

Synthesis of Benzoxazoles Using Electrochemically Generated Hypervalent Iodine

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Image of the electrochemical cell

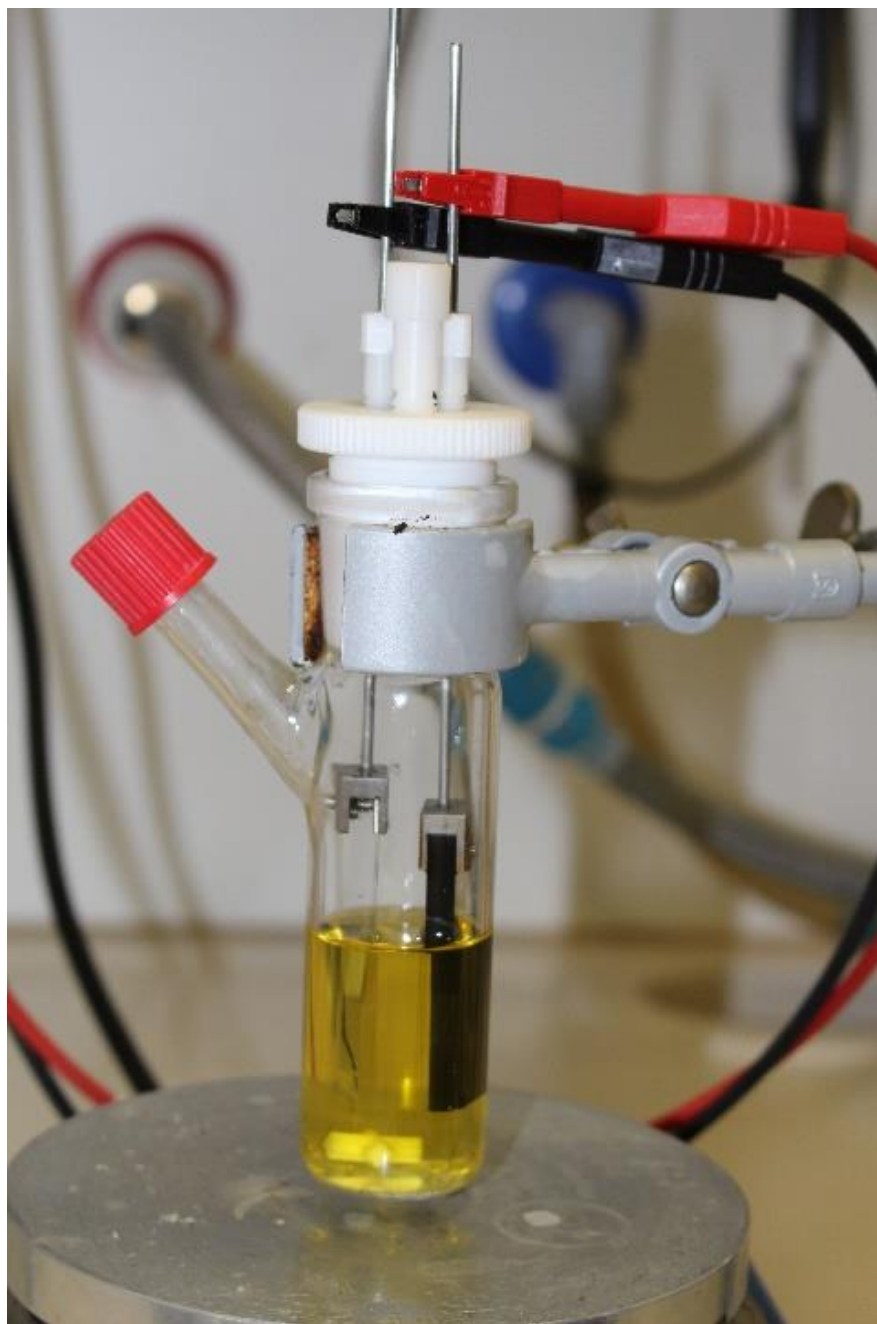


Figure S1. Undivided electrochemical cell used for the generation of iodine(III) reagent **2**.

Working electrode: glassy carbon plate. Counter electrode: platinum sheet.
Specific details are provided in the Experimental Section.

Cartesian coordinates for optimized structures

7a-A

G = -10692.20263855 Eh

#(imaginary frequencies) = 0

I	0.00363031772562	0.33041604818875	-0.40024062596684
O	0.24322990950808	0.16746404662364	1.72925583601985
O	-0.11932417017239	0.34667108336379	-2.58005782015562
C	1.99109599143298	1.40683818546979	6.06859965231720
C	1.02225903442322	0.44968780230983	5.72633952199654
C	-0.32107070095546	0.67147652506417	6.08309575229460
C	-0.68300991522510	1.83653266770507	6.74854159795409
C	0.28655953175011	2.79412090090553	7.06773890816493
C	1.62335636946638	2.57638053659445	6.72995191659661
C	1.43847047282545	-0.73599969884191	4.97606770781076
N	0.59314166052852	-1.53456787469578	4.42205634341812
C	1.09755597460974	-2.65723800171581	3.72447885156418
C	2.05151049941351	-2.55462078239361	2.68545110302262
C	2.56433512401253	-3.70981327585063	2.09666578655439
C	2.11878765123349	-4.96725629505256	2.49913363465513
C	1.12152323393541	-5.07612117403788	3.47043181577291
C	0.60750945728673	-3.92514225164292	4.06359292964509
O	2.50813315529793	-1.34061553554883	2.22520132886237
H	3.30100762040942	-3.60293093972333	1.30637079771424
H	2.53094195220471	-5.85688772729931	2.03245880552651
H	0.74823462177477	-6.05062954797530	3.76997957844045
H	-0.15690195858046	-3.98925437692310	4.83284357715527
H	-1.06429449781418	-0.08026900344323	5.83402091808550
H	-1.72055394011103	2.00404358653902	7.02174465245628
H	-0.00173972880975	3.70618385208678	7.58220685866095
H	2.37612796429650	3.31838971156867	6.97864415554768
H	3.02945108665910	1.23458799475557	5.79715596251935
H	1.76459745738757	-0.69148558359405	2.24717582300751
H	2.52076633496478	-0.90295375971011	4.90644142956245
C	1.14170833033155	-2.36691960424026	-1.18056925374332
C	0.18837710819546	-1.77836473107421	-0.35735666343905
C	-0.66949714463527	-2.48863034969935	0.47170457648264
C	-0.56774768782621	-3.87685767359751	0.45961874403675
C	0.35998381539730	-4.51894689417220	-0.37087548856175
C	1.21099277272848	-3.75530557495415	-1.18215299232481
H	1.79743524488504	-1.77451163375317	-1.80772857642686
H	-1.38835363487618	-1.99300969931041	1.11103743719830
H	-1.22145623141985	-4.44439150599147	1.11077841086311
C	0.49069592929580	-6.01391723081268	-0.40291043793440
O	1.38230108820374	-6.53681763721606	-1.06974589541049
C	-0.51157704093869	-6.84680087921812	0.36155669672024
H	-0.65024108069025	-6.43704756018814	1.36853843933297
C	-1.87905699694918	-6.90018480974239	-0.36097701579636
H	-0.10275321883308	-7.85610282170632	0.45740424065475
C	-2.91221529402777	-7.68309507092458	0.45338722094683
H	-2.24334813380526	-5.88193009185437	-0.53918344696307
H	-1.74044031486197	-7.36408343436749	-1.34410188851827
H	-3.87029348255303	-7.72562474497064	-0.07494350142576
H	-2.57452068230290	-8.70995287190303	0.63159052627334
H	-3.08048214053498	-7.20830803640418	1.42677606586005
C	-0.38108564620417	1.07715858585129	2.59090505659277
C	-1.25015805137188	0.08737561639085	-3.37278023029934
H	1.93768602694569	-4.26147250446685	-1.80860310935693
C	0.29181946623285	2.45895564749829	2.50640632238678
C	-1.91428405094421	1.14943046232808	2.42687197636066
C	-2.58800670159385	0.47817446239944	-2.71046780663592
C	-1.24370849559655	-1.36712355070557	-3.88537352116621
F	-2.19042368534950	-1.55024941764754	-4.83635131312362

F	-0.04479992545978	-1.64077577257196	-4.44265012873858
F	-1.45994328317700	-2.28199006008581	-2.91556575829090
F	-3.59744850974805	0.48779325577300	-3.60242525801102
F	-2.94653564826059	-0.33478107613956	-1.69057984059566
F	-2.48628070564815	1.73369911900108	-2.19669139537748
F	-2.49081229438079	1.71938227732710	3.50602623451127
F	-2.31000685562068	1.85682476809578	1.33697046531943
F	-2.42275154611744	-0.09645869795164	2.29862139584641
F	-0.24431446920676	3.35523331569752	3.35708725123328
F	1.60524131110139	2.34300206236943	2.79375980804819
F	0.20773111816049	2.98391163838888	1.24999510833653
H	-1.18103280358435	0.71242807836544	-4.27238612608103
H	-0.21911316531335	0.70719255303095	3.60962511449532
C	1.05517830499724	4.52079170011170	-2.39722259424226
C	0.20643636907066	3.50068312467301	-3.17541669570010
O	1.05040237025368	2.49349770964265	-3.66588942101247
C	-0.57708750480818	4.11450627205599	-4.34973707715309
H	-0.54500305319870	3.12374826095333	-2.47233541483315
F	1.67152265900375	3.88557194552550	-1.37041205322305
F	2.01458954611625	5.09185786130138	-3.15485641061946
F	0.30266027002662	5.51162100529299	-1.86448448302582
F	-1.32382805127720	3.14346530121203	-4.93920202707165
F	-1.42868515575383	5.08462899971935	-3.94756635949567
F	0.22634639713658	4.63370027911089	-5.29987132317149
H	0.74262404930889	1.63010152082683	-3.27814438293373

TS-2

G = -10692.19116989 Eh

#(imaginary frequencies) = 1

I	-0.307528	0.758197	-0.288548
O	-0.338053	0.552522	2.365963
O	-0.565110	0.436558	-2.571351
C	0.840593	0.500522	6.200736
C	0.684948	-0.602064	5.343436
C	-0.398629	-1.476410	5.537102
C	-1.305036	-1.243512	6.562047
C	-1.145499	-0.140126	7.408774
C	-0.069778	0.729402	7.229378
C	1.604731	-0.755970	4.224417
N	1.565371	-1.759835	3.418468
C	2.387434	-1.783362	2.302608
C	2.588502	-0.624535	1.467420
C	3.504658	-0.724556	0.389270
C	4.169806	-1.907334	0.125654
C	3.919159	-3.050154	0.904504
C	3.024636	-2.985076	1.963144
O	1.943576	0.509970	1.643514
H	3.650553	0.157909	-0.224672
H	4.867157	-1.958545	-0.705125
H	4.417877	-3.986759	0.677208
H	2.823413	-3.856559	2.578410
H	-0.515918	-2.314855	4.858275
H	-2.148836	-1.912599	6.701684
H	-1.864719	0.043152	8.201440
H	0.053550	1.587809	7.882567
H	1.670524	1.184574	6.041146
H	0.845038	0.522197	2.209608
H	2.350731	0.040923	4.103558
C	0.848975	-1.973210	-0.874090
C	-0.119754	-1.314828	-0.114614

C	-0.946456	-1.971649	0.794276
C	-0.787909	-3.344103	0.944056
C	0.170368	-4.043220	0.196033
C	0.978461	-3.347109	-0.712193
H	1.475402	-1.435293	-1.574274
H	-1.670403	-1.424653	1.383529
H	-1.415435	-3.862513	1.660454
C	0.383816	-5.524223	0.347366
O	1.324210	-6.069285	-0.215870
C	-0.604444	-6.314796	1.183836
H	-0.771639	-5.812182	2.145273
C	-1.957787	-6.493794	0.458813
H	-0.155770	-7.290747	1.386393
C	-2.991137	-7.197096	1.342634
H	-2.342547	-5.516029	0.146385
H	-1.788948	-7.069941	-0.458040
H	-3.936257	-7.332454	0.807191
H	-2.635472	-8.184156	1.657162
H	-3.196778	-6.611383	2.246236
C	-0.912887	1.417085	3.288625
C	-1.765269	0.439326	-3.271674
H	1.722157	-3.901506	-1.274366
C	-0.347946	2.845455	3.168378
C	-2.442644	1.347392	3.140798
C	-2.426865	1.831637	-3.238248
C	-2.701503	-0.704241	-2.829799
F	-3.789282	-0.803996	-3.624858
F	-2.036382	-1.879236	-2.898642
F	-3.137187	-0.559923	-1.554177
F	-3.546989	1.890509	-3.986019
F	-2.745652	2.222054	-1.980310
F	-1.556473	2.746340	-3.730769
F	-3.074876	2.001151	4.139722
F	-2.884976	1.854912	1.968208
F	-2.840933	0.051270	3.191676
F	-0.929038	3.711690	4.025375
F	0.977446	2.817592	3.456503
F	-0.474568	3.352835	1.918275
H	-1.537111	0.243691	-4.331042
H	-0.698077	1.096479	4.319828
C	3.214210	2.177214	-3.348440
C	1.919099	1.680943	-4.009587
O	1.772847	0.315728	-3.723407
C	1.869730	1.884769	-5.533647
H	1.103912	2.284080	-3.592448
F	3.076971	2.086240	-1.997611
F	4.291741	1.446787	-3.692941
F	3.478868	3.472296	-3.634833
F	0.690284	1.396560	-6.000837
F	1.921806	3.193203	-5.876496
F	2.859991	1.244498	-6.183259
H	0.888075	0.223216	-3.277484

III

G = -10692.21162334 Eh

#(imaginary frequencies) = 0

I	-0.32456570290913	-0.96403106372546	0.72788055738455
O	-2.07437657556189	-1.01580552468866	4.36839931018032
O	-0.30363003217629	-0.06876691554721	-1.30069669535049
C	3.85801740805747	2.68892590731736	2.81239852545942
C	2.79297029579578	1.96809051305836	3.37931116588926

C	1.80182798853034	2.66084933722556	4.09531520069058
C	1.86689676471467	4.04138526107747	4.22542702877175
C	2.92469068841304	4.75199824203679	3.64618305216746
C	3.92034759554475	4.07384881896812	2.94098462720087
C	2.77348596164950	0.52110359536567	3.21679726967059
N	1.77235027321180	-0.23194997082007	3.53432106399213
C	1.96326260036529	-1.62407816458226	3.48978790847728
C	0.91563946145296	-2.45700917249652	3.03828143240864
C	1.06183940583009	-3.84457755360142	3.01292443025091
C	2.23887974658787	-4.43137924046662	3.47439978880020
C	3.27662997146828	-3.62364152046931	3.94555683966197
C	3.13985713825395	-2.23731131656218	3.95202589711245
O	-0.27958497882964	-1.91302630077545	2.62527784459505
H	0.23882289344556	-4.44695485890193	2.64198934846003
H	2.34081032411738	-5.51209831073885	3.47129868938069
H	4.19151627591205	-4.07337036055161	4.31945702604955
H	3.93151970604353	-1.61216120811482	4.35499254192422
H	0.99189608133373	2.10483987721945	4.54991876249194
H	1.09775063213287	4.57090549025515	4.77995991019632
H	2.97184198804234	5.83229917103457	3.74877325048921
H	4.74204887728985	4.62443838419315	2.49297263783304
H	4.63073362345197	2.15463842605796	2.26532515883101
H	-1.49424360061418	-1.50880879968686	3.73384961907353
H	3.68537339964756	0.08333854522020	2.78932089196513
C	0.81137767803423	-3.28935476685250	-0.85577232721744
C	-0.30687774288803	-2.88867228682763	-0.13031367951381
C	-1.42361960857454	-3.69302148757611	0.06915131354080
C	-1.42662658422108	-4.95363146590217	-0.52000149787698
C	-0.33341676535669	-5.38739077236998	-1.28412132843023
C	0.78452971706224	-4.55486623877109	-1.43316332951209
H	1.66738459856353	-2.63729393242559	-0.98451039715260
H	-2.27143056455014	-3.35515834806133	0.65331379529548
H	-2.29456360957108	-5.58764406408692	-0.37930319679087
C	-0.33111742321720	-6.72278709848976	-1.97406125754024
O	0.71313434430358	-7.16243069083976	-2.45058149844763
C	-1.64227680791702	-7.46021510446182	-2.11590196679047
H	-2.14055731219151	-7.52837434695995	-1.14108610682489
C	-2.58699521055810	-6.75773741287494	-3.12093660289532
H	-1.42086382254272	-8.47522182004260	-2.45576663316624
C	-3.94233207049262	-7.46389319573384	-3.20884625622462
H	-2.73405591063269	-5.71366796056498	-2.82186092299670
H	-2.10453347947342	-6.74042160798519	-4.10488142578207
H	-4.59234624622757	-6.96305683694256	-3.93380025646465
H	-3.82258501256609	-8.50702276423517	-3.52130461944974
H	-4.44809228871498	-7.45727640027490	-2.23654235287852
C	-1.39494232929623	0.18202743485828	4.65563647715253
C	-1.32262565431498	0.01231164798721	-2.25369245495730
H	1.62985916180677	-4.90473790934945	-2.01627491179707
C	-2.21874024300886	1.35362749947057	4.09960459151830
C	-1.15250070688517	0.25350749872097	6.16948826962303
C	-2.74284374922499	0.02007630033514	-1.65354271550434
C	-1.14685814187752	-1.05990195192446	-3.35332956280744
F	-1.90639140440260	-0.76621835751237	-4.43715795410974
F	0.14203424922195	-1.08204286926278	-3.75444825790203
F	-1.47142396376800	-2.30921800927359	-2.95659581242383
F	-3.67795510952588	0.28628289940396	-2.58722187224169
F	-3.08114613765781	-1.14430906002689	-1.05404770373391
F	-2.82318336180148	0.99054671419095	-0.70455384083804
F	-0.47096331144462	1.37180066779073	6.52619205600655
F	-2.29398900359010	0.22704147992366	6.89417118581923
F	-0.40655973406601	-0.80900703761256	6.55258322046426

F	-1.65634941358900	2.55930576861121	4.35258925936752
F	-2.30594640796657	1.22979098650817	2.74820044807008
F	-3.48223186435473	1.38471881539317	4.57692878633451
H	-1.23176469428236	0.97262361585880	-2.78474464501489
H	-0.40079256539470	0.21998317583617	4.18186443206640
C	0.26385901305056	3.46409974928304	0.47640898567260
C	-0.08942858270780	3.08297952772239	-0.97229895281309
O	0.91426533898089	2.26275823908827	-1.50761479560640
C	-0.25513943538063	4.28317811206742	-1.91258053925329
H	-1.06784163834216	2.59083597030591	-0.92048119291222
F	0.41194379515139	2.31778130106376	1.19334889911537
F	1.41390473239960	4.15713910064144	0.57223603867070
F	-0.71113991583031	4.18422579550011	1.07722084606740
F	-0.71458268528655	3.84403701045851	-3.11151483622910
F	-1.14747082365571	5.18413096834042	-1.44245122791677
F	0.90613279737142	4.93250643541900	-2.13804764145673
H	0.60409970020265	1.31814179516116	-1.41125011536948

TS-3

G = -10692.19033623 Eh

#(imaginary frequencies) = 1

I	2.64643076133896	-2.80753134153063	-1.13514628000808
O	-0.34414447257239	0.45154672717805	3.49176256297542
O	2.91050942188394	-2.51798040889368	-3.90579002035043
C	0.08486860133874	-4.78047378939797	3.20852667240306
C	0.15781514779886	-3.40409664980633	3.53600686165629
C	-1.02187078161121	-2.71702595453311	3.91279987516165
C	-2.24018080370672	-3.39291411187367	3.95482062874954
C	-2.31022564918126	-4.75100946097137	3.59046454742469
C	-1.14676652277287	-5.44305162378365	3.21663291638346
C	1.45286001012732	-2.75761050651373	3.43211638114599
N	1.62595320432429	-1.46046477749431	3.41603098569023
C	2.76692998624148	-0.86391692645510	2.96301540699222
C	3.62117696930483	-1.53291694380185	1.95065145468262
C	4.72977704862851	-0.78291360291370	1.40985870332953
C	5.00715160929784	0.49448712057412	1.84470697721477
C	4.22132642385175	1.09179801424144	2.87736406529762
C	3.13396530021176	0.42237043321137	3.42305185390382
O	3.36454516185420	-2.72209734858397	1.57741755235277
H	5.30665593998768	-1.25421183113591	0.61680056232081
H	5.82862093207361	1.05618068259196	1.40015315836849
H	4.47079022405064	2.09139163919100	3.23352556103097
H	2.54500051496101	0.88965947968416	4.20676695890679
H	-0.97313520260079	-1.668711995651223	4.19023507789318
H	-3.14175583189389	-2.86483471494783	4.26573584215618
H	-3.27015523595076	-5.26796152999743	3.60619940233968
H	-1.20044781538586	-6.49594537903310	2.93964589459513
H	0.99431140225513	-5.31151040381425	2.92392317565427
H	0.35942682624920	-0.26147248493469	3.46619472769885
H	2.32673787060178	-3.41402054573475	3.36678177853535
C	-0.20785333489469	-3.40306164148826	-0.24426165757459
C	0.74919782592930	-2.37515696007590	-0.32851247776557
C	0.47660507799191	-1.06748332127064	0.10609338012434
C	-0.77284141779858	-0.79841873231126	0.67806975449698
C	-1.75665773544809	-1.80722660807891	0.76335178201613
C	-1.46270396886877	-3.10174275405957	0.28839319363451
H	0.02159574972071	-4.41087856851084	-0.58688044353554
H	1.21766630218599	-0.27566344761671	0.00478295921870
H	-0.96615163390190	0.20264294534856	1.05962977957428
C	-3.12579170793269	-1.57126565243824	1.34395991406573
O	-4.00546626622597	-2.42009037867224	1.19468982967060

C	-3.39058430417135	-0.28900161110387	2.10830853419084
H	-2.49751318878056	0.01323231595947	2.67140971372722
C	-3.83977597839036	0.87255056980755	1.18467727287547
H	-4.19621729957338	-0.50563118396692	2.82364994940793
C	-4.11426881931063	2.15761691205147	1.97879953196374
H	-3.06635492800732	1.06469704018611	0.42487053819071
H	-4.74502868942139	0.56189475899647	0.64073418043233
H	-4.44211130712513	2.96665939766859	1.31059067418676
H	-4.90290052608350	1.99392175732710	2.72827376017732
H	-3.21248621652021	2.48998019901785	2.50917613813050
C	-0.19534976617456	1.20662116426206	4.66069714766558
C	2.18852438160607	-1.63378386844361	-4.67023131470128
H	-2.23264216315874	-3.86928798115819	0.36320001189545
C	0.06469092984101	2.66566103300052	4.28266530523297
C	-1.44375978625854	1.03910427202885	5.52829577485995
C	1.28971248014521	-0.69419057191478	-3.84864523263967
C	1.36314668052524	-2.41722222960106	-5.69609032458207
F	0.63237766477734	-1.61585218129631	-6.49465979303538
F	2.19460195457798	-3.12431909049832	-6.47851687448721
F	0.52389458963229	-3.28070531499459	-5.10507884555343
F	0.72274224547202	0.23876105349705	-4.62525574860628
F	0.31226056346760	-1.35138588095778	-3.20596897627182
F	2.01369564519727	-0.04313442283274	-2.90770654009606
F	-1.39337469171004	1.80483195175403	6.62651255646878
F	-2.56363060810319	1.34461138217290	4.85689691863239
F	-1.54235351908343	-0.24466377100360	5.92246594277827
F	0.32302266728390	3.41243856293665	5.36574747975183
F	1.12892697103488	2.73709285004492	3.46687173853338
F	-0.97970372795729	3.21297005268741	3.63952207101263
H	2.84427284493521	-0.94830122635571	-5.24553870046832
H	0.65481974211033	0.87630219251040	5.27694484748613
C	6.09256674657412	-0.67007339209880	-2.32378060102279
C	5.12032044968619	-0.53982263400613	-3.49109170677364
O	5.24005231900181	-1.64138572671619	-4.33921302541742
C	5.32663382981264	0.73931086975643	-4.29472317554552
H	4.11629886453528	-0.47220924553405	-3.04634902795357
F	5.85954605274895	-1.84031305011203	-1.68577870904053
F	7.37176310096308	-0.66848296945515	-2.71460265591844
F	5.93096760044090	0.31488555546926	-1.42039861859034
F	4.34101207065597	0.86186656729304	-5.20819158657902
F	5.29127585841506	1.83167677764201	-3.51293798280608
F	6.49163292854742	0.73719467283130	-4.95430487548604
H	4.37145640637894	-2.15755424168637	-4.18740507045575

IVa

G = -10692.22341263 Eh

#(imaginary frequencies) = 0

I	-4.59021914623304	-1.94672188413203	-0.69845264154303
O	-0.12245491601786	-0.62872349285415	2.95617473747348
O	-0.27926059213769	-5.26586539527738	-4.21202664577410
C	-1.73393382688047	-3.96942218820529	3.10612426976484
C	-1.90063675483704	-4.17605784894718	1.73407739823135
C	-2.96493600535916	-4.93668371354131	1.24924885521384
C	-3.86411961692647	-5.50300560012906	2.15396132340673
C	-3.70274013417369	-5.30626419815905	3.52450973789422
C	-2.63832948627559	-4.53763211262897	3.99929619469132
C	-0.87377390608848	-3.56036400035261	0.79907861262631
N	-0.91814518646421	-2.12346404666728	0.75916417685754
C	-1.11181786746438	-1.76137386313680	-0.47871174991439
C	-1.18913322882996	-2.95162309292040	-1.33298990957281

C	-1.28497871886552	-2.88370302977401	-2.72341922788818
C	-1.30881597596496	-1.59912605605102	-3.23102693444965
C	-1.25971839535349	-0.40473168551746	-2.42289684710669
C	-1.17139438632903	-0.45404116931214	-1.06412286966634
O	-1.06149402167167	-4.02537845224690	-0.59012311696814
H	-1.23596652042508	-3.78229795496884	-3.34378275037160
H	-1.36148988684353	-1.46683765838164	-4.30665522098652
H	-1.28913285981635	0.55285660572778	-2.93030696544345
H	-1.10925451816670	0.43588061035608	-0.44992583252342
H	-3.08564540167959	-5.10471866297412	0.18560693312693
H	-4.68953998104218	-6.10051507663338	1.77958068115952
H	-4.40595640094092	-5.74881406819267	4.22317775130274
H	-2.51042626076511	-4.37692800888477	5.06501362937968
H	-0.90431928921679	-3.37598946731794	3.47870901358485
H	-0.62214210495504	-1.12665846399365	2.26197905304842
H	0.14564660847937	-3.87528501116901	1.06041028232564
C	-4.85180085148021	-2.15546408730630	2.33656769077431
C	-4.28522104714182	-1.39038751462661	1.31584214739166
C	-3.48350537055763	-0.28216939092357	1.59179056874699
C	-3.19554707523773	0.02830363050259	2.91723828340810
C	-3.72222164311808	-0.74301824517309	3.96193976425148
C	-4.57303966124772	-1.81579445773479	3.65467212555779
H	-5.48206686957414	-3.00667077471093	2.11038117410645
H	-3.08973894201743	0.33059490208976	0.79007551812305
H	-2.54635938314770	0.87139978714816	3.12094163146276
C	-3.37576619840747	-0.48042496287041	5.39337023429687
O	-3.96012879267265	-1.08681585174732	6.29219093291936
C	-2.30162928132605	0.53820551803797	5.70539109660760
H	-1.49166025484804	0.46737136332867	4.97093029280070
C	-2.86293646727198	1.98058120981136	5.72425778868416
H	-1.89425856053506	0.29667394213897	6.69135889536070
C	-1.75247117887594	3.00796500485144	5.95910914014296
H	-3.37175270367116	2.19580900138317	4.77753359716088
H	-3.61998027146624	2.05272126738372	6.51325206796414
H	-2.16212872043726	4.02301020642939	5.98804190979280
H	-1.23902011612839	2.81927379886258	6.90837394816947
H	-1.00635680561653	2.96488879467424	5.15738126647683
C	1.18479425176363	-0.48515275211948	2.46544709750002
C	-0.77121898280490	-6.53800278623961	-4.27297516142912
H	-4.99073421254870	-2.40171608723036	4.46639041741067
C	1.49094054883275	1.01373667430892	2.32387083473835
C	2.14773724199204	-1.24122667850246	3.39490937581999
C	-2.29046022682461	-6.54832978881517	-3.99141739341932
C	-0.00007192190428	-7.45268743579536	-3.29863737231562
F	-0.43069817896309	-8.74621610070805	-3.29967551900796
F	1.31117290470582	-7.48231289497876	-3.65362686496605
F	-0.04804375346804	-7.02365743353803	-2.01279546213970
F	-2.86409323014788	-7.77518475286564	-4.11701196707629
F	-2.61055690933001	-6.08798049747341	-2.75215428343138
F	-2.92267695751951	-5.73390460410697	-4.87931922713719
F	3.43360975299119	-1.15943353992567	2.98427288386663
F	2.09295912835618	-0.80663457483624	4.67127219402782
F	1.80853785857228	-2.55628114327000	3.40034622832999
F	2.73595881974549	1.24363488890265	1.84876246519881
F	0.61511017186428	1.55772656669811	1.43936848651722
F	1.35977467613364	1.68778748881255	3.48567892496521
H	-0.66421029384950	-7.02183194537186	-5.26222406933797
H	1.30999162633697	-0.92320377714144	1.46876365487483
C	-0.26156511156000	-2.65191285979551	-7.48459543949620
C	-0.6030999272602	-4.08038483147233	-7.02827688413688
O	0.51419394667463	-4.64935893022734	-6.44496507520494

C	-1.11151492492972	-4.96557916117760	-8.18294787916853
H	-1.44883268308750	-3.98685058838026	-6.33007500928169
F	0.05720547951733	-1.89806052888704	-6.39691752093200
F	0.80181674065575	-2.60558134572530	-8.31885218384038
F	-1.29067955036324	-2.02201644116663	-8.10801990231820
F	-1.38142498051046	-6.21089965172445	-7.71671373522919
F	-2.26034329535201	-4.49836754226400	-8.73975501943003
F	-0.20802742703109	-5.10559344885624	-9.18236018681848
H	0.21380846080247	-4.93088765139086	-5.42909841921060

8a

G = -10692.31009801 Eh

#(imaginary frequencies) = 0

I	0.97982981333991	-2.52396215216456	0.80990052714882
O	-1.08152150365078	0.73880078213482	1.89026391684877
O	-7.41555593065506	-2.25870019990619	3.11031823994932
C	-2.40583928740372	-2.44984628212073	2.68126692132447
C	-1.93408540437715	-2.67446580905774	3.98573338031864
C	-2.05233198076893	-3.95338945674378	4.55680451506578
C	-2.63018656858857	-4.98823615728869	3.82849972424748
C	-3.09154803198590	-4.76230215434778	2.52989036029395
C	-2.97979980907172	-3.49090831518430	1.96240419694116
C	-1.32800558823728	-1.58805678741792	4.73309615988041
N	-1.13999112738598	-0.33991321169904	4.36365829183793
C	-0.53910082061142	0.29110777626157	5.45902670152973
C	-0.39485277277157	-0.65482886369723	6.47998764039129
C	0.15487503090810	-0.38438433006608	7.72085859805072
C	0.57598664587834	0.93496336350368	7.90902974002081
C	0.44438730937231	1.90588492480544	6.89941883022013
C	-0.11320674342610	1.60594940491454	5.65741758644604
O	-0.89806420094325	-1.85540558685566	6.01092655863611
H	0.25144483289365	-1.14016906474738	8.49204255136051
H	1.01615944572020	1.21643609993469	8.86035692018571
H	0.78708172910747	2.91701579631812	7.09510569457161
H	-0.20860231436117	2.36063380564833	4.88540910638145
H	-1.69147189263515	-4.13095206627751	5.56364241724399
H	-2.71659586547241	-5.97451618457718	4.27320172994241
H	-3.53555076237849	-5.57374454787513	1.96194981278006
H	-3.32488146028065	-3.31312151842172	0.95021348356099
H	-2.30553096771200	-1.47083575770378	2.22678381931917
H	-1.08172139895936	0.30632302985159	2.80478495336279
H	-6.72844454933443	0.50002341876331	4.25674266262813
C	-1.03150472750084	-4.01555723151882	-0.93698150212790
C	-0.73065753828428	-2.75804496315185	-0.40784443949387
C	-1.56309268430026	-1.65991715898663	-0.62231795894634
C	-2.73056419743616	-1.83531673305063	-1.36131898174932
C	-3.06257007170330	-3.08809743533479	-1.90025745193344
C	-2.19257611723031	-4.16868439229776	-1.68529105316598
H	-0.37811808553629	-4.86271040132590	-0.76109944349633
H	-1.31901021383563	-0.69283843815431	-0.19893606418699
H	-3.38297256829969	-0.98135878828369	-1.50627345666958
C	-4.31188007465178	-3.31624808221563	-2.68736911847442
O	-4.53938476914600	-4.42027756148270	-3.18530520843015
C	-5.27258156063266	-2.16454634780777	-2.89282378081631
H	-5.36493932725745	-1.57139192194899	-1.97643334287319
C	-4.82023649071976	-1.24774173991309	-4.05377127899340
H	-6.25374428510690	-2.58886260006347	-3.12371280923821
C	-5.76828413583497	-0.05898476874102	-4.23241827585658
H	-3.80239432176954	-0.88679127902844	-3.86510997863696

