

Supplementary information

Catalyst-free nucleophilic substitution of hydrogen in quinoline ring by acylethylnylpyrroles: a stereoselective synthesis of 2-(*E*-2-acylethylnylpyrrolyl)quinolines

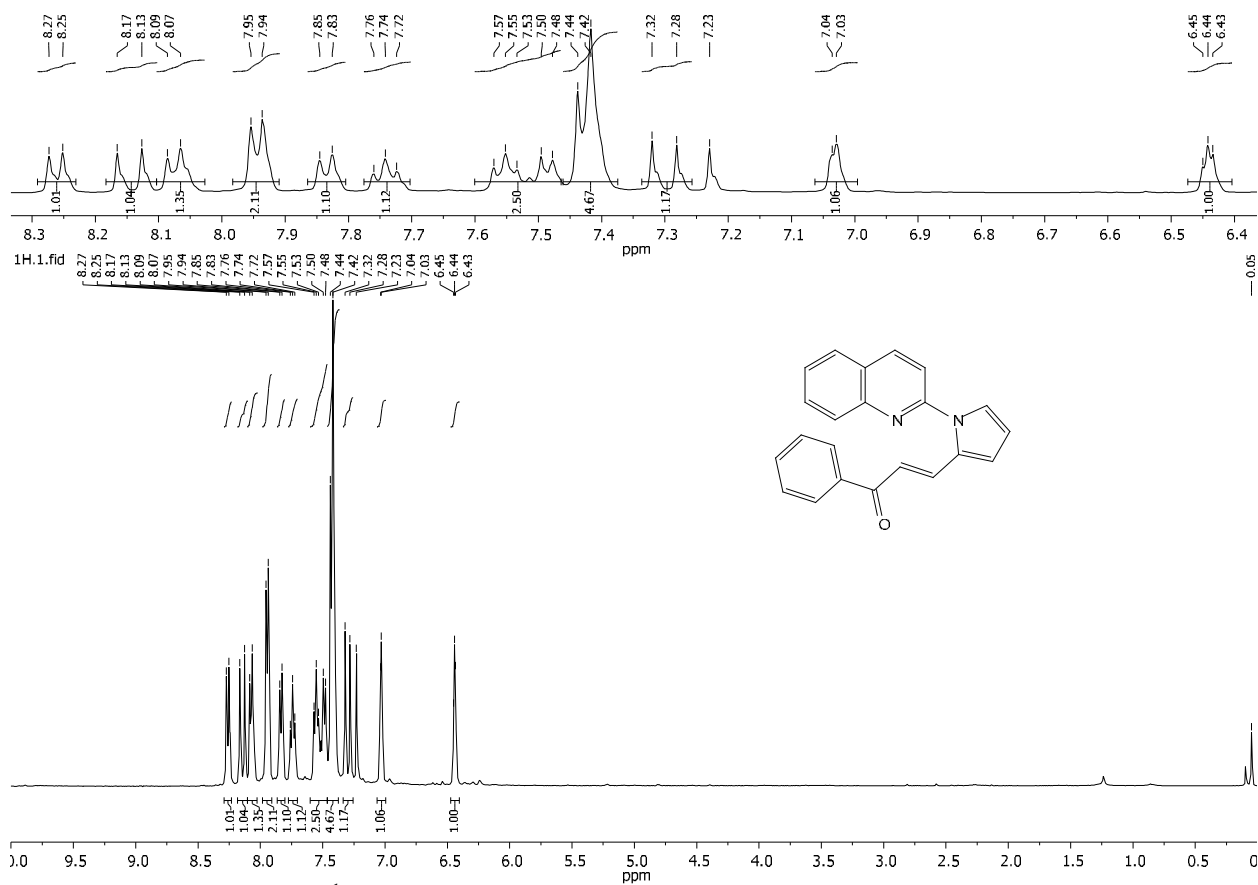
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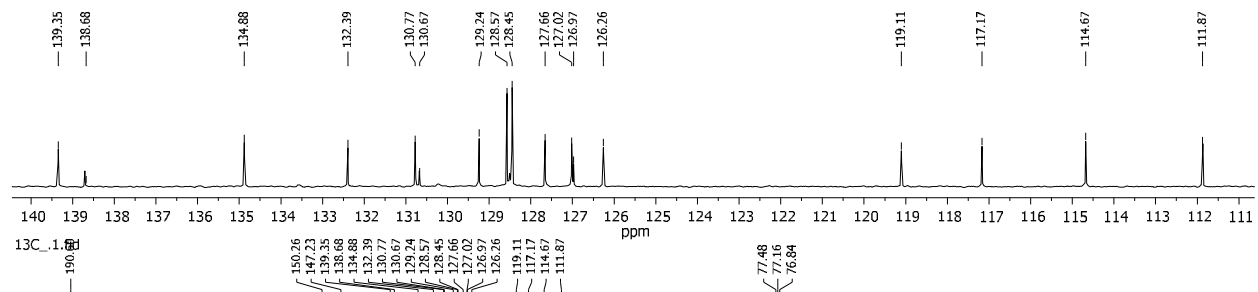
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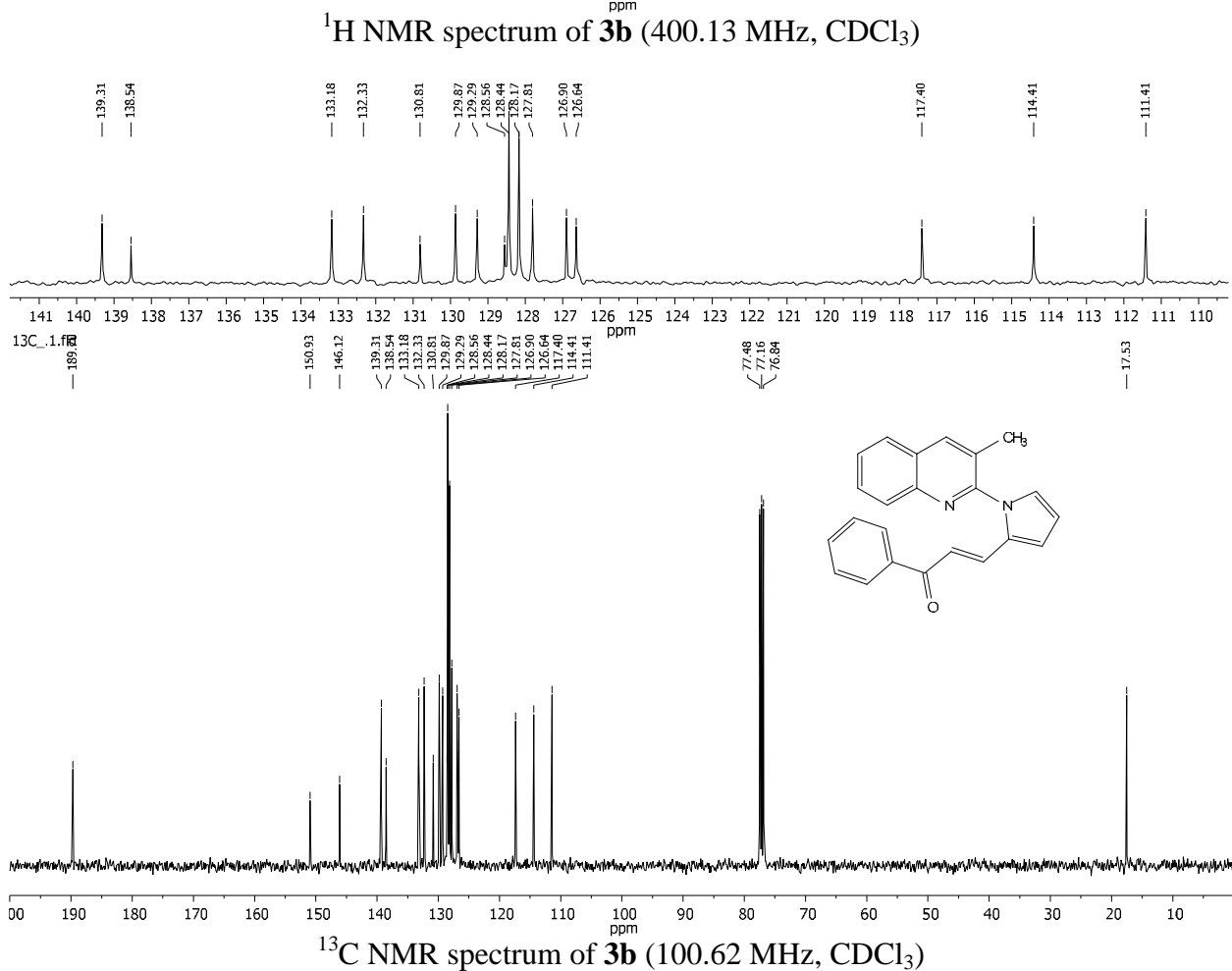
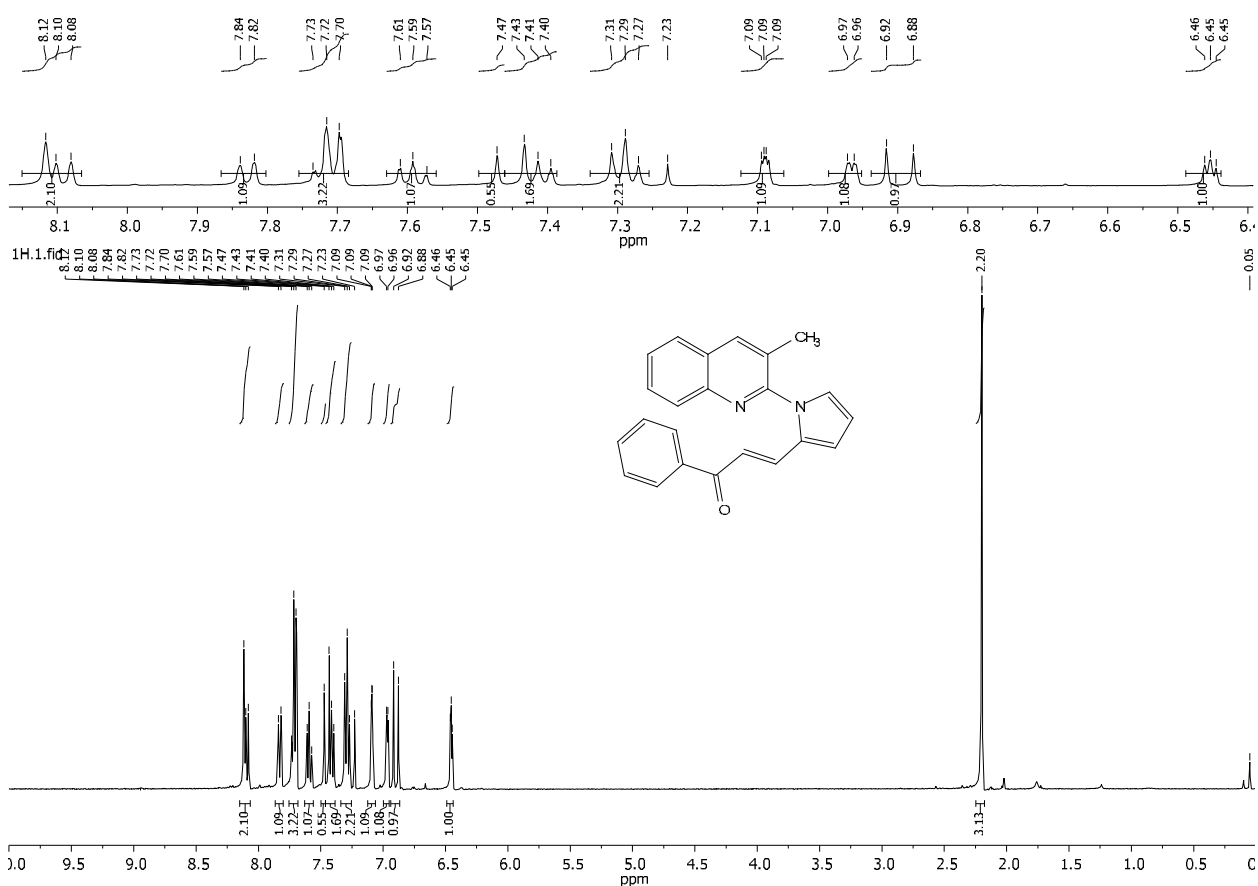
^1H , ^{13}C and ^{19}F spectra of compounds 3 and 5

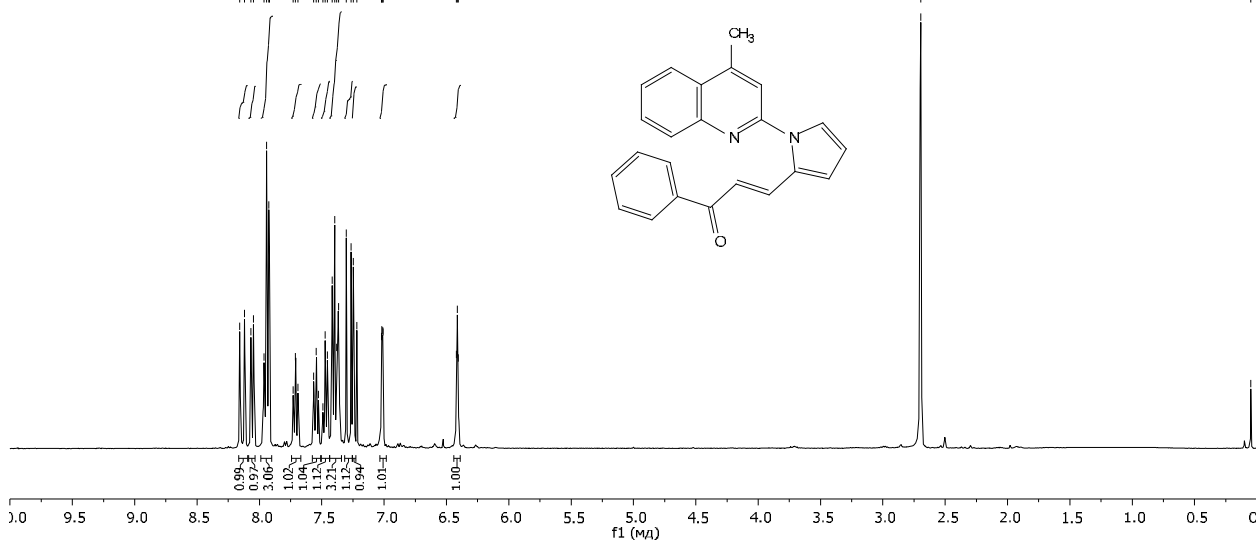
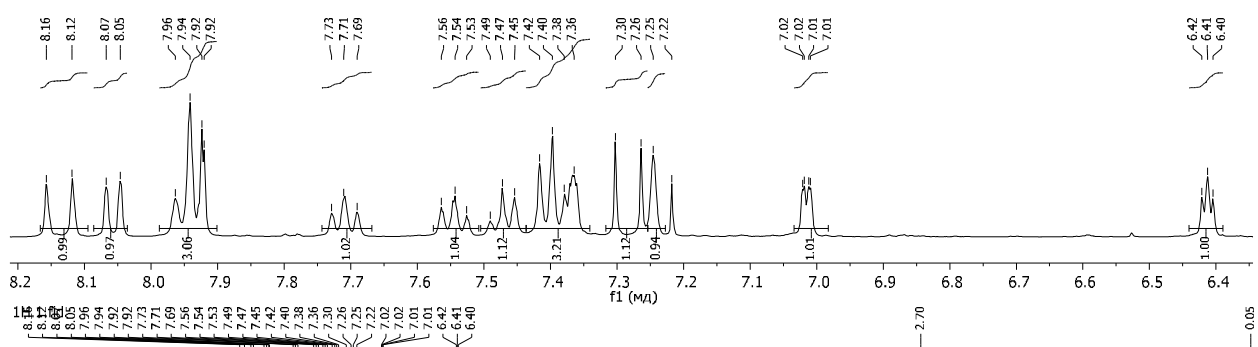


^1H NMR spectrum of **3a** (400.13 MHz, CDCl_3)



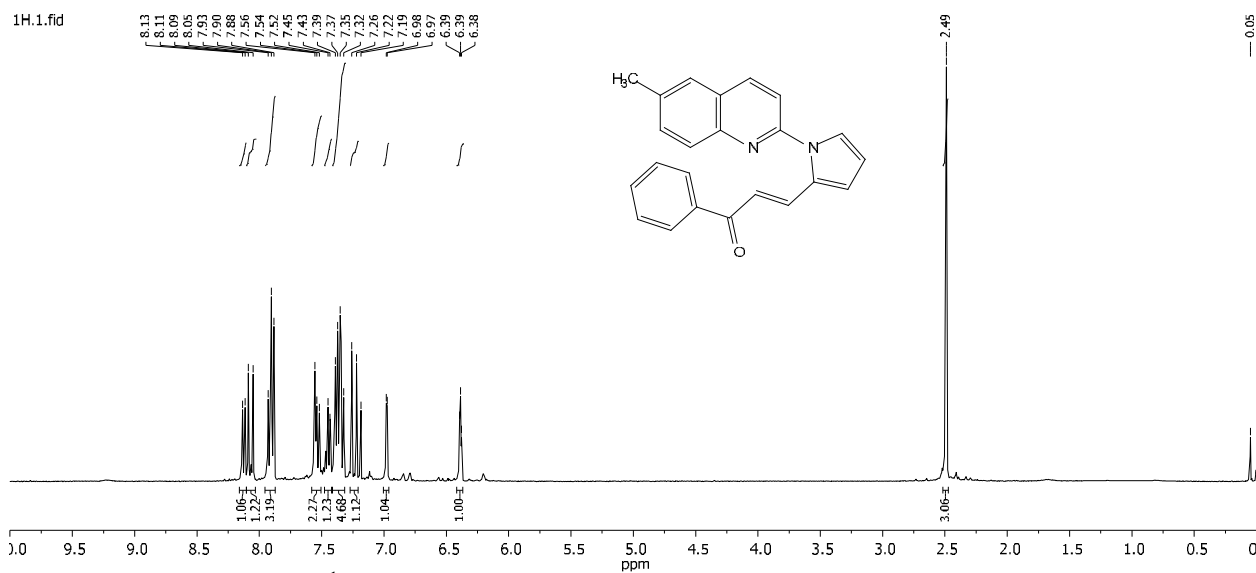
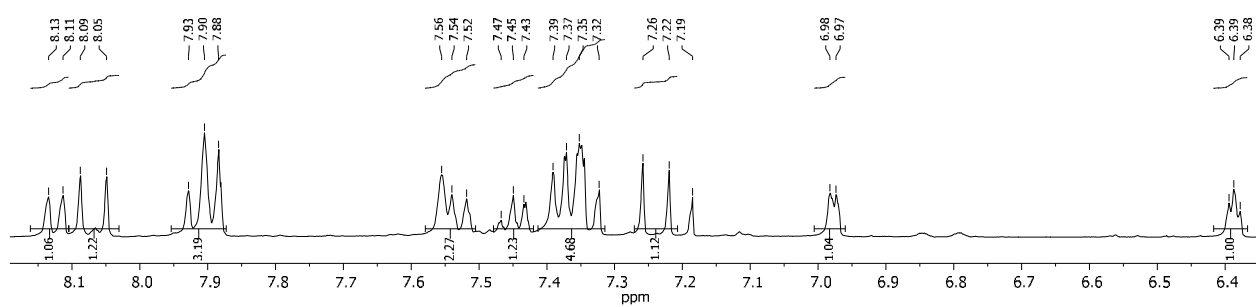
^{13}C NMR spectrum of **3a** (100.62 MHz, CDCl_3)



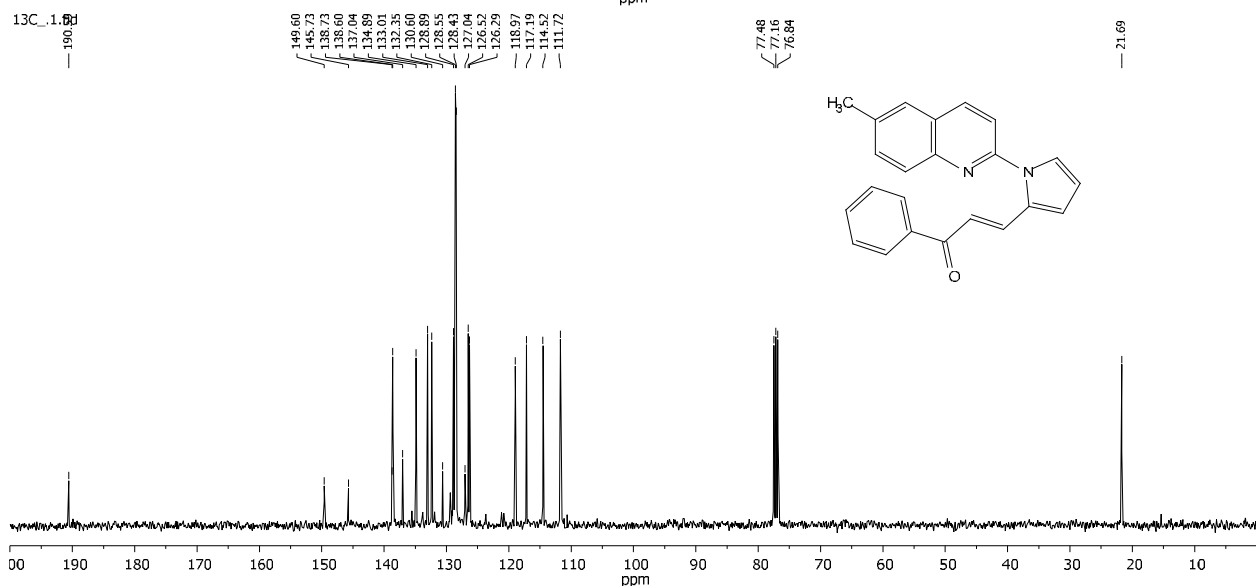
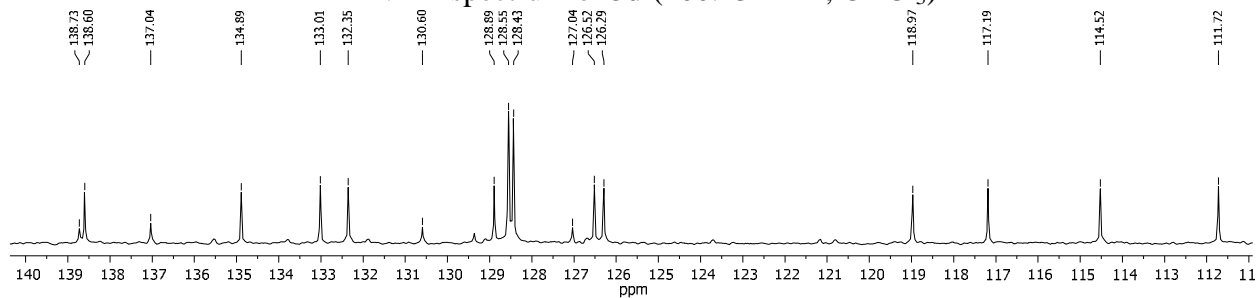


