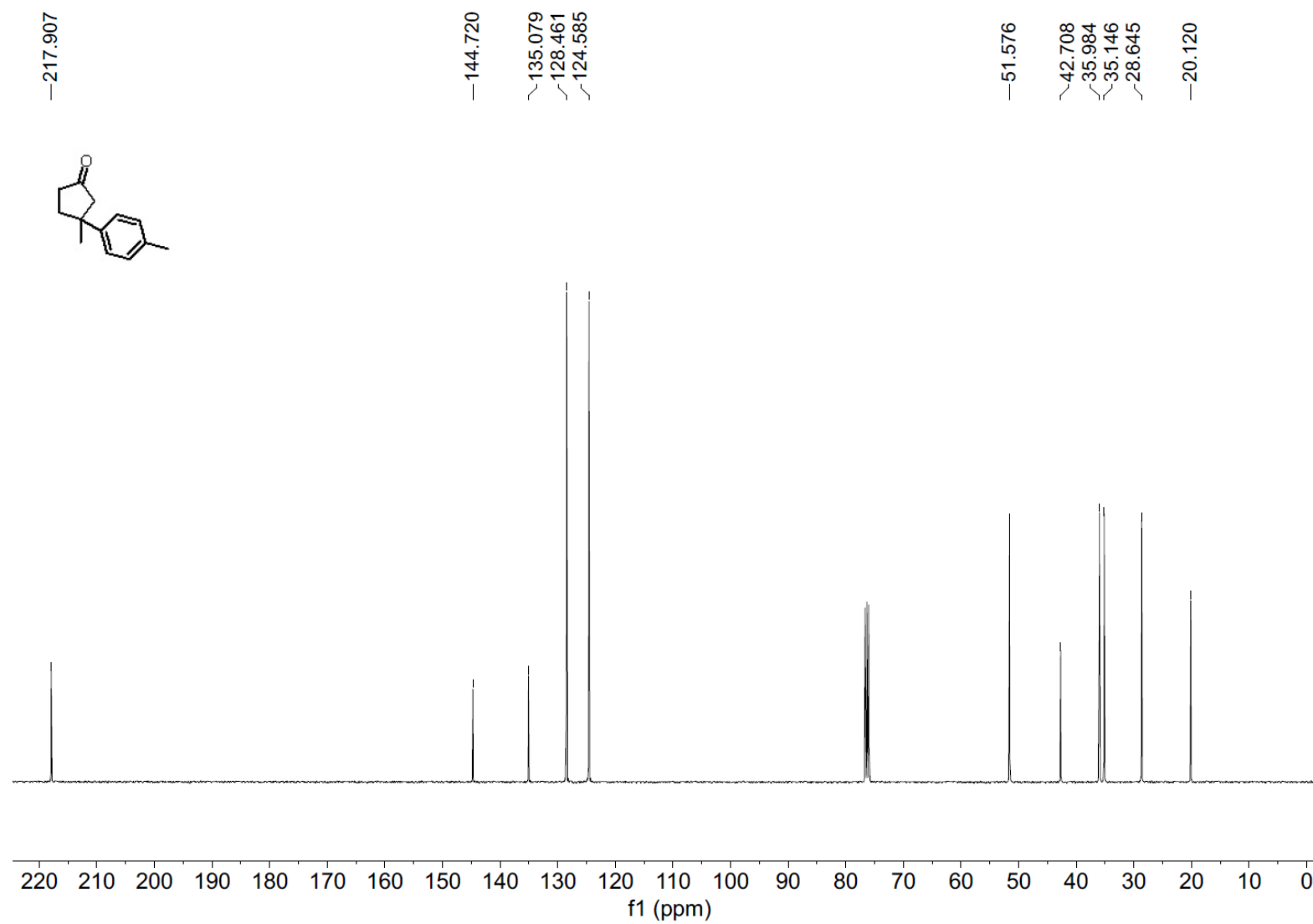
$^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of Compound 3v (CDCl_3 , 100 MHz)



¹H NMR Spectrum of Compound 3w (CDCl₃, 400 MHz)



¹H NMR Spectrum of Compound 3x (CDCl₃, 400 MHz)



¹³C{¹H} NMR Spectrum of Compound 3x (CDCl₃, 100 MHz)