H	-4.78024350386239	-1.84128403414759	-4.97408299913294
H	-5.44535430943228	0.57320062056818	-5.06603057821072
H	-6.78904171102490	-0.40012680781168	-4.43741349095642
H	-5.79469737594039	0.55937660560045	-3.32760890464349
C	-1.87595896613562	1.88605691504102	1.95688236913985
C	-6.61689153438116	-3.24463126624235	2.51021087589323
H	-2.44771757813892	-5.13740317341135	-2.10299551071352
C	-1.02087069955249	3.10147765060659	1.56064792648263
C	-3.11385871856719	1.70012144180967	1.05691186746340
C	-6.64084528989771	-3.05684050619684	0.98041666635794
C	-7.15145263919499	-4.60594323467186	2.97858388679556
F	-6.50104034206170	-5.63680610428356	2.39005942324658
F	-6.97278358132957	-4.72447933224911	4.31454984577443
F	-8.47014478249065	-4.75691987151215	2.72996050017838
F	-5.89983757320189	-3.98024881467135	0.32277652584222
F	-7.88742101424408	-3.09139495211387	0.46770727964629
F	-6.11367092846889	-1.83832312721900	0.68961707390183
F	-3.96667381543569	2.74666930305830	1.11645843977537
F	-2.79240269733318	1.50880707004426	-0.24344922029399
F	-3.79879355101068	0.59905398631501	1.46233382869627
F	-1.73607377974512	4.25081396981976	1.53871134544275
F	-0.02605295666412	3.26285999356360	2.46821881555439
F	-0.44094139298105	2.95618117671147	0.35043377316325
H	-5.56467489811591	-3.19929268310020	2.81537402973406
H	-2.25209041771200	2.09212549199069	2.96614562073864
C	-4.66721017078511	1.52634784437135	5.19137805473867
C	-4.86404957653381	0.07677230190748	4.71321024874936
O	-5.98547573967221	0.01097795186023	3.85355073539971
C	-5.00899346826625	-0.93823975951270	5.86430982842278
H	-3.98329613125337	-0.21111016065413	4.13426670630755
F	-4.38083193524102	2.31689305138989	4.13138372727197
F	-5.79989574431049	2.00725556301407	5.75628782926481
F	-3.66616654189135	1.65136793276824	6.08016932161536
F	-5.16761695525953	-2.17655602996824	5.34072297365985
F	-3.91720751396468	-0.96817246483638	6.65520240862116
F	-6.08522057390854	-0.67955448319948	6.63614432887037
H	-6.84493624895395	-1.49429217731764	3.35147355180120

7a-B

G = -10692.21174142 Eh

#(imaginary frequencies) = 0

C	0.70488187381011	-2.04887584208470	-3.90979858844355
C	-0.06022676262016	-0.91100326778737	-4.13308070831475
C	-1.44826669218696	-1.00578073623170	-4.25553567653861
C	-2.12438429461421	-2.20861364057173	-4.18416549571991
C	-1.34771993535255	-3.36358484375435	-3.97403609730616
C	0.03707445360610	-3.28148089893673	-3.83154996811379
N	0.32225668529450	0.43257788053226	-4.29809260832017
C	-0.93374631369353	1.22546985406990	-4.33049333425238
C	-1.10130286406202	2.10404334084625	-3.10465580870288
C	-0.21318285873846	3.17144428802247	-2.91841888003491
C	-0.31645053221760	3.98487888766250	-1.79068310103658
C	-1.31801153500768	3.74774298651057	-0.84494531016400
C	-2.21082737760740	2.69280307783946	-1.03219590477721
C	-2.10378815811754	1.87320603717227	-2.15890751671050
O	-2.00806031890134	0.24421874518390	-4.44475999109275
H	-3.20489041185497	-2.25709256220346	-4.27117143550044
H	-1.84213516100817	-4.32666395851699	-3.89869863084754
H	0.61208227675397	-4.18361493190097	-3.64599444320052

H	1.78142124075791	-1.98650588093036	-3.78891909483999
H	-2.81324416818286	1.06794675170000	-2.31956498652167
H	-2.99398280527989	2.50549224585126	-0.30423467141554
H	-1.40227088459085	4.38533649019127	0.02909985838277
H	0.37812506755496	4.80867057445473	-1.65411458282756
H	0.55985024739308	3.36886958607151	-3.65613112470101
H	-0.97560791815894	1.83219866911808	-5.24093423682785
H	0.98420901446244	0.75582018632028	-3.58403715323873
C	-0.71805749117024	-1.26419579792130	-0.86630211129396
C	0.48500163787053	-0.95117834259889	-0.23736441821914
C	1.27094698269218	-1.89530338696462	0.41521748981530
C	0.80367314650464	-3.20654062991377	0.46456070181129
C	-0.41902929797753	-3.55439417821240	-0.12789499919630
C	-1.16270545714473	-2.58065336877405	-0.80660723661875
H	-1.30074298301017	-0.50186103008003	-1.36812723384176
I	1.04233909299295	1.08160838298889	-0.18214139592068
H	2.20790297882502	-1.62918760893060	0.88718241295829
H	1.40460840626224	-3.94915674183627	0.97721479112997
C	-0.98336968765022	-4.94537660212247	-0.04078688751327
O	-1.96248887074626	-5.24670782281525	-0.71858078171436
C	-0.36821200448423	-5.91452867590045	0.94096133811558
H	0.72293475911742	-5.92558930885181	0.83281464238577
C	-0.73260517223917	-5.54135630979194	2.39848725640636
H	-0.74524880874788	-6.91329768161301	0.70613405601111
C	-0.09437600219599	-6.50239944426375	3.40419626319234
H	-0.40664749760483	-4.51643849025960	2.60926730298382
H	-1.82347561883551	-5.55490979000246	2.50336278999946
H	-0.37217425726089	-6.22989687805627	4.42767160663985
H	-0.42170873225122	-7.53223065466002	3.22434451660783
H	0.99860287857648	-6.47551907825911	3.32900150255613
O	-0.22182579124099	1.10410073981605	1.63199133535506
O	2.06150896165769	0.79580341679877	-2.05214025084679
C	0.22154499970522	1.56421674765377	2.87586776483613
C	3.44421414330075	0.91321399787522	-2.22315820130139
H	-2.10022946903089	-2.86346457421540	-1.26916492493667
C	1.46162023041288	0.81078967403341	3.40028091710208
C	0.41196647252828	3.09295243159560	2.85455492531359
C	4.24151692036983	-0.13451927057210	-1.42157719275817
C	3.91862867329041	2.36015645582610	-1.97942019640957
F	5.25171268363095	2.50658294332310	-2.12198362110578
F	3.31663253378207	3.18780440943017	-2.86158687898843
F	3.59057311768212	2.80207637152209	-0.73456608811307
F	5.53808653856293	-0.17594362748766	-1.79599086585630
F	4.21136805602769	0.09075550695862	-0.08172936164921
F	3.71518667260049	-1.36050482667051	-1.63201307050279
F	0.92475728735525	3.57761825090913	4.00438914430856
F	1.23254973560208	3.48727563217348	1.84316501791857
F	-0.78241384118901	3.69132504536696	2.65146618050766
F	1.65396003626055	1.03336693521150	4.71880148040433
F	1.29407810444888	-0.51927921458177	3.23202052019921
F	2.60646534694052	1.15652399181247	2.75760107925097
H	3.65693428871682	0.70048626305585	-3.27827344254882
H	-0.57030034537137	1.36950170467001	3.61001347626368
C	-2.87056713654329	-1.30489353036195	3.32966417924530
C	-2.83900172226202	-0.72231114752552	1.90385583261606
O	-2.79386945723215	0.67724600828794	1.95663438642306
C	-4.05257550633967	-1.12682399693126	1.05213367507811
H	-1.95515113718509	-1.15082627991210	1.41746807286492
F	-1.76616259192139	-0.89244031113123	4.00349060349578
F	-3.94546802173811	-0.90840868317756	4.04220543292494
F	-2.85113224133200	-2.65931531050750	3.32749141347923

F	-3.90850809680488	-0.63016980752809	-0.20119213225275
F	-4.17450221149165	-2.47074305236312	0.94101897719113
F	-5.21551865001755	-0.64668092495791	1.54101146489912
H	-1.85989745213585	0.94179043181422	1.72222523236370

TS-1

G = -10692.19959183 Eh

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C	-2.77671764900842	0.51526546672932	-1.21287865632833
C	-4.19760490102265	0.46099388438006	-1.34592569285204
C	-4.91482364938577	-0.71858876349045	-1.23364171071080
C	-4.16747056174902	-1.86581334121353	-0.96212131727146
C	-2.76005809207846	-1.82958215318733	-0.80290789406527
N	-2.36332388103756	1.77623403333307	-1.43259666734994
C	-3.54342798226954	2.61361841734791	-1.64459957269481
C	-3.69882191727404	3.73076824740763	-0.62971362355088
C	-2.75252295517998	4.75952493634029	-0.62610890827913
C	-2.82172962294236	5.76164211523841	0.34003700999193
C	-3.84734318370640	5.75281281068984	1.28882087381259
C	-4.80922384691670	4.74459284667272	1.26138114563126
C	-4.73779609400732	3.73252745347461	0.30242607479913
O	-4.68370444567727	1.69347991918306	-1.60032731039210
H	-5.99289863771234	-0.74527096860209	-1.33958503169340
H	-4.68193987978310	-2.81442380846666	-0.85470327363097
H	-2.23588559550868	-2.75442039185412	-0.58726106077606
H	-0.96841736826157	-0.61826354632804	-0.79734084789193
H	-5.48999778725883	2.95341412802766	0.27914228853043
H	-5.60657883897760	4.72596597625249	1.99658234378498
H	-3.89416553422784	6.52962238555907	2.04605555947866
H	-2.07520226977043	6.55021723177206	0.35012903244687
H	-1.95387870623871	4.76915223973135	-1.36009455955368
H	-3.52499052861738	3.01631642471045	-2.66545424118968
H	-1.40902433224979	2.17284663305641	-0.86102757468359
C	-3.59925694726325	0.56201640199115	1.95902757345792
C	-2.27590699304906	0.86847646553689	2.30688927714022
C	-1.36604384148426	-0.13060337018445	2.67031283326171
C	-1.80269481102071	-1.44840797636967	2.70706650623340
C	-3.13758152291091	-1.77519202307461	2.40938921842481
C	-4.02511663628881	-0.75493627871475	2.03863940693325
H	-4.28116554720253	1.35410389738705	1.67739179623531
I	-1.72300625693082	2.86146253343166	2.37456452173925
H	-0.34270135200201	0.11576681928818	2.92670566792687
H	-1.09277630839672	-2.22050231100377	2.98171256894731
C	-3.65840838769141	-3.17877711405181	2.49344857885693
O	-4.82559018825516	-3.41952688086618	2.18673689641895
C	-2.74496397786804	-4.26506808713116	3.01254366873293
H	-1.74726654391042	-4.17351738093530	2.56750587103931
C	-2.62384440584150	-4.20705264373059	4.55482187679549
H	-3.16731589487138	-5.22769078435122	2.71200892946493
C	-1.67382129638179	-5.28372611413650	5.08526329784411
H	-2.26898332452759	-3.21592244197761	4.86045846443138
H	-3.62157020857155	-4.33558503049092	4.98979397772626
H	-1.60921183482799	-5.23836725812978	6.17734412977136
H	-2.02084017249169	-6.28441083384596	4.80504015691751
H	-0.66529355391901	-5.14843804892892	4.67826423487569
O	-3.55844776311137	3.06254169708214	4.32515667784922
O	-0.47084630952713	2.49617631572581	-0.01073034839799
C	-3.23349569913593	3.11748275616747	5.65478398314368
C	0.82103194931949	2.53475015449728	-0.48570822923306

H	-5.05011004477685	-1.02086179046460	1.80599415188740
C	-2.51096618832425	1.83336050555896	6.12854537102748
C	-2.43548985319073	4.39774289136171	5.98449686653573
C	1.69964064801181	1.52071548222830	0.27603220525669
C	1.36776303061245	3.97514290481777	-0.40860347174011
F	2.65438264236720	4.08589525239893	-0.82647708191914
F	0.62330765218637	4.78150987546808	-1.20654962996869
F	1.30539608645944	4.48815664803406	0.84307683085779
F	2.97724071781560	1.47238166733673	-0.17722272660884
F	1.75425682418263	1.77029615612942	1.60648327079050
F	1.18185729948473	0.27467278095496	0.12776913809042
F	-2.10680308328984	4.49364921575168	7.29995094217058
F	-1.28058937234715	4.50584825425267	5.28024596422972
F	-3.18395819251921	5.48524374736544	5.68081135167712
F	-2.39382624624820	1.76611269566377	7.48070074517667
F	-3.21669690426226	0.74262816353486	5.74104541403017
F	-1.26233153902011	1.69701954283635	5.61499796741571
H	0.88205167361834	2.24542225266799	-1.54781770583077
H	-4.13471725803400	3.18289580349964	6.28809852655434
C	-6.89541446105021	1.21022606507015	5.51338129660941
C	-6.33123668946670	1.53393680331125	4.11218236161644
O	-6.06329246015509	2.89472888065526	3.99011584182829
C	-7.30821950298795	1.12972338019220	2.99397176679844
H	-5.43261233726241	0.91375359408642	3.99484160696173
F	-6.05428881997490	1.68189604376753	6.46577633034730
F	-8.10467288135698	1.77103336375993	5.74081120763918
F	-7.01732158056421	-0.12491607659764	5.71885372259316
F	-6.72315919450726	1.30366909624970	1.77981225234582
F	-7.67025349309219	-0.17467899262262	3.07031748123500
F	-8.43596183436052	1.86995958025954	2.99420221763414
H	-5.04384433025870	3.02004580746697	4.08396431512045

IVb

G = -10692.22436237 Eh

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C	1.26882094502197	-1.99689875670347	-2.47071194104996
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C	-0.89807555550900	-0.82994940406497	-2.92962714810235
C	-1.60720435088473	-2.02329223572382	-2.99991053257811
C	-0.85524488507571	-3.16914156293830	-2.79211881614287
C	0.55741572909839	-3.16224123983241	-2.54046922642848
N	0.95793886692354	0.45341506396957	-2.71287255305980
C	-0.17251591369742	1.29125355285314	-3.03137621579056
C	-0.39027572498675	2.44605813881484	-2.08052705962574
C	0.54202408463393	3.48741783750153	-2.11995147649692
C	0.44212560162021	4.53006620708587	-1.20214411335073
C	-0.59423662961658	4.53984678702738	-0.26483819685691
C	-1.53005116240387	3.50858883210459	-0.24908153368866
C	-1.43166385806965	2.45170409138351	-1.15462146420773
O	-1.34809878652059	0.39689288879535	-3.10984064852987
H	-2.67039085175638	-2.05556196196380	-3.19829292453696
H	-1.35693340916887	-4.13066815052118	-2.82995504556409
H	1.05961486303302	-4.11424678845467	-2.41588244037375
H	2.33664658944845	-1.97269157124046	-2.29113591803767
H	-2.15774247626553	1.64840706516751	-1.11318128389198
H	-2.33141606596406	3.49928551235347	0.48030472219688
H	-0.66786021336032	5.35184122816328	0.45222960471733
H	1.16995383574320	5.33543787699722	-1.22438355879902
H	1.34658005131027	3.48050418458678	-2.84987238626186
H	-0.03836363975876	1.65232997672262	-4.06164908892736
H	2.66884451079333	0.97819421719870	-2.68933239440158

C	-0.41249974867579	-1.22351570344918	0.33373400038889
C	0.97005239938160	-1.04695465968894	0.48745889848863
C	1.83017382883928	-2.13749403580377	0.67893459707572
C	1.29434896788486	-3.41813217445237	0.70305095810034
C	-0.08462066439297	-3.62247994689418	0.51819075420875
C	-0.92549162039282	-2.51166479875711	0.34914481630482
H	-1.06156343236243	-0.36255253644683	0.24319385937295
I	1.75018080221476	0.89064586965995	0.41914166232971
H	2.89651113396604	-1.98643530622153	0.80285420729102
H	1.96503049627802	-4.25886480177176	0.84096058647299
C	-0.69929574234875	-4.99178200505539	0.49348682391758
O	-1.88294731995656	-5.12180558957132	0.18398638952813
C	0.15029044451734	-6.17765470498883	0.88452437913869
H	1.11826030617290	-6.13350647583336	0.37037457750231
C	0.38935917264403	-6.23054965110657	2.41252503324702
H	-0.36842611082892	-7.08251022220812	0.55709260734819
C	1.28973520116593	-7.40671182429156	2.79870616110530
H	0.84218064728676	-5.29069058935939	2.74854976024139
H	-0.57992093354966	-6.31431798446103	2.91701632330160
H	1.43867380340617	-7.43972524159529	3.88288632351746
H	0.84670112442747	-8.35857100813772	2.48578628678598
H	2.27265408115671	-7.31751313683356	2.32215619805033
O	-1.41539619693019	1.21185762952753	2.09250706178276
O	3.61157634678754	1.10657425746180	-2.97458263994761
C	-1.55071238361219	1.36205745004493	3.45489234310038
C	3.70261256319477	0.56215306686875	-4.26465197305436
H	-1.98874823613168	-2.68549777003041	0.22442365914627
C	-0.99862738303499	0.11201561420125	4.16659089329001
C	-0.85263897492274	2.65977185512101	3.90434455713125
C	4.97412656505162	-0.29422695470854	-4.32259826920360
C	3.65608523872363	1.69504574108467	-5.30640466284095
F	3.72453071148567	1.23978592764563	-6.57757029779225
F	2.47228924258878	2.35349505669434	-5.17920151737369
F	4.63861913465055	2.60376389071798	-5.13791066443955
F	5.16801965756653	-0.84341815047699	-5.54320442779635
F	6.08486675862433	0.40154149589454	-4.00123870009396
F	4.86260305589373	-1.31448709912570	-3.43461850423345
F	-0.94677525568203	2.88229335500767	5.24517898770900
F	0.46316919713541	2.69518121601807	3.58871138235556
F	-1.43807463352742	3.72036289518335	3.29301682903447
F	-1.09137389475318	0.17880330442293	5.52281713590822
F	-1.71123145655035	-0.97898280531628	3.78279710230429
F	0.29830214857394	-0.14097571648132	3.86949129665847
H	2.86652211952772	-0.10483540186295	-4.50409066165878
H	-2.59606094801748	1.45904027151664	3.78462940344429
C	-5.28736541964279	-0.10012291252432	2.23136828186772
C	-4.11051514993217	-0.05273586986275	1.22980246995647
O	-3.64404121419936	1.21642728390318	1.08823314288668
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F	-4.85668581852494	0.31685830344437	3.45343419599369
F	-6.31689034107272	0.71003486796834	1.88407107464714
F	-5.80999263589711	-1.34636857934351	2.41338554204603
F	-3.45005143867883	-0.57705276014542	-0.98849111371843
F	-4.87928016536581	-1.95359113373424	-0.09169729528755
F	-5.52726344664292	0.02860939898273	-0.74188092526989
H	-2.41540294960157	1.25421159831339	1.62981842508205

8a

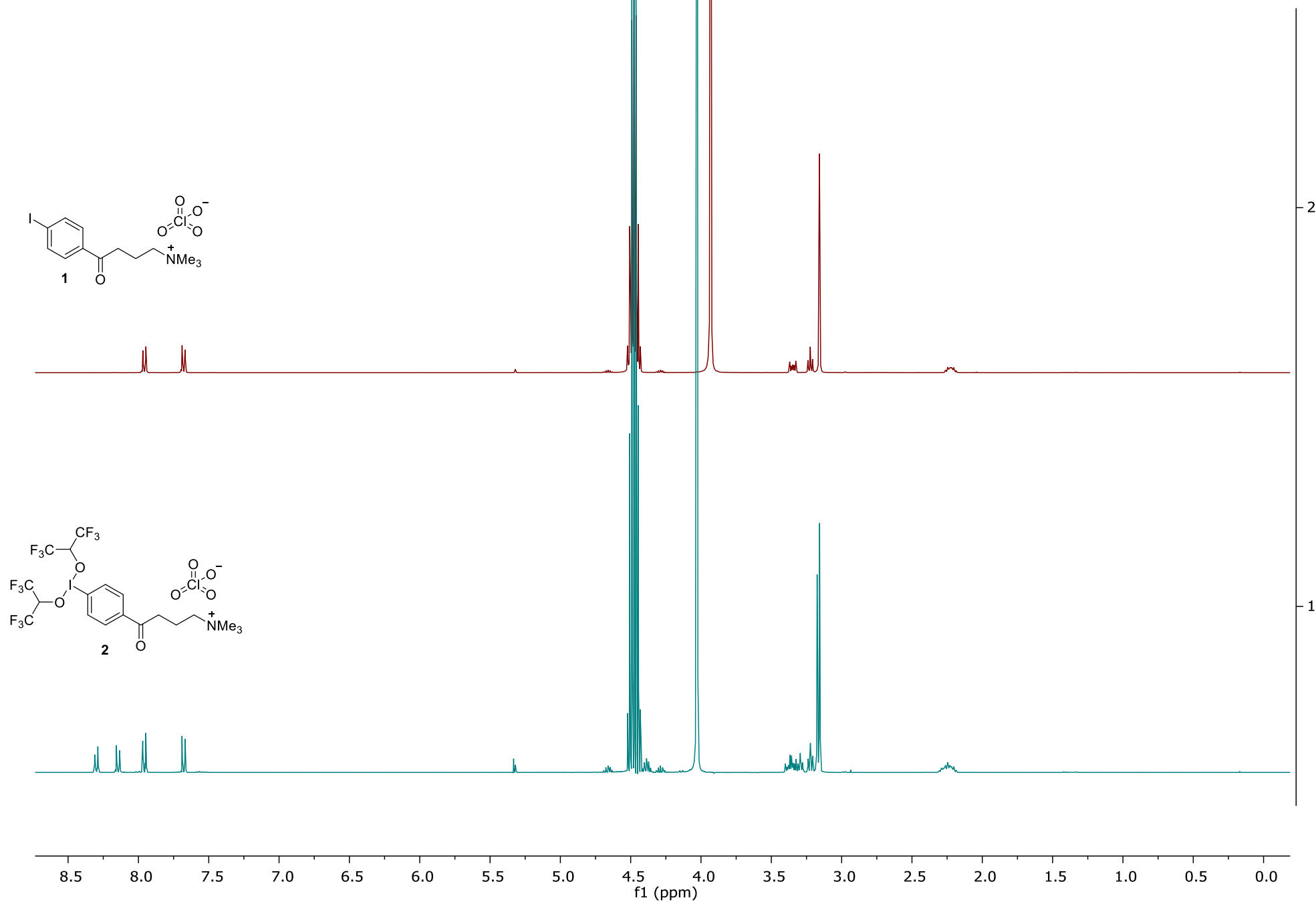
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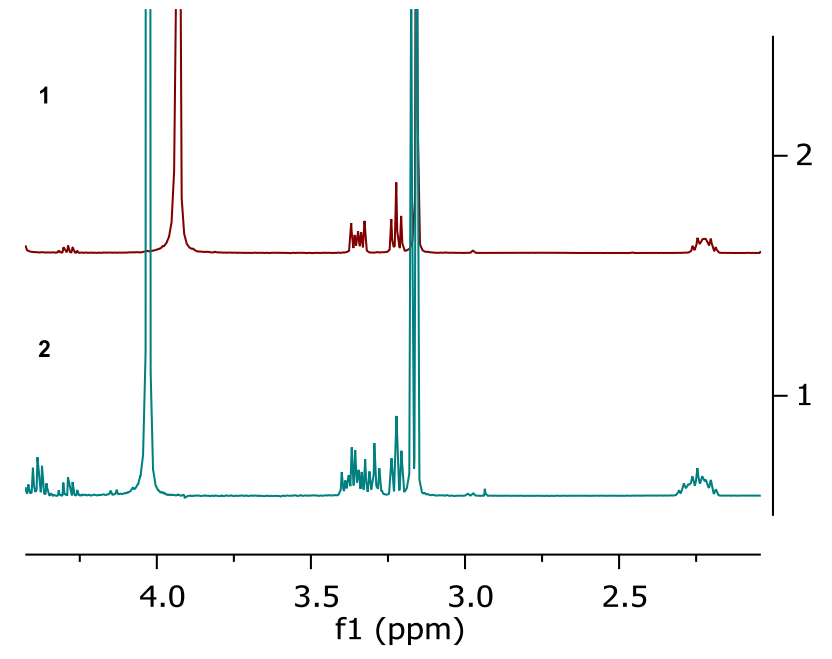
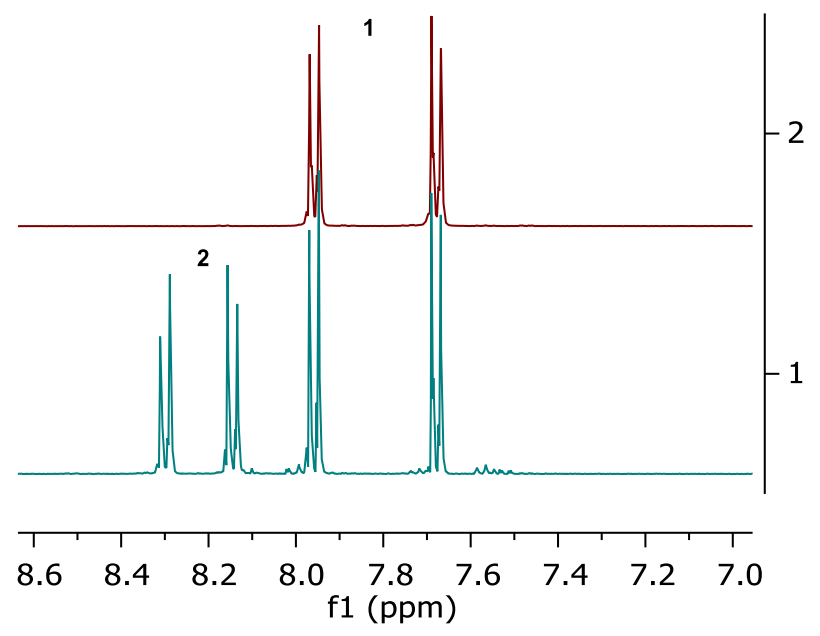
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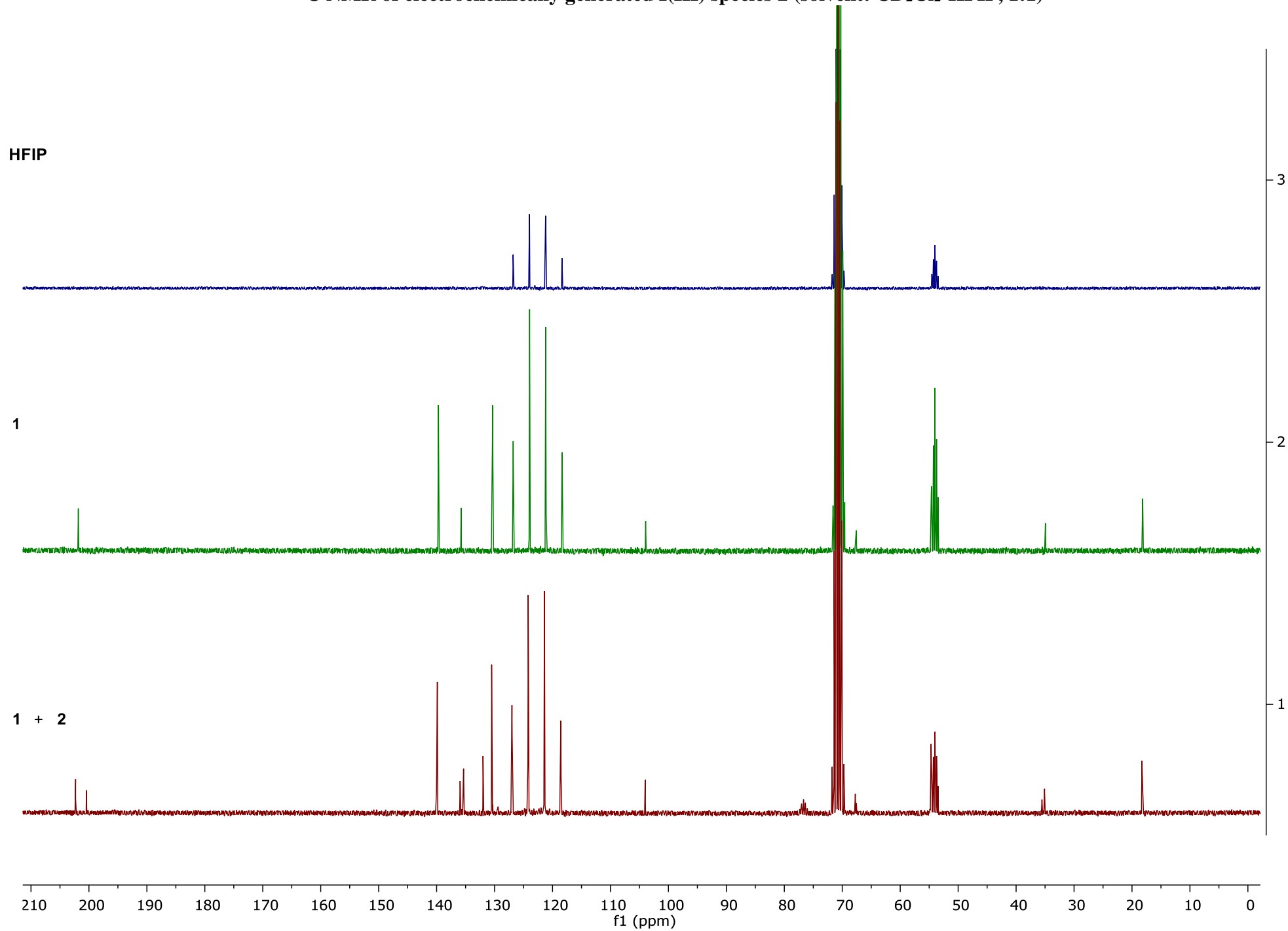
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C	-2.90911250298420	-2.32531556837264	-2.63074109515650
C	-3.34082158402611	-3.56435416496096	-2.18856957049377
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C	-1.64896516943935	-3.33389171909155	-0.42873091405184
N	-1.71151441727906	-0.40094085743687	-2.74280883853243
C	-2.59680835679036	-0.44928550570091	-3.71042832072754
C	-2.83839829056283	0.54422905210899	-4.74481708510827
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C	-2.67160140950956	2.83753707843081	-5.49564296543297
C	-3.31301877014220	2.49011820652831	-6.68957812073462
C	-3.70189053269665	1.16636745099020	-6.91744258968477
C	-3.47628389724077	0.19521422910073	-5.94734465522804
O	-3.36702988856918	-1.59155326734489	-3.71358185061393
H	-4.13448700381989	-4.11524276063962	-2.68044451189585
H	-2.96671440472107	-5.02384152778013	-0.66096291540389
H	-1.17037816291210	-3.76069457232444	0.44677692774491
H	-0.43877610098146	-1.53097169378620	-0.41474699156649
H	-3.78398973332234	-0.83086001618282	-6.11816786787006
H	-4.19417096687878	0.89558620796701	-7.84604149125036
H	-3.54536671844240	3.25434820468792	-7.42765396440338
H	-2.38215566863774	3.86717314110027	-5.30903289826417
H	-1.94151651593827	2.13089807561907	-3.59440857817332
H	-1.25457349994550	3.23080715306340	-7.76867547839080
H	-0.09140653220614	0.11822657406012	-3.17197267064793
C	1.24552477451305	-0.74002038567306	1.61805871861715
C	1.78634635110985	-0.31904639806995	0.39915467489865
C	2.36053078230010	-1.22552096478165	-0.49217325522118
C	2.39093910658602	-2.57642036455098	-0.15388366863284
C	1.84521517271443	-3.02804907613633	1.05696062178228
C	1.27556968332029	-2.09252059638710	1.93494983147048
H	0.80159574056574	-0.02648546926578	2.30322699963831
I	1.68777633049627	1.72361911059066	-0.12732396371196
H	2.76145561374971	-0.88992162656890	-1.44109826084140
H	2.82978615044211	-3.27530753621769	-0.85777361081402
C	1.83416880548220	-4.47077444977804	1.44357823955738
O	1.19899609070330	-4.84120716351895	2.43342427129476
C	2.64945308202107	-5.45485026824701	0.63387199272028
H	2.47918386235954	-5.30372396208911	-0.43870630579267
C	4.16088625611548	-5.31839950716529	0.93345186680512
H	2.30902425081011	-6.46083561284382	0.89436765479165
C	4.98942321422840	-6.32158978232044	0.12670272392662
H	4.48885835679795	-4.29736878418421	0.70737827913551
H	4.32265476891449	-5.47444178709645	2.00648590500418
H	6.05476426035308	-6.21952705244554	0.35872993293562
H	4.68832592080854	-7.35027797399062	0.35410525539387
H	4.85809070641879	-6.16034098580411	-0.94934284539814
O	0.28653983600642	5.35597964429371	-5.66694034117846
O	0.79207005084439	0.17829546691422	-3.64053489916216
C	1.26610477967326	4.39954866154349	-5.34158612924692
C	0.73305617122280	-0.67705562592191	-4.74410256091452
H	0.85376550370590	-2.44196857356097	2.87187810111934
C	2.61376659664023	4.78355023049629	-5.98571519938456
C	1.33051482658842	4.31557727897251	-3.81072181572774
C	1.58620180131960	-1.93215720155184	-4.47706822544147
C	1.17746380518205	0.10852556554286	-5.98741445228932
F	1.18231025248831	-0.64672679251956	-7.10923832545369
F	0.30693487643201	1.13035448866485	-6.20113390170618
F	2.40569245292675	0.65300997655019	-5.85239247134885