¹H NMR spectrum of 3c (400.13 MHz, CDCl₃)

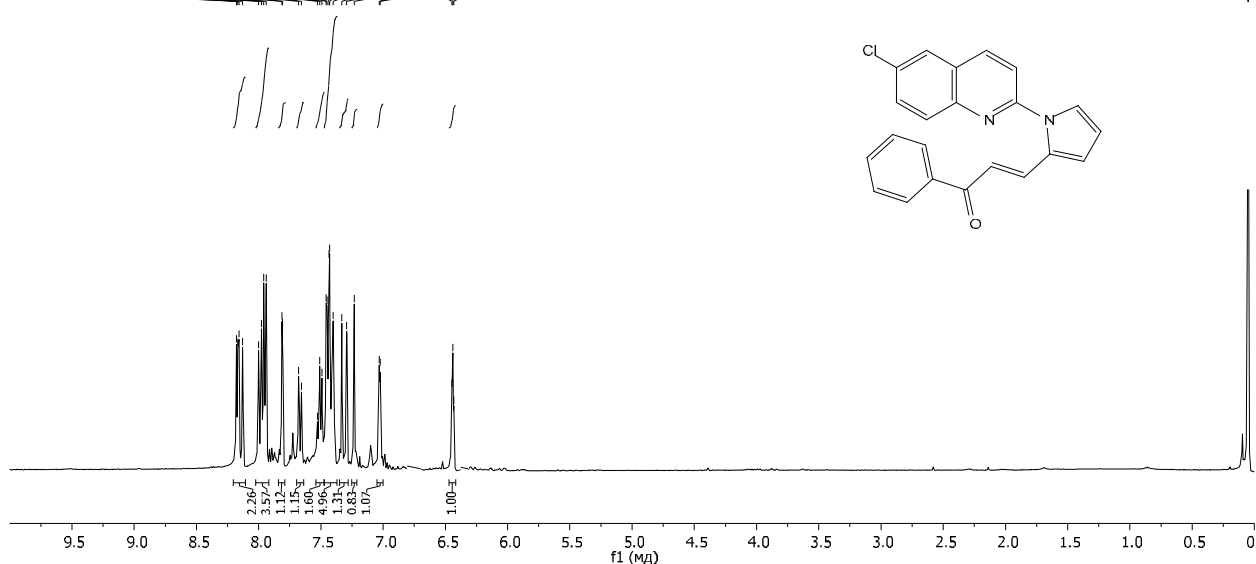
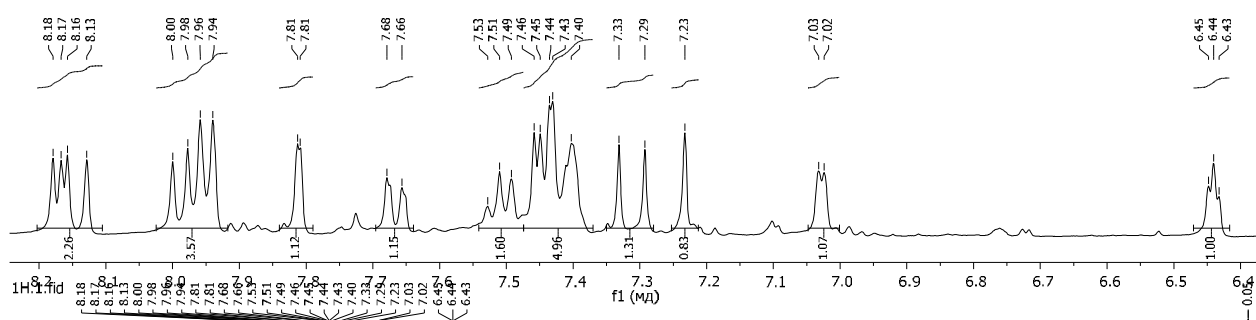
¹³C NMR spectrum of 3c (100.62 MHz, CDCl₃)



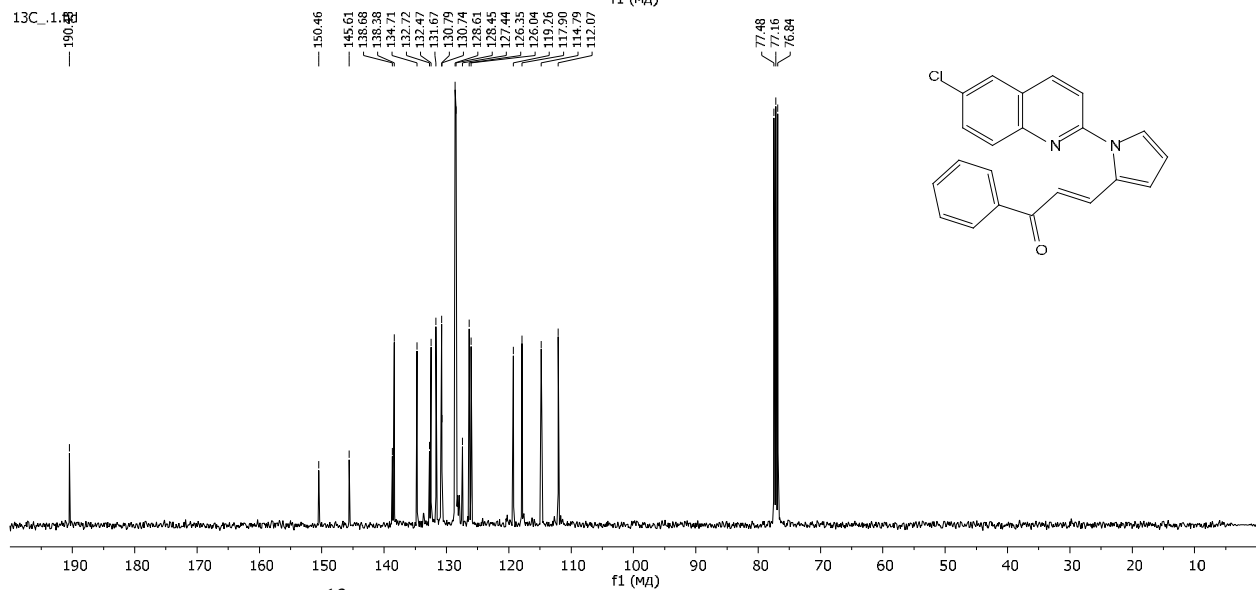
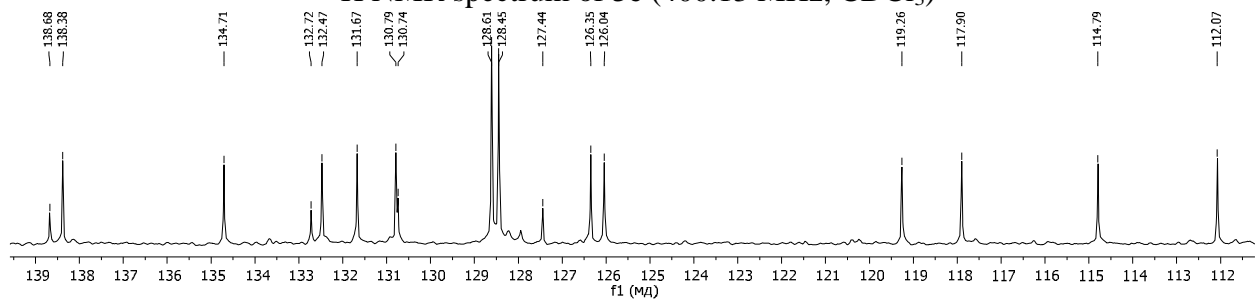
¹H NMR spectrum of **3d** (400.13 MHz, CDCl₃)



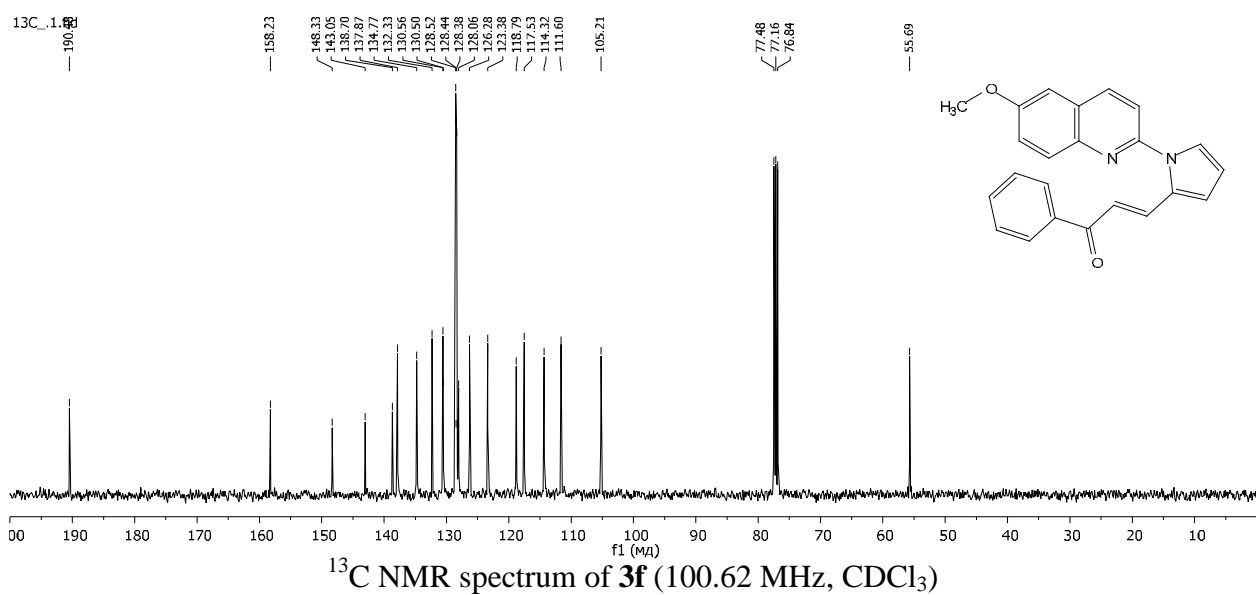
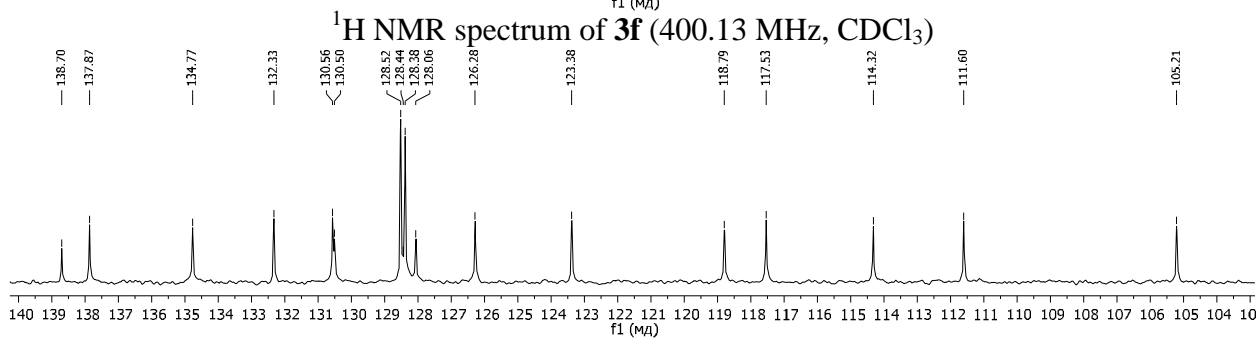
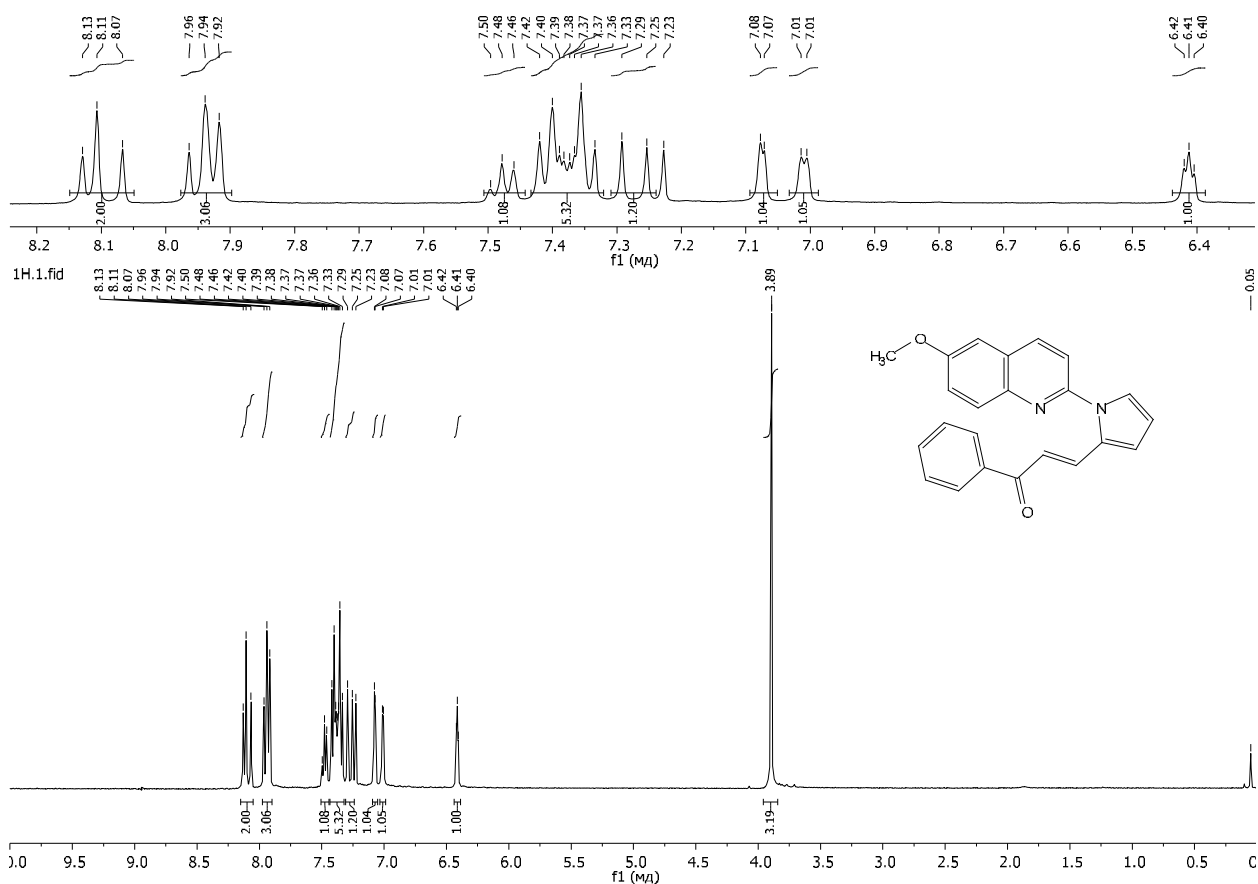
¹³C NMR spectrum of **3d** (100.62 MHz, CDCl₃)

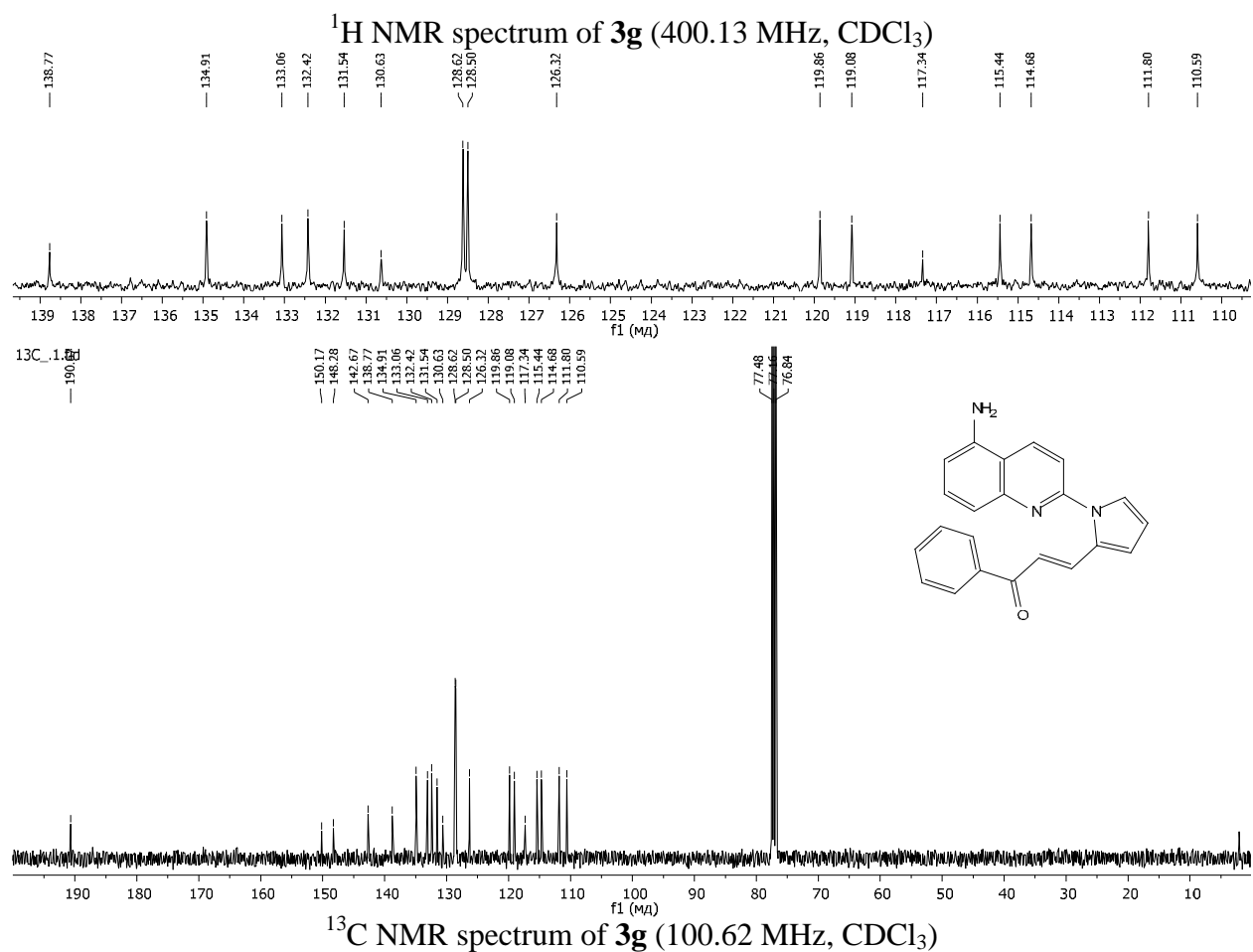
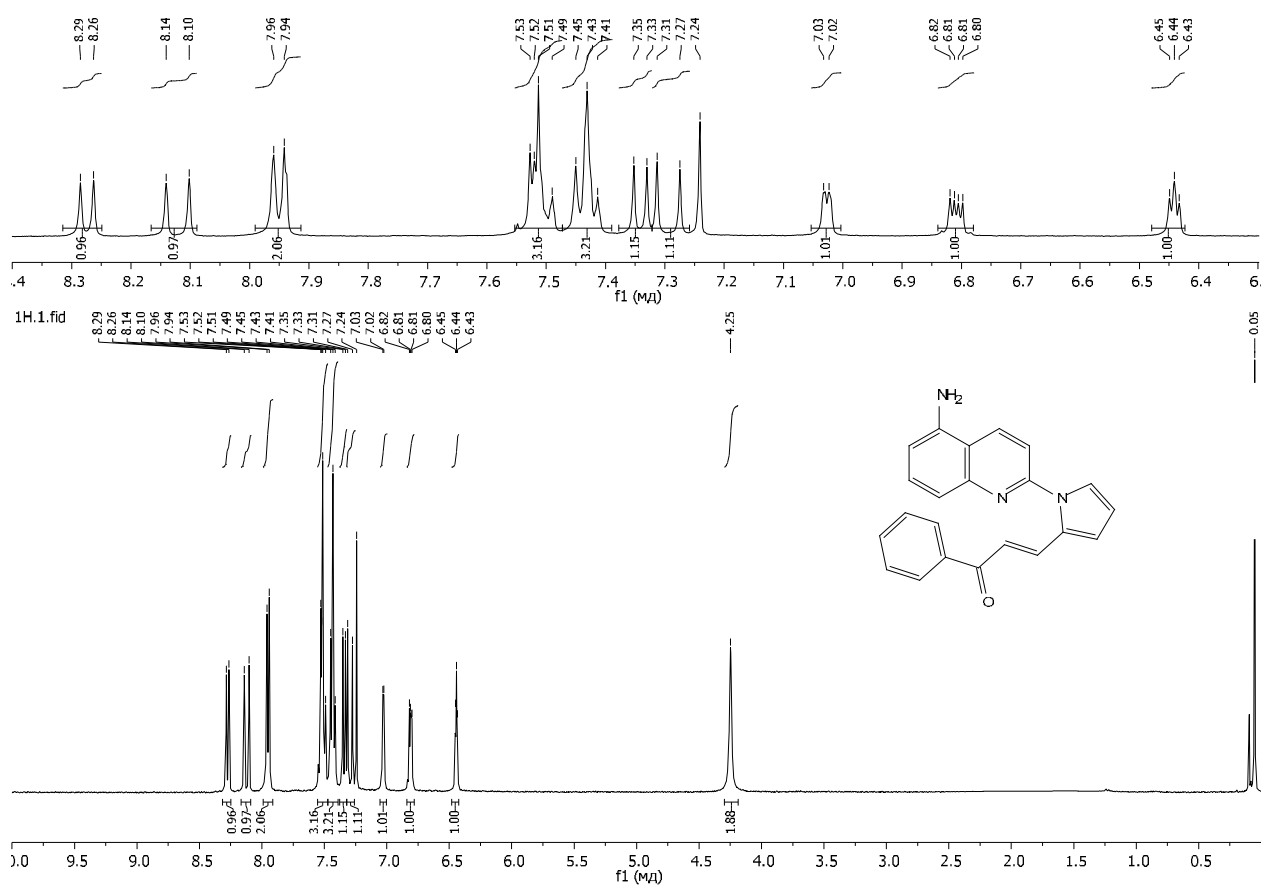