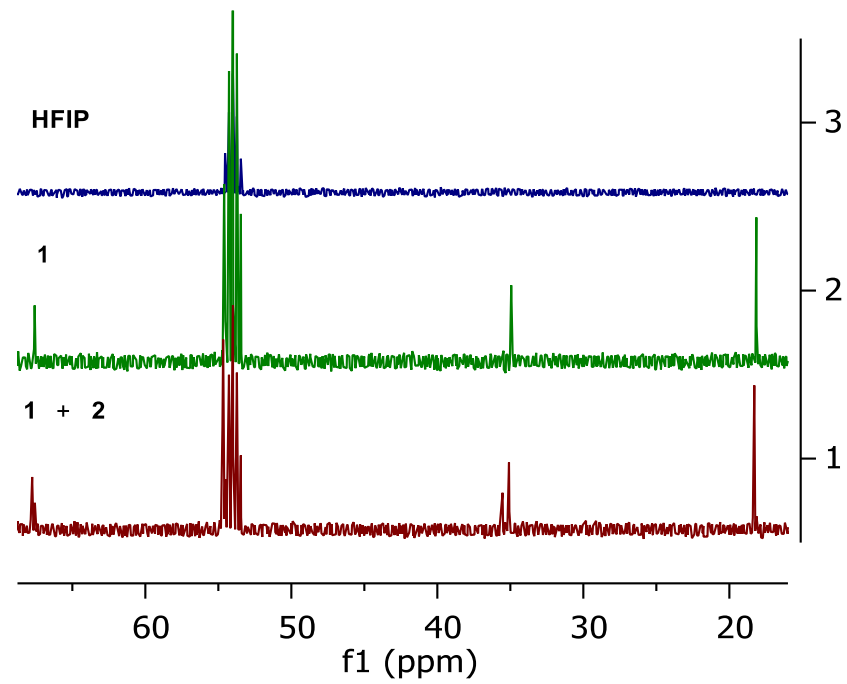
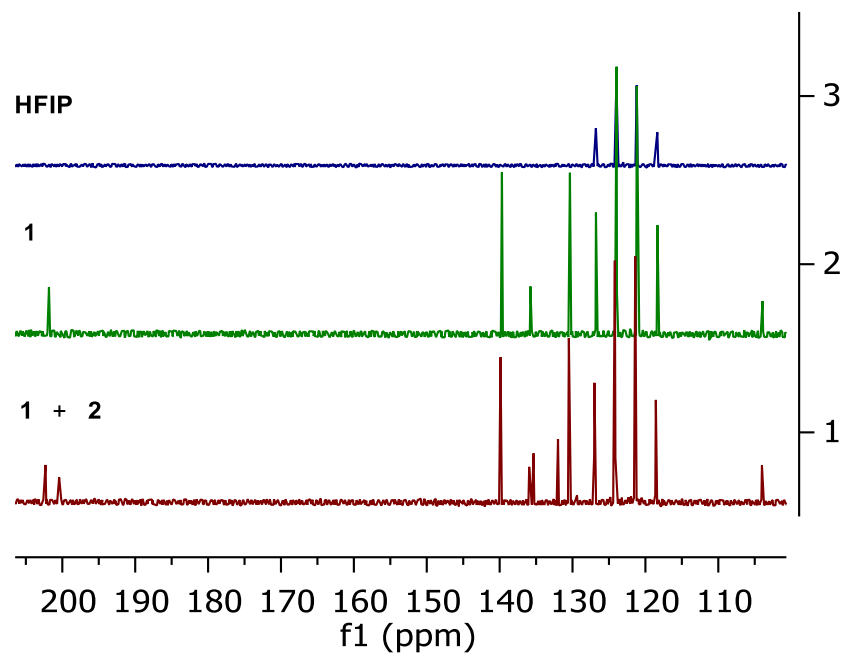
F	1.59091964435919	-2.79214750776701	-5.52506015182787
F	2.87316921248643	-1.63746912446579	-4.18606060825971
F	1.07467276476219	-2.60081451329618	-3.41541266462981
F	2.32507820930482	3.50422530888348	-3.39183039842810
F	1.51597388127934	5.52550842623177	-3.23597059234647
F	0.16485260943527	3.82101464045387	-3.33326553626204
F	3.55320466043225	3.82627782984625	-5.81742354126649
F	2.43902276444462	4.94146167362210	-7.32407979873595
F	3.11411423550916	5.94407001985375	-5.51120126140102
H	-0.28053500397016	-1.03758151977645	-4.95641713675912
H	1.01395145314997	3.39963691298360	-5.70870275028370
C	0.42480347813151	2.67760936799019	-9.68495486392020
C	-0.12334688845941	4.02908132695228	-9.19094542381965
O	-0.54776596513883	3.90277442035093	-7.84745776867494
C	-1.26606749256847	4.60005404219727	-10.05025802729014
H	0.69490695626767	4.74956739443710	-9.20898899486230
F	1.51023792271102	2.33697858757354	-8.95941568134525
F	-0.49473837872511	1.69203711732560	-9.52652695194173
F	0.78572612749588	2.70568366986040	-10.98182189712496
F	-1.66661805034669	5.78230965126557	-9.53619809927366
F	-0.89602426445992	4.80721287982028	-11.32801184976507
F	-2.34528647344564	3.77627112473632	-10.05340390272041
H	-0.15945613369927	5.03304183645011	-6.48013011863623

Spectroscopic data

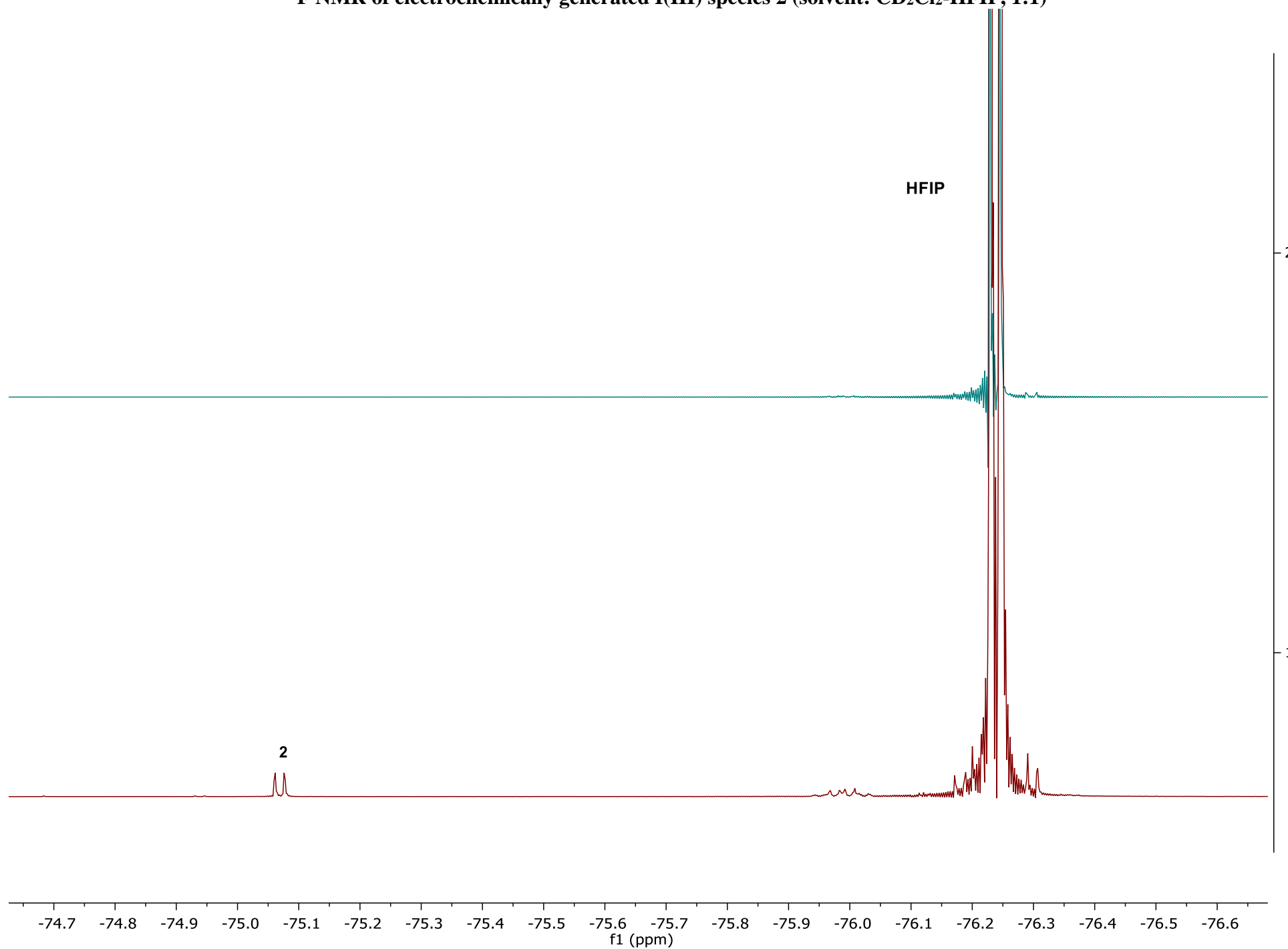
^1H NMR of electrochemically generated I(III) species **2** (solvent: CD_2Cl_2 -HFIP, 1:1)



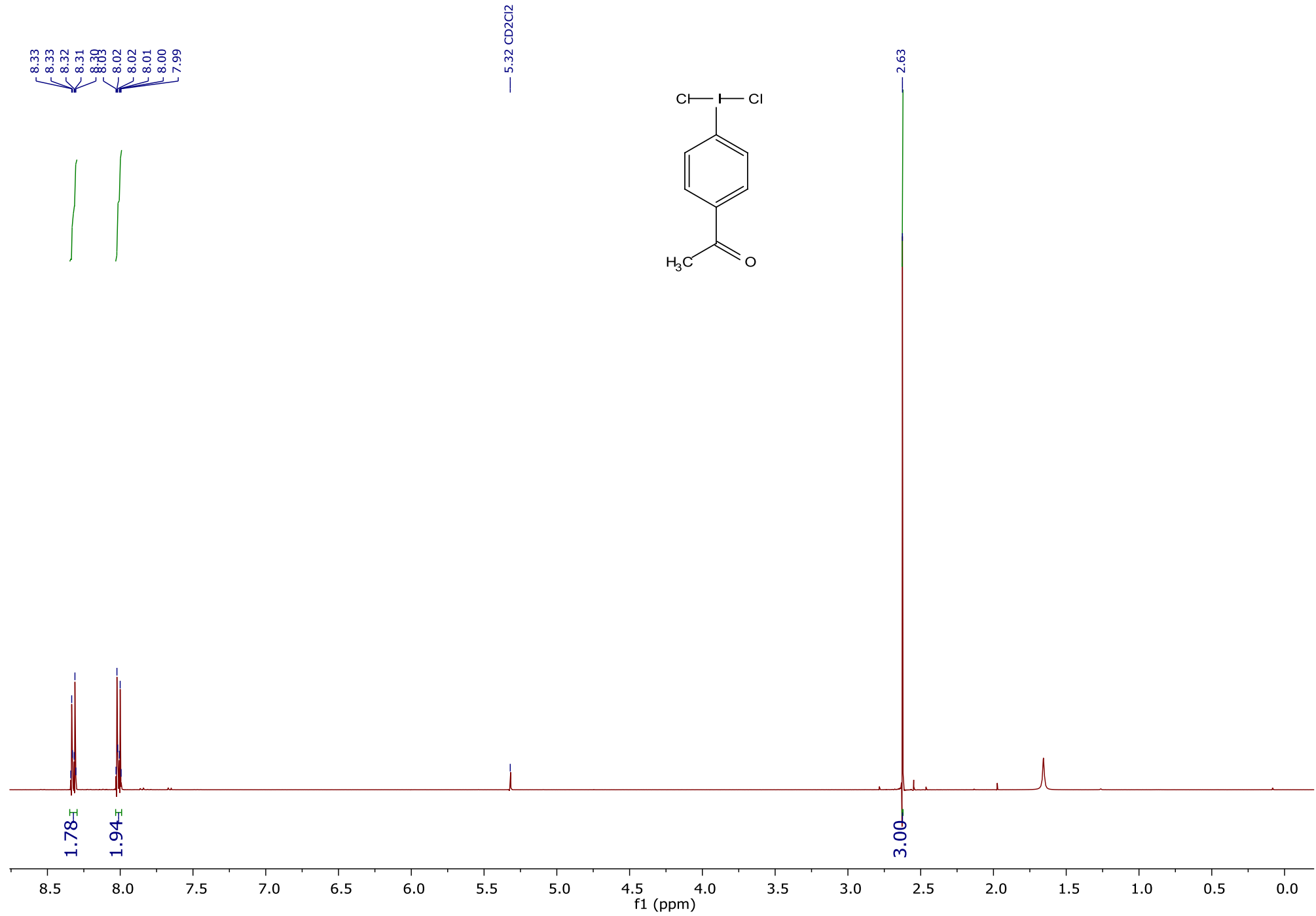
^{13}C NMR of electrochemically generated I(III) species 2 (solvent: CD_2Cl_2 -HFIP, 1:1)

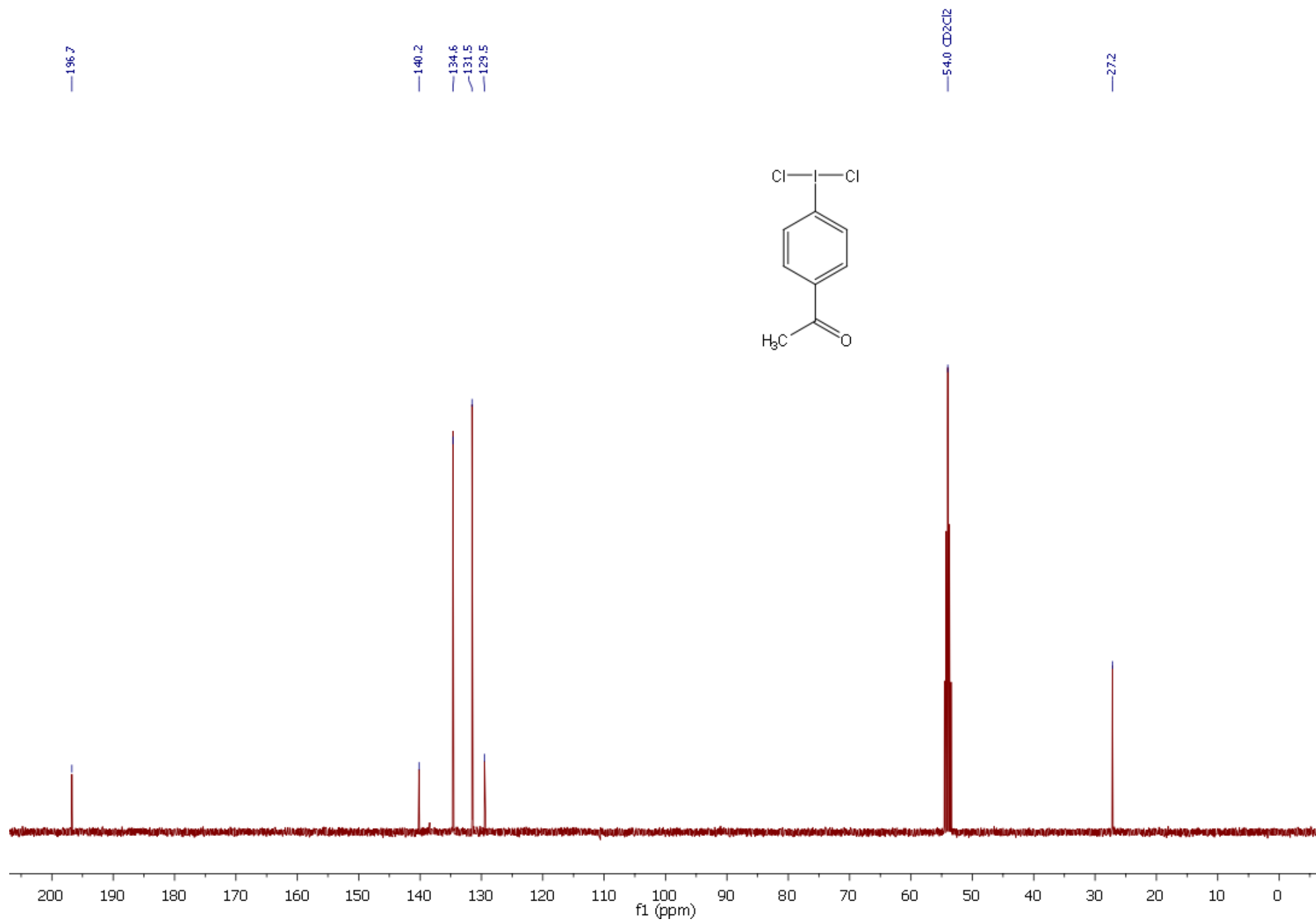


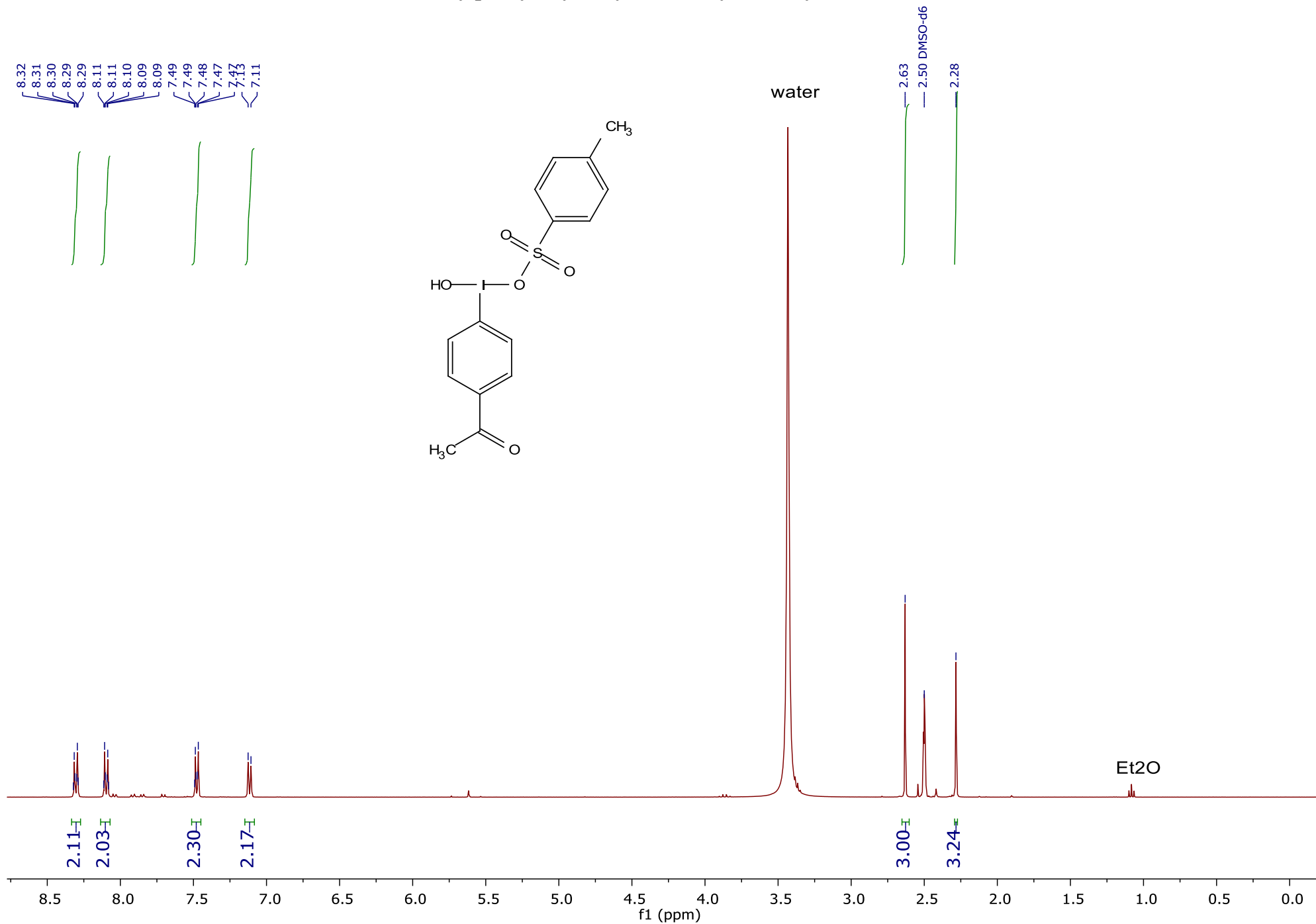
^{19}F NMR of electrochemically generated I(III) species 2 (solvent: CD_2Cl_2 -HFIP, 1:1)

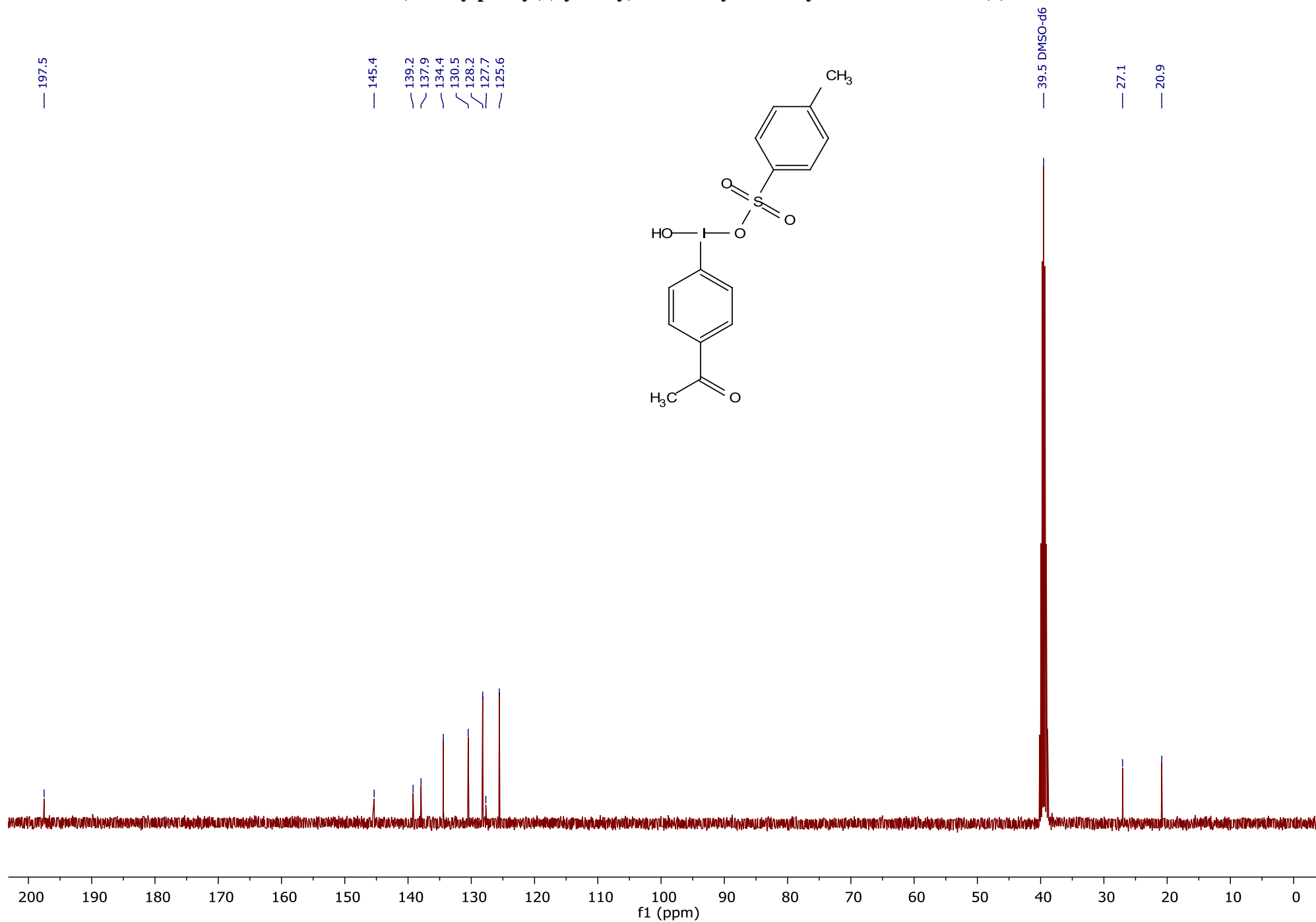


¹H NMR of 1-(4-(dichloro-λ³-iodanyl)phenyl)ethan-1-one (3)



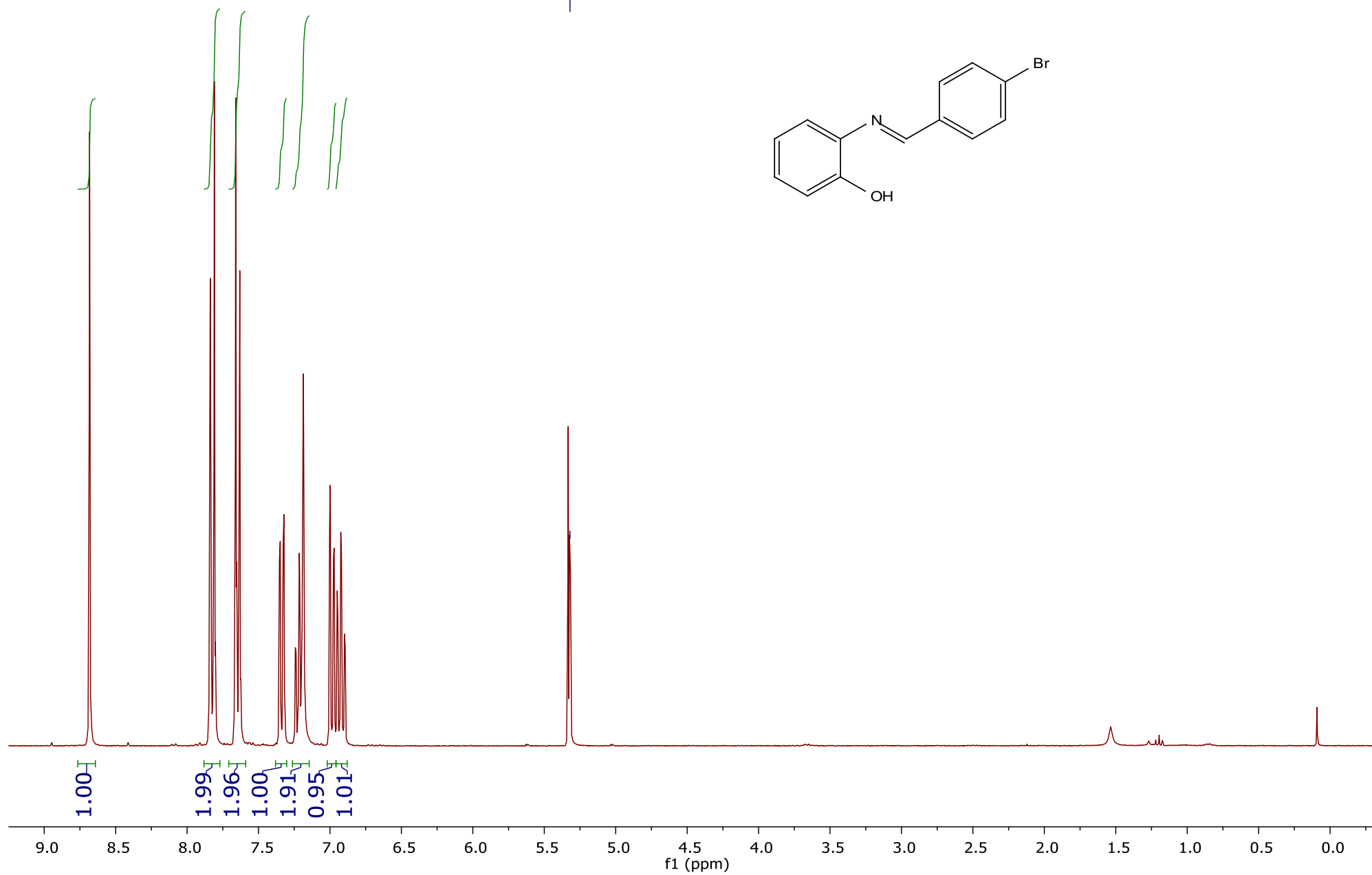
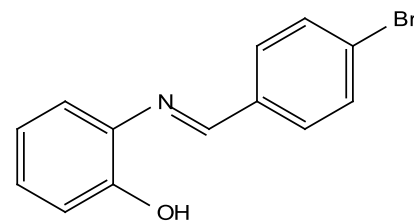
^{13}C NMR of 1-(4-(dichloro- λ^3 -iodanyl)phenyl)ethan-1-one (3)

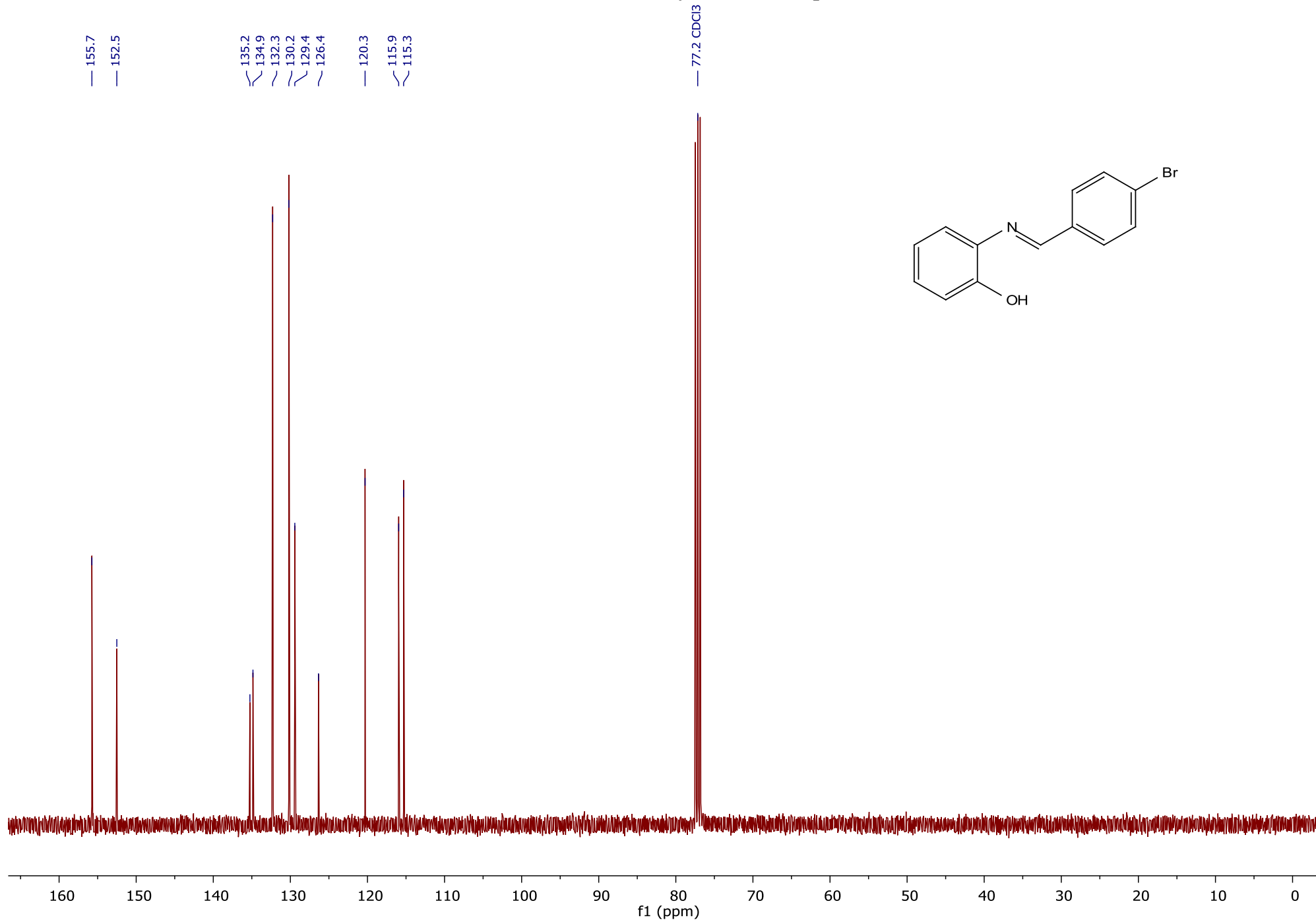
¹H NMR of (4-acetylphenyl)(hydroxy)-λ³-iodanyl 4-methylbenzenesulfonate (4)

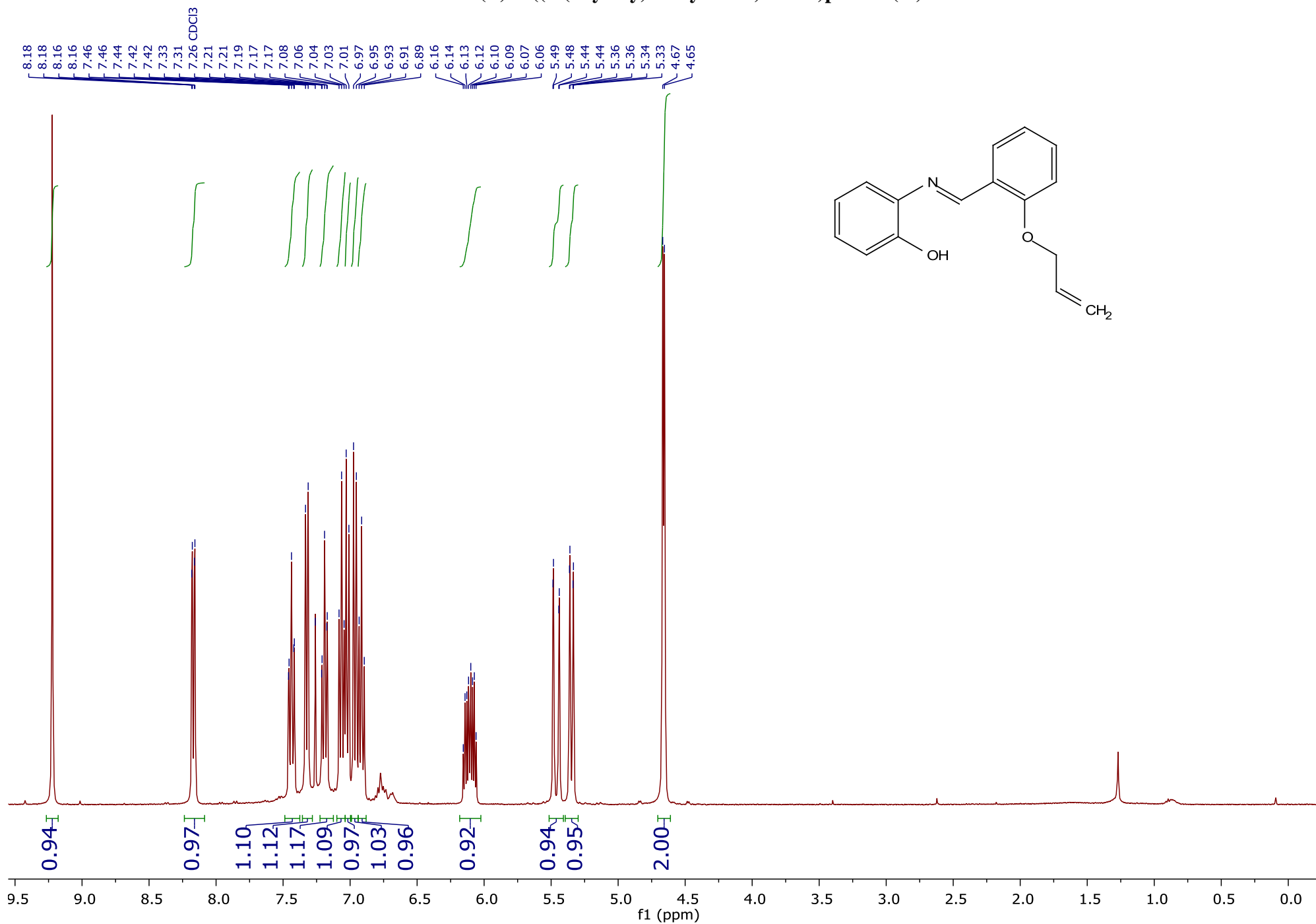
^{13}C NMR of (4-acetylphenyl)(hydroxy)- λ^3 -iodanyl 4-methylbenzenesulfonate (4)

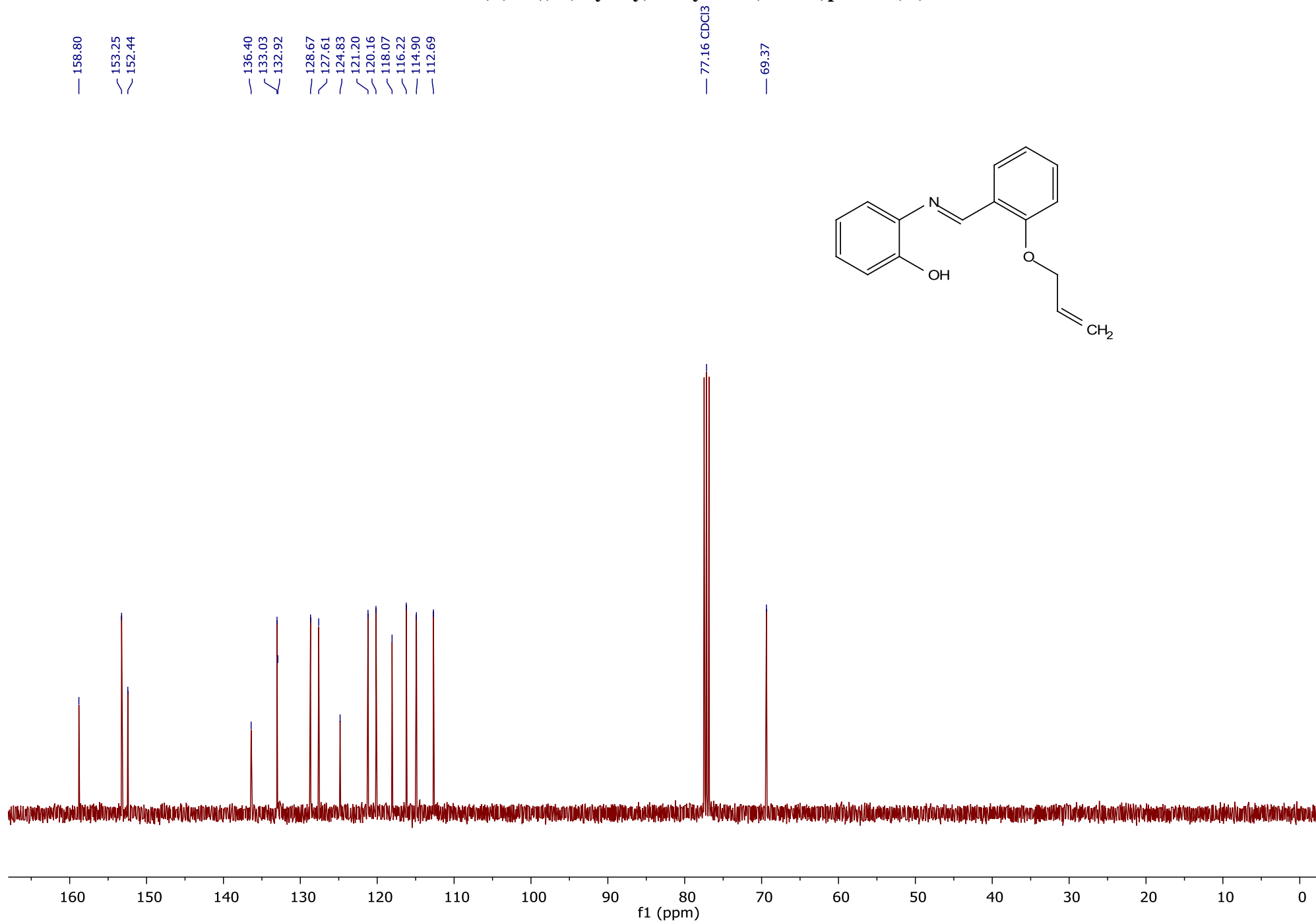
^1H NMR of (*E*)-2-((4-bromobenzylidene)amino)phenol (**7b**)

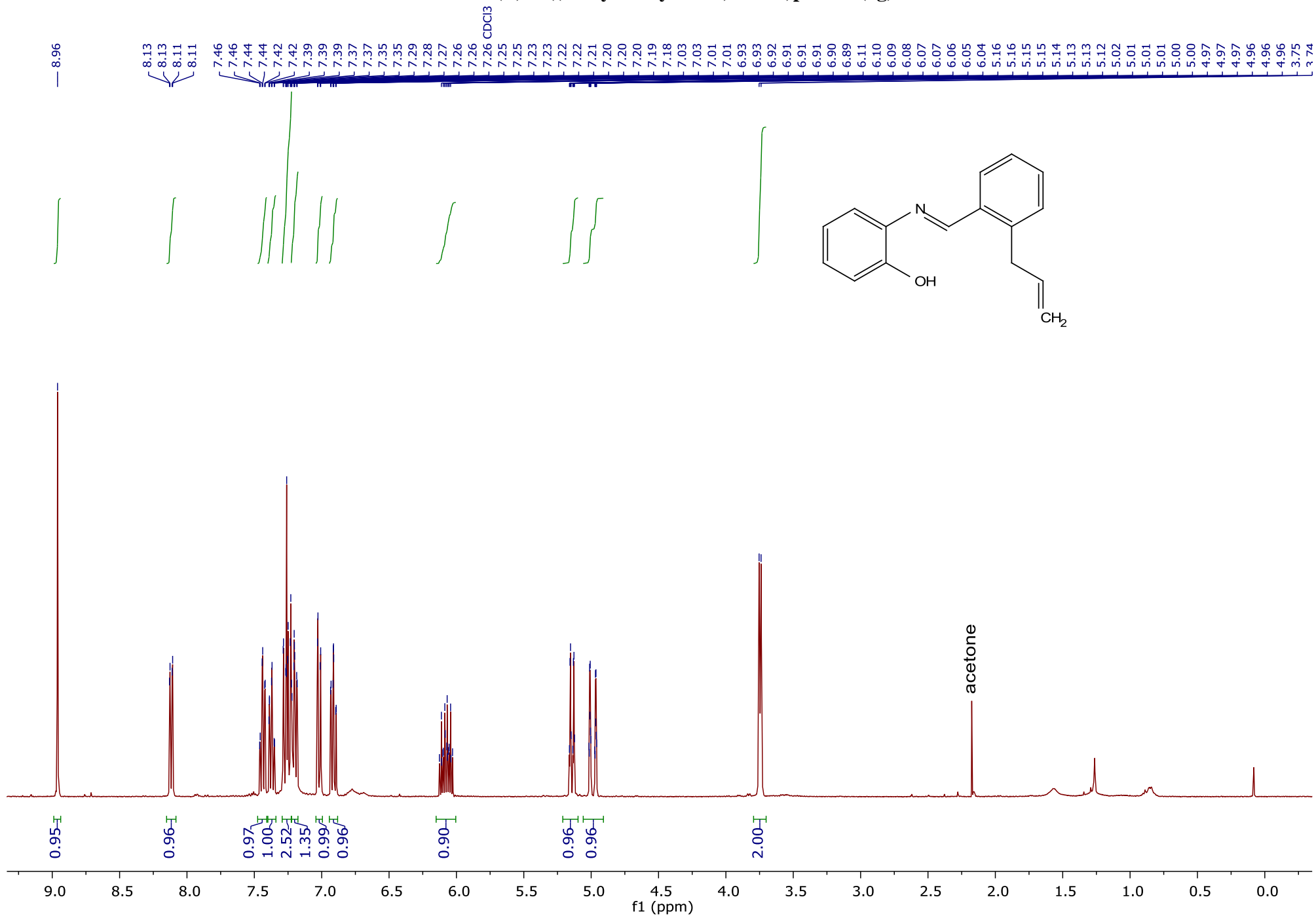
— 5.32 CD2Cl2



^{13}C NMR of (*E*)-2-((4-bromobenzylidene)amino)phenol (**7b**)

^1H NMR of (*E*)-2-((2-(allyloxy)benzylidene)amino)phenol (7f)

^{13}C NMR of (*E*)-2-((2-(allyloxy)benzylidene)amino)phenol (**7f**)

^1H NMR of (*E*)-2-((2-allylbenzylidene)amino)phenol (**7g**)

8.96

8.13
8.13
8.11
8.117.46
7.46
7.44
7.44
7.42
7.42
7.39
7.39
7.37
7.37
7.35
7.35
7.29
7.28
7.27
7.26
7.26
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7.23
7.22
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7.21
7.21
7.20
7.20
7.19
7.18
7.18
7.03
7.03
7.01
7.01
6.93
6.93
6.92
6.92
6.91
6.91
6.91
6.91
6.90
6.89
6.11
6.10
6.09
6.08
6.07
6.07
6.06
6.06
6.05
6.05
5.16
5.16
5.15
5.15
5.14
5.13
5.13
5.12
5.12
5.02
5.02
5.01
5.01
5.01
5.01
5.00
5.00
4.97
4.97
4.97
4.97
4.96
4.96
4.96
4.96
3.74

0.95

0.96

0.97
1.00
2.52
1.35
0.99
0.96

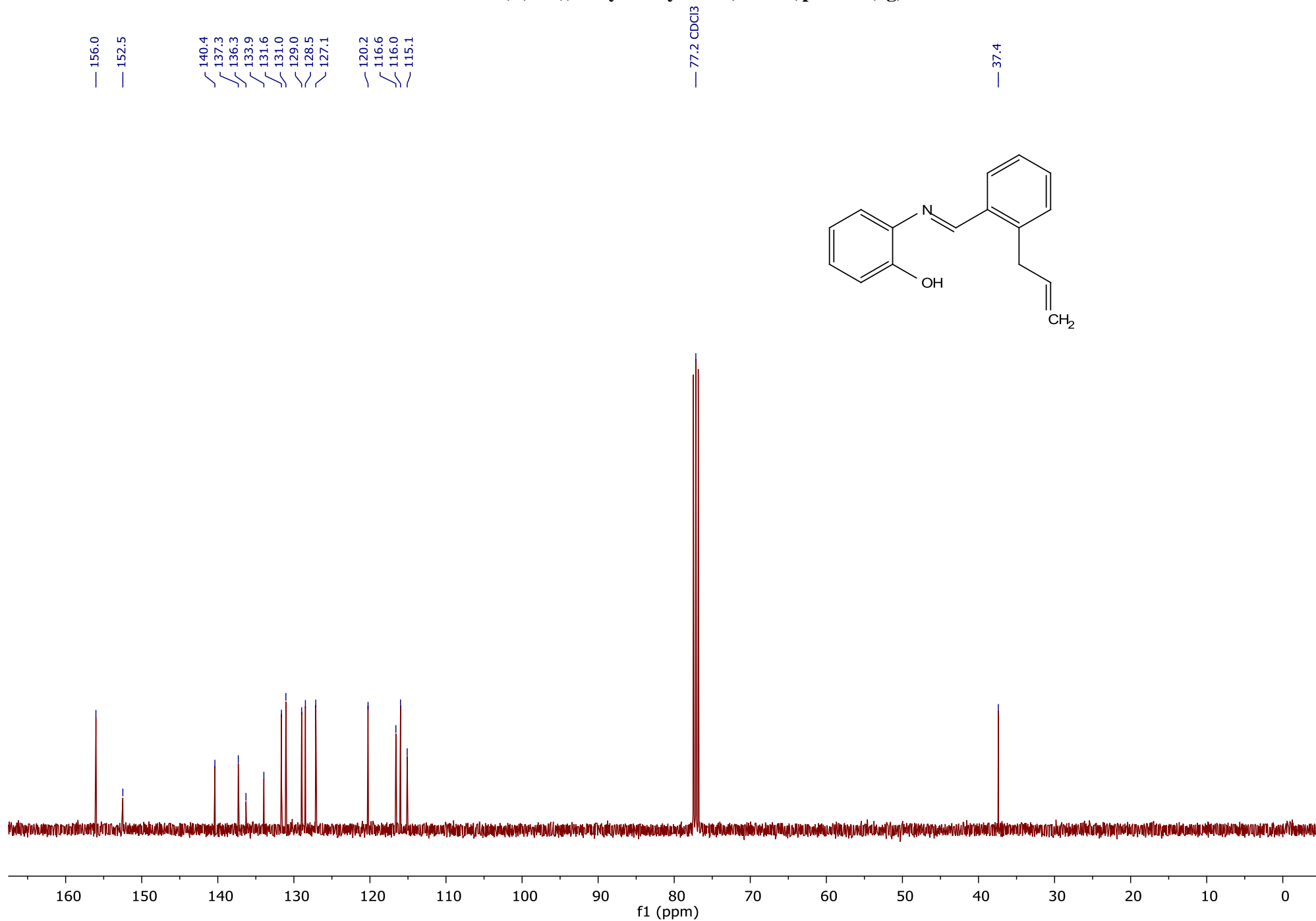
0.90

0.96
0.96

2.00

acetone

f1 (ppm)

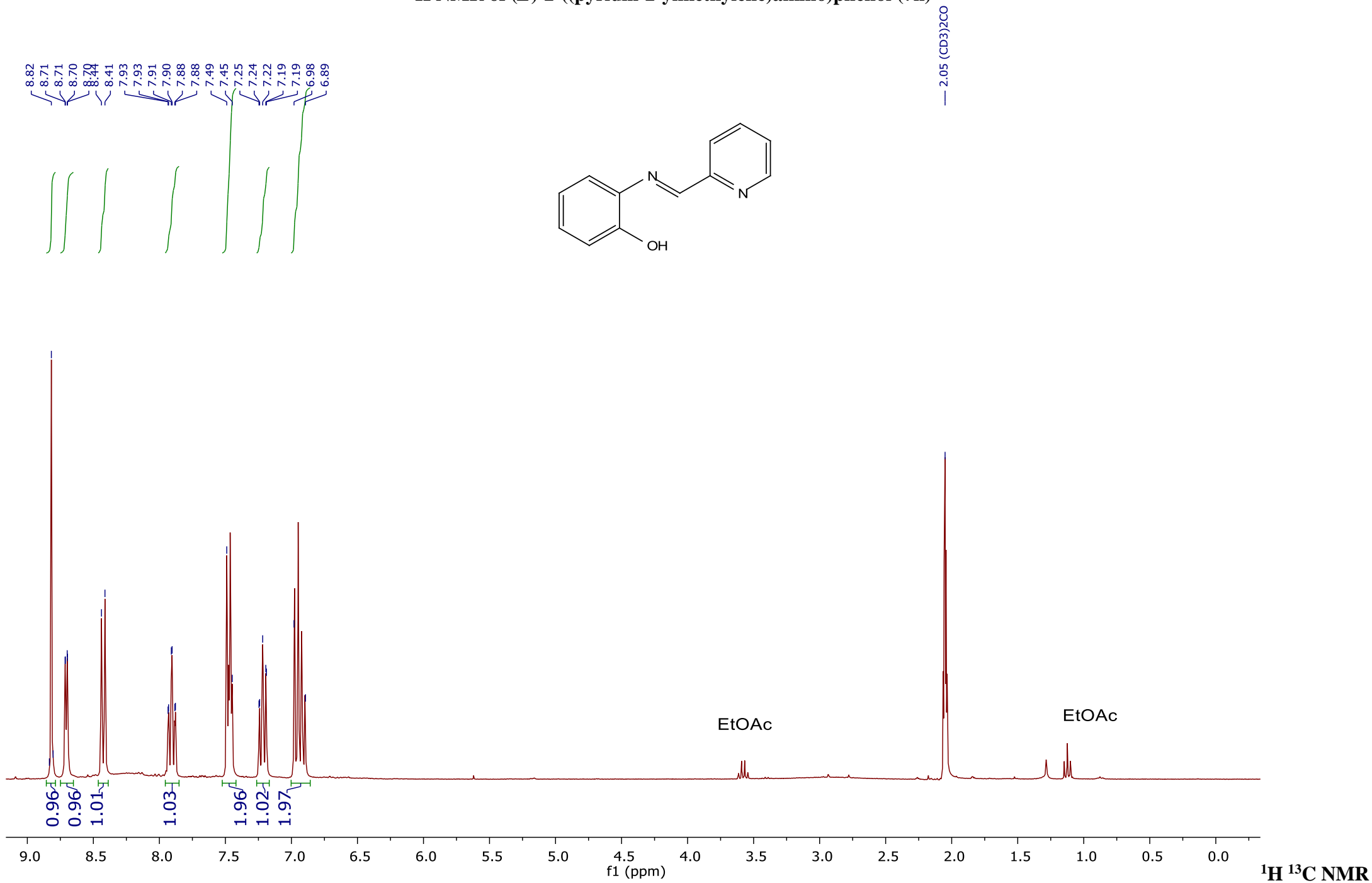
^{13}C NMR of (*E*)-2-((2-allylbenzylidene)amino)phenol (**7g**)— 156.0
— 152.5/ 140.4
/ 137.3
/ 136.3
/ 133.9
/ 131.6
/ 131.0
/ 129.0
/ 128.5
/ 127.1/ 120.2
/ 116.6
/ 116.0
/ 115.1

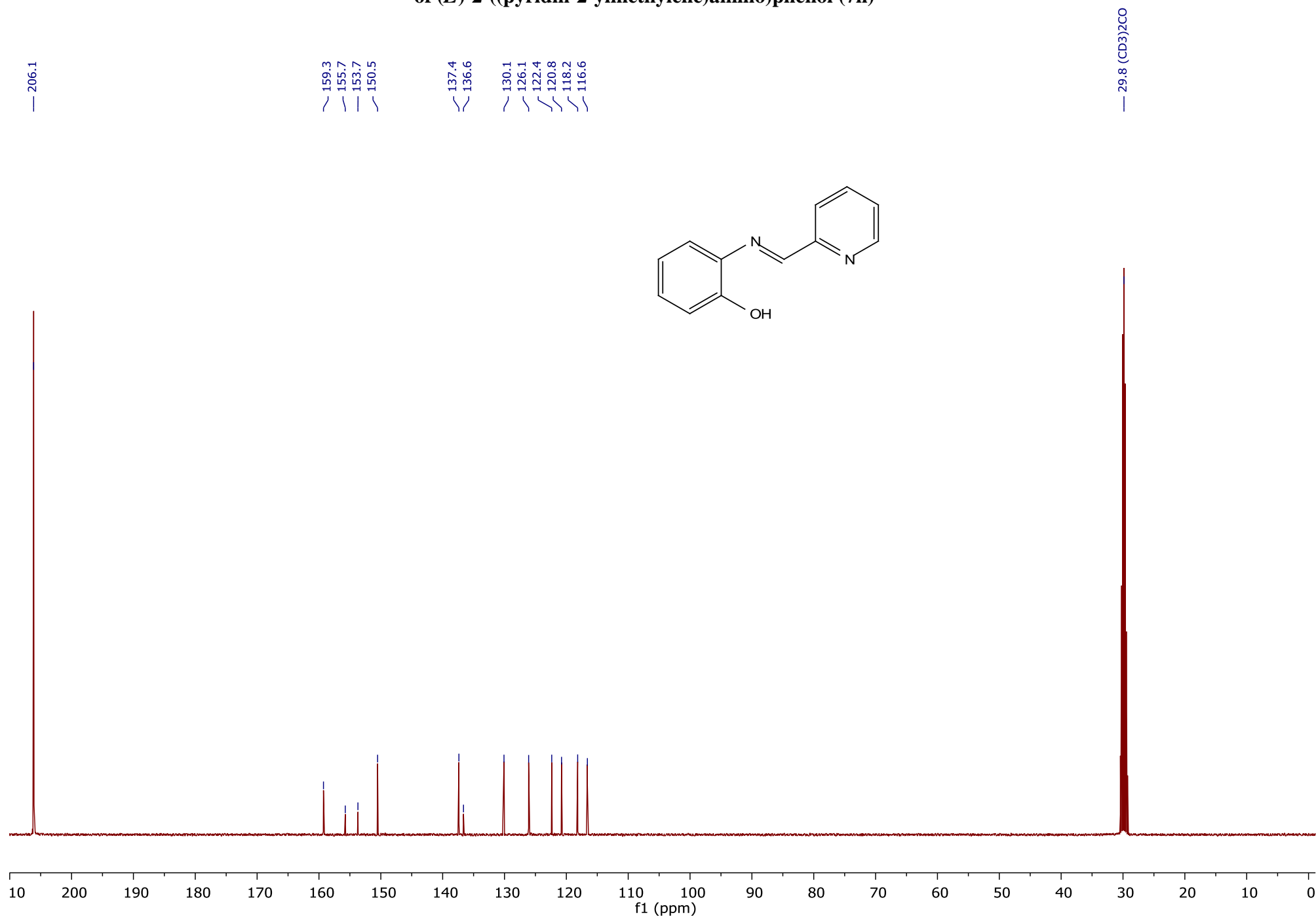
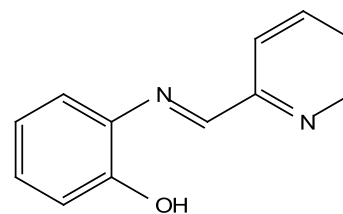
— 77.2 CDCl3

— 37.4

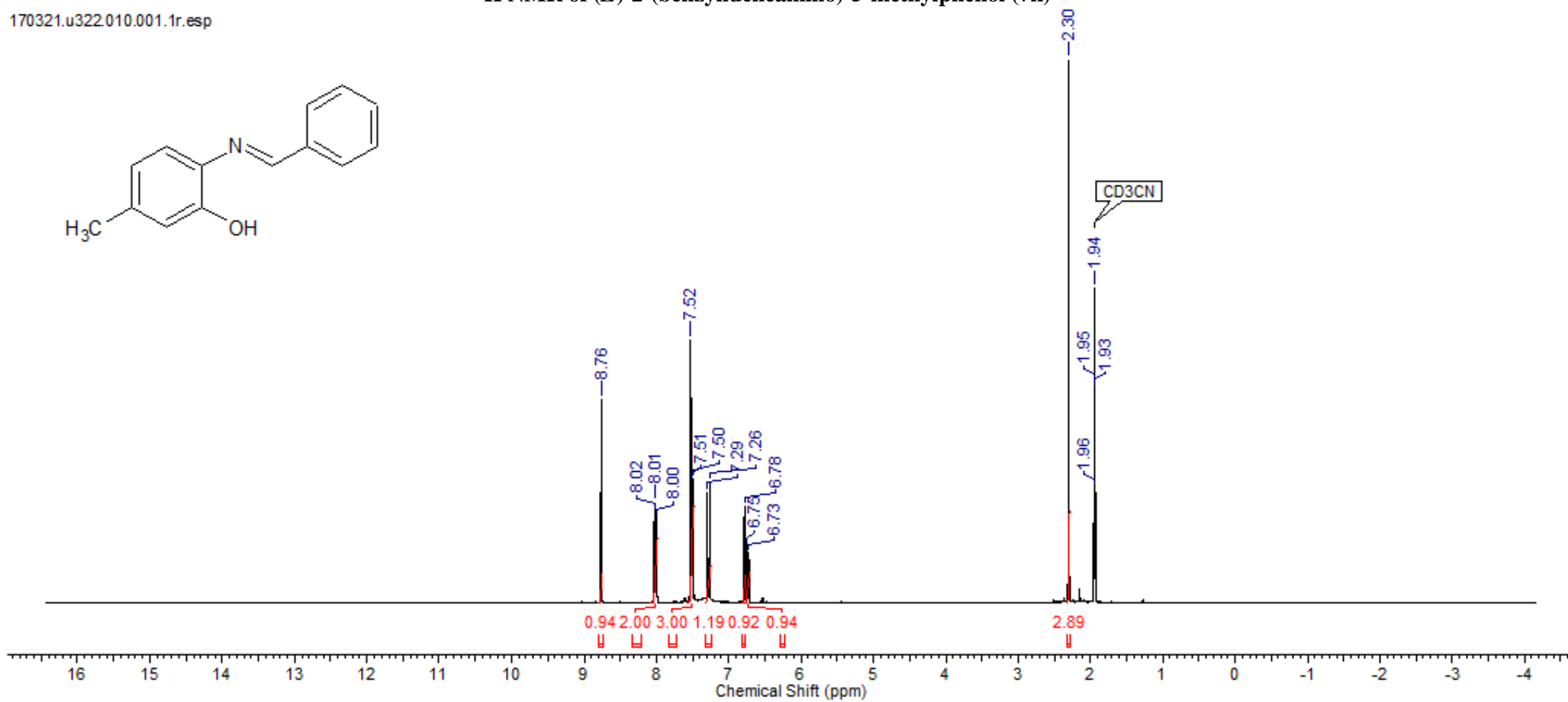
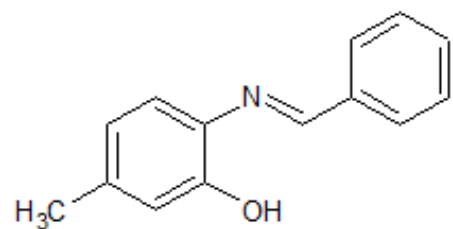
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)

¹H NMR of (*E*)-2-((pyridin-2-ylmethylene)amino)phenol (7h)

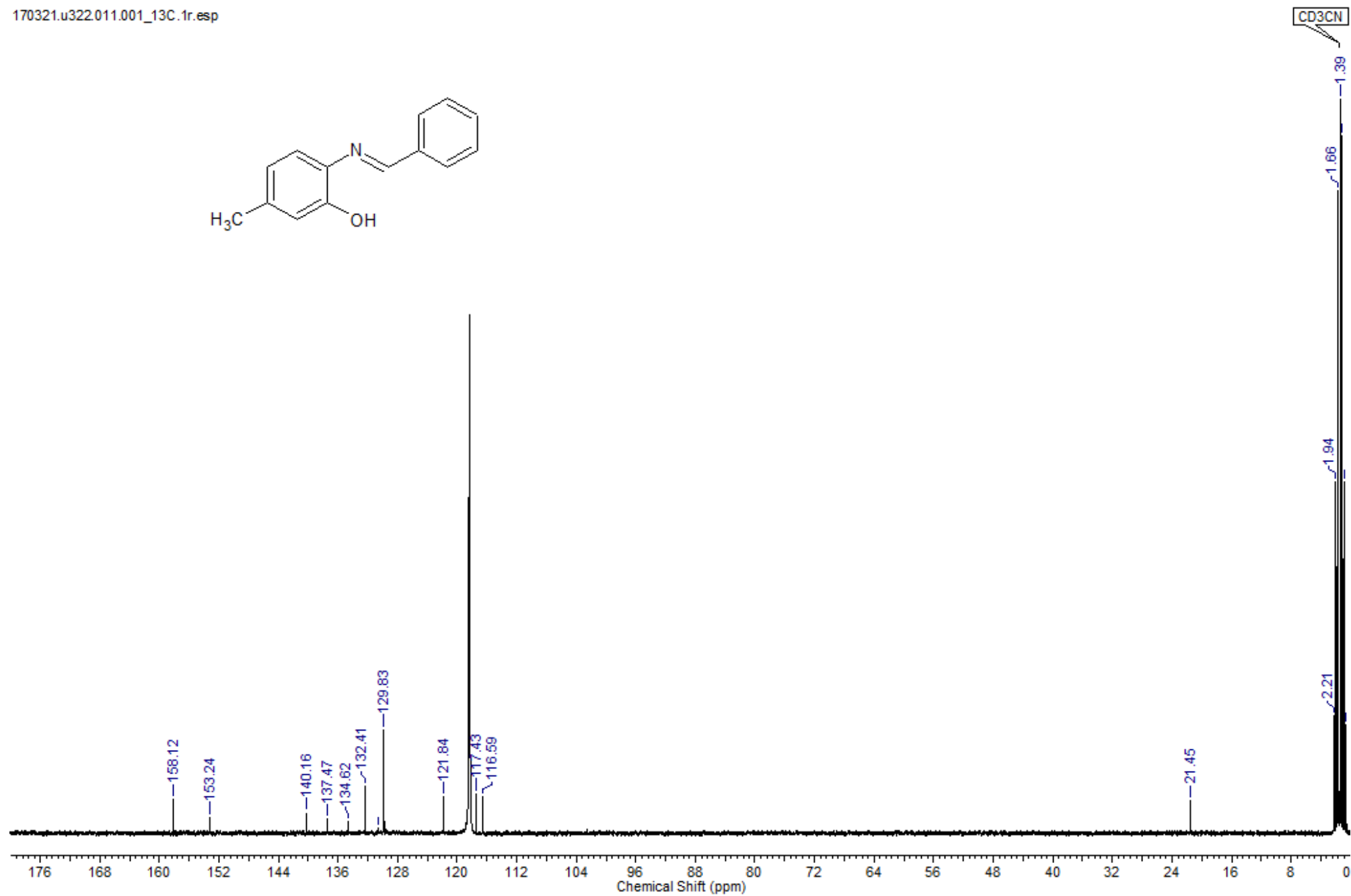
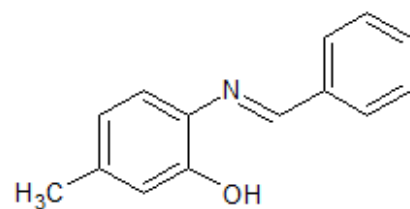
of (*E*)-2-((pyridin-2-ylmethylene)amino)phenol (**7h**)