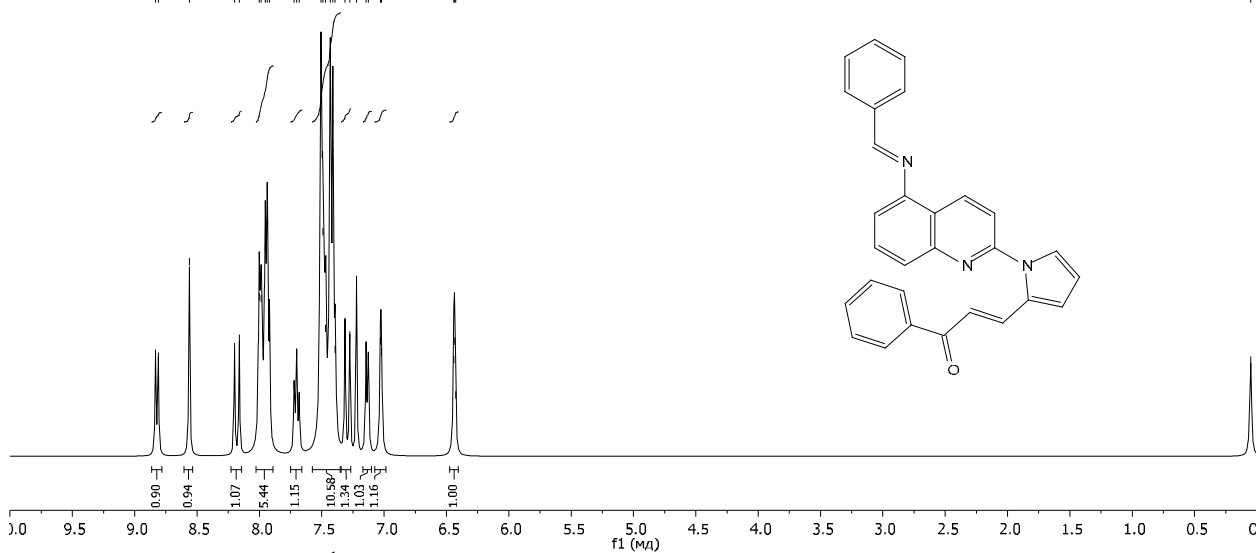
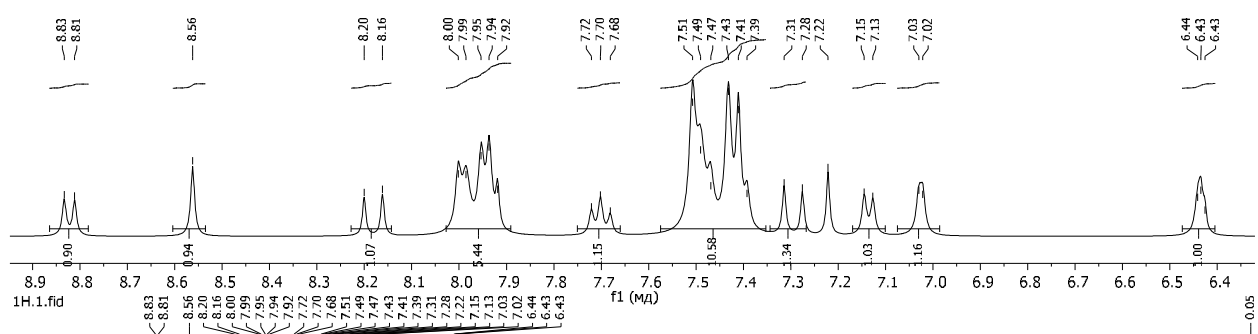
^1H NMR spectrum of **3e** (400.13 MHz, CDCl_3)



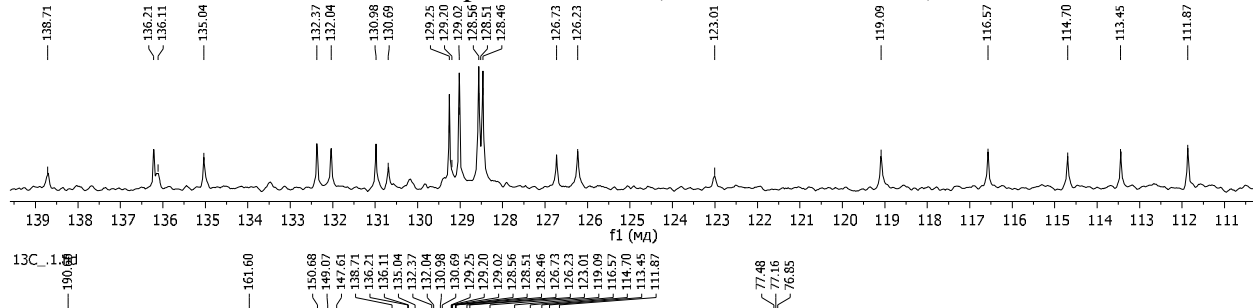
^{13}C NMR spectrum of **3e** (100.62 MHz, CDCl_3)



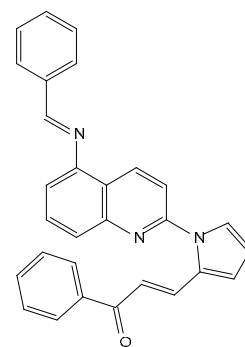
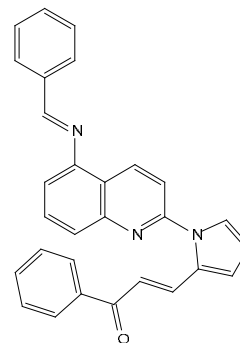


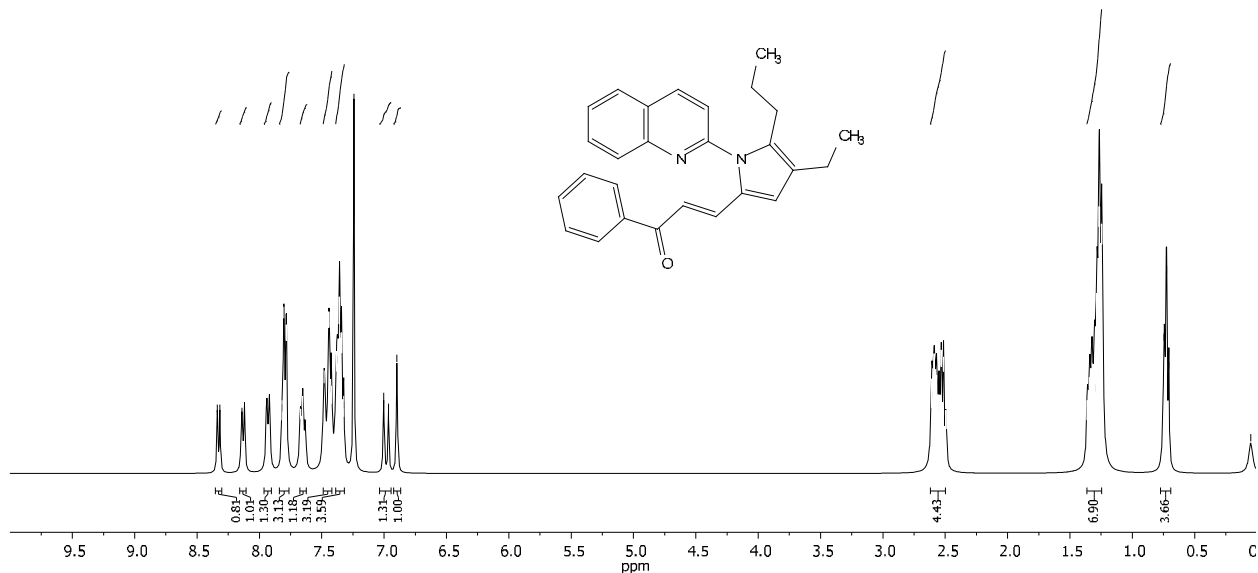
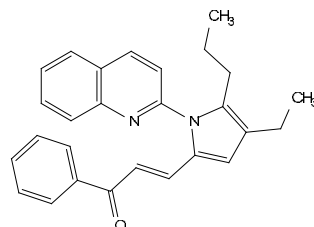
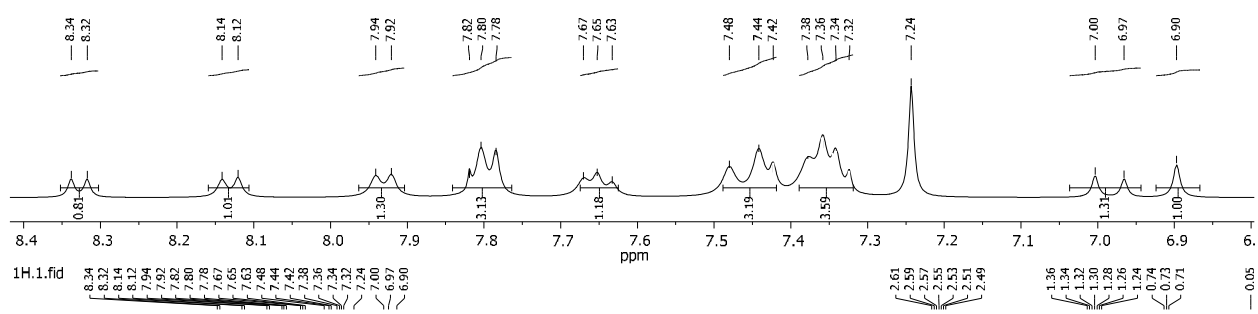


¹H NMR spectrum of **3h** (400.13 MHz, CDCl₃)

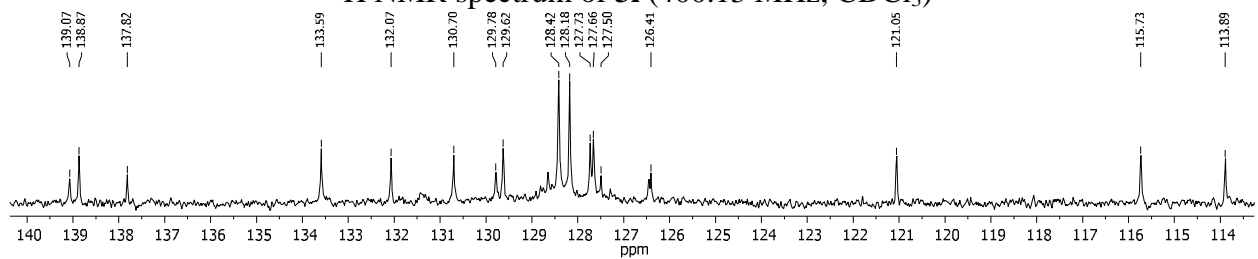


¹³C NMR spectrum of **3h** (100.62 MHz, CDCl₃)

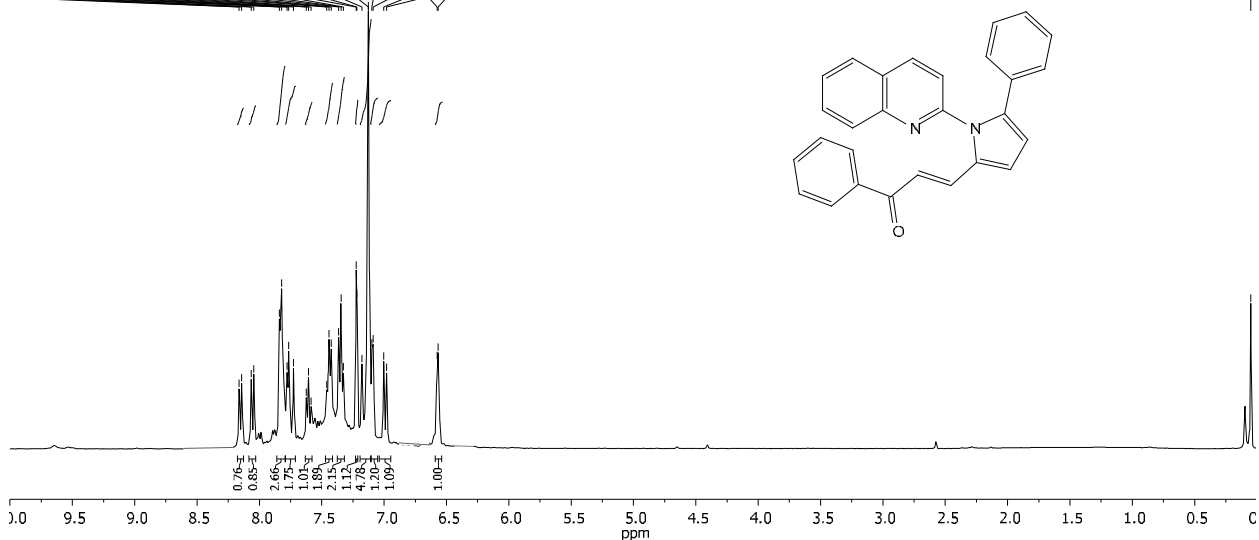
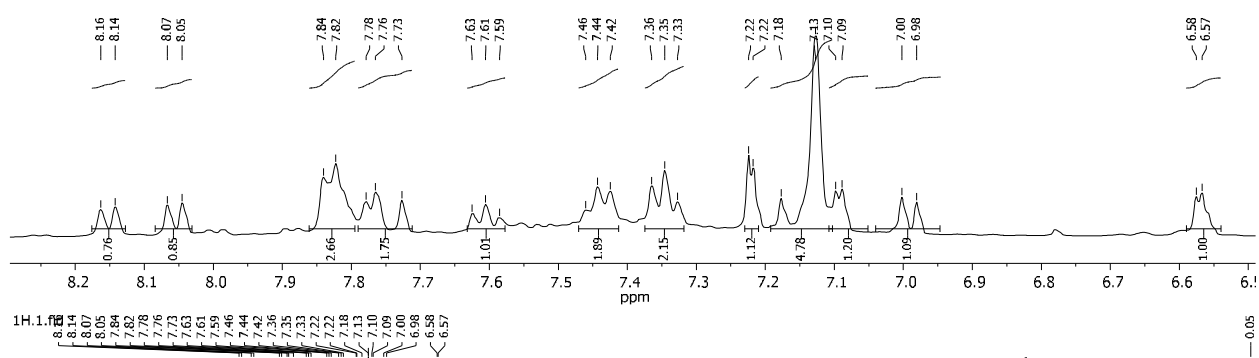




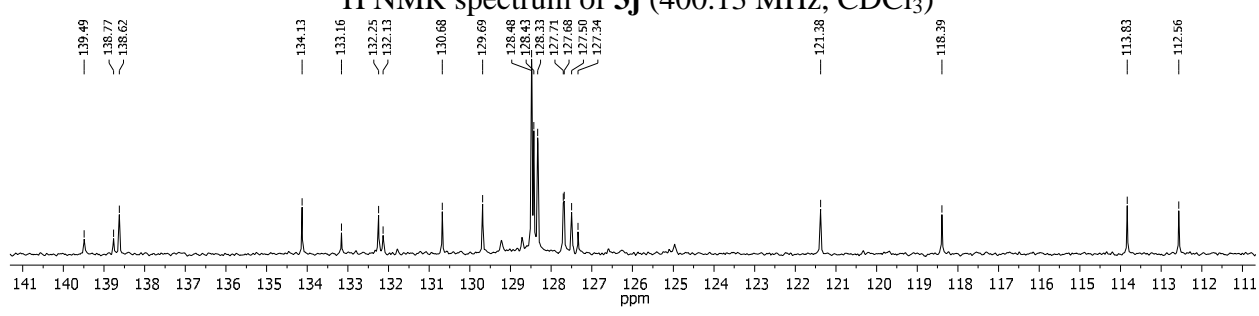
¹H NMR spectrum of **3i** (400.13 MHz, CDCl₃)



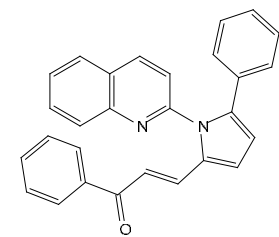
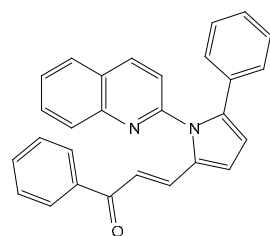
¹³C NMR spectrum of **3i** (100.62 MHz, CDCl₃)

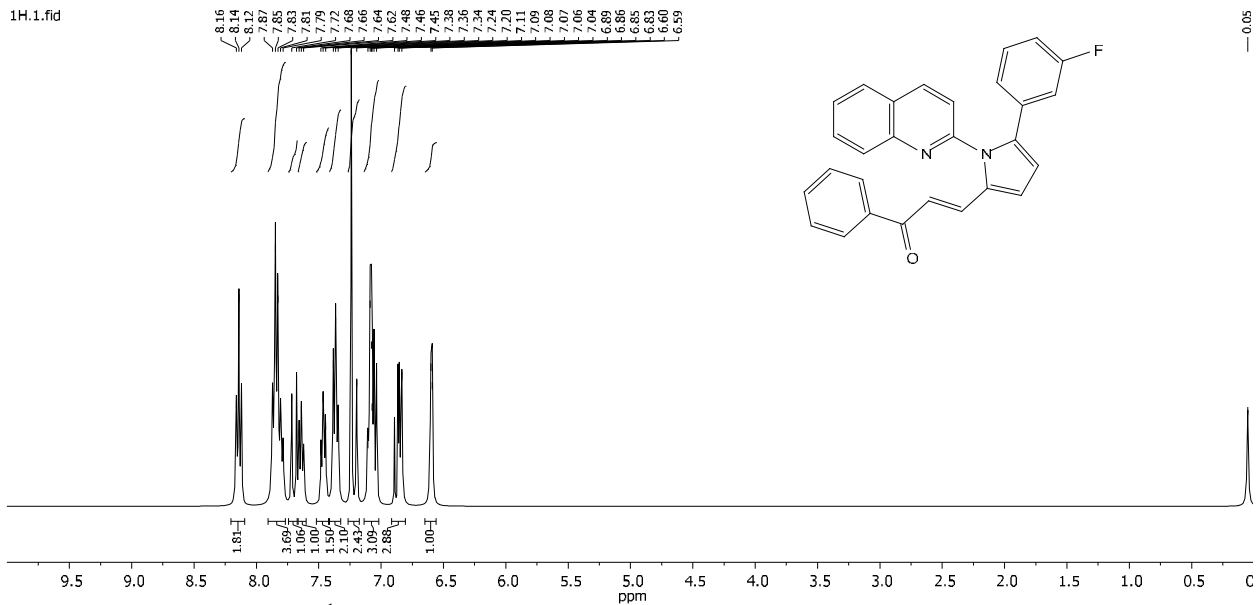
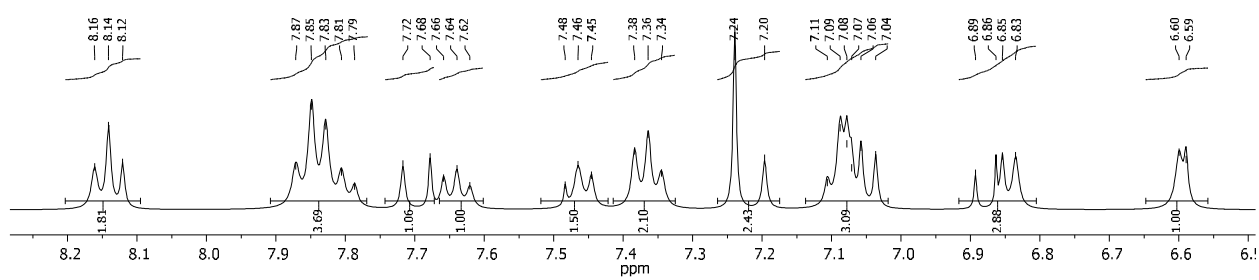