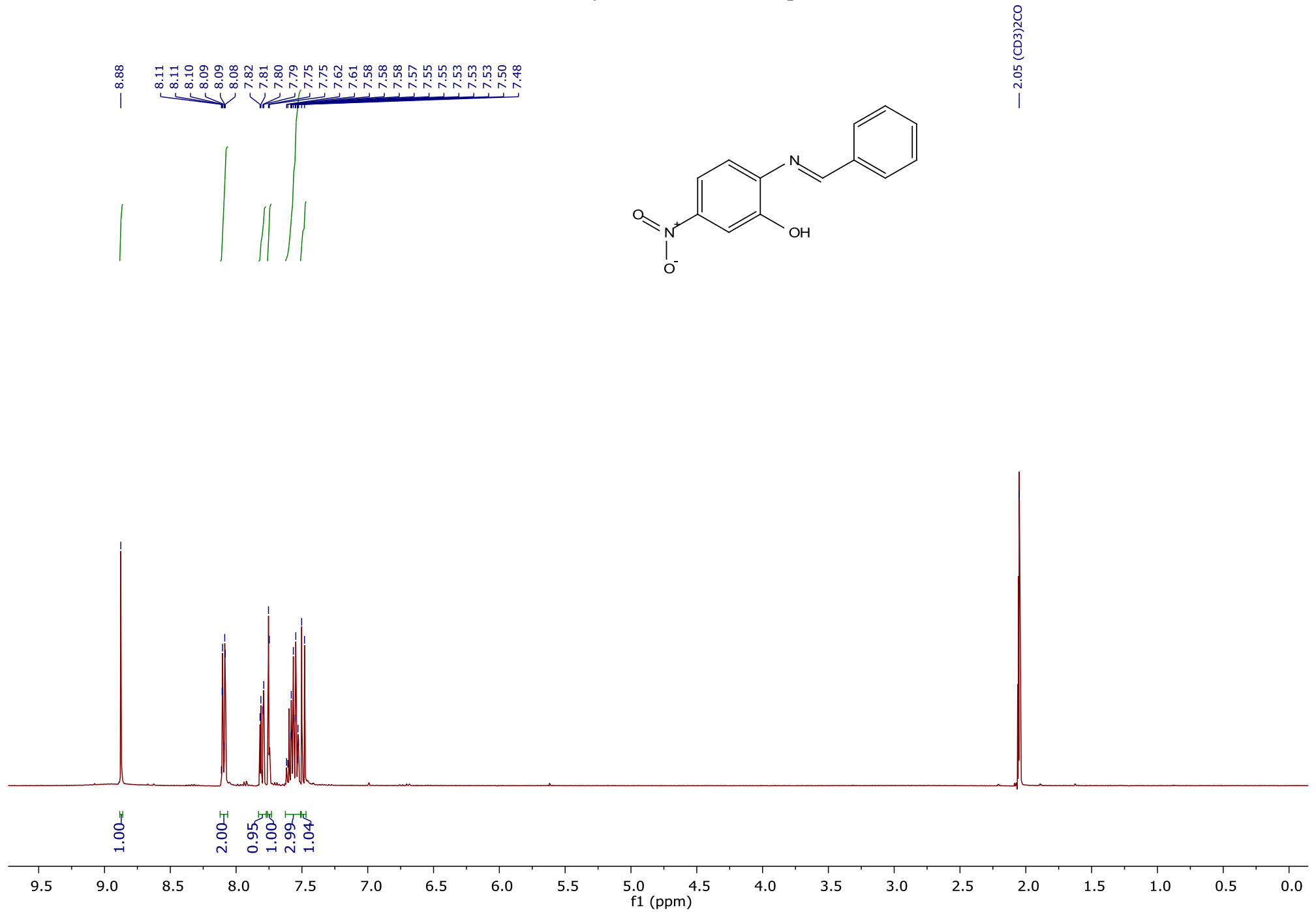
170321.u322.010.001.1r.esp

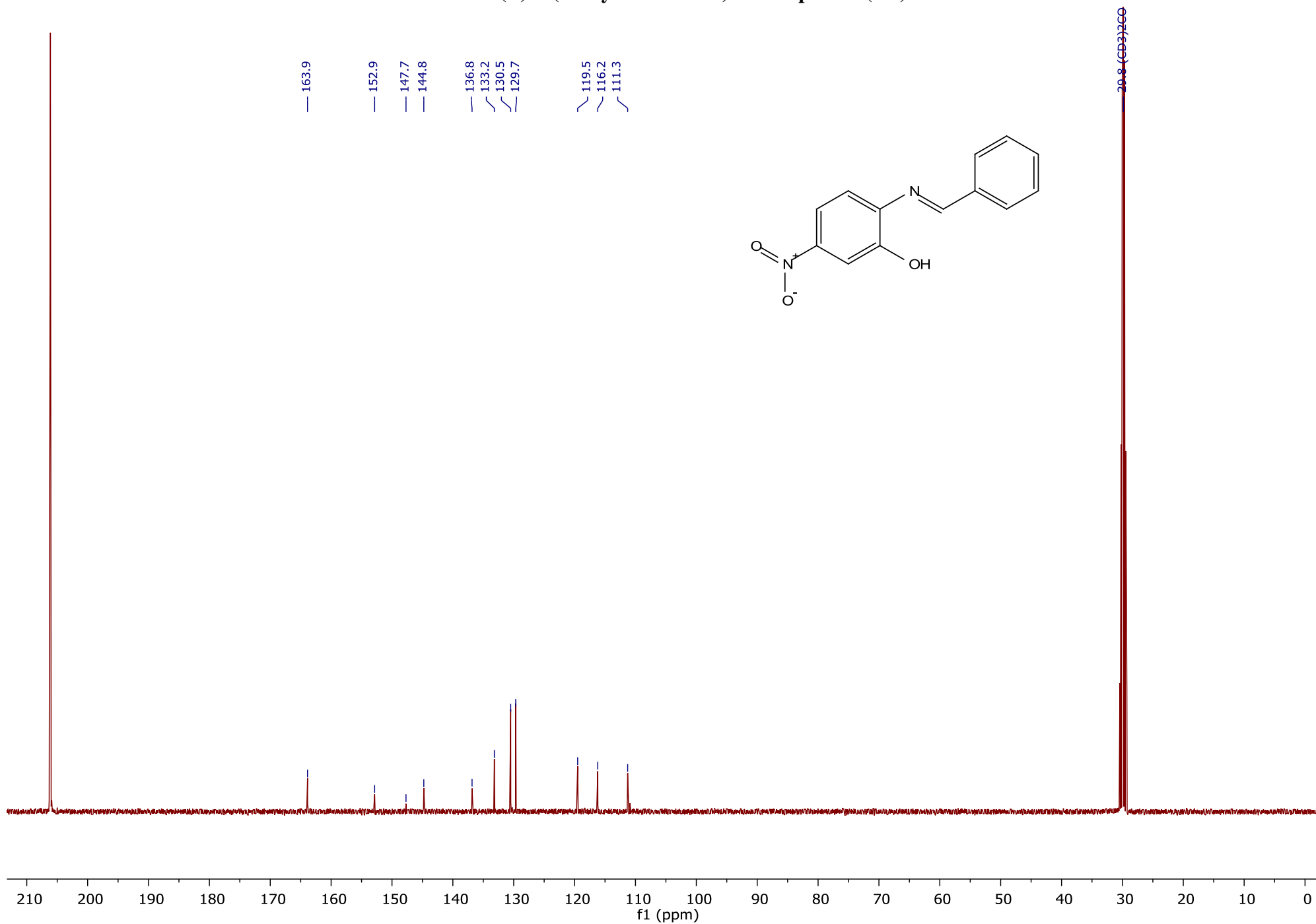
 ^1H NMR of (*E*)-2-(benzylideneamino)-5-methylphenol (7k)

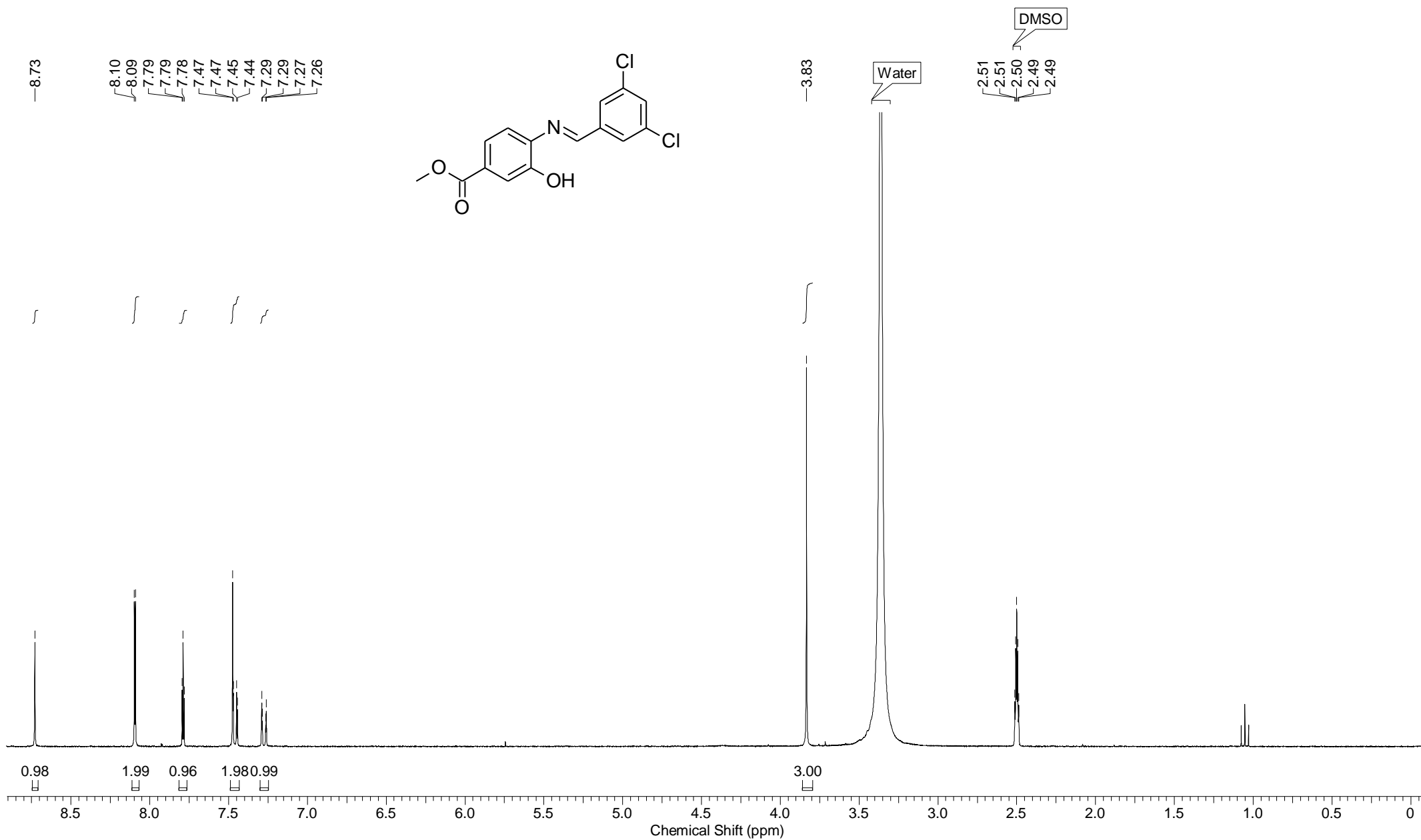
¹³C NMR of (*E*)-2-(benzylideneamino)-5-methylphenol (7k)

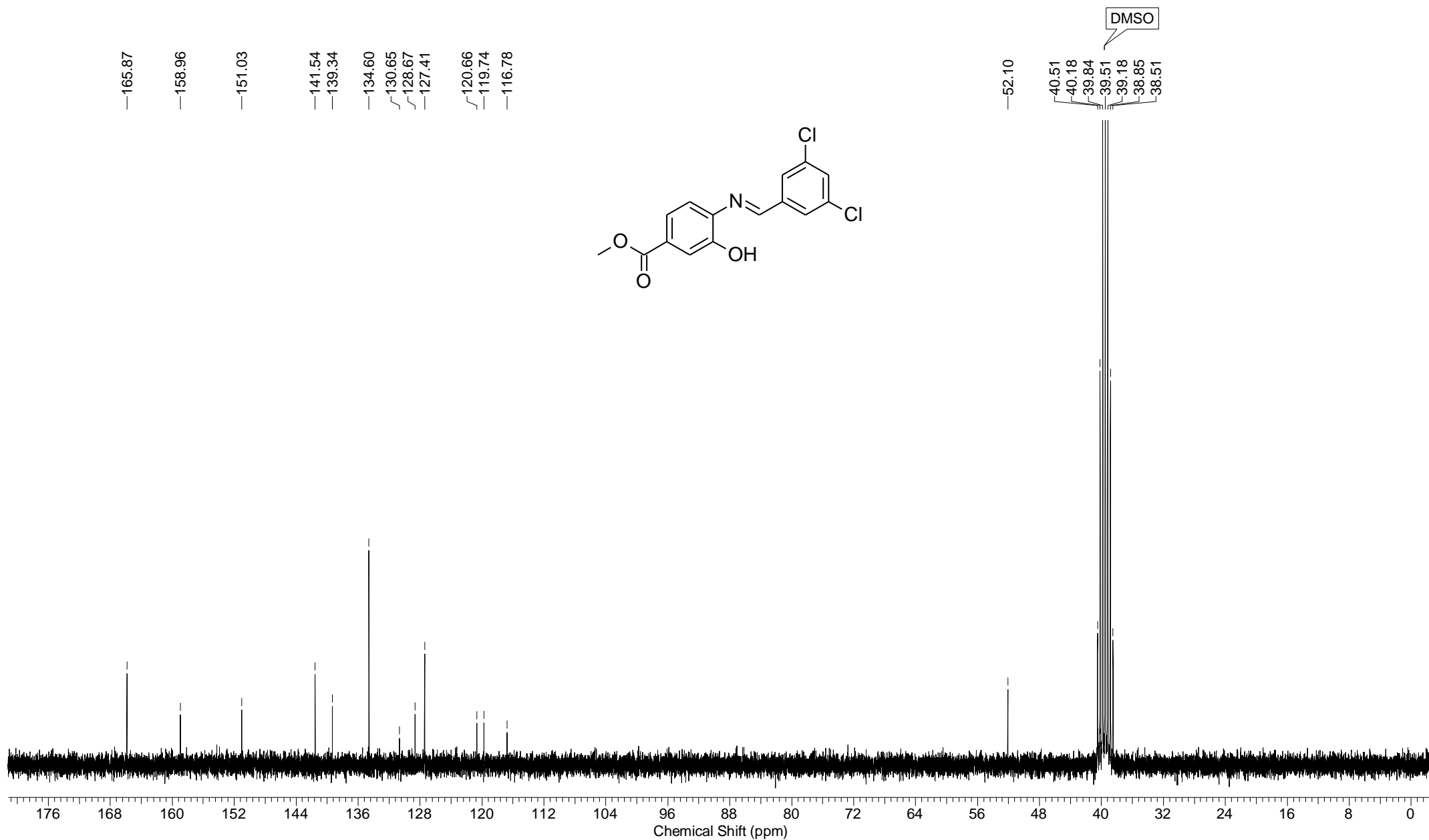
170321.u322.011.001_13C_1r.esp

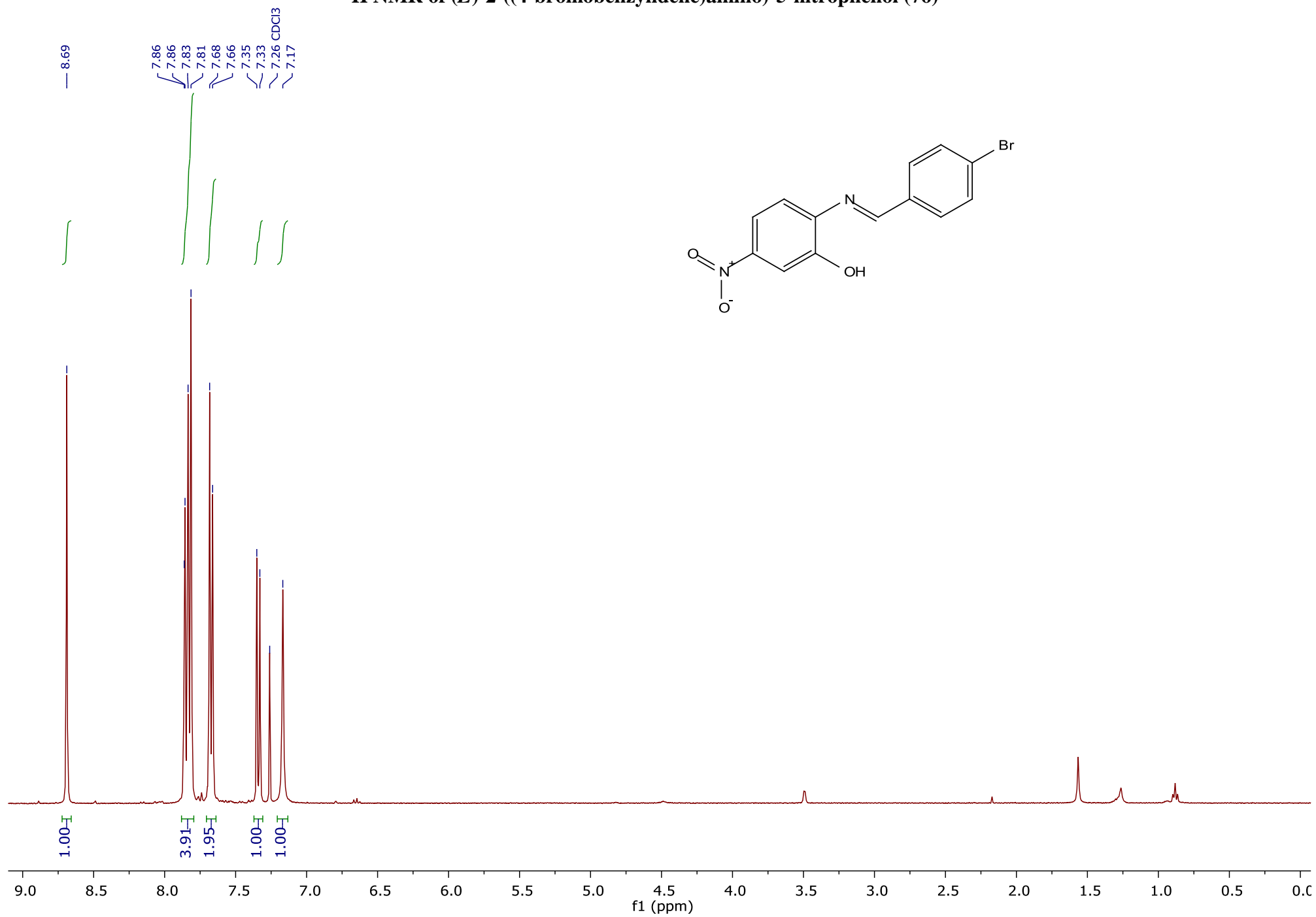


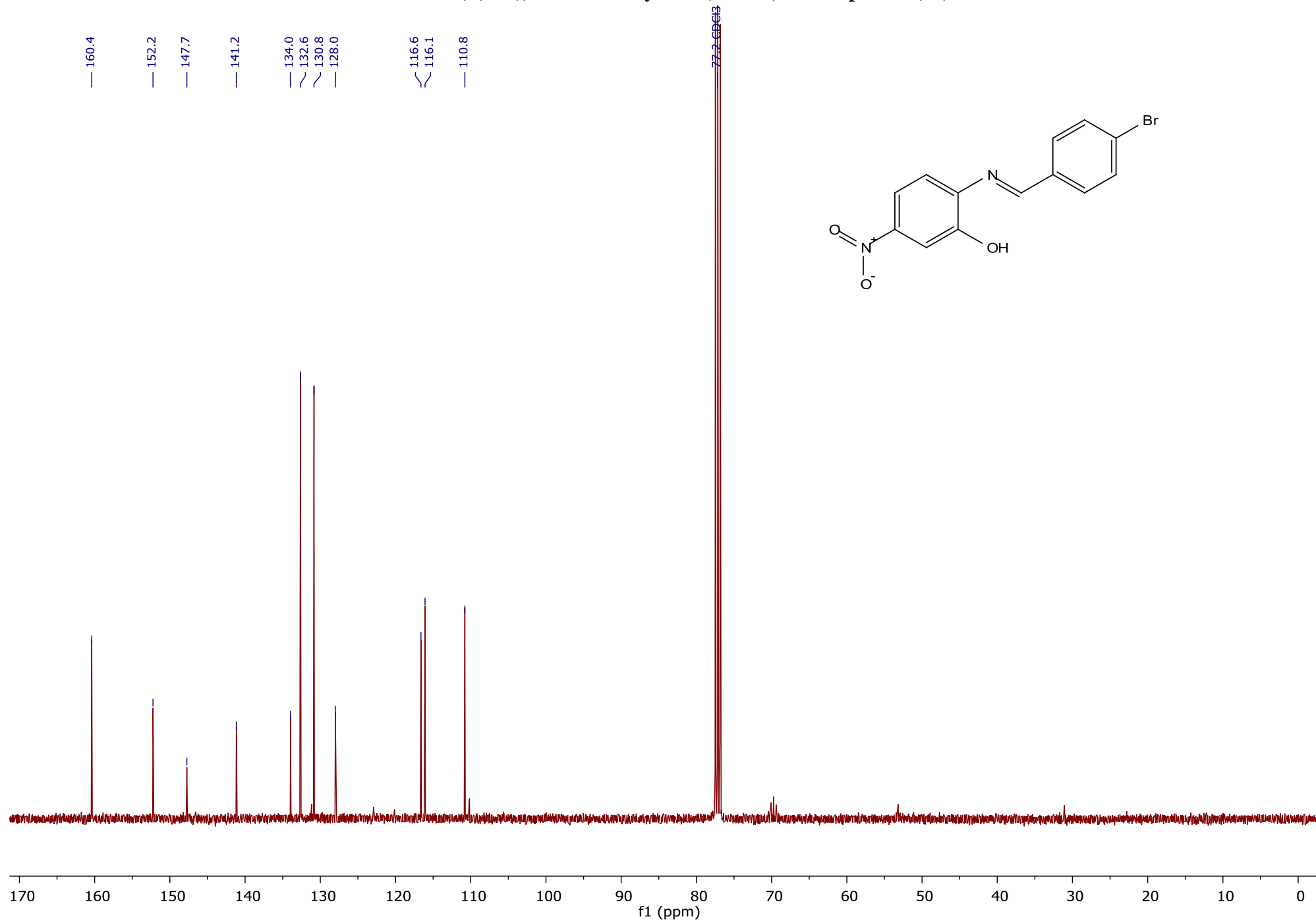
^1H NMR of (*E*)-2-(benzylideneamino)-5-nitrophenol (7m)

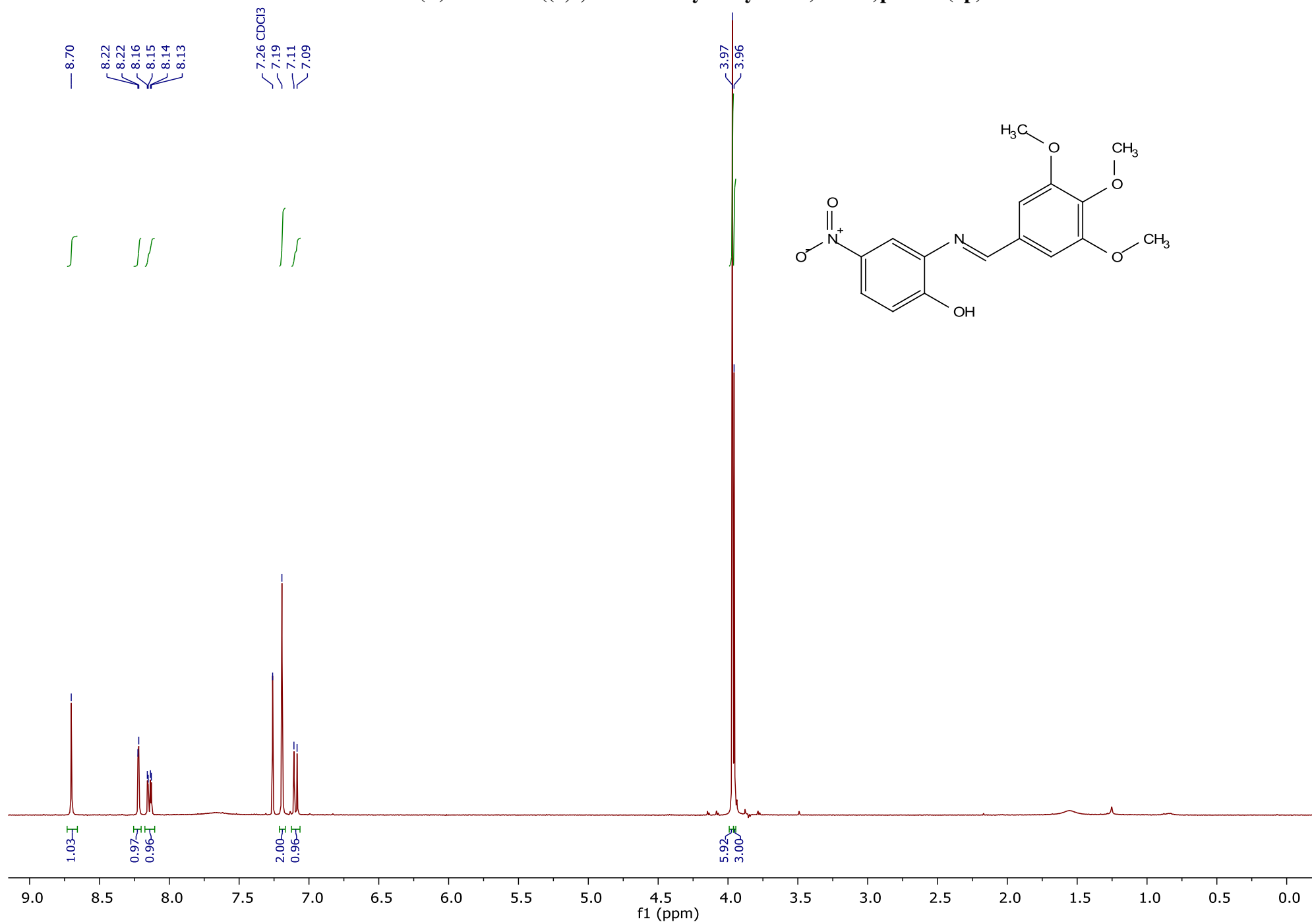
^{13}C NMR of (*E*)-2-(benzylideneamino)-5-nitrophenol (**7m**)

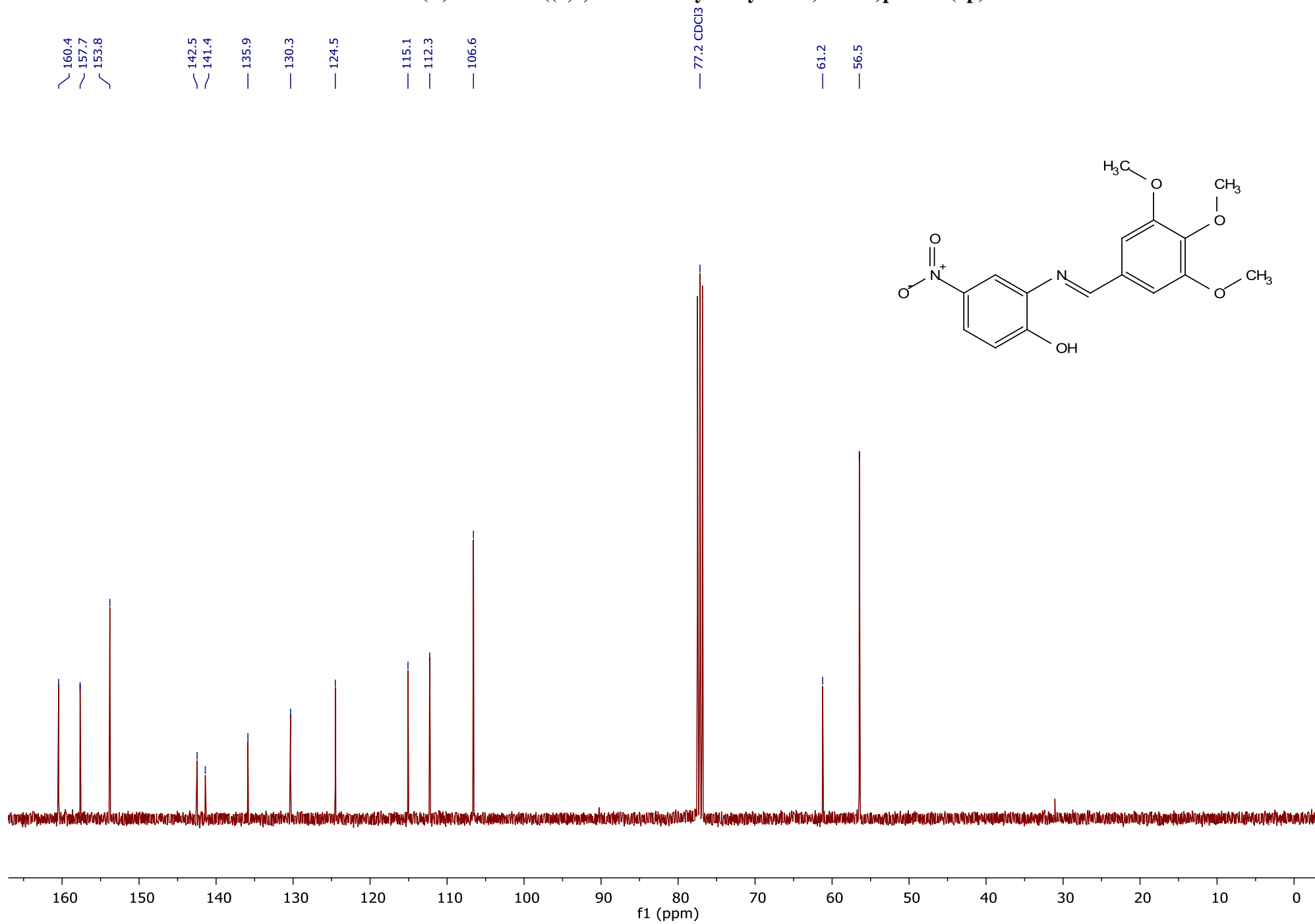
¹H NMR of (*E*)-methyl 4-(3,5-dichlorobenzylideneamino)-3-hydroxybenzoate (7n)

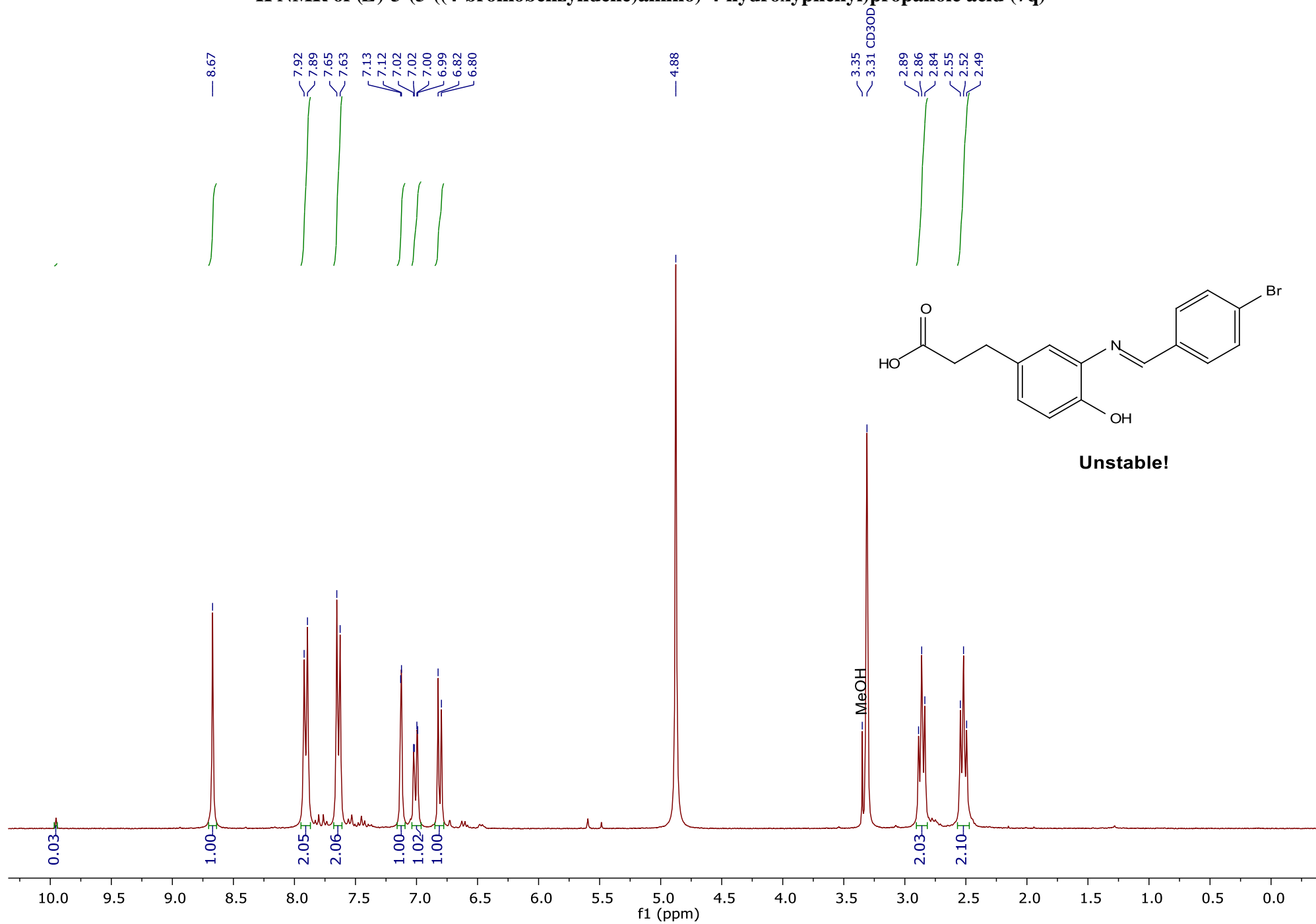
^{13}C NMR of (*E*)-methyl 4-(3,5-dichlorobenzylideneamino)-3-hydroxybenzoate (**7n**)