¹H NMR spectrum of **3j** (400.13 MHz, CDCl₃)

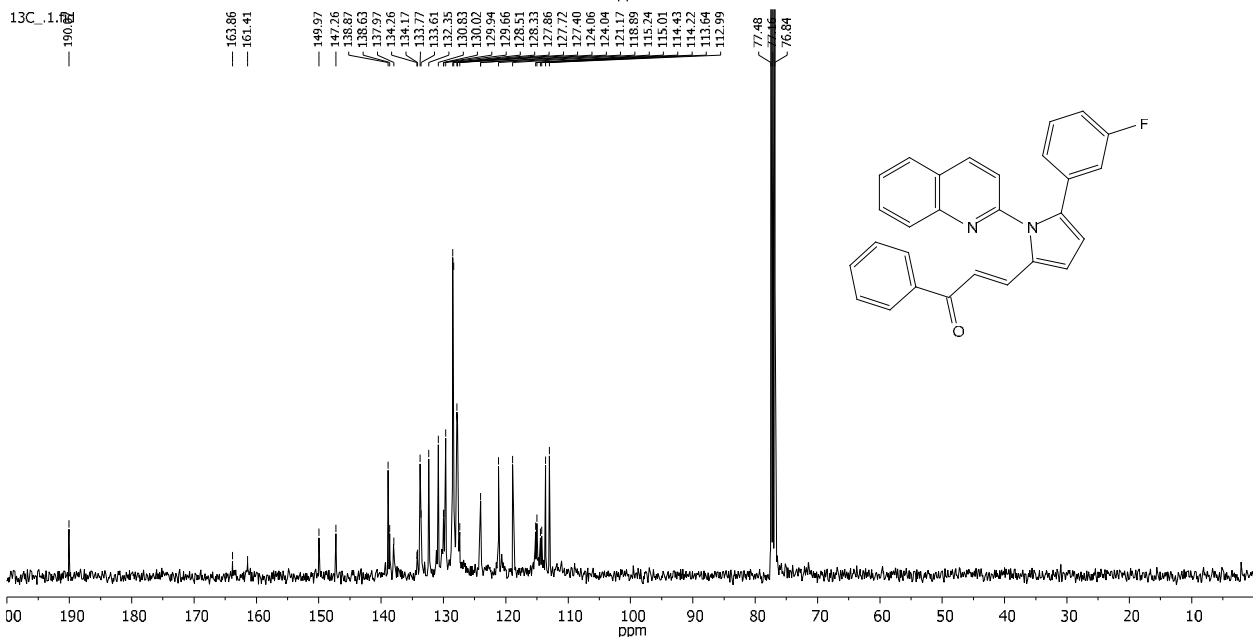
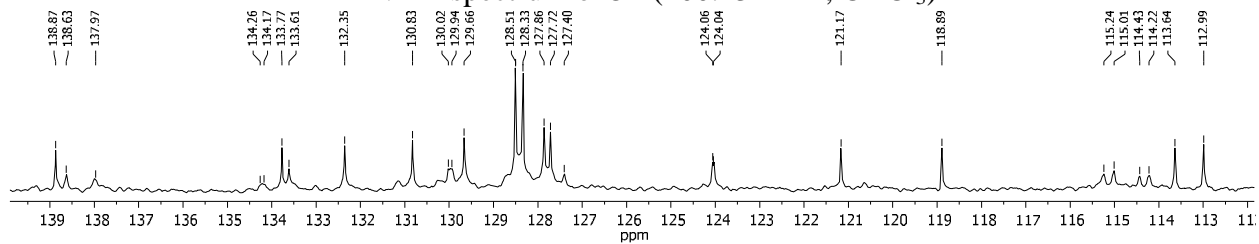


¹³C NMR spectrum of **3j** (100.62 MHz, CDCl₃)





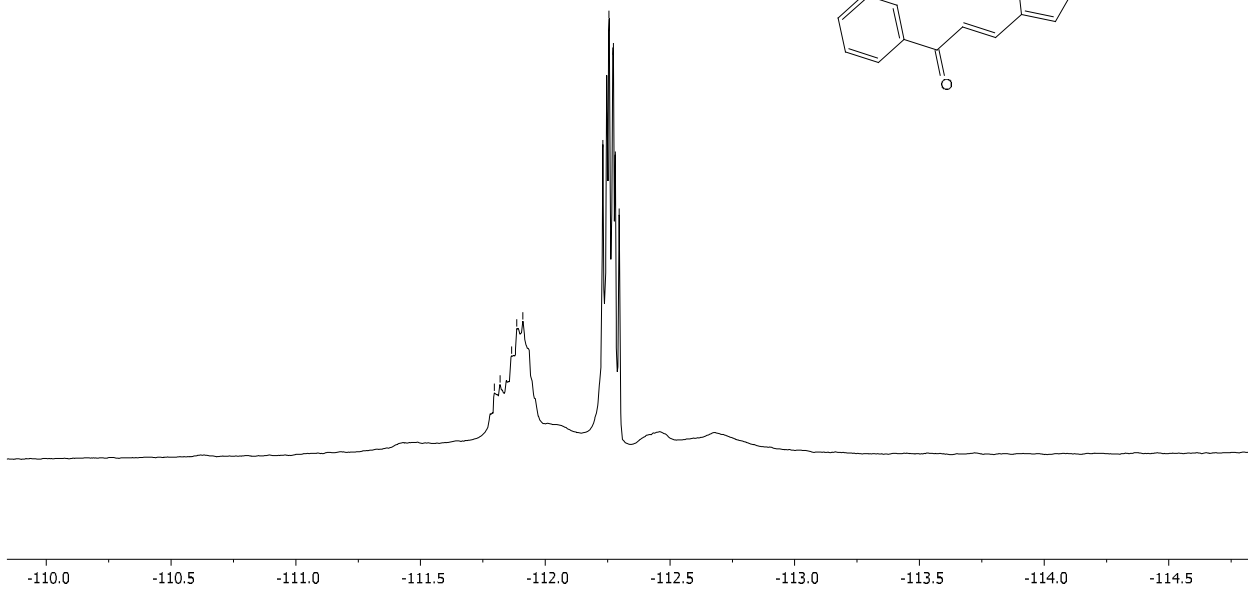
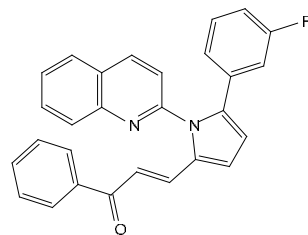
¹H NMR spectrum of **3k** (400.13 MHz, CDCl₃)



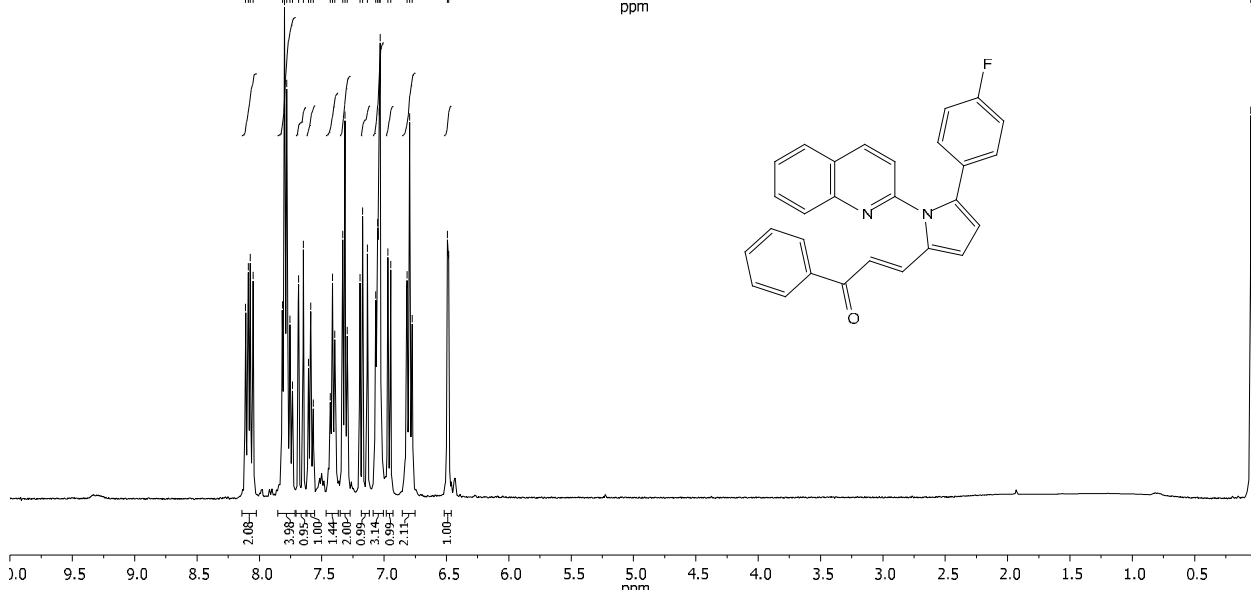
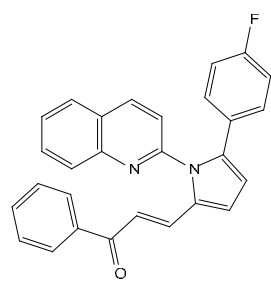
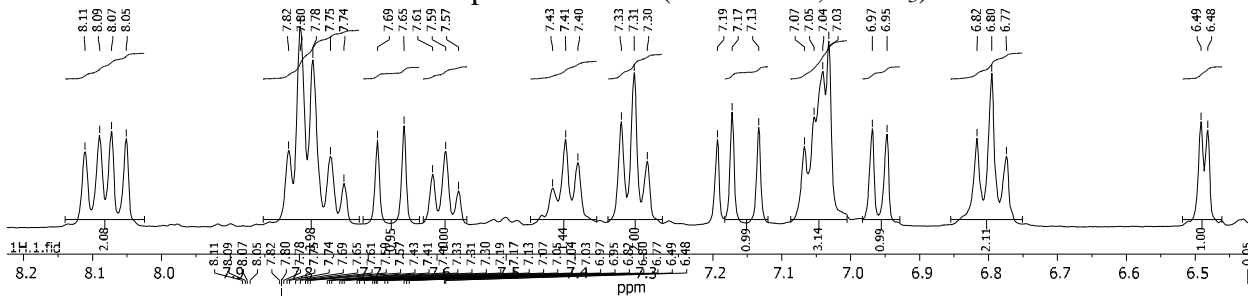
¹³C NMR spectrum of **3k** (100.62 MHz, CDCl₃)

19F_1.fid
F19

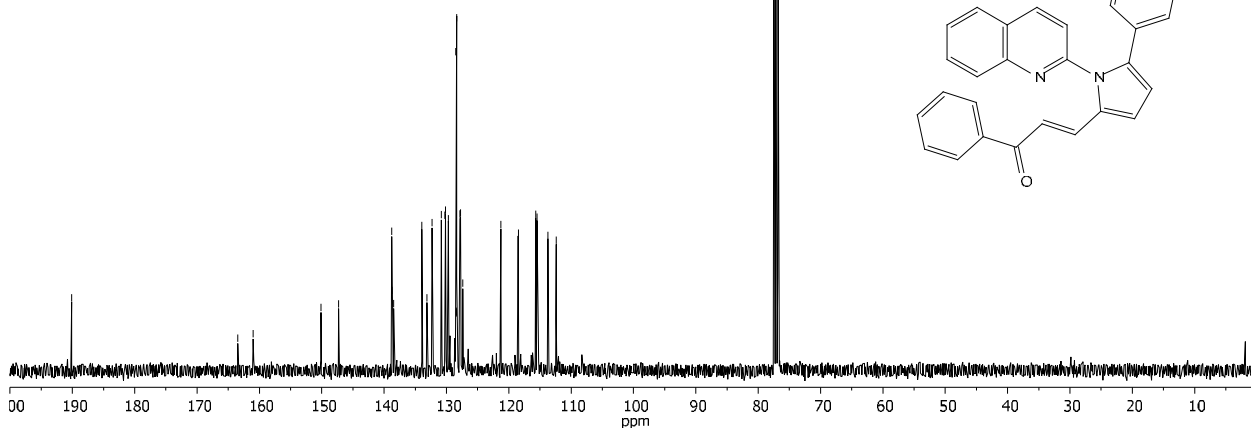
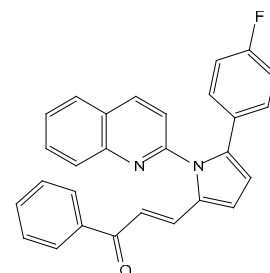
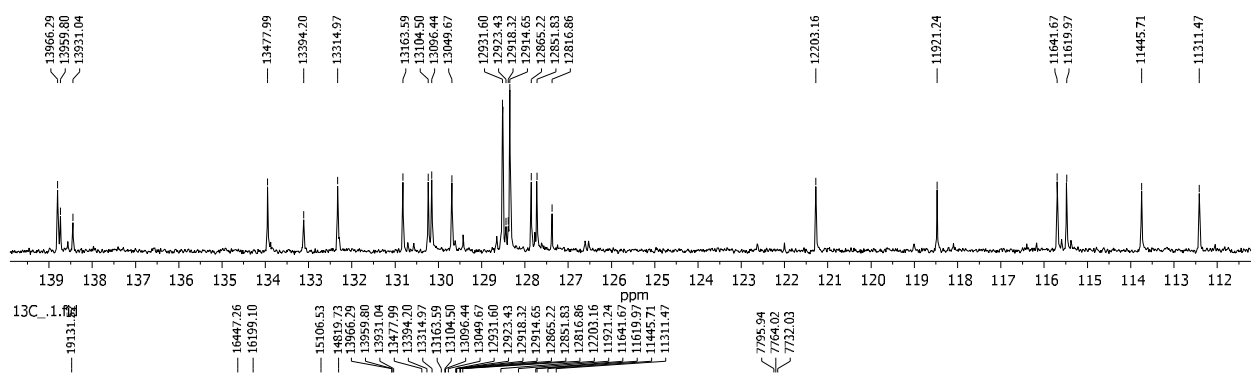
-111.89
-111.89
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-112.30



¹⁹F NMR spectrum of **3k** (376.5 MHz, CDCl₃)



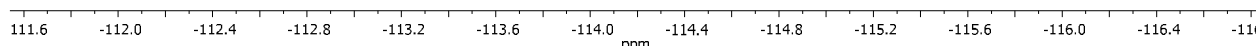
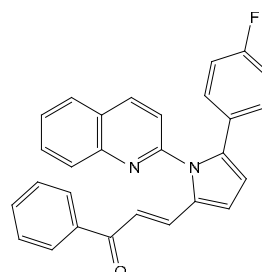
¹H NMR spectrum of **3l** (400.13 MHz, CDCl₃)



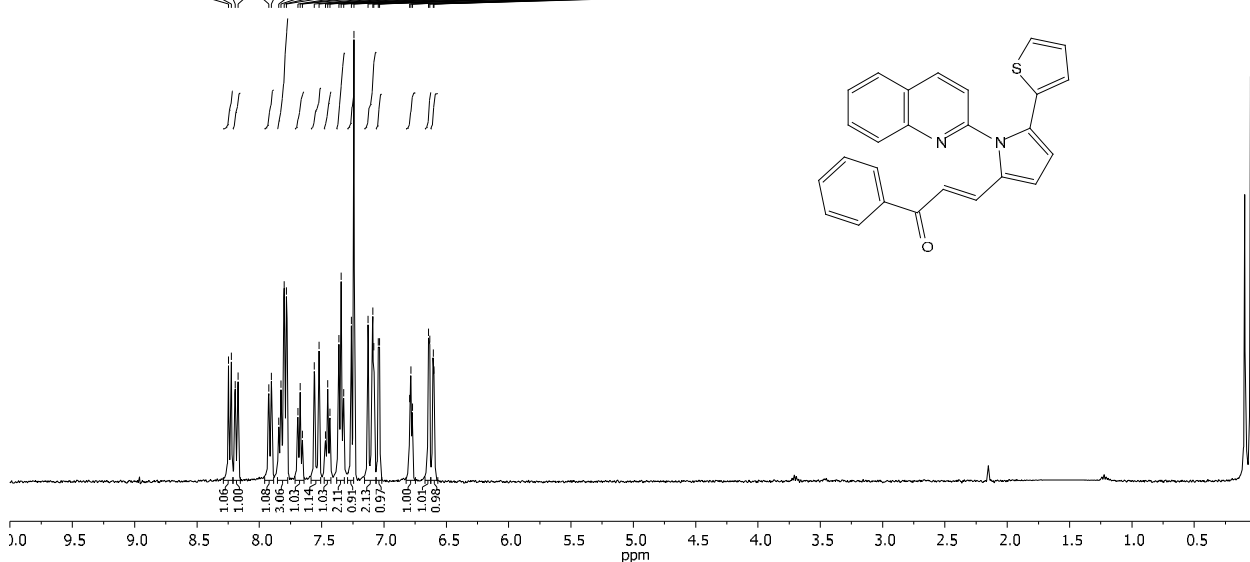
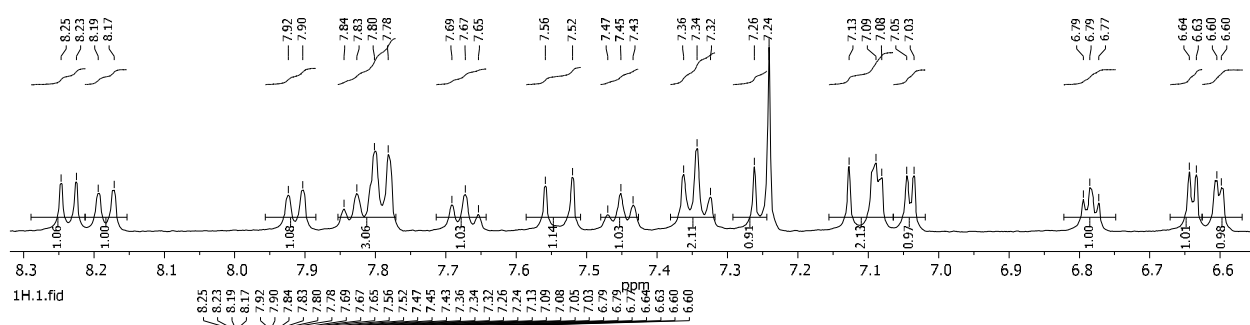
¹³C NMR spectrum of **31** (100.62 MHz, CDCl₃)

19F_1.fid
F19

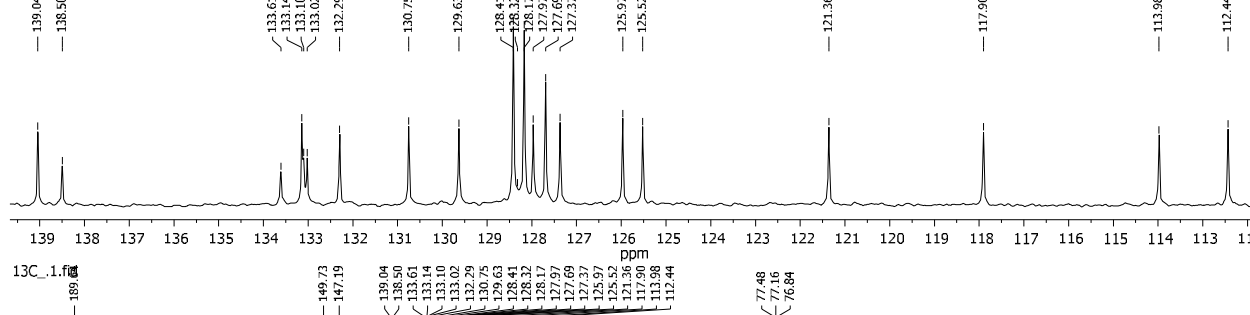
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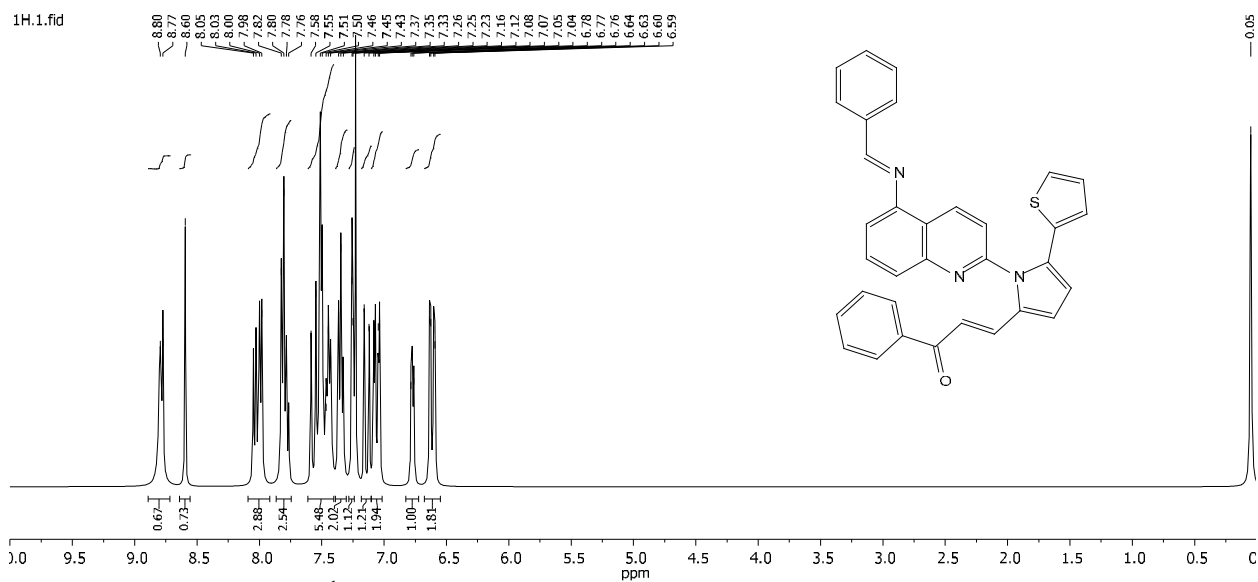
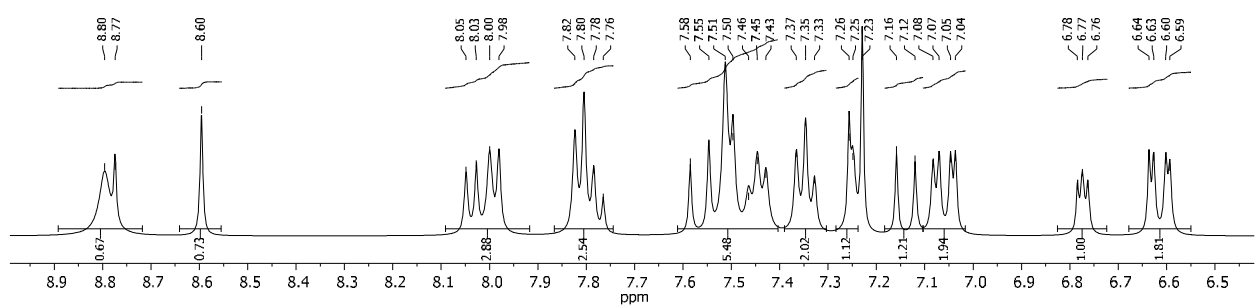
¹⁹F NMR spectrum of **31** (376.5 MHz, CDCl₃)



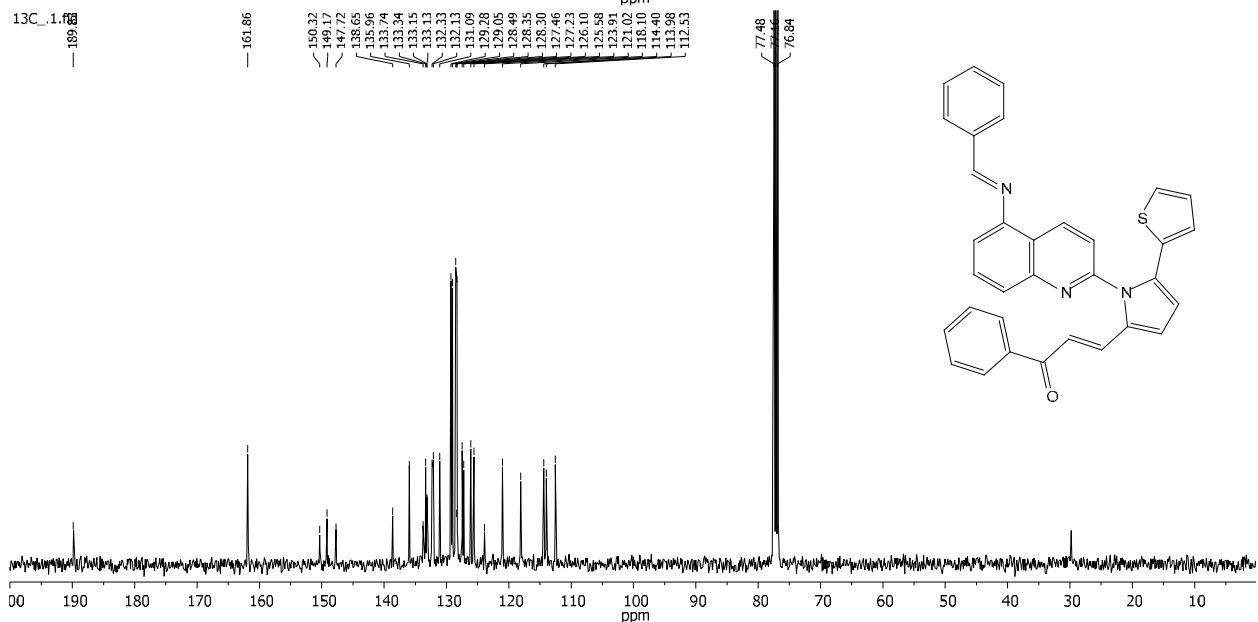
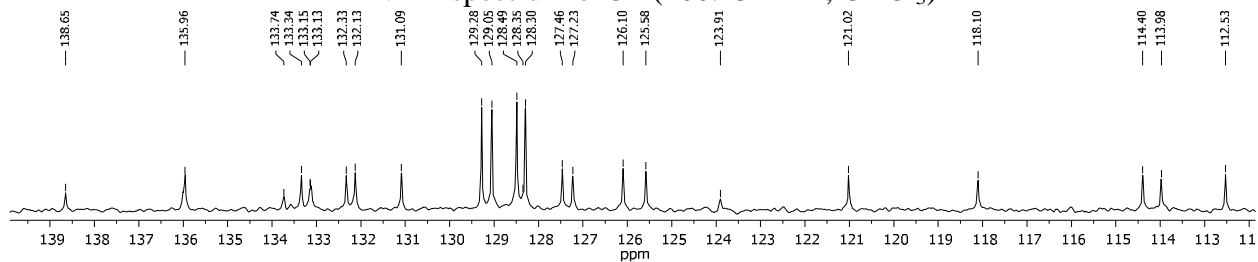
¹H NMR spectrum of **3m** (400.13 MHz, CDCl₃)



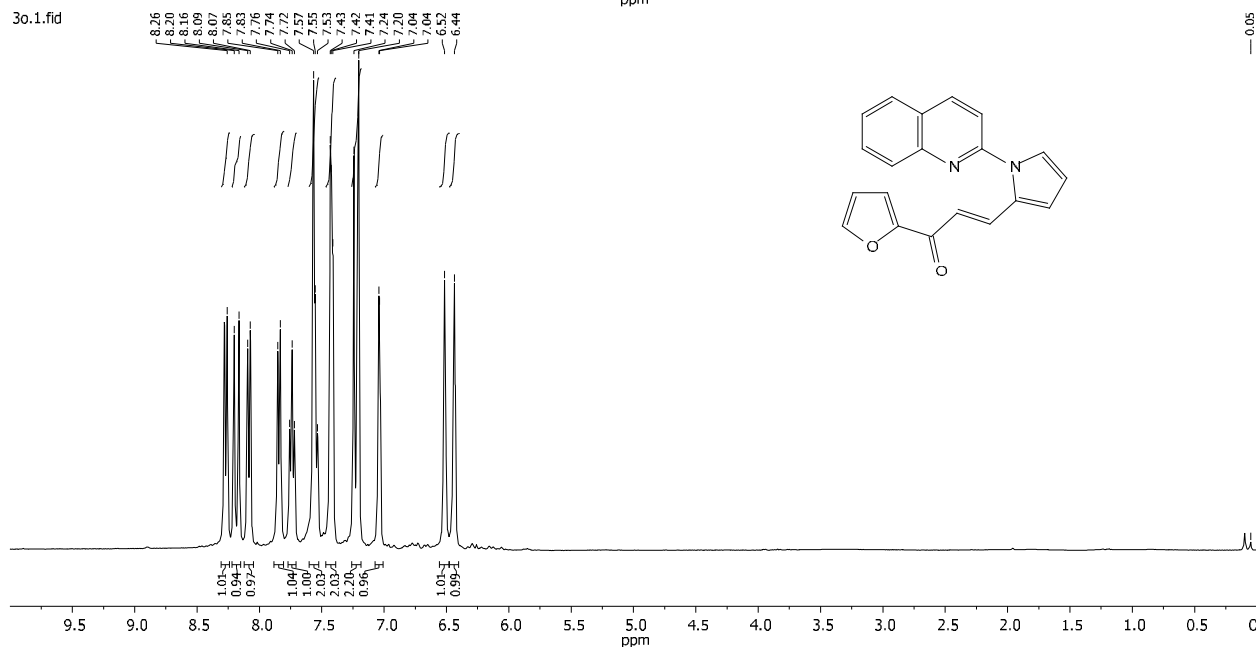
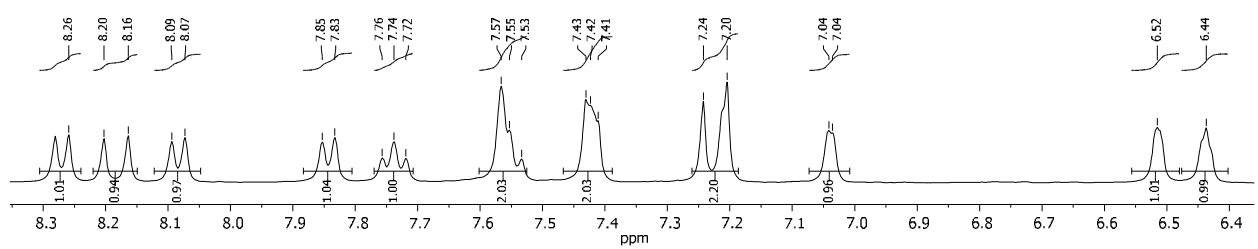
¹³C NMR spectrum of **3m** (100.62 MHz, CDCl₃)



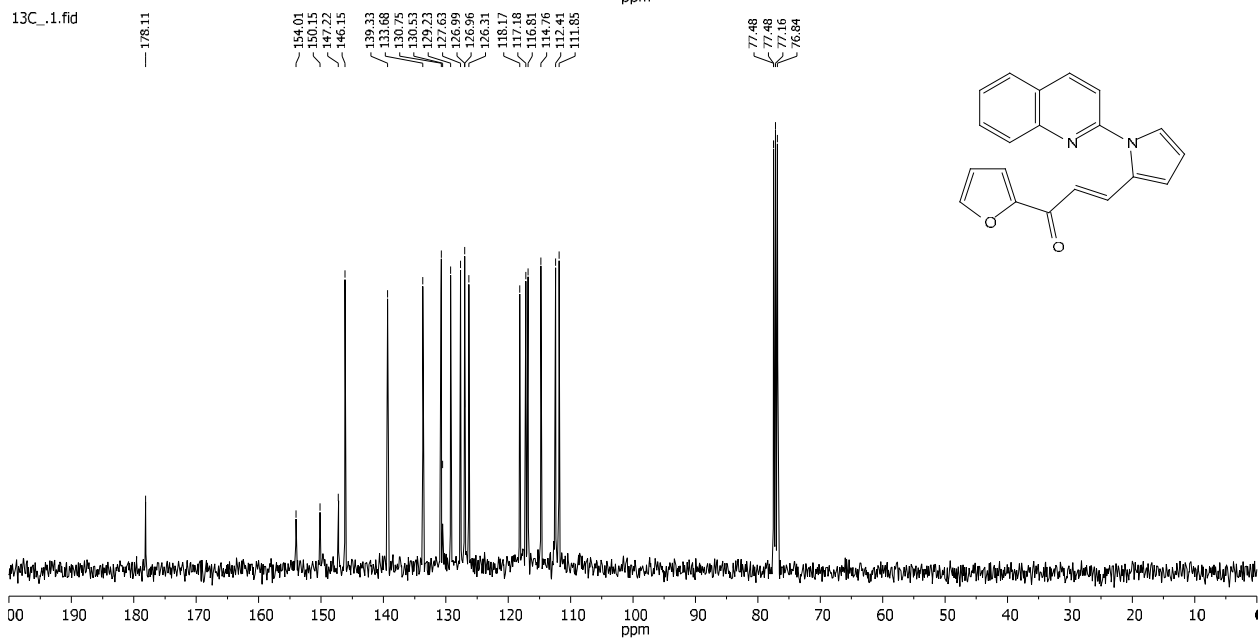
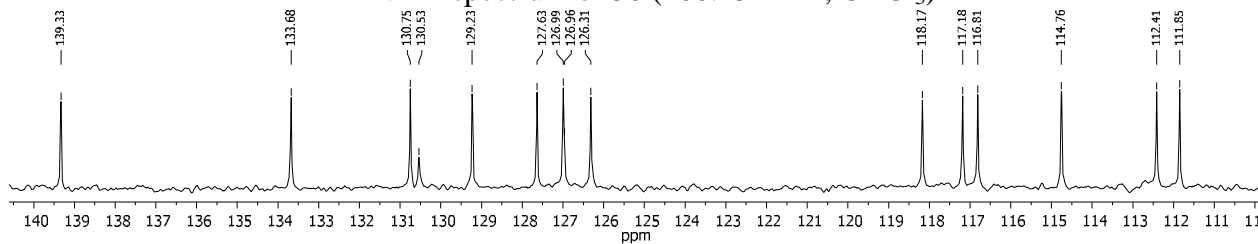
¹H NMR spectrum of **3n** (400.13 MHz, CDCl₃)



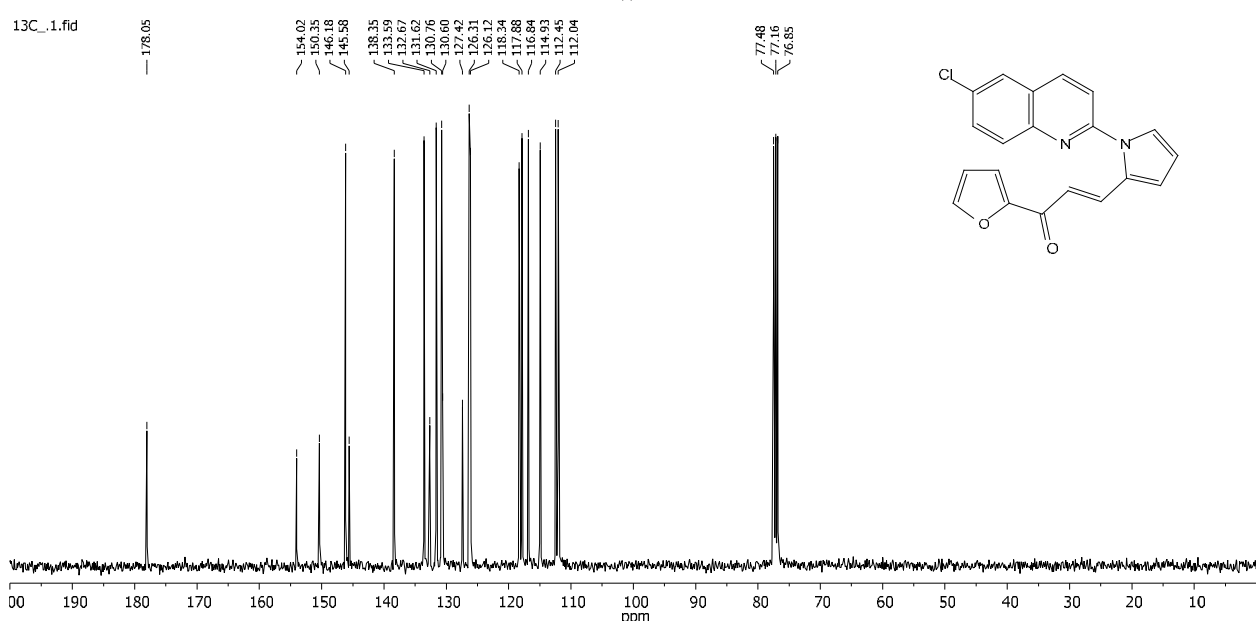
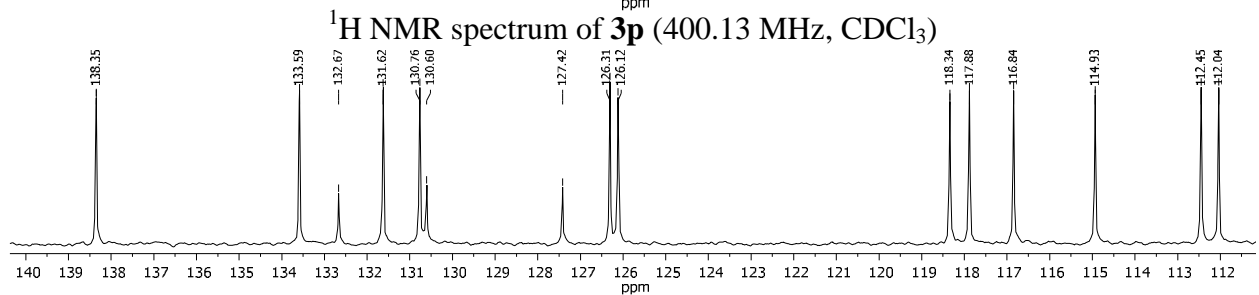
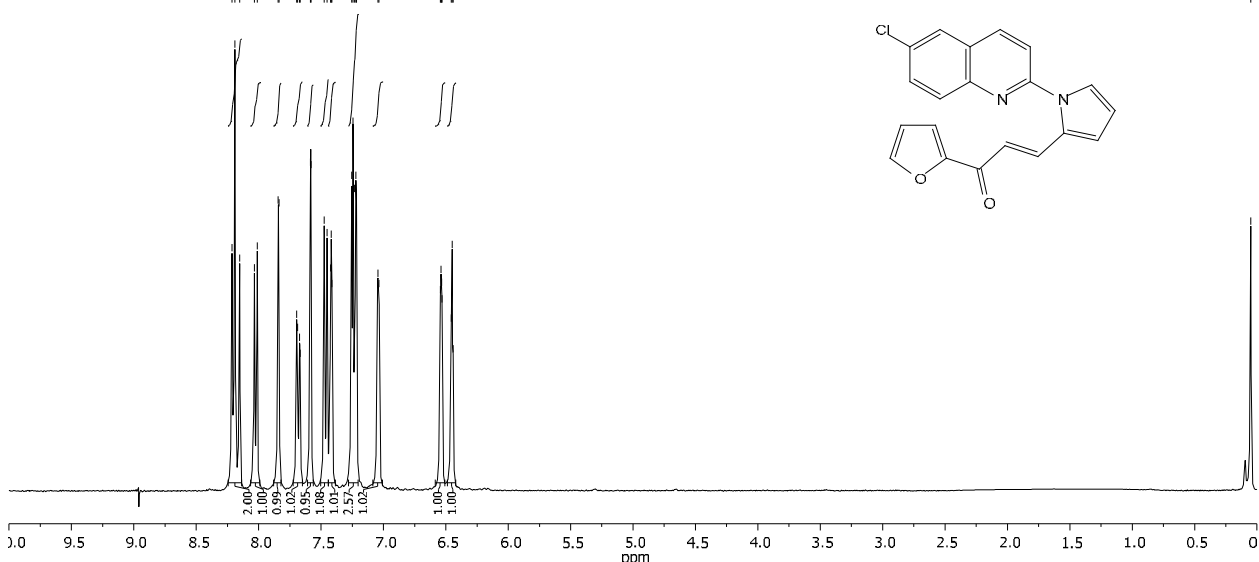
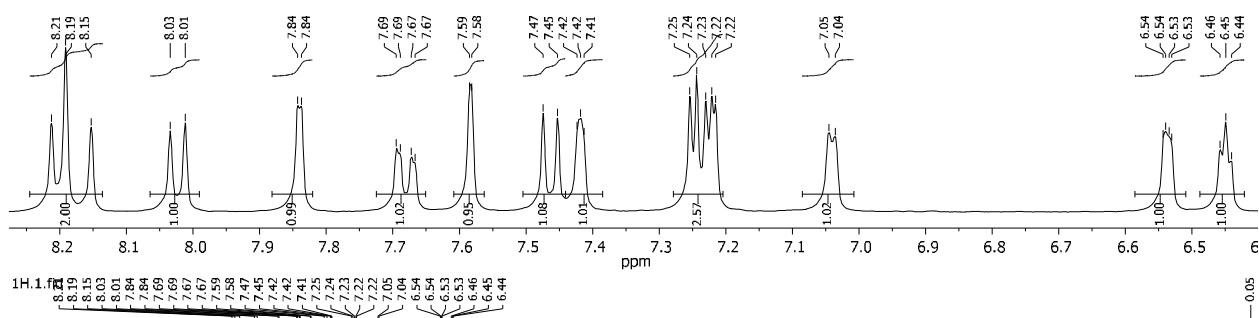
¹³C NMR spectrum of **3n** (100.62 MHz, CDCl₃)