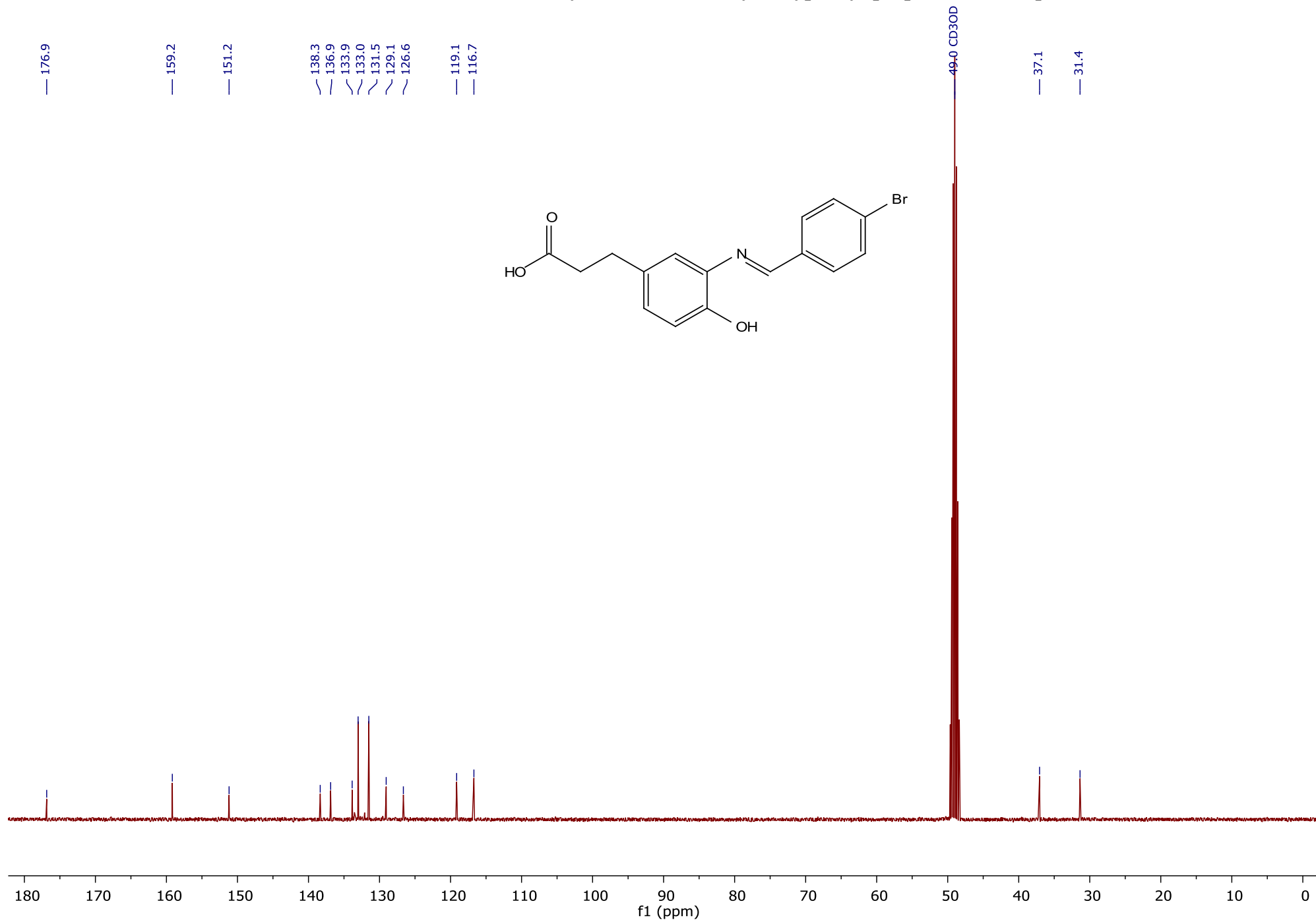
^1H NMR of (*E*)-2-((4-bromobenzylidene)amino)-5-nitrophenol (**7o**)

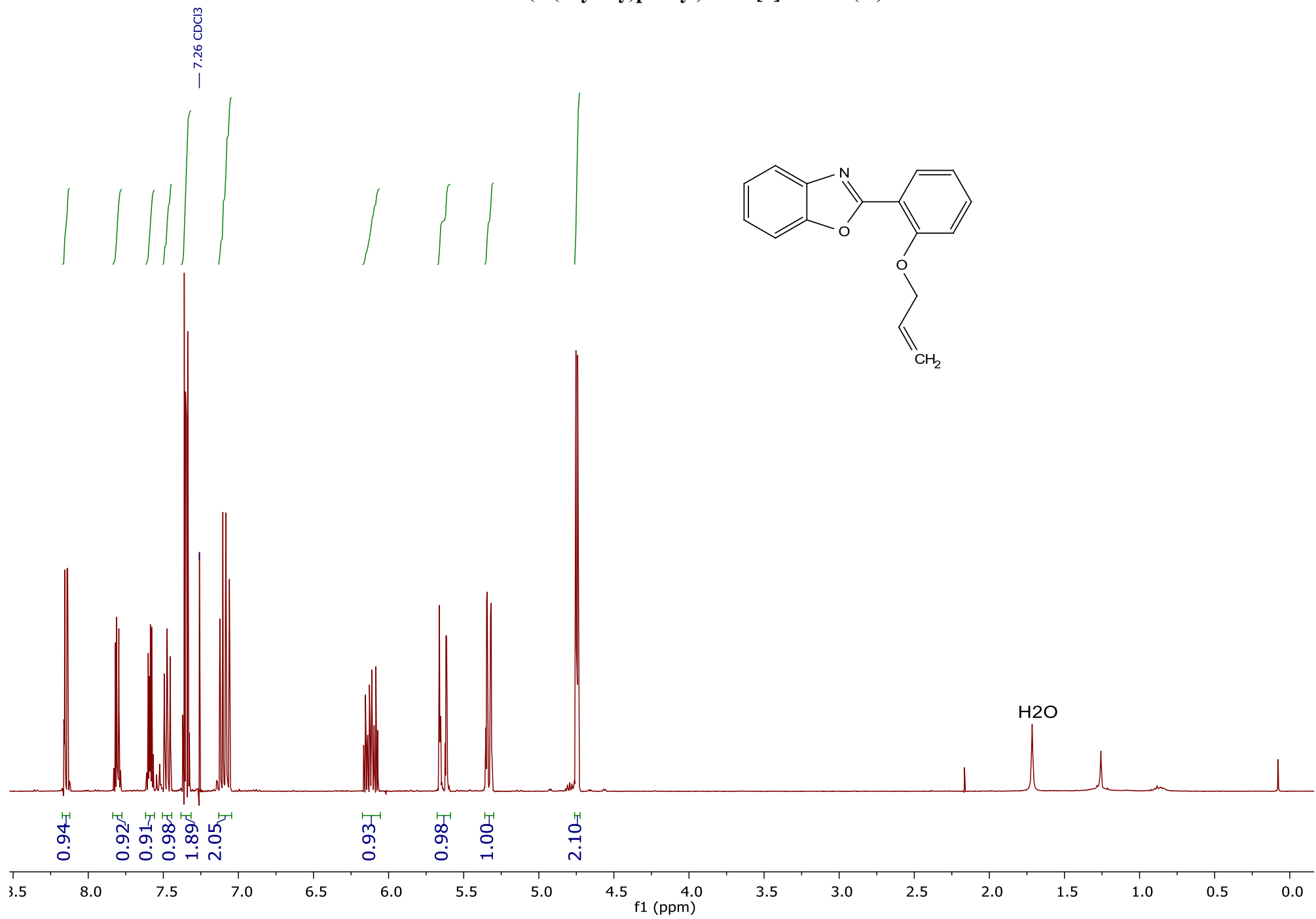
^{13}C NMR of (*E*)-2-((4-bromobenzylidene)amino)-5-nitrophenol (**7o**)

^1H NMR of (*E*)-4-nitro-2-((3,4,5-trimethoxybenzylidene)amino)phenol (7p)

^{13}C NMR of (*E*)-4-nitro-2-((3,4,5-trimethoxybenzylidene)amino)phenol (7p)

^1H NMR of (*E*)-3-(3-((4-bromobenzylidene)amino)-4-hydroxyphenyl)propanoic acid (7q)

^{13}C NMR of (*E*)-3-(3-((4-bromobenzylidene)amino)-4-hydroxyphenyl)propanoic acid (7q)

¹H NMR of 2-(2-(allyloxy)phenyl)benzo[d]oxazole (8f)— 7.26 CDCl₃

0.94

0.92

0.91

0.98

1.89

2.05

0.93

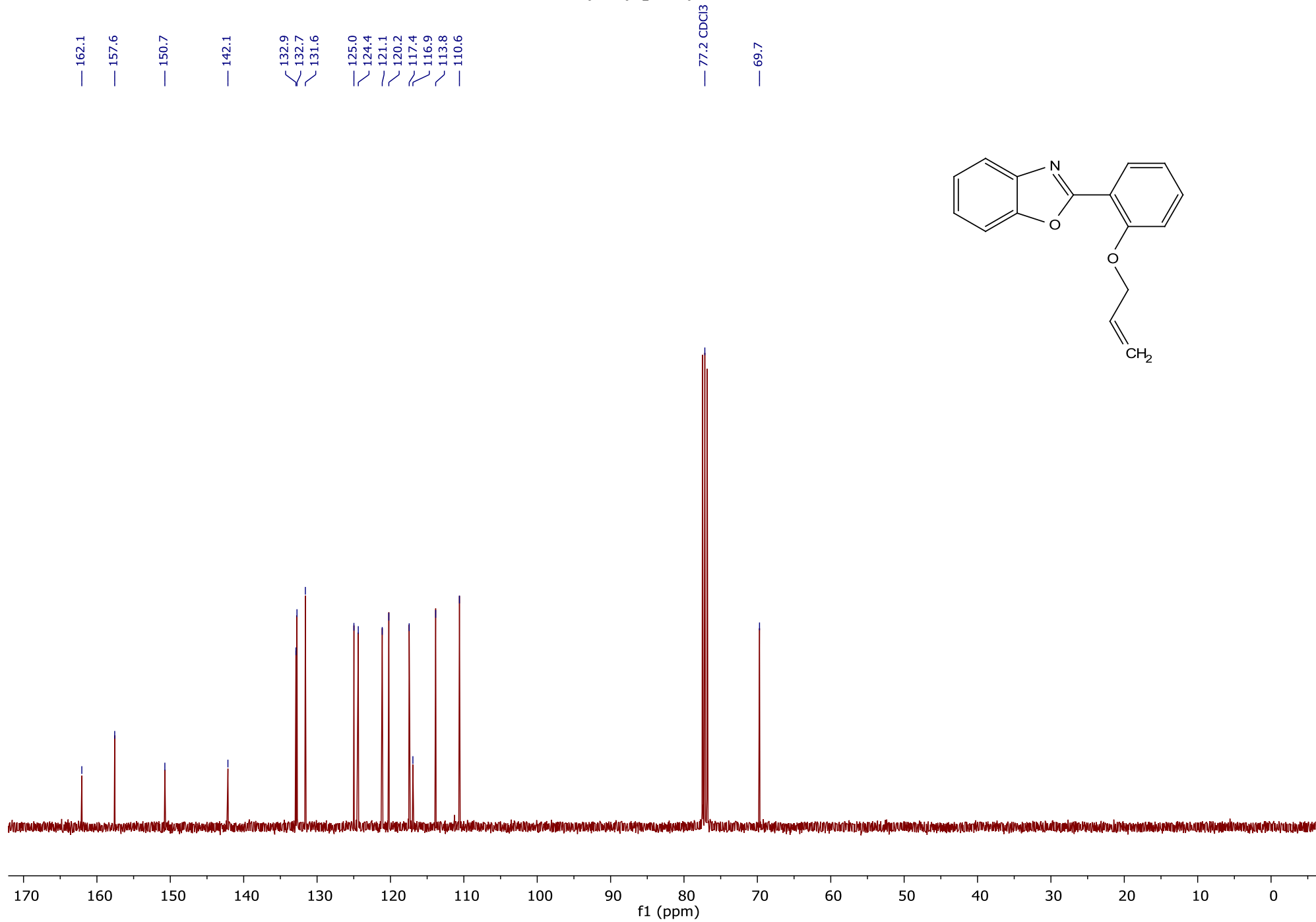
0.98

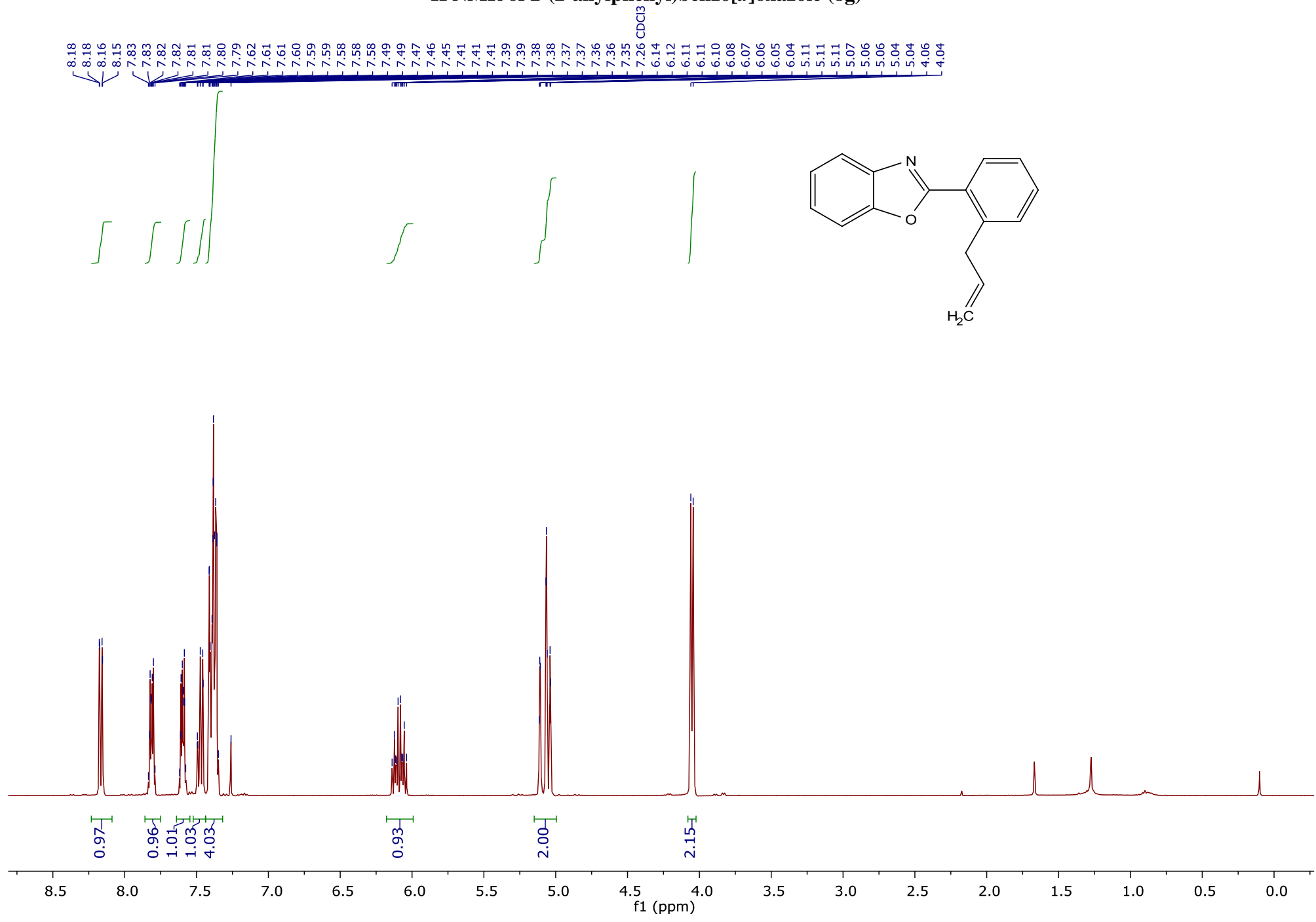
1.00

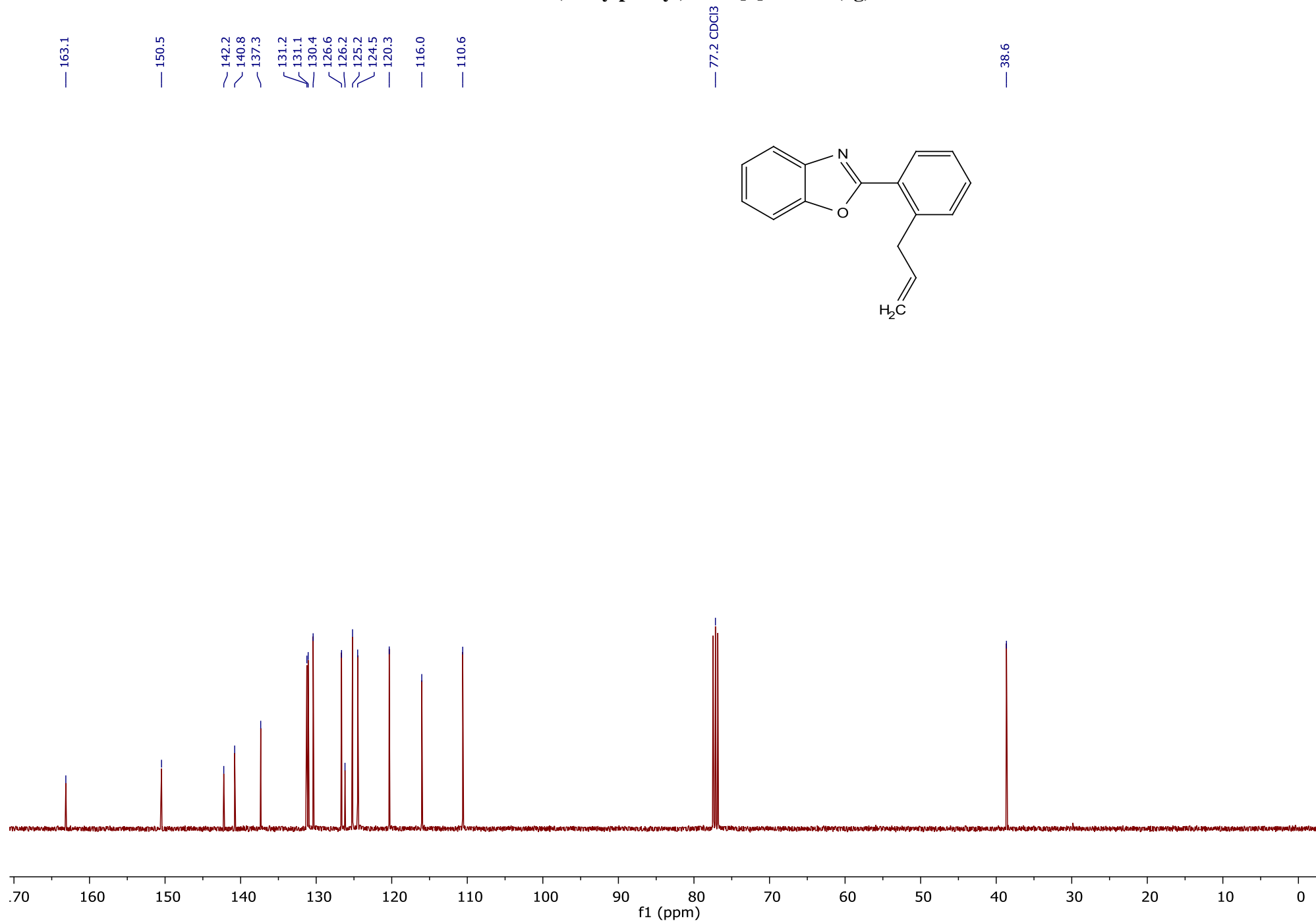
2.10

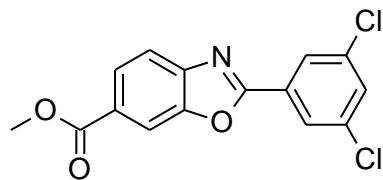
H₂O

f1 (ppm)

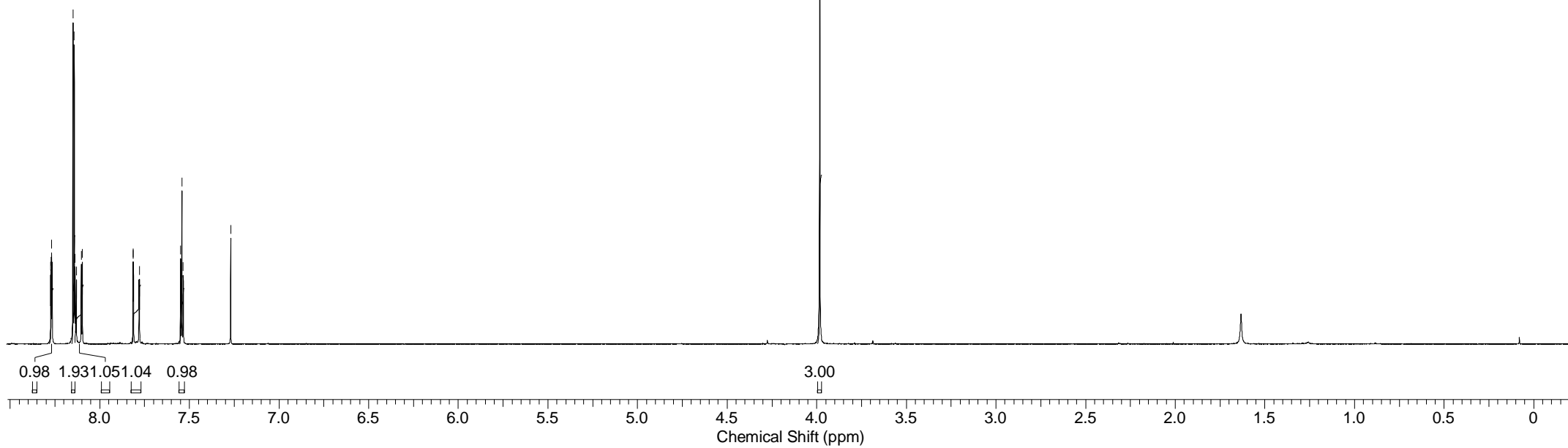
^{13}C NMR of 2-(2-(allyloxy)phenyl)benzo[*d*]oxazole (8f)

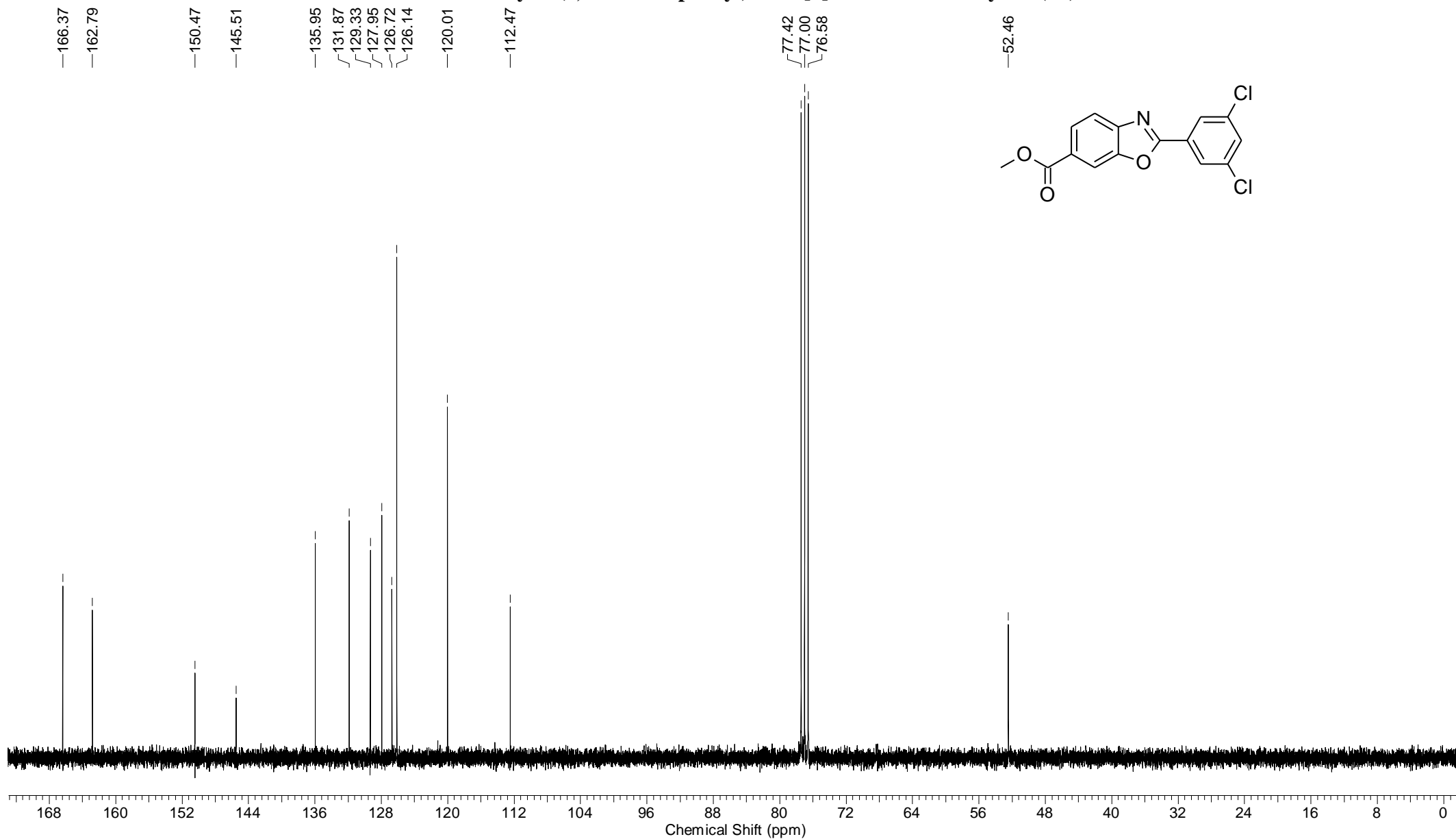
¹H NMR of 2-(2-allylphenyl)benzo[d]oxazole (8g)

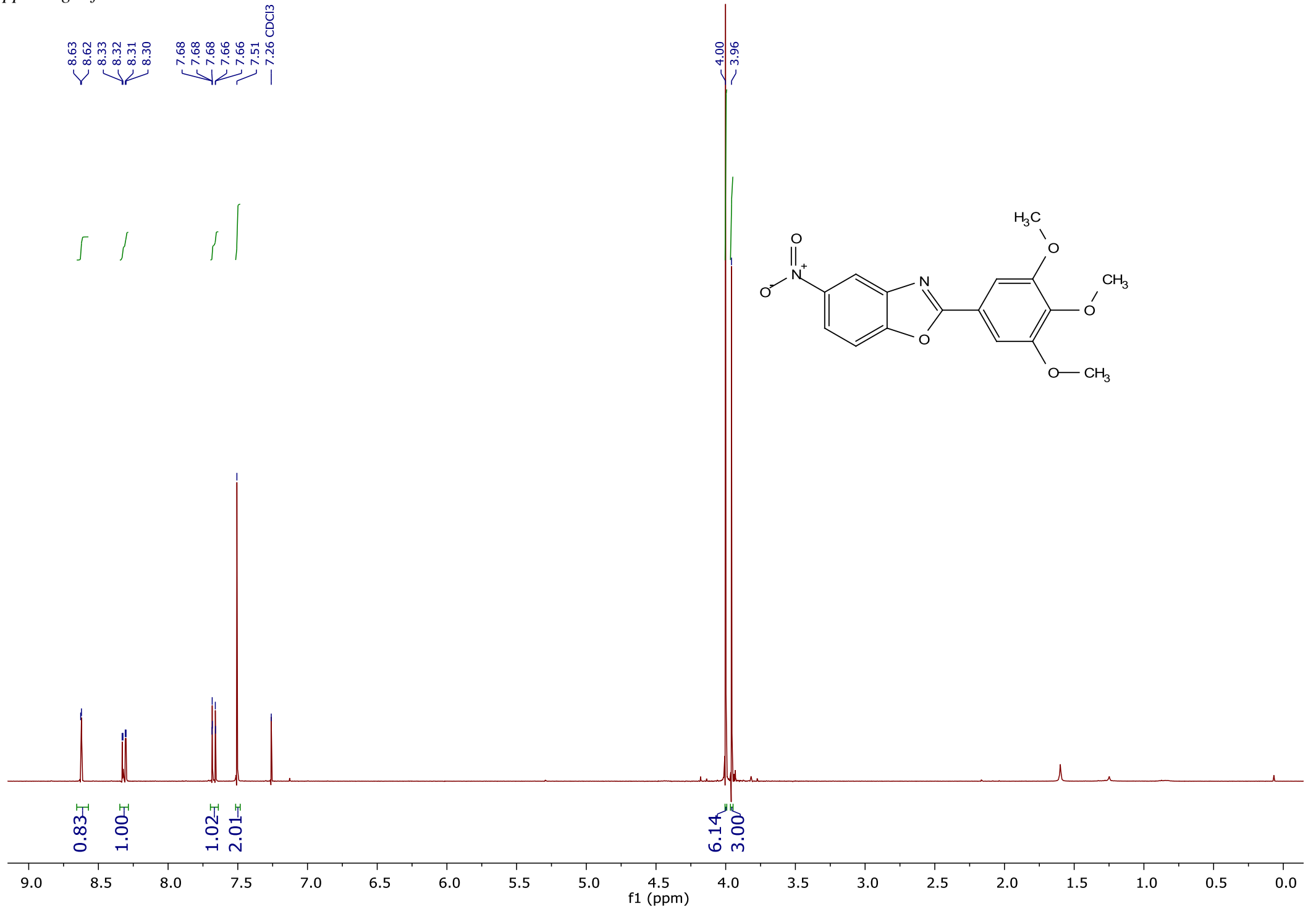
^{13}C NMR of 2-(2-allylphenyl)benzo[d]oxazole (8g)

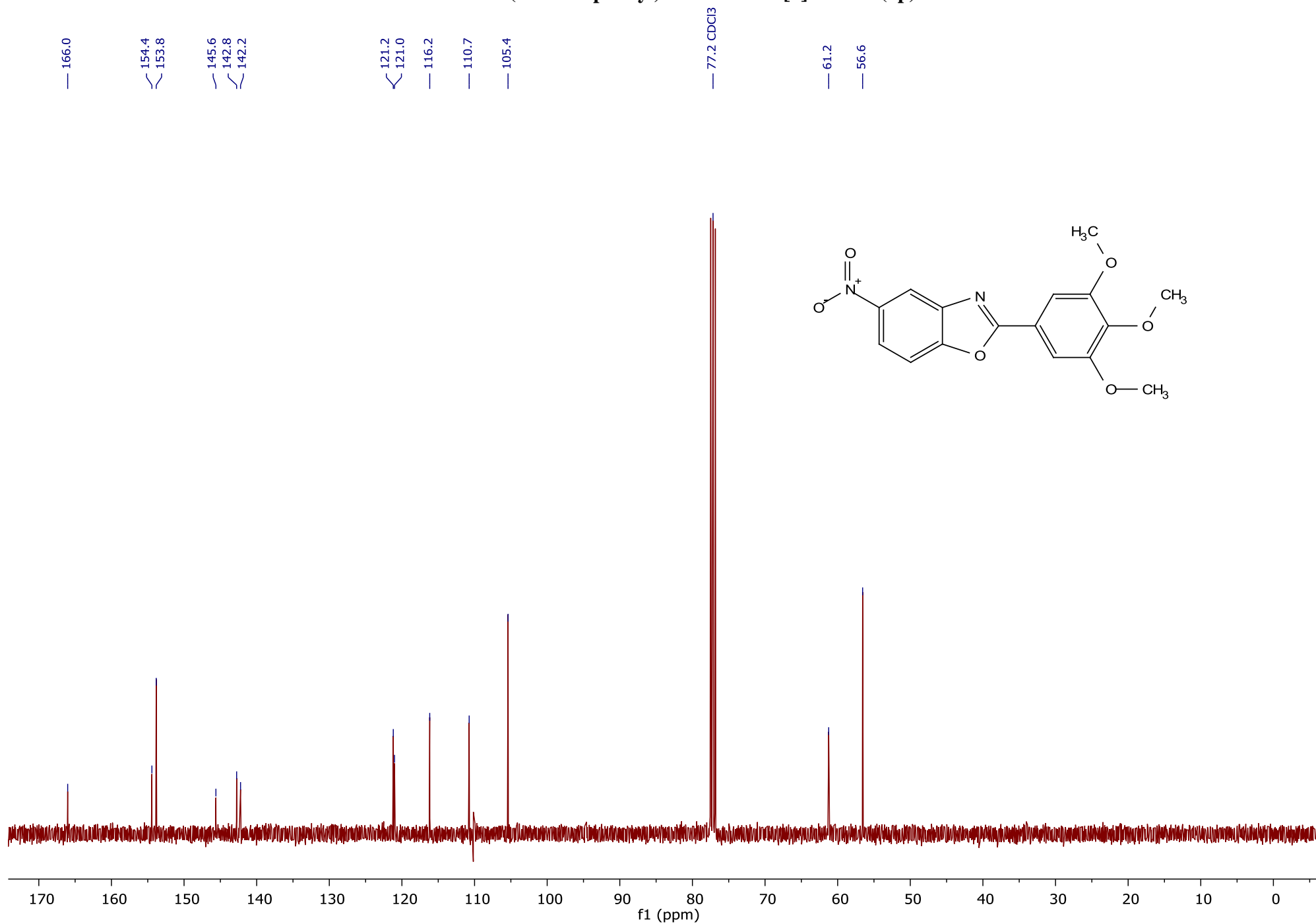
^1H NMR of methyl 2-(3,5-dichlorophenyl)benzo[d]oxazole-6-carboxylate (8n)CDCl₃8.27
8.27
8.27
8.15
8.14
8.14
8.10
8.10
7.82
7.81
7.55
7.54
7.53
7.27