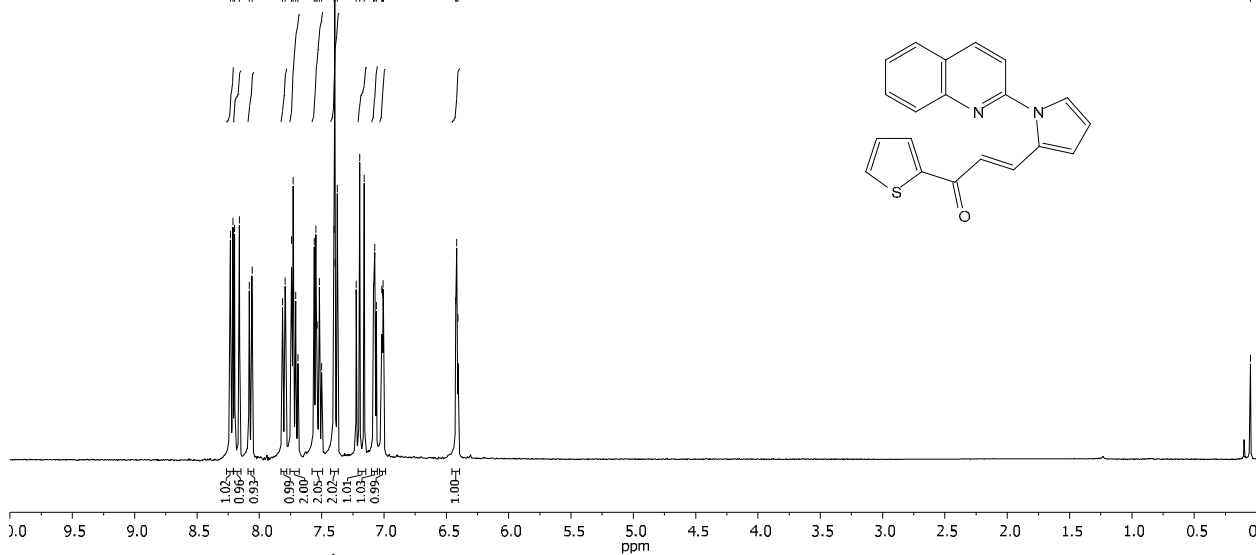
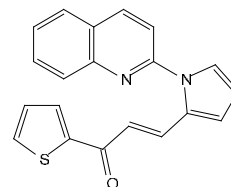
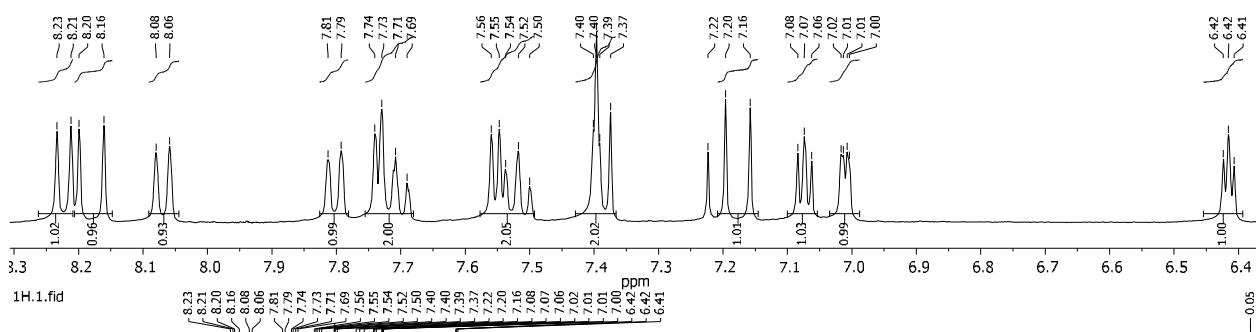
¹H NMR spectrum of **3o** (400.13 MHz, CDCl₃)



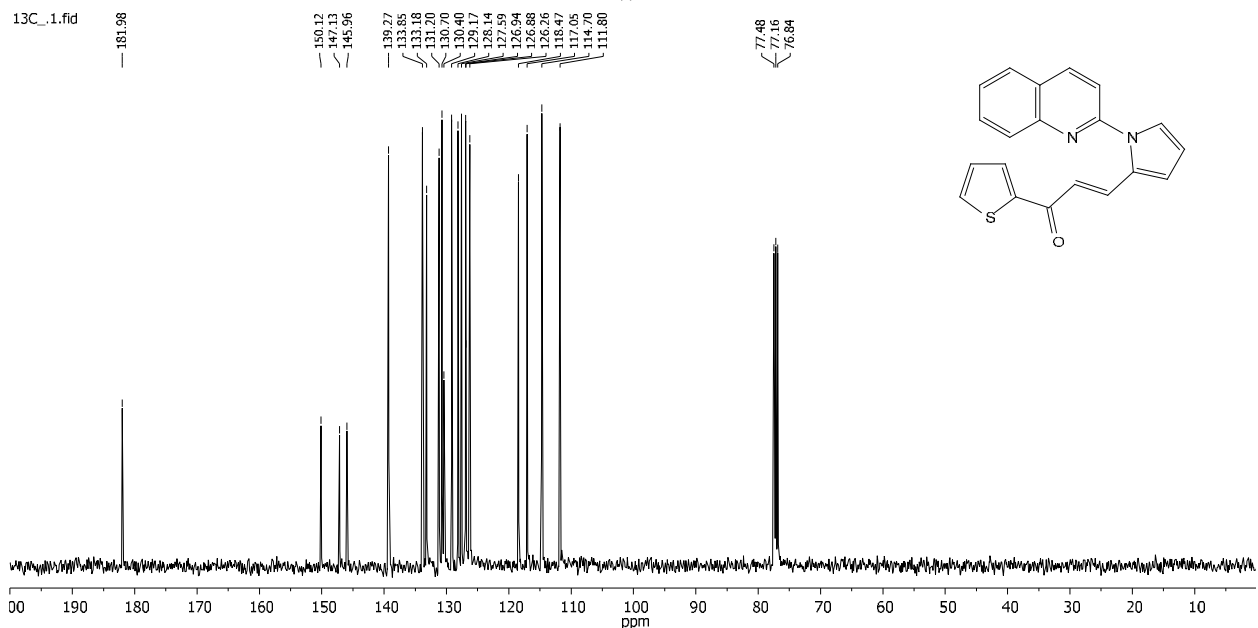
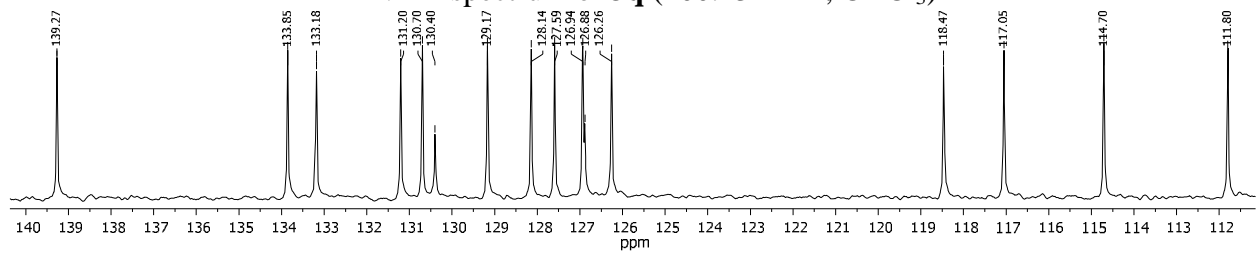
¹³C NMR spectrum of **3o** (100.62 MHz, CDCl₃)



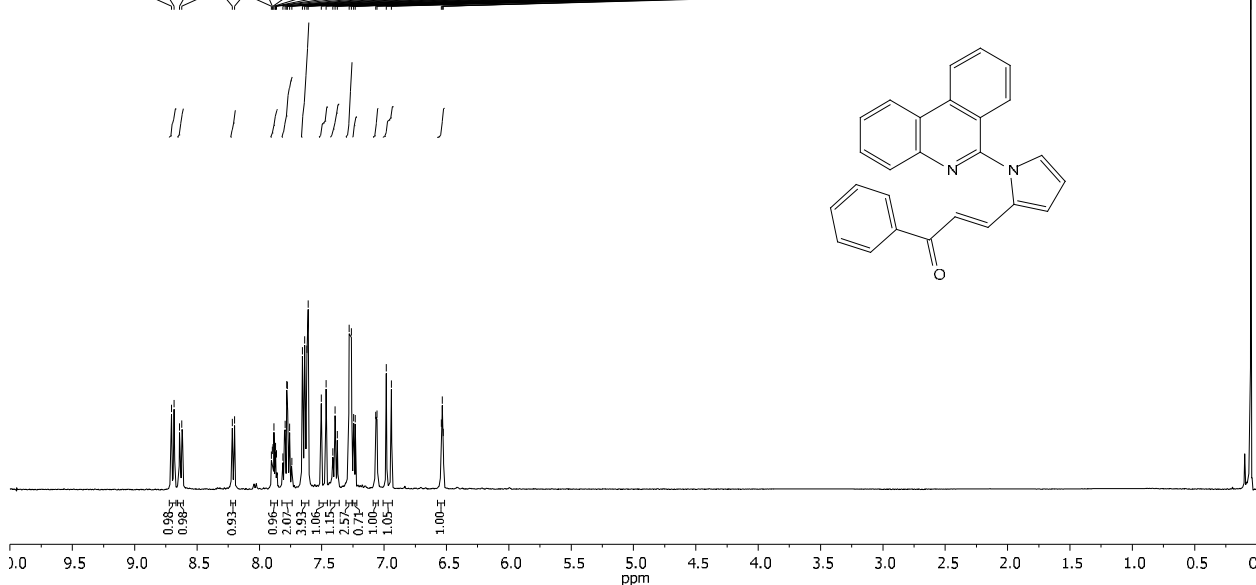
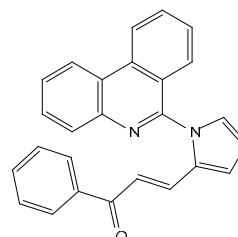
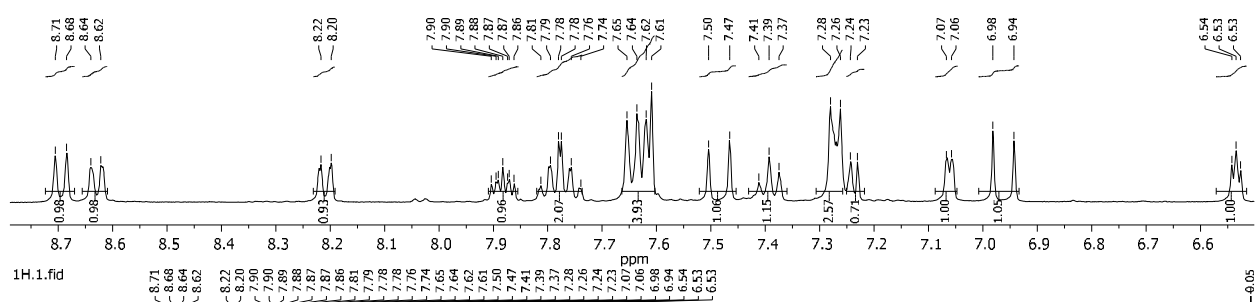
¹³C NMR spectrum of **3p** (100.62 MHz, CDCl₃)



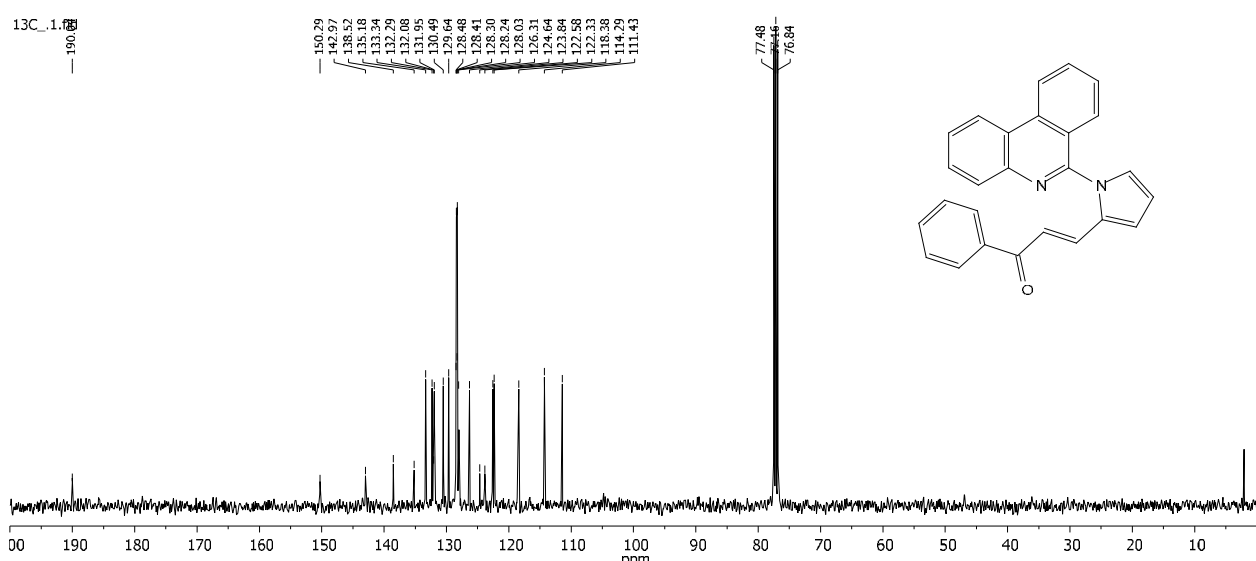
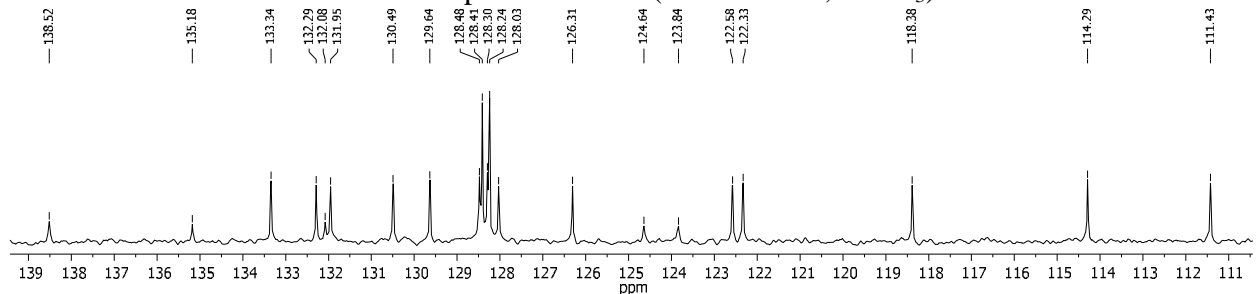
¹H NMR spectrum of **3q** (400.13 MHz, CDCl₃)



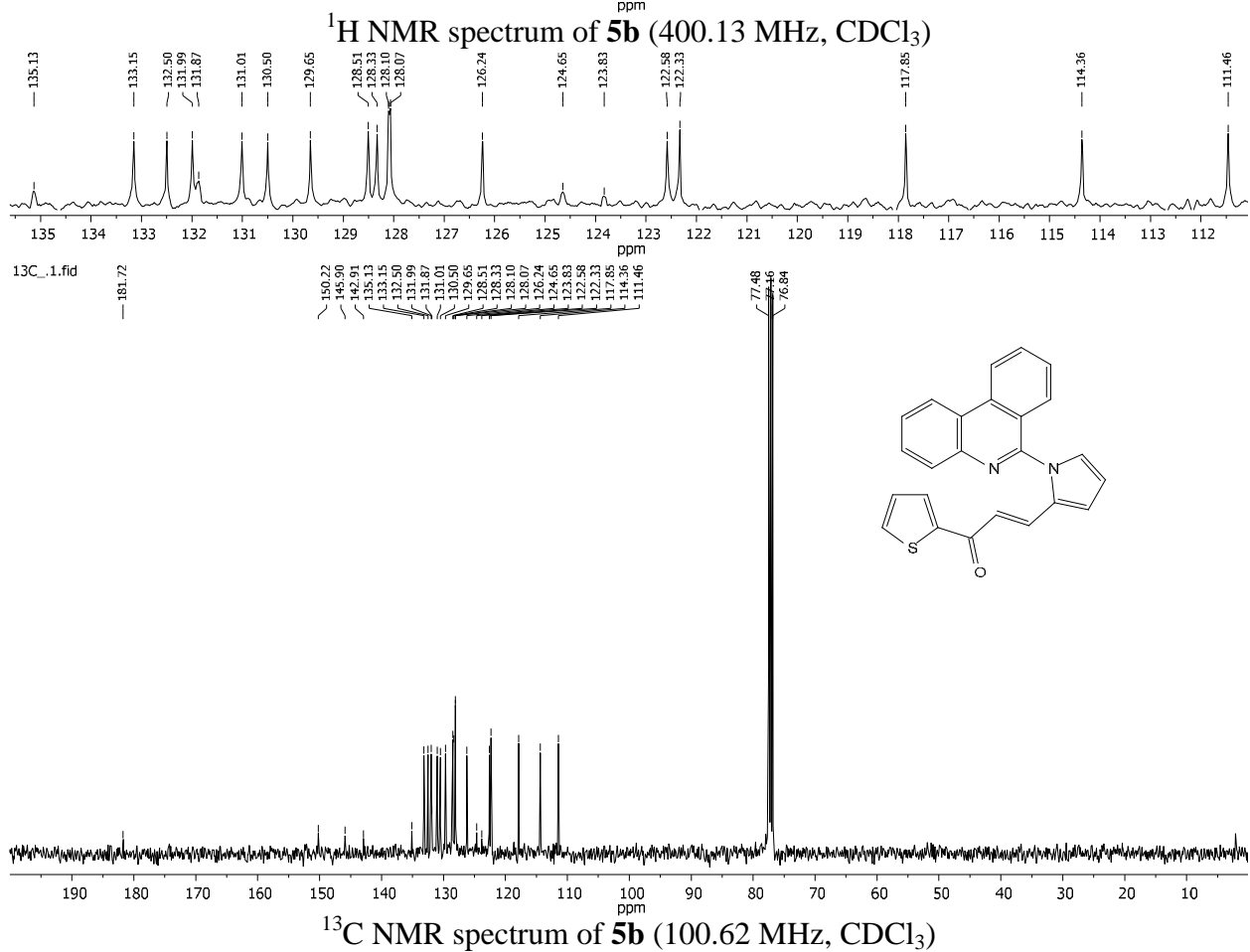
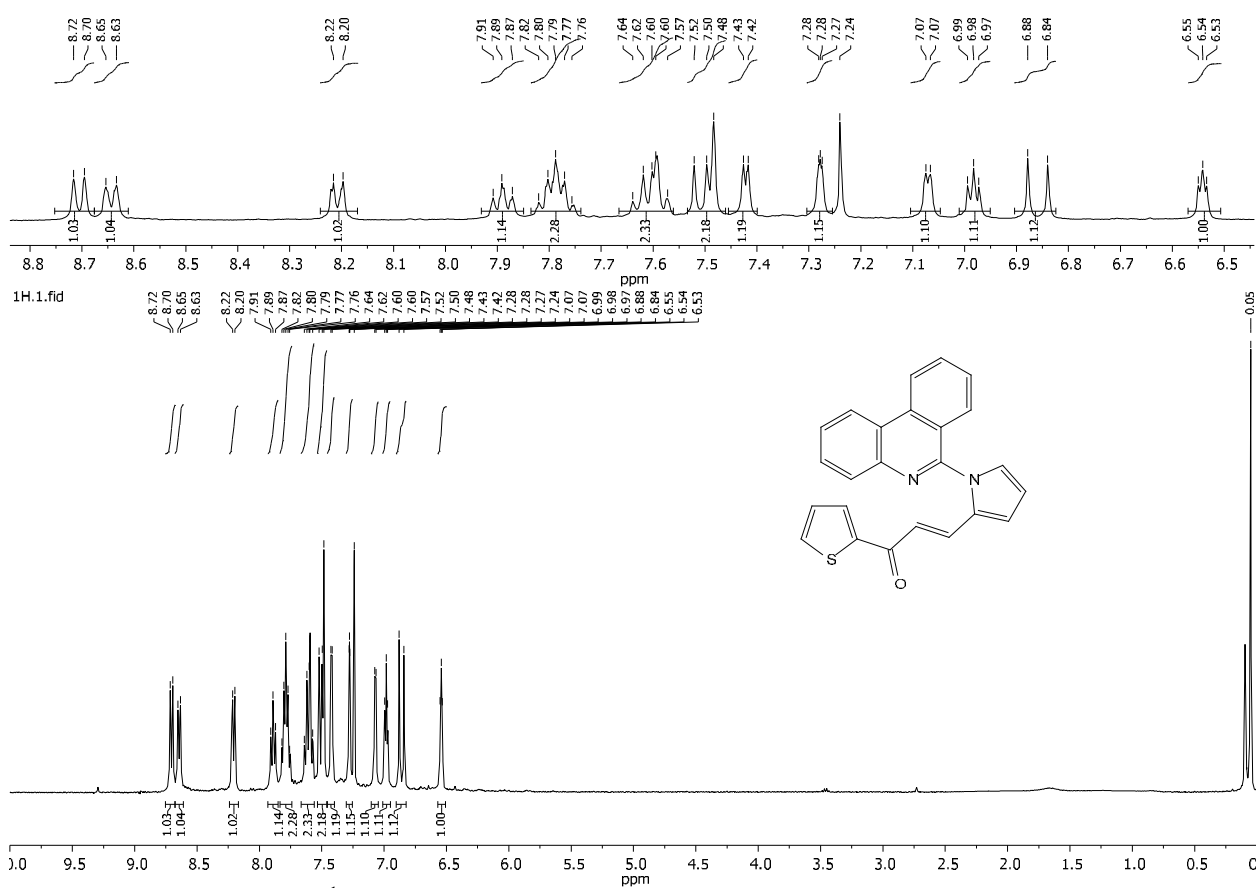
¹³C NMR spectrum of **3q** (100.62 MHz, CDCl₃)

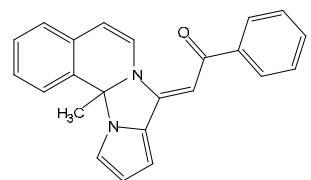
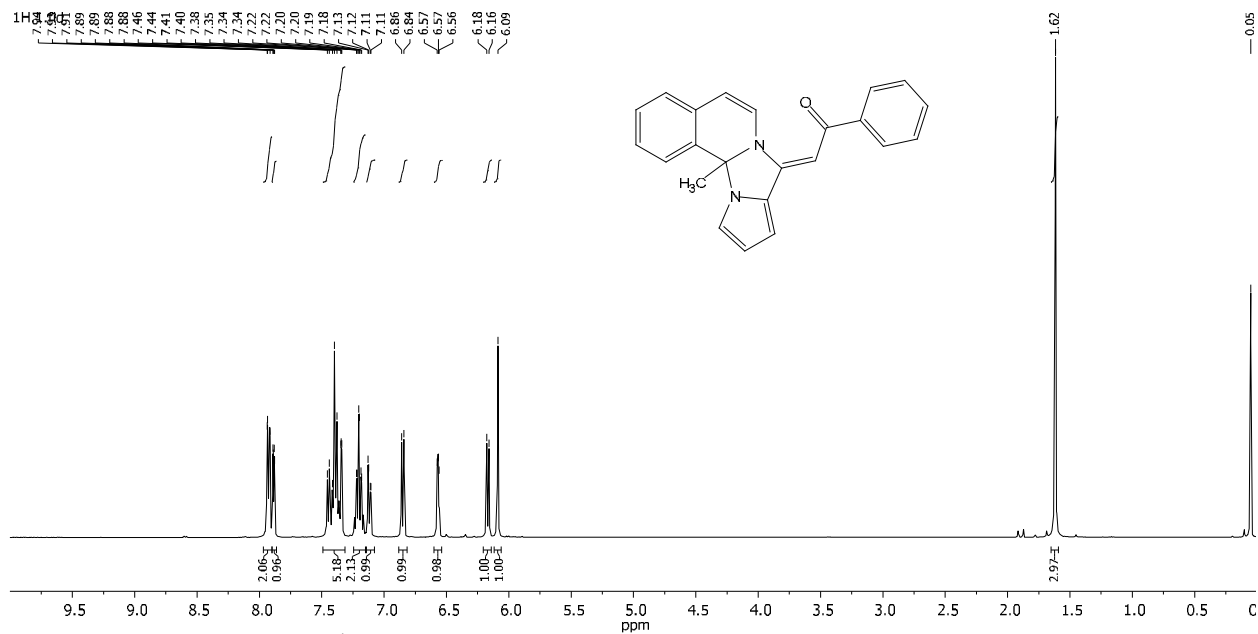
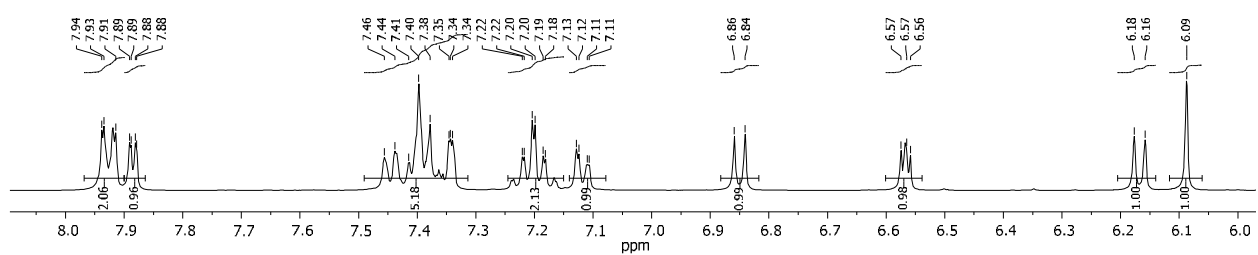


¹H NMR spectrum of **5a** (400.13 MHz, CDCl₃)

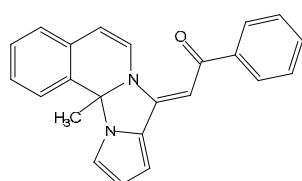
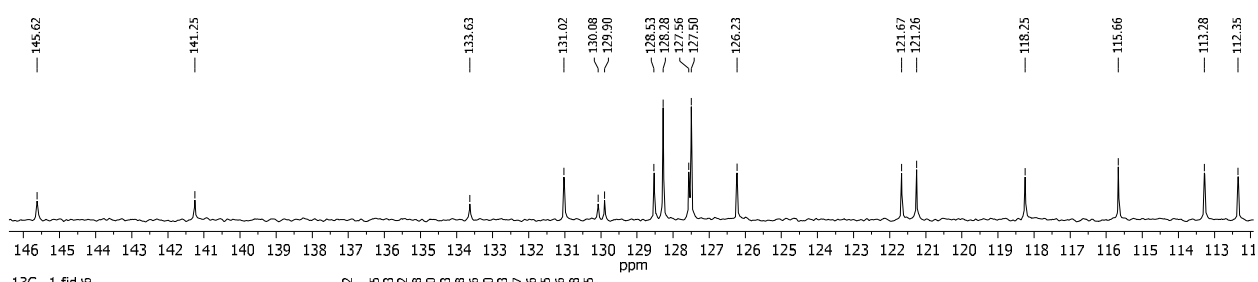


¹³C NMR spectrum of **5a** (100.62 MHz, CDCl₃)





¹H NMR spectrum of **7** (400.13 MHz, CDCl₃)



¹³C NMR spectrum of **7** (100.62 MHz, CDCl₃)

Cartesian coordinates, the number of imaginary frequencies, and computed total energies of target and optimized structures

1a; E_CEPA = -401.308470990223; E_M06-2X = -401.91455909; ZPVE_corr = 0.13701155; Q_corr = 0.00659387; H_corr = 0.00094421; G_corr = 0.10592643

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C	1.19442144841190	-0.21633479782309	0.08469117063627
C	0.35905415392670	-1.26633578777542	0.32957823974808
C	-1.03568039984908	-1.06691804529514	0.20552693590225
N	-1.58664151454423	0.07085906446131	-0.13253054397272
C	-0.76630859854837	1.13108419436217	-0.38120629198907
C	1.43971808545093	2.17244988786518	-0.55500073663472
C	0.85449141961562	3.35606841387406	-0.90863561964473
C	-0.55328922724267	3.45355073645937	-1.00667441712340
C	-1.34587786819513	2.36942236924393	-0.74962817898338
H	2.26965337374412	-0.31978220673718	0.16642035627085
H	0.73716011010626	-2.23813732785174	0.61349493599751
H	-1.70953647960749	-1.89526577475268	0.39782690296006
H	2.51645904775821	2.08539437833860	-0.47687476452914
H	1.46539968745302	4.22447334715677	-1.11530857462409
H	-1.00267533446669	4.39677093997328	-1.28775200205220
H	-2.42413579999832	2.42835743847124	-0.82024401853638

2a; E_CEPA = -629.785271805542; E_M06-2X = -630.70908612; ZPVE_corr = 0.18547628; Q_corr = 0.01211979; H_corr = 0.00094421; G_corr = 0.14707517

C	-0.05392629245082	0.03117960327025	-0.48264970448946
C	-1.30302880762199	-0.05082299264435	0.13322134668067
C	1.10201053629449	0.08547328407511	0.29345853050053
C	-1.39300878030704	-0.07742845464764	1.51466896267287
C	1.00921396961881	0.05710264577408	1.67771920481877
C	-0.23639988764714	-0.02366779159707	2.28756280527950
H	-2.19187646996308	-0.09177096202083	-0.48124103287746
H	2.07083728387584	0.14901138035566	-0.18456530419659
H	-2.36136719064688	-0.13999876328636	1.99231527210471
H	1.90687463415532	0.09830709024273	2.27941787863003
H	-0.30806354663333	-0.04501284939238	3.36701015321574
C	0.00502934610676	0.05868923906571	-1.96989494532729
O	-0.99591443736194	-0.00923553963650	-2.66131135787461
C	1.30829361175287	0.17253724128566	-2.57827990465629
C	2.38891194429161	0.26736127356471	-3.11082169256241
C	3.64341062698869	0.37879119092900	-3.73280732960045
C	3.97249462687903	0.43001727389802	-5.07956183946044
H	3.26489885196275	0.38789899515352	-5.89049020942016
C	5.37197410730727	0.54555549019219	-5.16313858532450
H	5.96438674007654	0.61046677186852	-6.05977880277429
C	5.85981034960450	0.56097638369435	-3.86989480223755
H	6.86834152469448	0.63597844213907	-3.50059582210882
N	4.81526666074485	0.46062300785328	-3.01934394426803
H	4.87740860827835	0.44863289986323	-2.01331389672446

A'; E_CEPA = -1031.108381523104; E_M06-2X = -1032.63635298; ZPVE_corr = 0.32351836; Q_corr = 0.02041716; H_corr = 0.00094421; G_corr = 0.27632199

C	1.89059825500642	-4.68229453838123	-3.05379460305038
C	0.75278569399533	-5.24103269695193	-2.47131931094559
C	2.50358686459864	-5.31645532391931	-4.13277088970941
C	0.23822577497375	-6.42933156353847	-2.96303777658487
C	1.97514088566409	-6.49715418692753	-4.63460927833520
C	0.84755298078458	-7.05640657589541	-4.04684600608347
H	0.28805347448517	-4.73987508365055	-1.63312638140616
H	3.38684987344834	-4.88231377168194	-4.58351340616768
H	-0.63753388673323	-6.86924885165953	-2.50532366427891
H	2.45073999589964	-6.98464465454736	-5.47651980282596
H	0.44217392779275	-7.98322634527978	-4.43145523214388
C	2.41778931332062	-3.39864603692181	-2.51217826901073
O	1.77052653475136	-2.69768308848604	-1.75439461631112
C	3.74835379877884	-3.02713508855676	-2.92384955906764
C	4.88114689617968	-2.76492975274010	-3.25453100747021
C	6.20200267914566	-2.50308028421584	-3.65577822742926
C	6.96459897249261	-1.34582170224835	-3.57413610039248
H	6.63022727269327	-0.40909497032275	-3.16054732564587
C	8.22007977741688	-1.64012511702914	-4.13509676122577
H	9.05636230037515	-0.96978298046260	-4.23910881857038
C	8.18835866332637	-2.96503889943442	-4.53604653100786
H	8.94778955247011	-3.57277311281060	-4.99842682890717
N	6.97143595497303	-3.47289818720733	-4.25201722554619
H	6.65817844796037	-4.44252466056714	-4.36990080677855
C	4.65890279870065	-8.25315830534582	-3.94235353378574
C	4.51470264718422	-8.20935691621147	-2.53645011188652
C	4.99345849784001	-7.13321525743207	-1.84760485799277
C	5.63487790124166	-6.10041923774484	-2.56783256394958
N	5.78987751315201	-6.10629121105299	-3.86755310618263
C	5.30066788154659	-7.16217949990249	-4.57671378531884
C	4.15891632158450	-9.31628057056688	-4.73109026046124
C	4.28353829603047	-9.28364631077120	-6.09240212928528
C	4.91691048391647	-8.18852713469303	-6.72462988168874
C	5.41833377774675	-7.15164214843385	-5.98630060973134
H	4.01870970689128	-9.02818155791143	-2.02937425730314
H	4.89844261304820	-7.05638515654811	-0.77402171486982
H	6.03153235461134	-5.24157018216983	-2.03493841601168
H	3.66872201833923	-10.14543769548470	-4.23586499714899
H	3.89445869721932	-10.09380540158636	-6.69421890375684
H	5.00296242161172	-8.17479356182092	-7.80300097216248
H	5.90529512753541	-6.30598453788720	-6.45474526356903

TS_A-A; E_CEPA = -1031.065811788683; E_M06-2X = -1032.59545579; ZPVE_corr = 0.32296133; Q_corr = 0.01956280; H_corr = 0.00094421; G_corr = 0.27692922; -354.71 cm⁻¹ ***imaginary mode***

C	1.86857102292916	-5.09682422557767	-3.66833862702672
C	1.14817369941077	-6.23644369462444	-3.31822888737300
C	1.77667841433783	-4.59326298271423	-4.96434166786653
C	0.36013815675880	-6.87959226877352	-4.26174949793917
C	0.97324782560626	-5.22526449667511	-5.90208963396553
C	0.27161079908994	-6.37444610802739	-5.55449415476190
H	1.22937158979625	-6.62098541608523	-2.31008351185260

H	2.33750515596637	-3.70730359356336	-5.23398356601588
H	-0.18282596132858	-7.77576365609527	-3.99174927265174
H	0.89853140222617	-4.82689449896244	-6.90524935795745
H	-0.34493575627726	-6.87489137682578	-6.28965498180812
C	2.77883126870072	-4.48333591195131	-2.64848585175151
O	2.55380359928084	-4.62455061891103	-1.44439628193484
C	3.89856314166507	-3.77242708510939	-3.14906561282072
C	5.11307308422805	-3.92741454489180	-3.42838471818525
C	6.31836629851235	-3.24766787602634	-3.82621636270908
C	6.63815922625614	-1.91048062238877	-3.69366191943869
H	6.02064224104003	-1.17162309525966	-3.21081934449074
C	7.89955724784360	-1.71750121782257	-4.30702732151189
H	8.44914680844404	-0.79404734225926	-4.37944169313427
C	8.31090663857490	-2.93988235750234	-4.78667055600018
H	9.20946269517603	-3.23138020024486	-5.30250412368288
N	7.34795993999477	-3.85378585384709	-4.49099860905743
H	7.38199766534800	-4.83415063096224	-4.72085172848623
C	5.05750707766728	-8.02430608848901	-3.11849794648980
C	5.71115134430766	-8.18501352223017	-1.87506886210823
C	6.34921696972676	-7.12331738775530	-1.29942525497032
C	6.31214046925634	-5.87929254744749	-1.95556900832891
N	5.70778709797197	-5.70560557798248	-3.10521283870794
C	5.08456077608889	-6.74800697972760	-3.72930982062773
C	4.39251488372087	-9.08643978233935	-3.77622823116637
C	3.79528856667898	-8.87913664764432	-4.98805245542316
C	3.84444205734809	-7.60601330693480	-5.59979064324922
C	4.47455566163269	-6.55769402764453	-4.98827875697090
H	5.69750270062922	-9.15568587226850	-1.39523171585062
H	6.86295112407713	-7.20954731253696	-0.35353037458084
H	6.77647172121335	-5.00181830225516	-1.51889664105661
H	4.37293103301308	-10.05934530551593	-3.30186767676167
H	3.28563018026432	-9.69094815629478	-5.48903220550417
H	3.37242966813170	-7.45916004248451	-6.56207478350199
H	4.50986824069101	-5.57832716334750	-5.44541654627884

A; E_CEPA = -1031.084765757220; E_M06-2X = -1032.61324088; ZPVE_corr = 0.32543172; Q_corr = 0.01943017; H_corr = 0.00094421; G_corr = 0.27966242

C	2.14890597967868	-5.24594939169563	-3.56053360713985
C	1.56949130654930	-6.45490412565719	-3.17764522654047
C	1.97466698529796	-4.78945436508265	-4.86680805789916
C	0.84531571202273	-7.20749760484340	-4.09193685996355
C	1.23493197771026	-5.53293932029153	-5.77628009698183
C	0.67606772492906	-6.74715102775891	-5.39336601749350
H	1.70827952853700	-6.80432945456062	-2.16289242303367
H	2.41765963411307	-3.84823036291739	-5.16480513887028
H	0.41302529814250	-8.15280777614979	-3.79104946707997
H	1.09580807954996	-5.16693853856857	-6.78505942203741
H	0.10730283185218	-7.33087402310296	-6.10517780901957
C	3.01604014763255	-4.52282895417824	-2.56668979363940
O	2.76013536772991	-4.60943244189342	-1.35354927281043
C	4.08082123123825	-3.76815021478576	-3.10926006069154
C	5.31768083109393	-4.18265389946089	-3.28596471811074

C	6.45843314942325	-3.47749452355252	-3.85668944574705
C	7.76760808856237	-3.86775512365865	-4.06053385458810
H	8.18573899550815	-4.82744282158883	-3.80220889788689
C	8.44220140006476	-2.77480988148108	-4.66778279624014
H	9.47729189158884	-2.73640047599186	-4.96351009941317
C	7.52569699094090	-1.76157693988551	-4.81263485043984
H	7.62511685321297	-0.77132464532903	-5.22277015956430
N	6.33254033686096	-2.20119950098787	-4.31949482658137
H	5.47044768588845	-1.67965751844303	-4.28777353518604
C	5.70255515207470	-7.93843945445888	-3.23502202553719
C	6.20263164299619	-8.10307158271709	-1.92628144381697
C	6.44007097868282	-7.01064800387870	-1.13814810104280
C	6.16737134666320	-5.74066245032860	-1.65003538319189
N	5.69440683335908	-5.56766569455334	-2.87304038018251
C	5.45523236671318	-6.63180604931548	-3.71386259700794
C	5.43491423500283	-9.03940356117311	-4.08295934223641
C	4.94856313240339	-8.83527073151452	-5.34233942137255
C	4.71715509381267	-7.52259805565612	-5.80929922290448
C	4.96395677009581	-6.43289773919183	-5.01873891849648
H	6.39181082885224	-9.10422231794226	-1.56016060608400
H	6.82246157758976	-7.09843862239163	-0.13294942389178
H	6.32128122515355	-4.83953374829741	-1.07313623596912
H	5.62307649199600	-10.03649182242763	-3.70703466782405
H	4.74004250033702	-9.67569674332942	-5.98962140179033
H	4.33594009682665	-7.37400384928364	-6.81061850505902
H	4.77760963131275	-5.43093588267473	-5.37568184763405

A-H₂O; E_CEPA = -1107.471633065241; E_M06-2X = -1109.06363958; ZPVE_corr = 0.34933435; Q_corr = 0.02250826; H_corr = 0.00094421; G_corr = 0.29984013

C	1.79143200673535	-5.57784299656403	-4.42498956529962
C	0.84389080333335	-6.59450308716986	-4.31991453207632
C	1.59234572145690	-4.38492269195537	-3.73027361588742
C	-0.28410838118675	-6.42423762058999	-3.53059083905383
C	0.46282313760266	-4.21241432340454	-2.94197913575094
C	-0.47630741150085	-5.23216182301197	-2.84018753562590
H	1.00730573235540	-7.51657925288034	-4.86103734097882
H	2.32146444226521	-3.58886829479297	-3.81495108460205
H	-1.01368008901917	-7.21929572898709	-3.45123883767443
H	0.31381999105497	-3.28270023598451	-2.40916535187255
H	-1.35672901647506	-5.09788088233447	-2.22553728832144
C	3.02573990186457	-5.81421707620348	-5.25582923264188
O	3.10539404007519	-6.84010893148924	-5.94236071720551
C	6.22358366971101	-7.91820017425388	-2.80663501770157
C	5.61386798473185	-7.74164004126676	-1.54775904200981
C	4.89103596132357	-6.60977831925730	-1.28534079795405
C	4.77135248795305	-5.64347424556354	-2.28427469988978
N	5.32696272425382	-5.79828697039135	-3.47551683703830
C	6.06963402903198	-6.91385598988954	-3.78947975969350
C	6.98421699349895	-9.07015068519465	-3.11972976268756
C	7.56050098357307	-9.19944623744283	-4.35005406156184
C	7.39793096376364	-8.18570911807958	-5.31984734661572
C	6.66617106274344	-7.05980211449572	-5.05697819199295

H	5.73015716798300	-8.51324193212832	-0.79723977767331
H	4.41517995888855	-6.43899281918971	-0.33207624578694
H	4.22119089830538	-4.72441753050696	-2.13696394537510
H	7.09353635226571	-9.83573650897925	-2.36309568922539
H	8.14260918336463	-10.07797395545169	-4.59085831627293
H	7.85917814141751	-8.30223065338105	-6.29101088043929
H	6.53673561761166	-6.29128428679756	-5.80438714646416
C	4.01816850530862	-4.79036284705412	-5.26365860978196
C	5.09169211321555	-4.73997395575539	-4.49941078097507
C	6.16981331886461	-3.75624087761023	-4.47452709274814
C	7.30152085906358	-3.68529178138827	-3.68397488745174
H	7.57958486341086	-4.38992011459614	-2.91643484827356
C	8.01652643089001	-2.52416995020488	-4.07593322218133
H	8.94647084984515	-2.16708029300227	-3.66616268942093
C	7.29906629929834	-1.93087958698465	-5.08708253115464
H	7.48850677316980	-1.03633273306026	-5.65548496682707
N	6.18783700322807	-2.68441451102337	-5.32022959281818
H	5.46183625870406	-2.47733011444493	-5.99982505953423
O	3.75162902608019	-2.53158852642305	-7.04256897944650
H	3.15120399441098	-1.89689979090508	-6.64023955091995
H	3.70599985352671	-3.33873294490870	-6.46402622109310

TS_{A-B}; E_CEPA = -1031.045488866601; E_M06-2X = -1032.57600011; ZPVE_corr = 0.32057390; Q_corr = 0.01901752; H_corr = 0.00094421; G_corr = 0.27490545; -1646.12 cm⁻¹ ***imaginary mode***