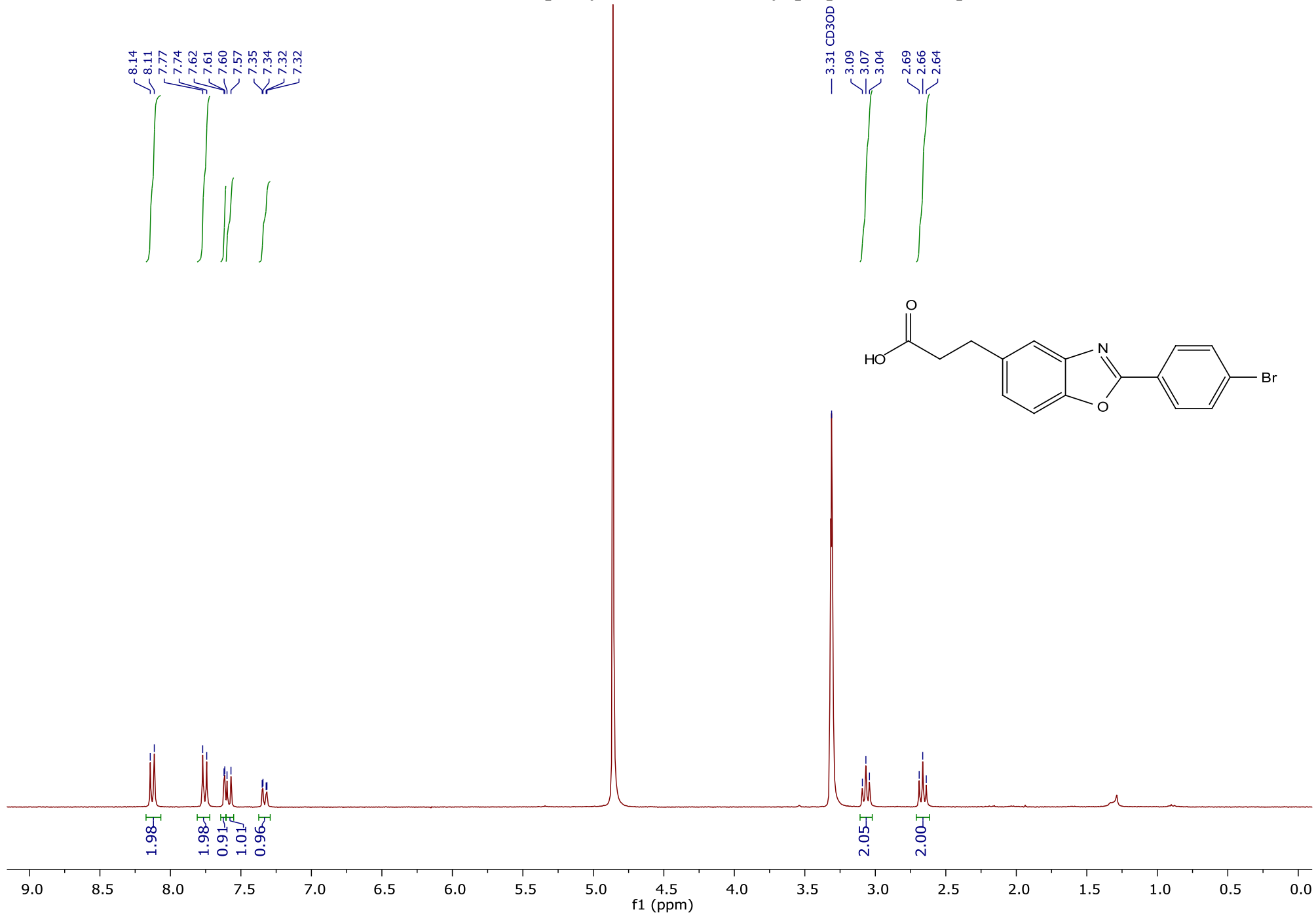
3.98

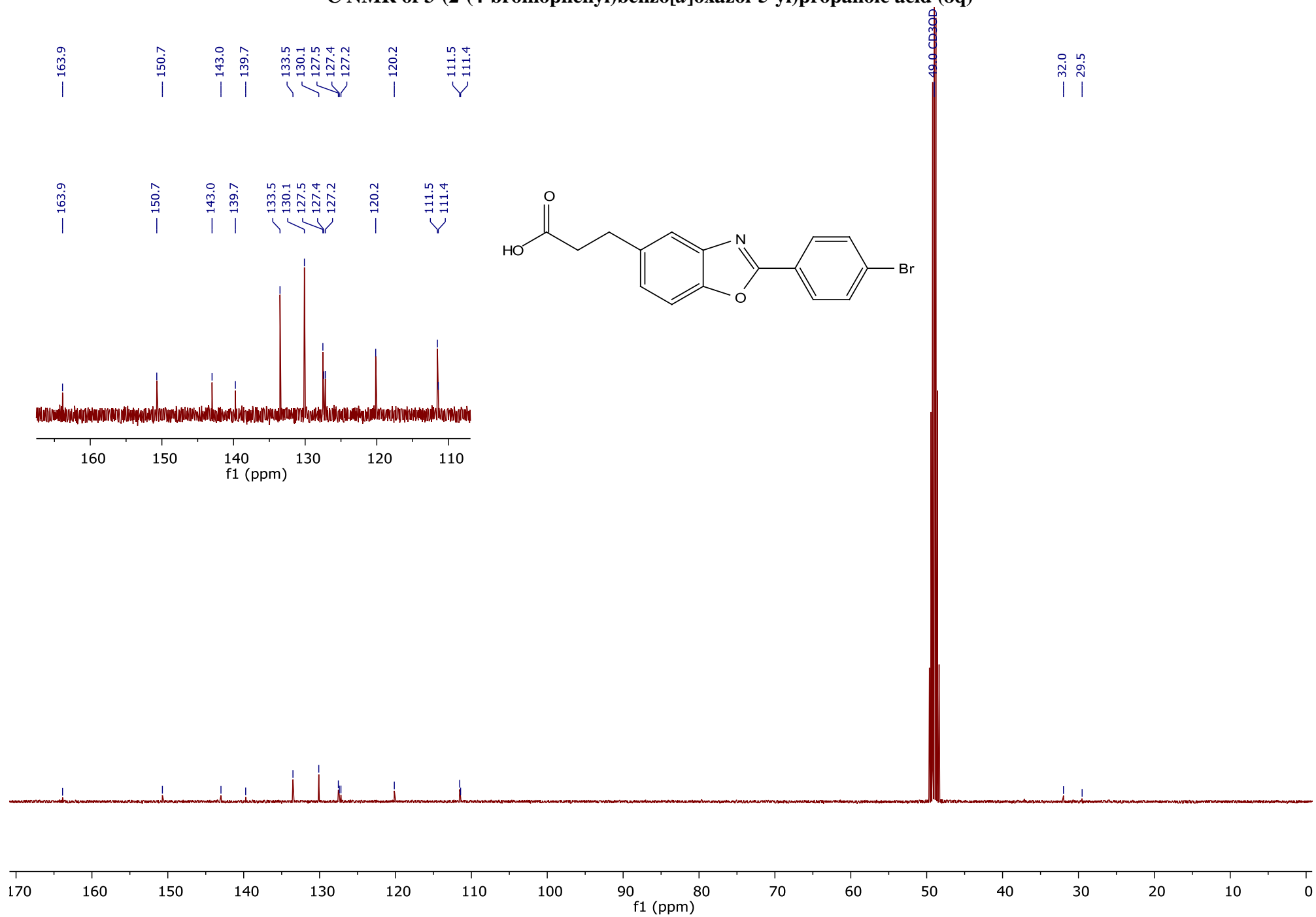


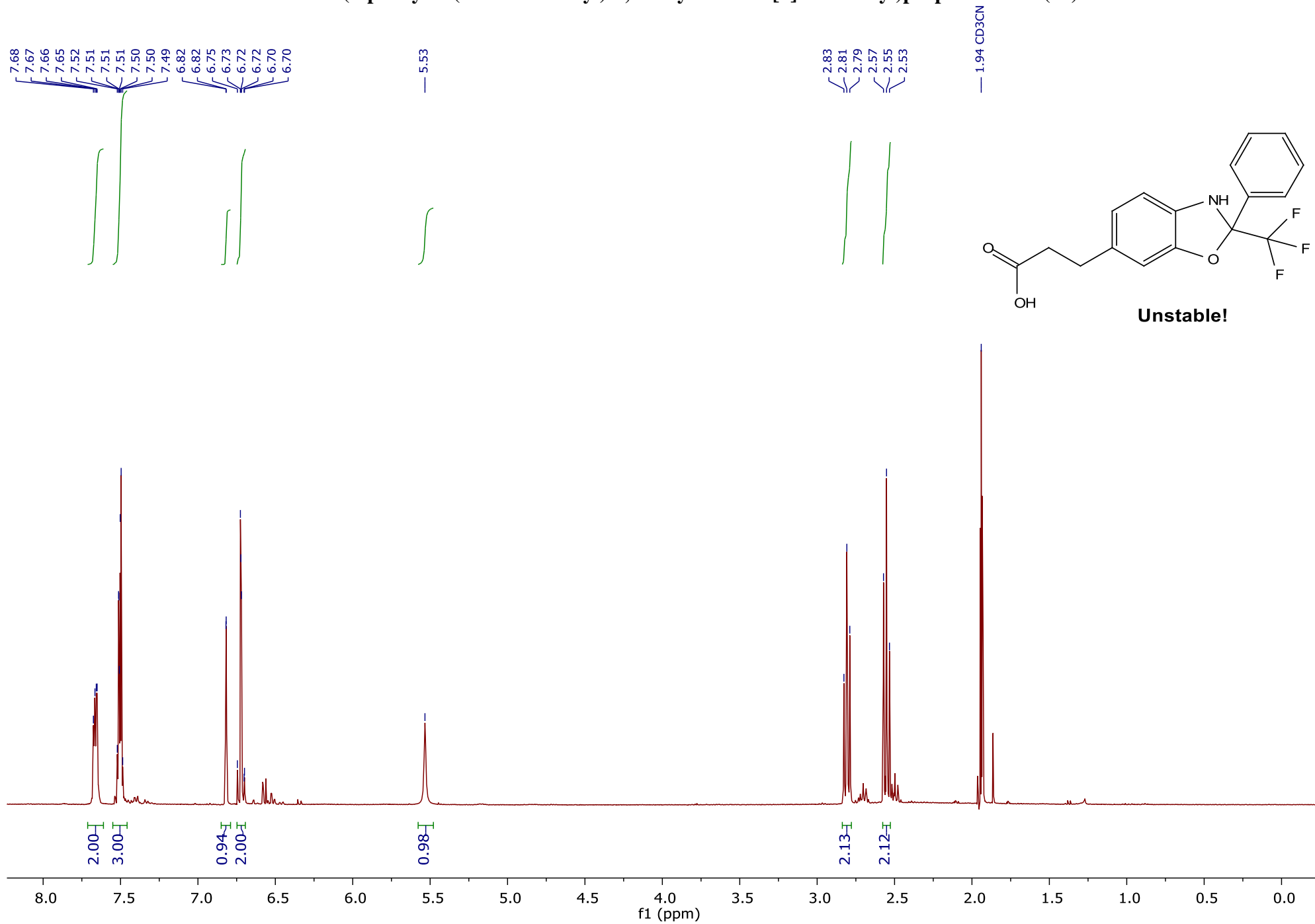
^{13}C NMR of methyl 2-(3,5-dichlorophenyl)benzo[*d*]oxazole-6-carboxylate (8n) ^1H NMR of 2-(4-bromophenyl)-6-nitrobenzo[*d*]oxazole (8p)

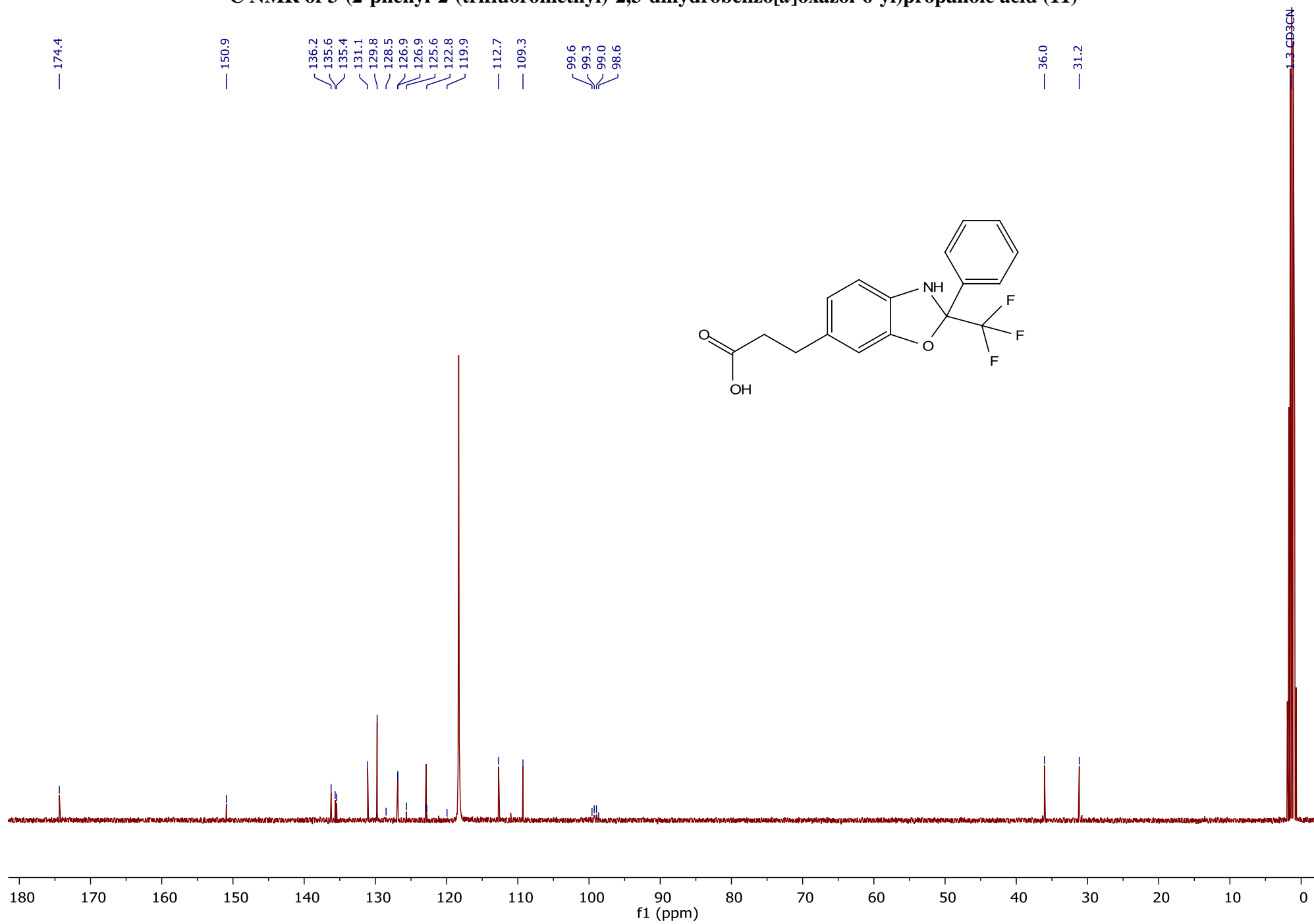


^{13}C NMR of 2-(4-bromophenyl)-6-nitrobenzo[*d*]oxazole (8p)

¹H NMR of 3-(2-(4-bromophenyl)benzo[d]oxazol-5-yl)propanoic acid (8q)

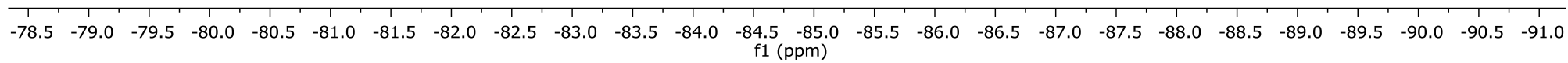
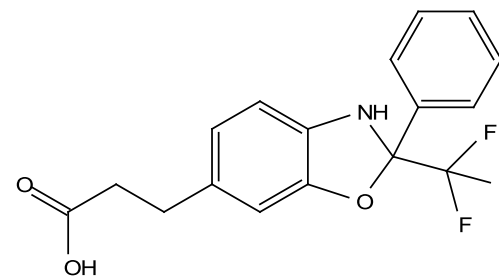
^{13}C NMR of 3-(2-(4-bromophenyl)benzo[d]oxazol-5-yl)propanoic acid (8q)

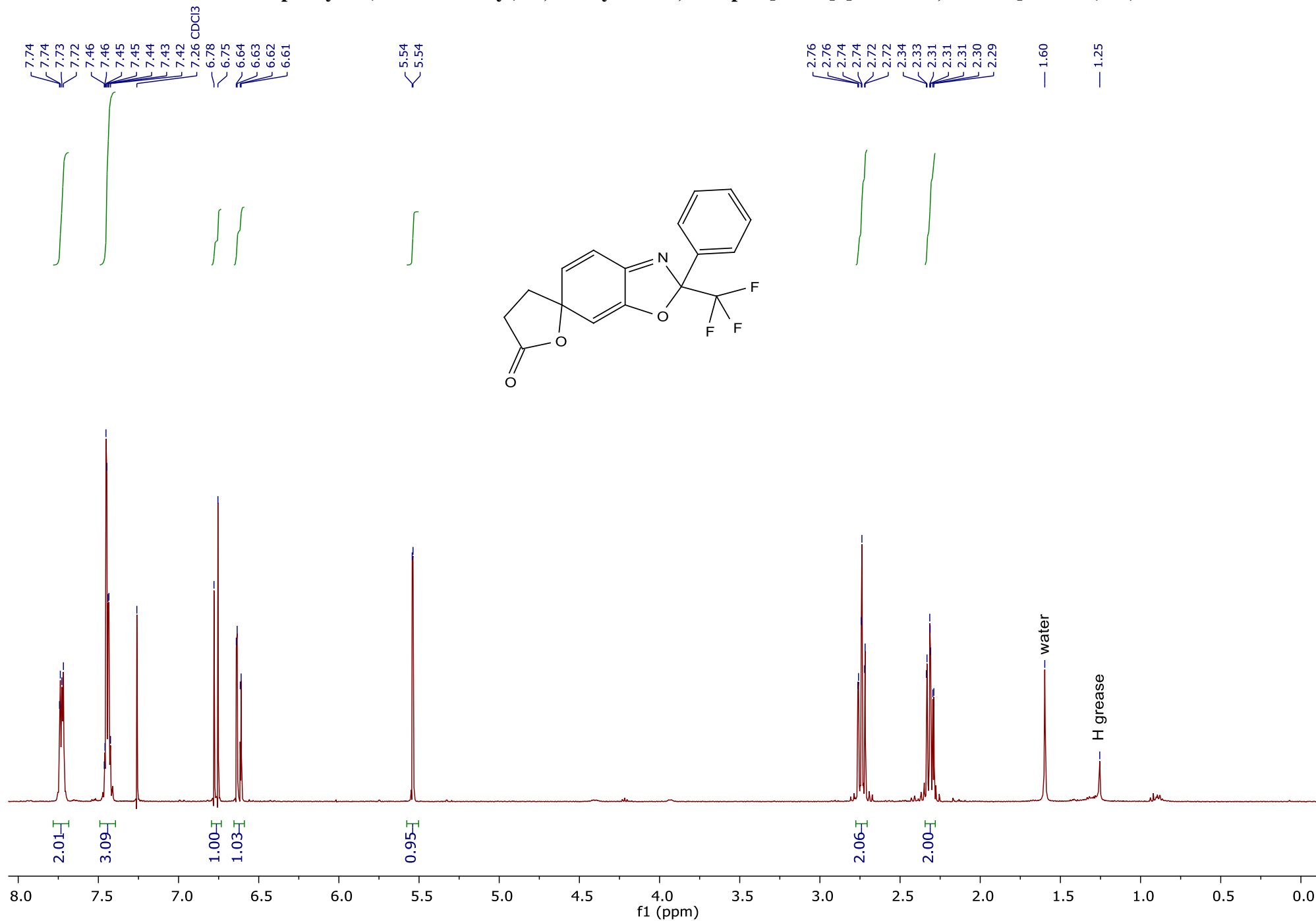
^1H NMR of 3-(2-phenyl-2-(trifluoromethyl)-2,3-dihydrobenzo[*d*]oxazol-6-yl)propanoic acid (11)

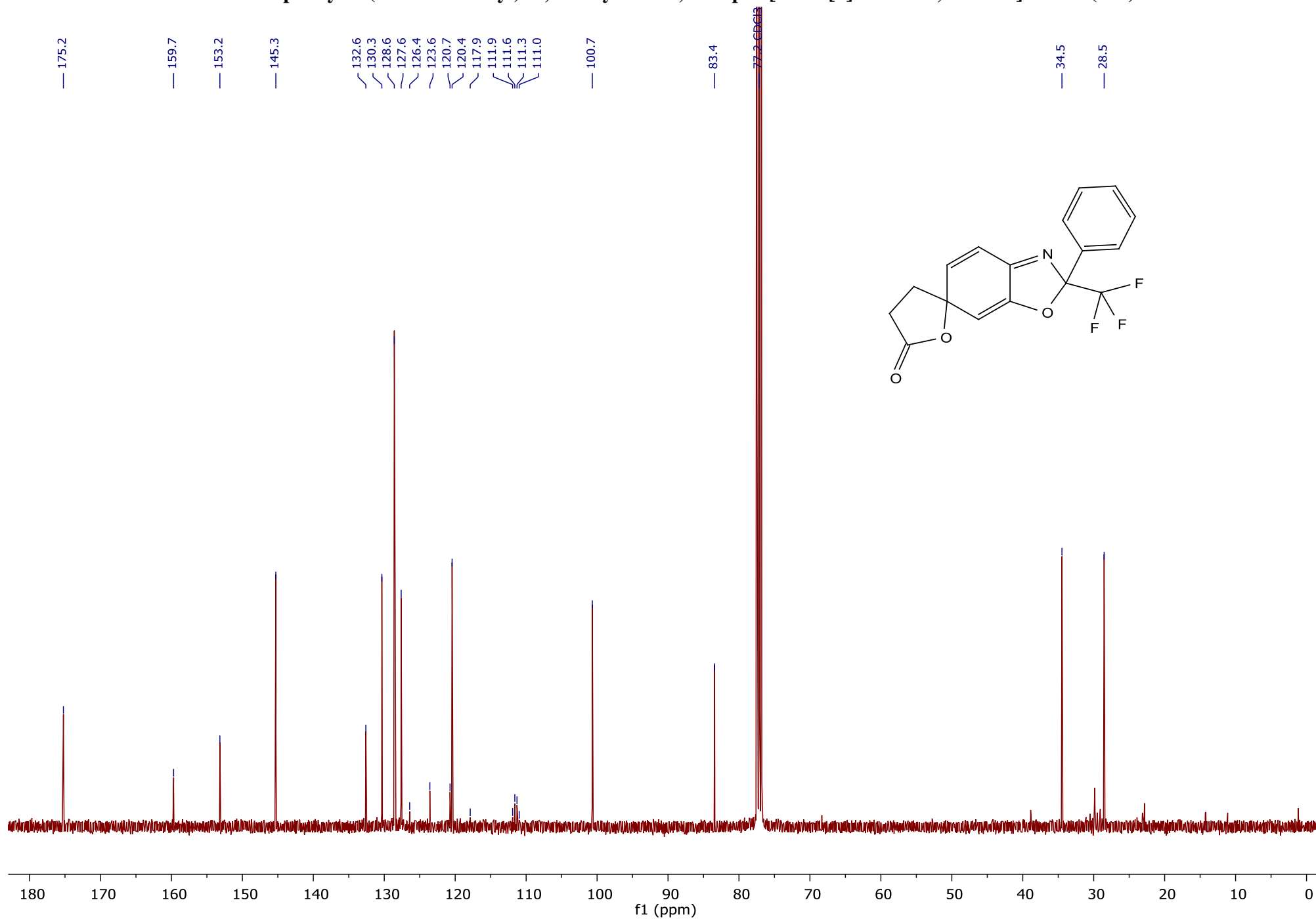
^{13}C NMR of 3-(2-phenyl-2-(trifluoromethyl)-2,3-dihydrobenzo[d]oxazol-6-yl)propanoic acid (11)

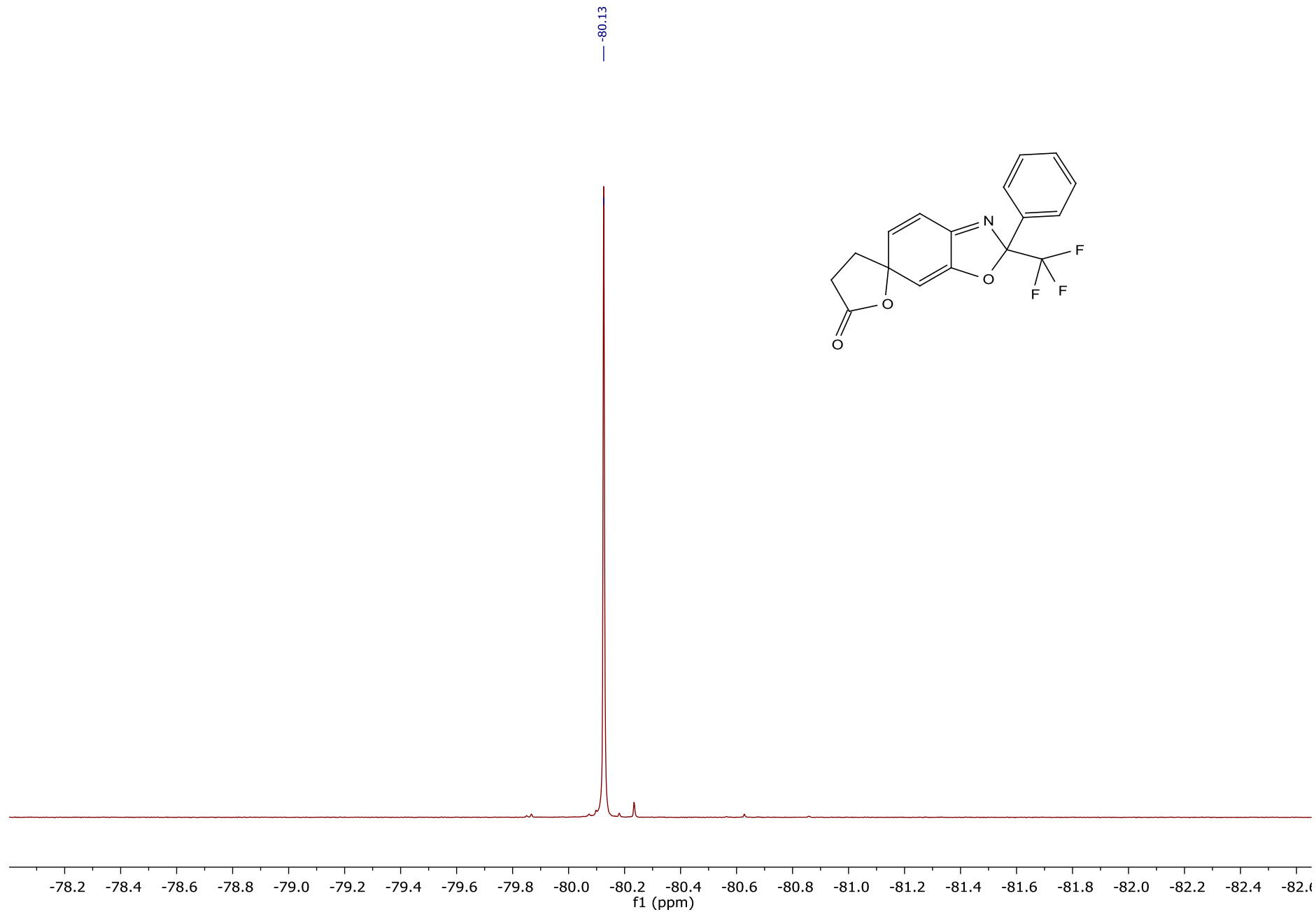
^{19}F NMR of 3-(2-phenyl-2-(trifluoromethyl)-2,3-dihydrobenzo[*d*]oxazol-6-yl)propanoic acid (11)

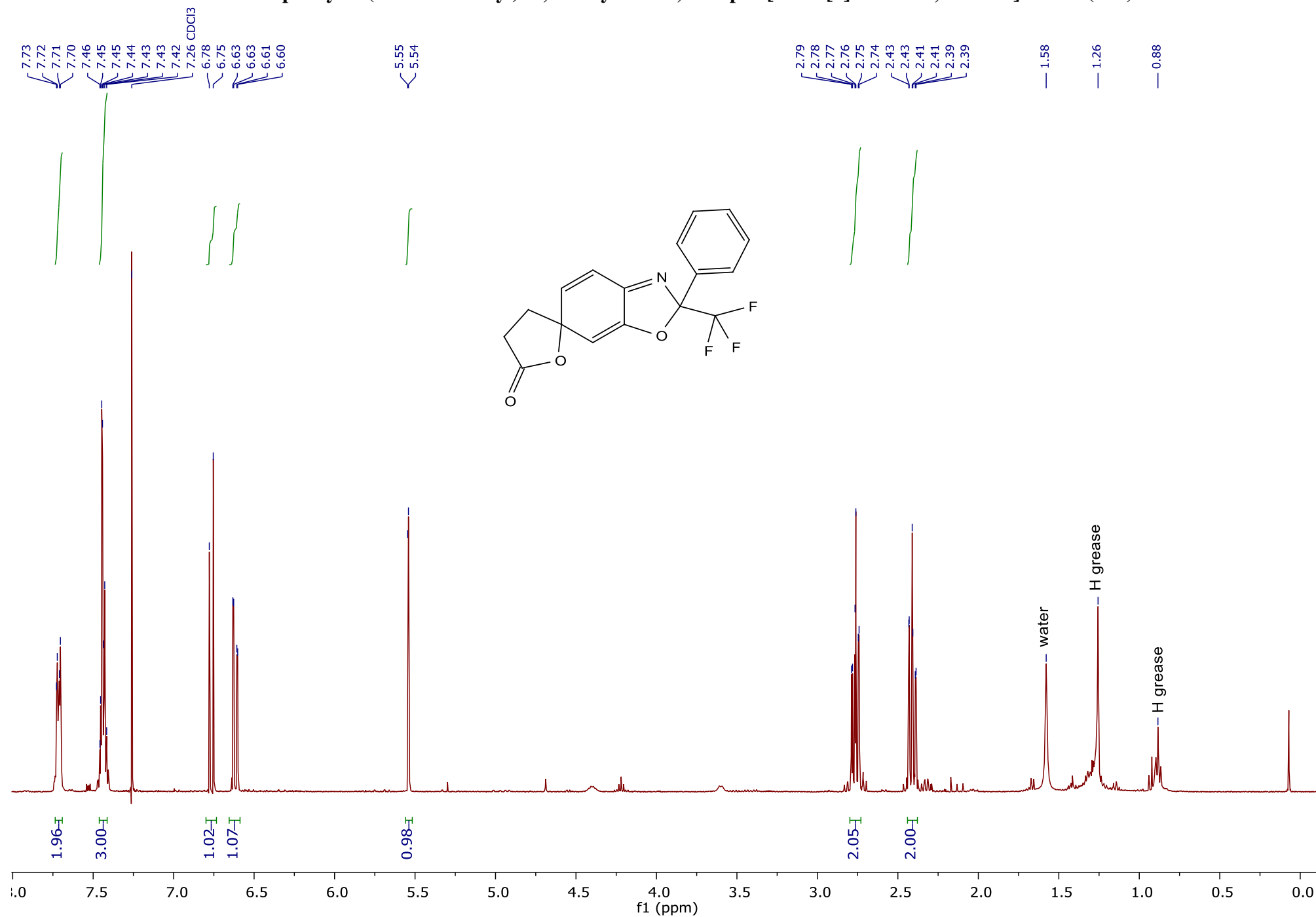
-84.56

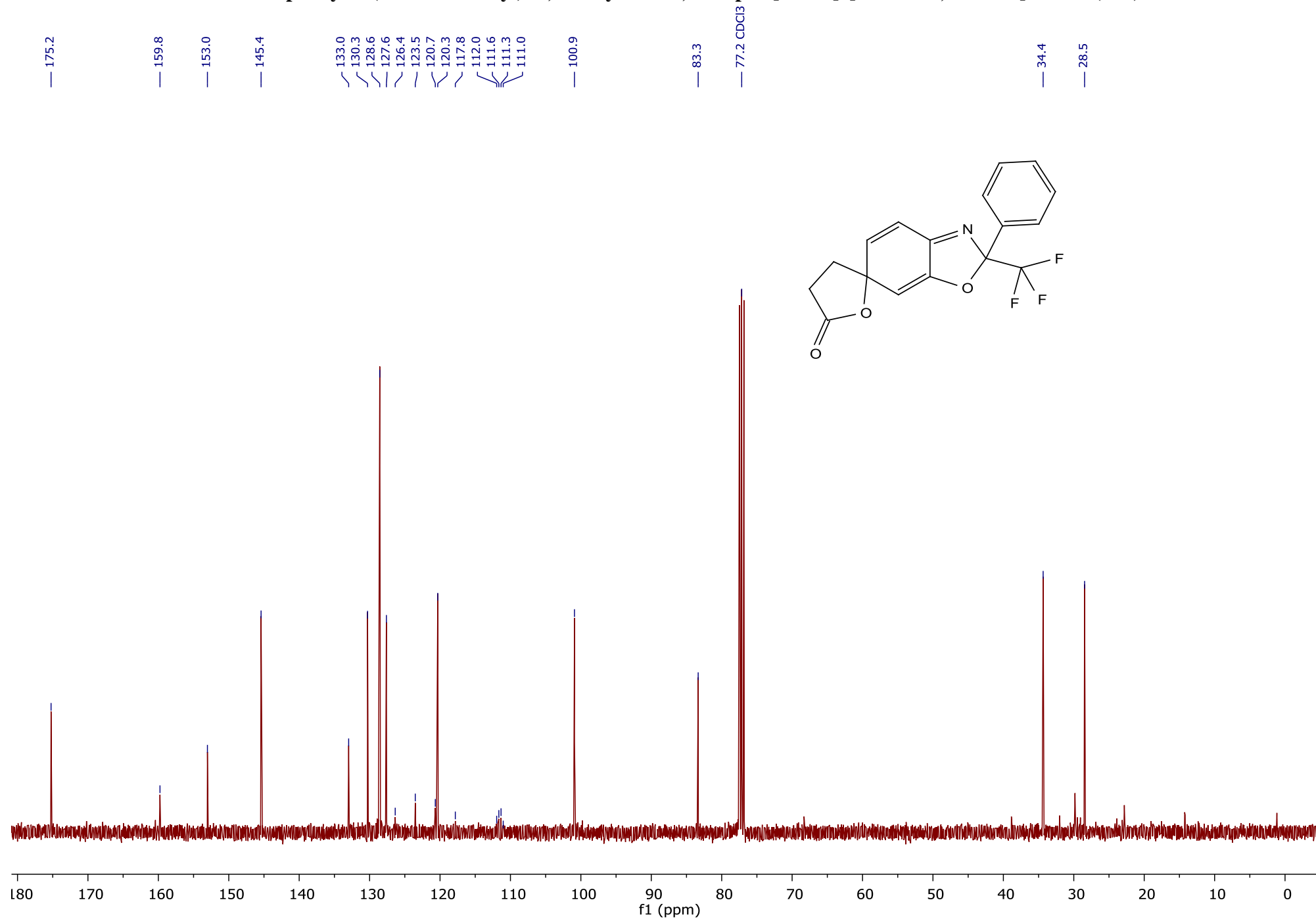


^1H NMR of 2-phenyl-2-(trifluoromethyl)-3',4'-dihydro-2*H*,5'*H*-spiro[benzo[*d*]oxazole-6,2'-furan]-5'-one (12a)

^{13}C NMR of 2-phenyl-2-(trifluoromethyl)-3',4'-dihydro-2*H*,5'*H*-spiro[benzo[*d*]oxazole-6,2'-furan]-5'-one (12a)

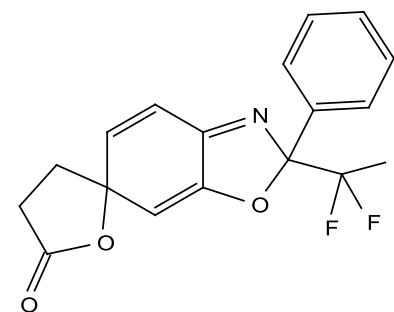
¹⁹F NMR of 2-phenyl-2-(trifluoromethyl)-3',4'-dihydro-2H,5'H-spiro[benzo[d]oxazole-6,2'-furan]-5'-one (12a)

^1H NMR of 2-phenyl-2-(trifluoromethyl)-3',4'-dihydro-2*H*,5'*H*-spiro[benzo[*d*]oxazole-6,2'-furan]-5'-one (12b)

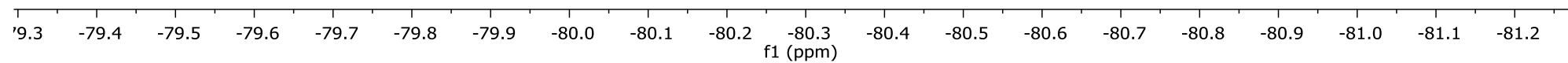
^{13}C NMR of 2-phenyl-2-(trifluoromethyl)-3',4'-dihydro-2*H*,5'*H*-spiro[benzo[*d*]oxazole-6,2'-furan]-5'-one (12b)

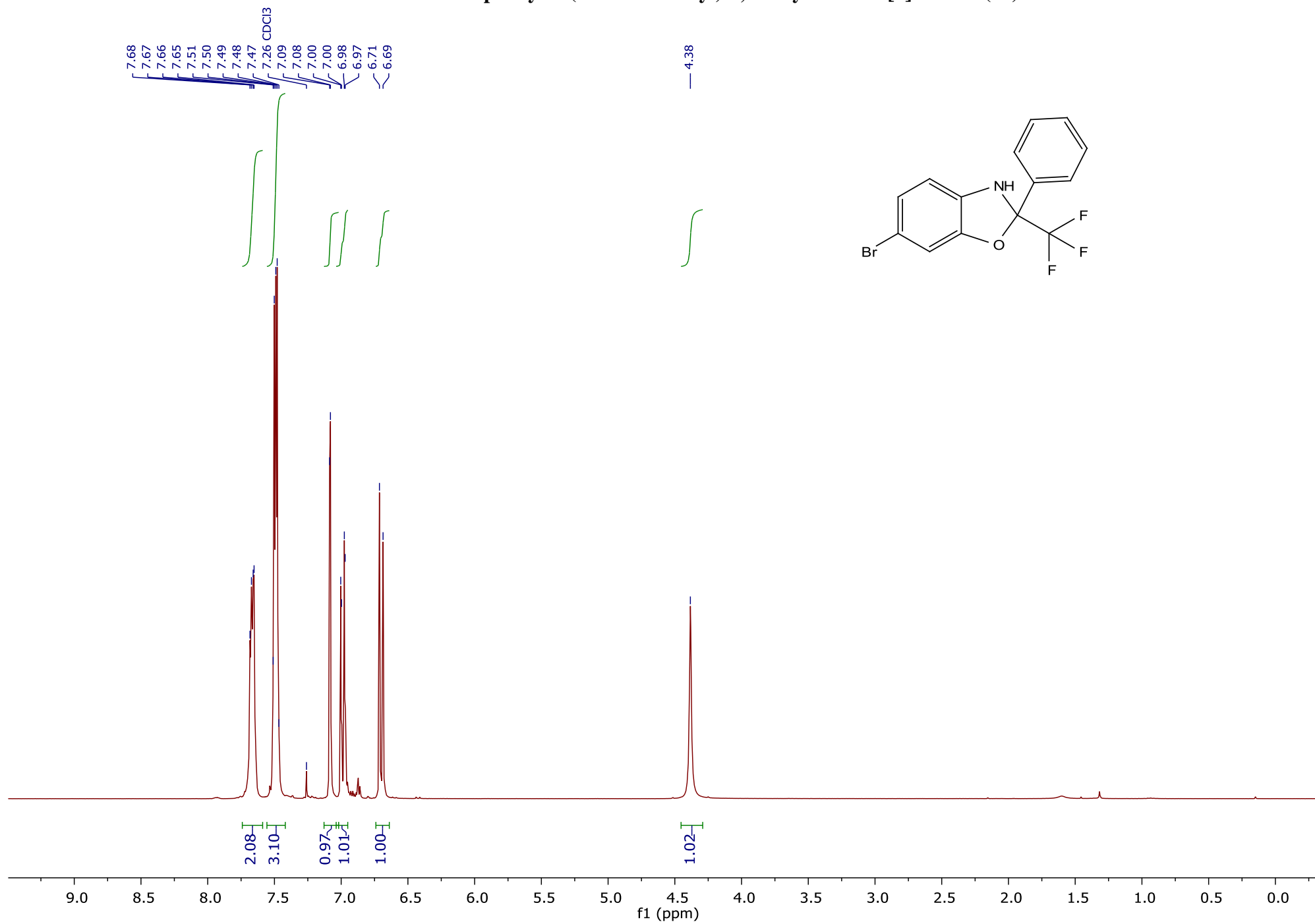
^{19}F NMR of 2-phenyl-2-(trifluoromethyl)-3',4'-dihydro-2*H*,5'*H*-spiro[benzo[*d*]oxazole-6,2'-furan]-5'-one (12b)

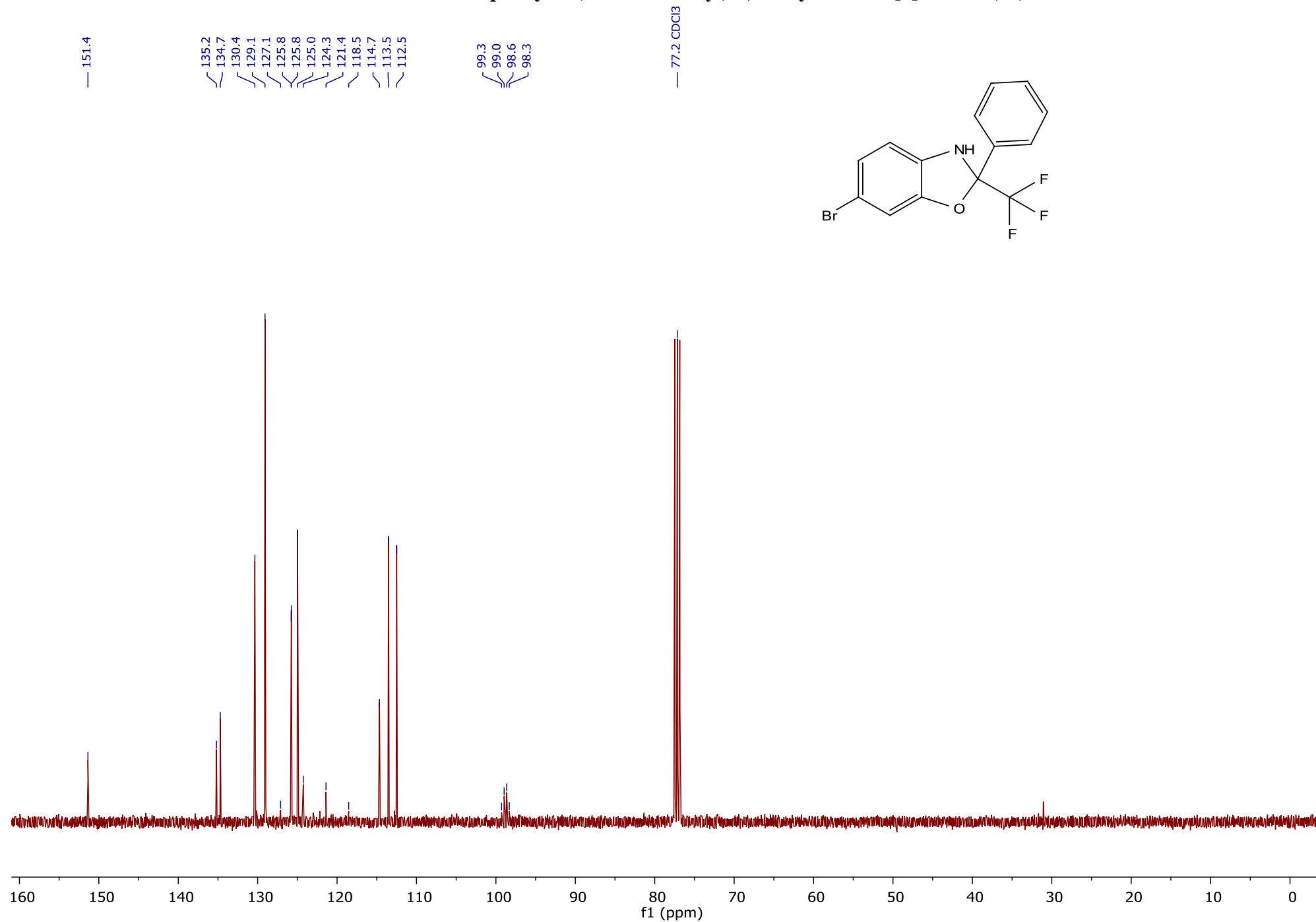
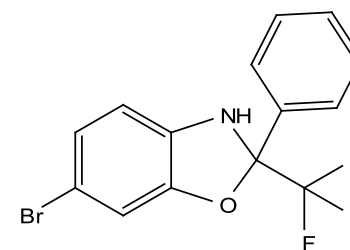
— -80.13
— -80.23

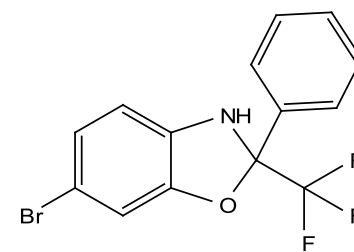


12a

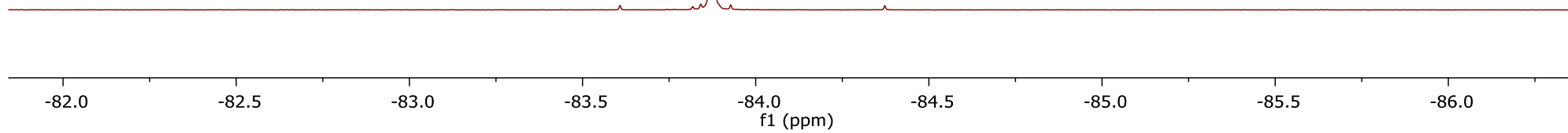


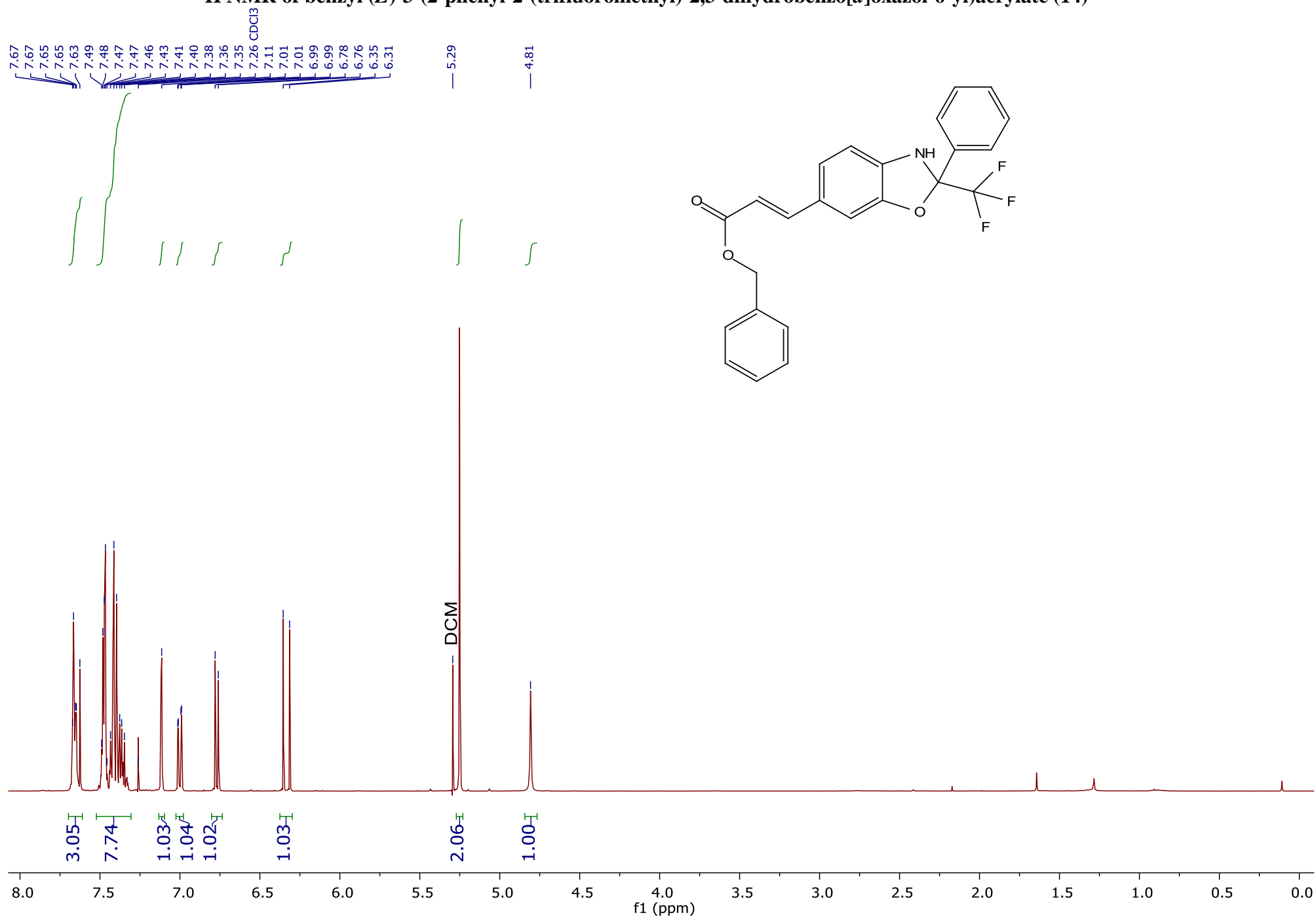
¹H NMR of 6-bromo-2-phenyl-2-(trifluoromethyl)-2,3-dihydrobenzo[d]oxazole (13)

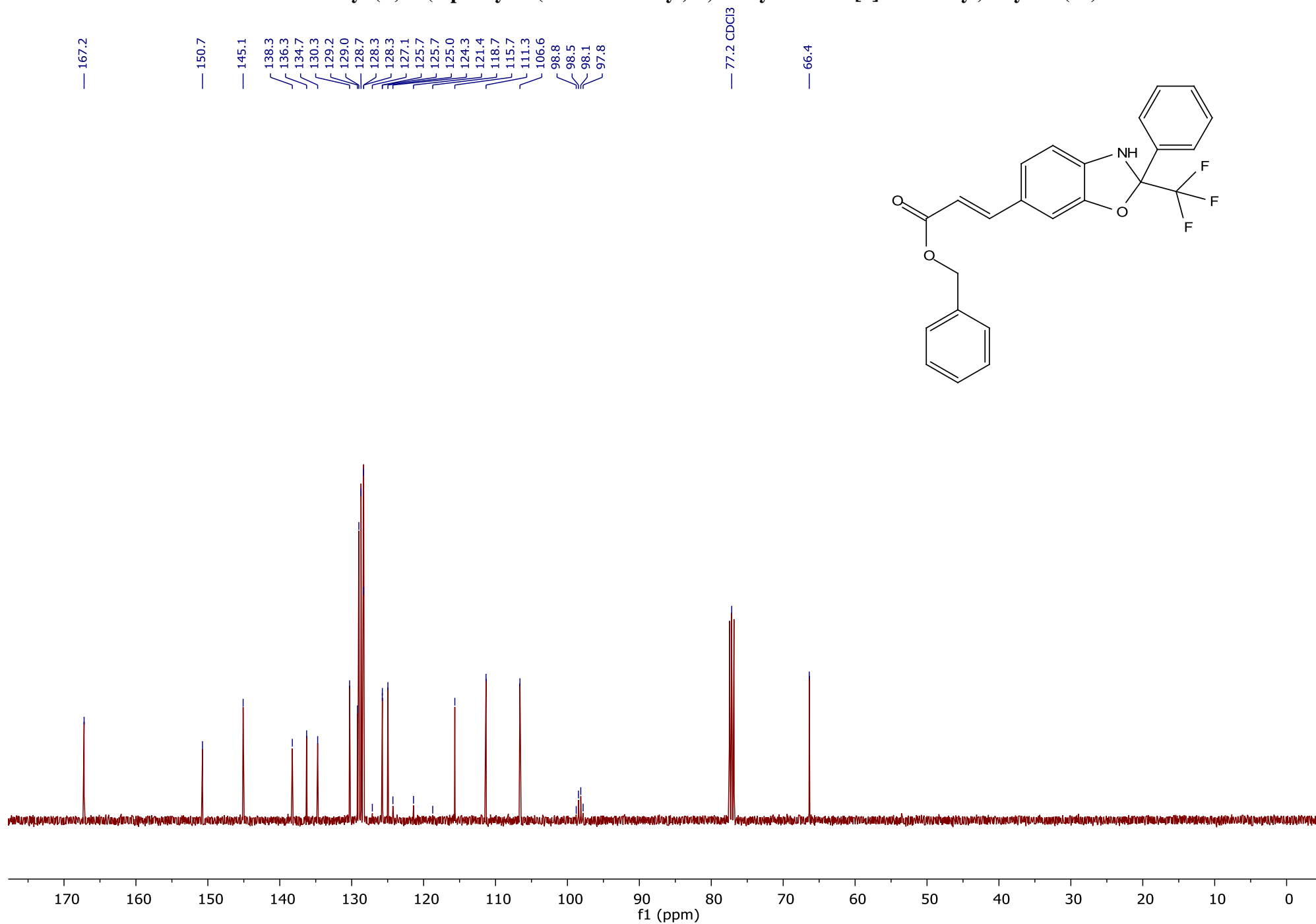
^{13}C NMR of 6-bromo-2-phenyl-2-(trifluoromethyl)-2,3-dihydrobenzo[*d*]oxazole (13)

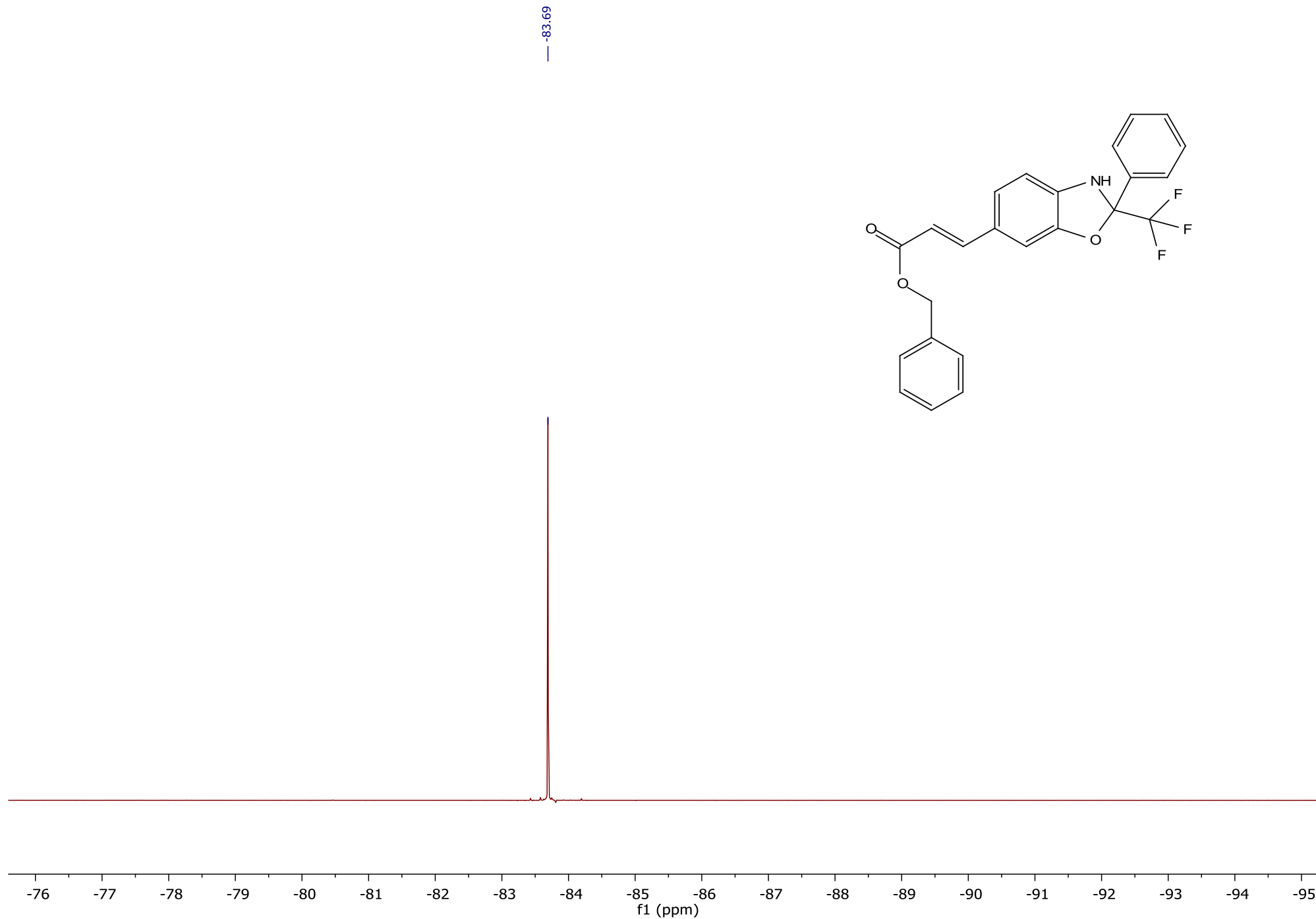
^{19}F NMR of 6-bromo-2-phenyl-2-(trifluoromethyl)-2,3-dihydrobenzo[*d*]oxazole (13)

-83.87

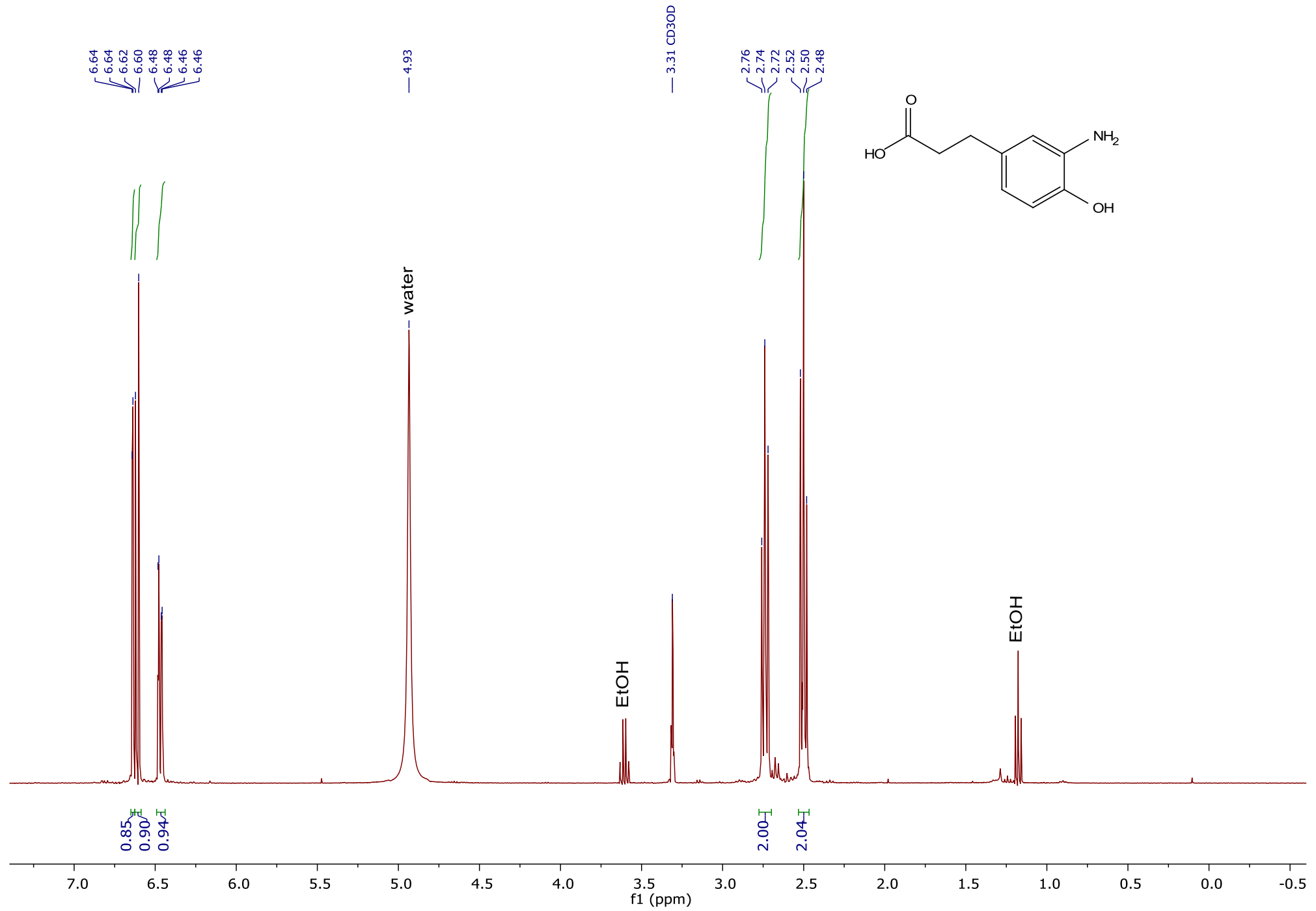


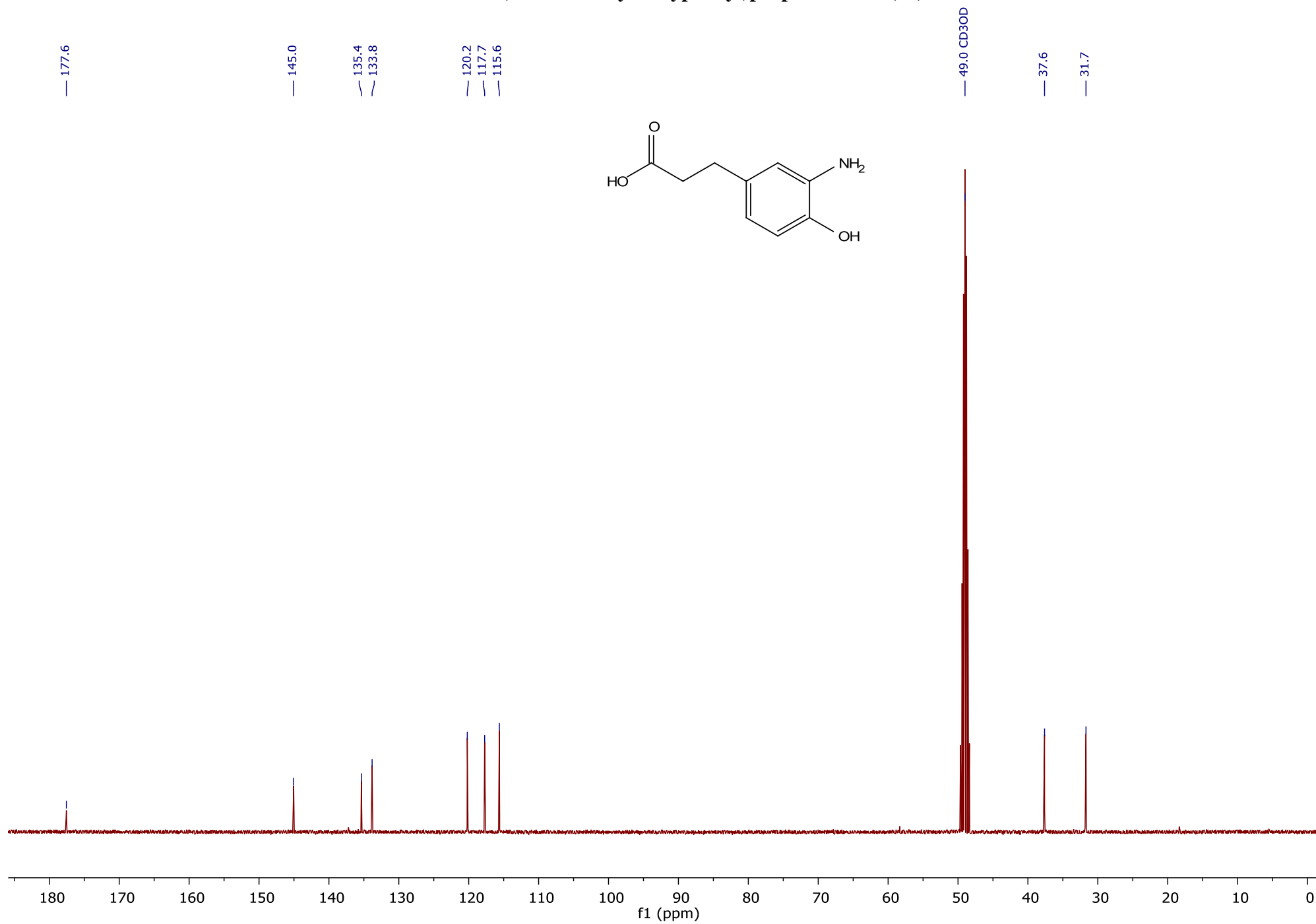
^1H NMR of benzyl (*E*)-3-(2-phenyl-2-(trifluoromethyl)-2,3-dihydrobenzo[*d*]oxazol-6-yl)acrylate (14)

^{13}C NMR of benzyl (*E*)-3-(2-phenyl-2-(trifluoromethyl)-2,3-dihydrobenzo[*d*]oxazol-6-yl)acrylate (14)

^{19}F NMR of benzyl (*E*)-3-(2-phenyl-2-(trifluoromethyl)-2,3-dihydrobenzo[*d*]oxazol-6-yl)acrylate (14)

¹H NMR of 3-(3-amino-4-hydroxyphenyl)propanoic acid (15)



^{13}C NMR of 3-(3-amino-4-hydroxyphenyl)propanoic acid (15)

^{19}F NMR of 1,1,1,3,3,3-hexafluoropropan-2-one; confirmation of its formation during the decomposition of the electrochemically generated I(III) species 2 and the iodane 3 (solvent: CD_2Cl_2 -HFIP, 1:1)