C	1.91649795523639	-5.00879841611081	-3.49693201119649
C	0.72329109566903	-5.48962724708369	-2.95985539976642
C	2.07867620566051	-4.96423196866048	-4.88079485255644
C	-0.29490601894227	-5.92123337366730	-3.79568304108863
C	1.06062330632116	-5.39991390369505	-5.71821151370424
C	-0.12636466226119	-5.87788920675708	-5.17629228412554
H	0.60738325032766	-5.52089245974660	-1.88500473341381
H	3.00301391022997	-4.58705851455095	-5.30034670201317
H	-1.21970645731513	-6.29274030607833	-3.37477685058268
H	1.19207673135775	-5.36523011161221	-6.79138910680145
H	-0.92077570502546	-6.21623557577656	-5.82853408545213
C	3.01683674257417	-4.57869421471607	-2.57157150066788
O	2.87302974786629	-4.67745388952623	-1.35615081380985
C	4.20589186895083	-4.01211195069690	-3.16874085123762
C	5.39788518665890	-4.58000587287608	-3.27819097294597
C	6.41756070973042	-3.78270317878784	-3.97042064886044
C	7.77190758987574	-3.80941883662901	-4.24595345309743
H	8.46918408304713	-4.59683883941759	-4.00560846507704
C	8.04691022520499	-2.57503016460697	-4.89369065737335
H	9.00145948765018	-2.23859476916706	-5.26780377005803
C	6.84601174234463	-1.88078263639726	-4.96757626615934
H	6.64638675977670	-0.91237050929952	-5.39896581618275
N	5.85877248233331	-2.63059094566337	-4.41556949910715
H	4.67430096283484	-2.85847022856047	-3.91862099903727
C	6.24107722374591	-8.22295061500632	-3.22908661458924
C	6.41241555472631	-8.40041608811944	-1.84051856824638
C	6.23462081187915	-7.34908448493975	-0.98328495673221

C	5.90174658759151	-6.10132872175395	-1.50882561187754
N	5.74282670049875	-5.91451037339629	-2.81240369817044
C	5.88809199367118	-6.94585320842090	-3.71847396201910
C	6.39564157499504	-9.28753224176243	-4.14807208376346
C	6.19534710750150	-9.07831480128099	-5.48235408747558
C	5.82598000945608	-7.79925515605808	-5.95150570689495
C	5.67139615386040	-6.74278855137521	-5.09428889822377
H	6.68243333170694	-9.38060404779488	-1.46821622523485
H	6.35363290088184	-7.45060436032336	0.08419596533467
H	5.76533735101682	-5.22689371454602	-0.88974412192581
H	6.66881365846818	-10.26197310571498	-3.76520987556637
H	6.31143327245602	-9.89089888545775	-6.18578214543095
H	5.65919700168566	-7.64979885537340	-7.00948521137698
H	5.38399470875152	-5.76830489759212	-5.46047964449144

TS_{A-B}-H₂O; E_CEPA = -1107.461955422994; E_M06-2X = -1109.05358849;
 ZPVE_corr = 0.34486779; Q_corr = 0.02153297; H_corr = 0.00094421; G_corr =
 0.29674059; -1375.38 cm^{**}-1 ***imaginary mode***

C	1.92381967967042	-5.38570757709355	-3.70421154528987
C	0.99699232783029	-6.28844167069207	-3.18271609698355
C	1.85326900001754	-5.02522540638645	-5.04944863062586
C	0.01131049865042	-6.82370027848206	-3.99582366271599
C	0.86299185413425	-5.55972399937350	-5.86303899987889
C	-0.05665247385292	-6.45872086256355	-5.33738086453549
H	1.06453667603765	-6.56485928811535	-2.13921750793228
H	2.56720402215976	-4.32036903050081	-5.45624507079940
H	-0.70429116795735	-7.52546525778941	-3.58864082633703
H	0.80863935677159	-5.27478035387108	-6.90510366771446
H	-0.82755687285930	-6.87598751564320	-5.97186178361557
C	2.99678474261854	-4.84771473454489	-2.81036892740765
O	3.00243987626538	-5.11916304337110	-1.61650198343278
C	6.07454210210864	-7.97170736225715	-3.17586571974636
C	6.43825830855910	-8.02695924179244	-1.81425918440250
C	6.42674137219974	-6.89254037177481	-1.04941116114470
C	6.05021250373923	-5.68723036614116	-1.64161437618022
N	5.70832016890055	-5.61780148802356	-2.91860752188566
C	5.70070095445433	-6.72902683758602	-3.73435434162275
C	6.06693011138378	-9.12122387541810	-4.00073067116426
C	5.70195837638142	-9.02369793982364	-5.31279427195280
C	5.33030845077170	-7.77383506501373	-5.85390095137368
C	5.32549955932624	-6.63869719491397	-5.08841934123755
H	6.72409190244642	-8.98052085857501	-1.38843827530769
H	6.69638019699046	-6.90000623157919	-0.00476040992421
H	6.01779459065577	-4.75646834476154	-1.09363788264762
H	6.35386257349709	-10.06905736748983	-3.56477051374259
H	5.69454631428752	-9.90102543217037	-5.94422109425260
H	5.04291703459203	-7.70993536164998	-6.89456992050439
H	5.03720656839340	-5.68662144803598	-5.50939882167527
C	4.00023996332762	-3.96832420649927	-3.41458074138550
C	5.28285230915099	-4.31281717861643	-3.45152840053500
C	6.39360178256453	-3.56516486245886	-4.01683278097561
C	7.74411139103576	-3.86836607335795	-4.06763080275346

H	8.20910332648661	-4.75644453445450	-3.66954056990893
C	8.38127105807467	-2.79478907988272	-4.73385024216817
H	9.43238536249800	-2.69703489628009	-4.94809802747654
C	7.39765931583136	-1.88520052652508	-5.06275809472205
H	7.46422470413543	-0.93953598350042	-5.57420624428517
N	6.20291349432610	-2.35906927276850	-4.62754311996251
H	5.26018645525217	-1.91994930576373	-4.72238491449949
O	3.57558485958974	-1.72705646572928	-4.68181623922051
H	3.27094158730810	-1.04668345828124	-4.07524925495140
H	3.68210962024478	-2.83064399244787	-4.00030771912167

B; E_CEPA = -1031.109522422710; E_M06-2X = -1032.63979357; ZPVE_corr = 0.32560782; Q_corr = 0.01912034; H_corr = 0.00094421; G_corr = 0.27993926

C	1.58587811312790	-5.39164522586197	-4.00896839331337
C	0.57704776405790	-6.06362086671939	-3.31756010007266
C	1.24360021208692	-4.58071903255502	-5.09105921043348
C	-0.75010251741984	-5.91714921815178	-3.68900871660784
C	-0.08496396441695	-4.44640606765364	-5.47331249833957
C	-1.08354034896936	-5.10868015180267	-4.77083189201541
H	0.84843942920499	-6.69695447153454	-2.48407721127065
H	2.00820995241781	-4.06764655727403	-5.65789852937749
H	-1.52514825084768	-6.43385206698132	-3.13870129202114
H	-0.33849154676655	-3.82502225149229	-6.32171969004399
H	-2.11857087747732	-4.99764356556365	-5.06617452056409
C	3.00605910214139	-5.60940715506653	-3.56943279630818
O	3.27320603434645	-6.61370572096596	-2.90972052559213
C	3.97976827325466	-4.60281025793034	-3.94299213280442
C	5.31786579388718	-4.66593559309544	-3.70319957231343
C	6.30891244673560	-3.72317705813082	-4.04910392326517
C	7.70751318741252	-3.82255430757981	-3.82222798851511
H	8.22752220492213	-4.63543570182264	-3.33755800962592
C	8.25419605478591	-2.66815244638603	-4.35178908664941
H	9.29367657159148	-2.38073065190702	-4.37065510354963
C	7.15988007267177	-1.93095024971790	-4.87322559391150
H	7.20614944384141	-0.96862089001729	-5.36610988889985
N	5.99840585845711	-2.55198487177165	-4.69822261224329
C	6.62770486305859	-8.10025131165640	-3.02502317424438
C	6.74591585508852	-8.02592285145044	-1.62241104196454
C	6.42168264112215	-6.87173953323583	-0.96154945874940
C	5.96359413665123	-5.78344660028790	-1.70070856203044
N	5.84384357638128	-5.84184772817973	-3.01651184849386
C	6.16381981617354	-6.97059841859057	-3.73403275844514
C	6.96049667571313	-9.27089224530390	-3.74744425726516
C	6.83268581279683	-9.29957564842541	-5.10605528454330
C	6.36967008714280	-8.15904684634651	-5.79831696350397
C	6.03763380404590	-7.00842116036634	-5.13521690064505
H	7.09920155141733	-8.89445826842838	-1.08095216309657
H	6.50405983423833	-6.77924610548571	0.11013430589763
H	5.67507092514836	-4.84875184237247	-1.24053752735739
H	7.31551078137896	-10.13185971457230	-3.19657341209423
H	7.08670035777431	-10.19262589531961	-5.65966378738722
H	6.27589049549124	-8.19366597388763	-6.87514246705980

H 5.68596385975444 -6.14057129134169 -5.67334672793586
H 3.64434857157719 -3.71184985276700 -4.44959504134329

B-H₂O; E_CEPA = -1107.497577822291; E_M06-2X = -1109.09083463; ZPVE_corr = 0.34984966; Q_corr = 0.02229188; H_corr = 0.00094421; G_corr = 0.30082065

C 1.57437502634520 -5.41120400908069 -3.95764184815435
C 0.58215690301884 -6.18044750363856 -3.34757915727623
C 1.20795882095245 -4.46911887102403 -4.92045586363043
C -0.75094765301066 -6.00738927371790 -3.68250040741225
C -0.12783985946042 -4.30520921520829 -5.26427574423058
C -1.10868790120854 -5.06843629650287 -4.64466221920007
H 0.87218267361799 -6.91134438313816 -2.60542460157067
H 1.95286566895981 -3.86574454819256 -5.42229230343579
H -1.51195828714786 -6.60311071374957 -3.19632768373246
H -0.40120506015622 -3.57906618992648 -6.01812426778587
H -2.14880170639875 -4.93417035725078 -4.91103606405091
C 3.00029719477886 -5.66037341687275 -3.55540357360936
O 3.27541171666448 -6.68469537737165 -2.93468581807816
C 6.69128471497439 -8.12642436351143 -2.99233884192568
C 6.77591006217599 -8.05342598538484 -1.58730580581042
C 6.40294390385098 -6.91158282202468 -0.93035951812180
C 5.93306442113086 -5.83331235461172 -1.67629419667185
N 5.84754005738084 -5.88979920426723 -2.99513358217618
C 6.21219178804686 -7.00773355413491 -3.70864574541429
C 7.07033532048177 -9.28553107036599 -3.71039844502611
C 6.97005391985274 -9.31417785747276 -5.07127544195942
C 6.48796512420867 -8.18587646092616 -5.77025747917586
C 6.11209024475346 -7.04607807583289 -5.11176440160735
H 7.14177314915425 -8.91342134618496 -1.04059733211706
H 6.45734418454133 -6.82094876538220 0.14325767212038
H 5.60954443566056 -4.90792308174908 -1.22053250564518
H 7.43738077442395 -10.13798999226475 -3.15425493626016
H 7.25920769462363 -10.19848203001674 -5.62163197581086
H 6.41407738937466 -8.22135789730429 -6.84858120272393
H 5.74538753476953 -6.18785350000997 -5.65536146797506
C 3.98138766024083 -4.65301156138542 -3.92198063314988
C 5.31654019575325 -4.72440975240520 -3.69326981209262
C 6.30788204280701 -3.78473386734133 -4.06471920252528
C 7.69791517729577 -3.84830245337220 -3.80857672265493
H 8.22042617991736 -4.62997142266510 -3.27780330288623
C 8.23962530291980 -2.70450265743565 -4.37545929285614
H 9.27468579862425 -2.40221274777264 -4.38289512793515
C 7.15276712367363 -2.00830510920802 -4.94918158400651
H 7.18737407350697 -1.06985062158494 -5.48577993317953
N 5.99717498720170 -2.64662494910338 -4.76774750298687
H 4.47927212274428 -2.14322069287834 -5.53768940621979
O 3.63721755433281 -1.90215339260356 -6.00181702071445
H 3.12359473731744 -1.41023890726599 -5.35586501341083
H 3.64693122130466 -3.76146416285862 -4.42733640691341

TS_{B-C}; E_CEPA = -1031.087626608169; E_M06-2X = -1032.61850532; ZPVE_corr = 0.32564982; Q_corr = 0.01814381; H_corr = 0.00094421; G_corr = 0.28105834; -290.13 cm^{**}-1 ***imaginary mode***

C	1.43900108711268	-5.37098112957934	-4.21720217238012
C	0.38093291044409	-5.99114215233148	-3.55160566371783
C	1.16660504907566	-4.53655052447901	-5.30094490136108
C	-0.92713009147690	-5.77010771732477	-3.95092044699684
C	-0.14374811861286	-4.32782238353708	-5.71119139816244
C	-1.19152303933306	-4.93825302426960	-5.03447839483337
H	0.59963848445278	-6.64253319284773	-2.71646126713723
H	1.97013536019906	-4.06266855186280	-5.84755998298422
H	-1.74166311090855	-6.24590126135335	-3.42130860773151
H	-0.34472105781746	-3.68825818111269	-6.56006568502671
H	-2.21223261215133	-4.76821019066982	-5.35064479957354
C	2.83439117821824	-5.66695866549887	-3.75110362064141
O	3.04370257045170	-6.67560244560478	-3.08796923515612
C	3.87618034337189	-4.70847483024580	-4.09362862346029
C	5.17366372527436	-4.79607321331227	-3.72579145312261
C	6.20017777336803	-3.80858757860215	-3.90329477333508
C	6.24951200344296	-2.54463898232989	-4.50176660543406
H	5.47343330203700	-2.07978274020444	-5.08889584800720
C	7.50052038811991	-2.01661113315712	-4.17027309334276
H	7.90728131894110	-1.06554173201183	-4.47742481754466
C	8.15010732338878	-2.97939477955995	-3.37815006099755
H	9.13509158094687	-2.93393841432806	-2.93885829905458
N	7.37736533603656	-4.06443026902402	-3.25204869342200
C	6.98310317284326	-7.99053466568422	-3.16555116638067
C	7.71489267697837	-7.59563806624576	-1.99803626642519
C	7.53659816955562	-6.37848139846931	-1.45426672460154
C	6.59499258433587	-5.47855507670874	-2.04486269161442
N	5.76812018813712	-5.91199514502854	-3.03481694927435
C	6.02473877119364	-7.11448695071324	-3.70636926187052
C	7.22322367082424	-9.22314964821652	-3.79261817369466
C	6.55247913327306	-9.56912637117424	-4.94188944165102
C	5.62564524657845	-8.67522766276685	-5.48859283809585
C	5.35632299134519	-7.46556689025893	-4.88348157176390
H	8.41407597736140	-8.30094845410655	-1.56612992172308
H	8.07323801315666	-6.04773868799084	-0.57818178717137
H	6.20300676882801	-4.67580163953952	-1.44064643449231
H	7.95801828845088	-9.88715187524578	-3.35538524156194
H	6.74364744270177	-10.51728631833105	-5.42449028917027
H	5.10379665859269	-8.93289560548760	-6.40047064827902
H	4.63736074669552	-6.79349005960399	-5.32441107821390
H	3.59569879456650	-3.80182939118125	-4.60846907059263

C; E_CEPA = -1031.116276566028; E_M06-2X = -1032.64599013; ZPVE_corr = 0.32740525; Q_corr = 0.018332231; H_corr = 0.00094421; G_corr = 0.28276480

C	1.44443783209271	-5.37121567358781	-4.30402773515941
C	0.33441263608790	-5.84085675172354	-3.60217377828719
C	1.25837523170460	-4.72918849424622	-5.52742494492251
C	-0.94307035311066	-5.65896239266585	-4.10747425729319
C	-0.02066201438240	-4.56104180243450	-6.04153928640154

C	-1.12208350956414	-5.01960622609537	-5.33028157499929
H	0.48767271044685	-6.34373581572430	-2.65696103786351
H	2.11017815083088	-4.37774646569423	-6.09443333846655
H	-1.80014857115837	-6.01580029267637	-3.55207665597782
H	-0.15619702391082	-4.07268357323387	-6.99719414264265
H	-2.11876470301708	-4.88116059760866	-5.72813695625323
C	2.80948518718445	-5.61778130009665	-3.73388299462029
O	2.96869219884576	-6.51527840960686	-2.91386849064247
C	3.87586880012773	-4.72287557249387	-4.14909385793654
C	5.17136765362741	-4.78474316679777	-3.74561767089093
C	6.07672762448851	-3.65160613540615	-3.74021270179320
C	6.18707495247274	-2.32313263652110	-4.09913713729573
H	5.48720913950597	-1.75494811956553	-4.68845947847949
C	7.41326585442239	-1.87277451608640	-3.55484078705431
H	7.84193222735330	-0.89079783350576	-3.66871743612876
C	7.99521611134269	-2.92421897296557	-2.86445405337864
H	8.91256136834614	-2.98039541924939	-2.30326604954350
N	7.18392280852484	-3.99603094025981	-3.02110500873064
C	7.04698522060673	-7.96921577039903	-3.33120485300849
C	8.16764733856687	-7.40359618032428	-2.59153624554379
C	8.17892138350357	-6.13687451301623	-2.19978434662468
C	6.97390007923792	-5.28233843877193	-2.35469628423414
N	5.88585848428299	-5.84647689815778	-3.17833754112957
C	5.95473566894728	-7.15387050470225	-3.69328247459279
C	7.11704881093981	-9.27869612289242	-3.79757568141105
C	6.15306777697242	-9.79456658338194	-4.64880029911729
C	5.12668305909732	-8.96192678469534	-5.06859002493854
C	5.02550705485836	-7.65726523000410	-4.60214364297858
H	9.02435003384065	-8.04289145813970	-2.41792028548313
H	9.02078632368230	-5.69015700360180	-1.68740509527645
H	6.56462083058459	-5.05821897139822	-1.36329774416600
H	7.96658391621289	-9.88158302492340	-3.50093051574326
H	6.21789719100707	-10.81473131964196	-5.00049655660329
H	4.38383522003493	-9.32220461113696	-5.76790070276930
H	4.22916558254842	-7.03836894110121	-4.97306755487287
H	3.59061271281432	-3.80280753546568	-4.63891077674525

TS_{C-D}; E_CEPA = -1031.092031529759; E_M06-2X = -1032.62018816; ZPVE_corr = 0.32556822; Q_corr = 0.01793462; H_corr = 0.00094421; G_corr = 0.28133003; -205.33 cm⁻¹ ***imaginary mode***

C	1.55700154550604	-5.09963148803024	-4.45606556391012
C	0.36076613107298	-4.70671267810525	-3.85784745539845
C	1.52775211010671	-5.54104842632280	-5.77934757251287
C	-0.83299163455212	-4.73307496478127	-4.56669934885417
C	0.33401534905858	-5.57883204889592	-6.48797458773970
C	-0.85053376476122	-5.17016515810875	-5.88574786396398
H	0.38069307583580	-4.37944396893814	-2.82726315833762
H	2.43868962017716	-5.87702956909867	-6.25739963894315
H	-1.75080800335876	-4.41569714788956	-4.08876937022173
H	0.32758199647719	-5.93385676530588	-7.51036592594446
H	-1.78026692744980	-5.19910377978110	-6.43860956777457
C	2.82424863606249	-5.04974024117195	-3.63664514292192

O	2.71574584878023	-5.12208889881010	-2.37358182252839
C	4.02437272266029	-4.94076865148946	-4.30350248478949
C	5.25138534399306	-4.86535722940834	-3.53235450434110
C	5.86388498780794	-3.69749933824185	-3.00324899492605
C	5.72385960487829	-2.32382304276300	-2.88347992838279
H	4.88449354315969	-1.73718523369772	-3.21663103717766
C	6.88993522643399	-1.87149991514693	-2.24521352679605
H	7.12865903214086	-0.85313039021652	-1.98893113551193
C	7.71354074815512	-2.96978918877395	-1.99650950208607
H	8.68432028345610	-3.02811301109486	-1.53334772971351
N	7.07482362973297	-4.05560200608147	-2.46119804870547
C	7.15780762517731	-7.82748281492668	-4.09826688682931
C	8.40291157166874	-7.05668870597198	-4.03338186834586
C	8.48614644012444	-5.93768087437659	-3.32011967716270
C	7.28200539001445	-5.48293609996162	-2.54373400800365
N	6.05113776360374	-5.88766670494953	-3.24489287206121
C	5.96047997548491	-7.23584347776355	-3.67550020246238
C	7.11404670075509	-9.13723036687110	-4.56674929213692
C	5.91468482966373	-9.83518779161125	-4.59373158772772
C	4.74464008372229	-9.23489678158206	-4.14316127772005
C	4.75950078949788	-7.92582424394143	-3.67813475716038
H	9.26486777914031	-7.44225554633390	-4.56249803802017
H	9.39549913129072	-5.36130042596967	-3.21595632793540
H	7.27581804027564	-5.92244932538788	-1.54077292552224
H	8.02946738637396	-9.60391213048016	-4.90719886704985
H	5.89369785956617	-10.85323819473675	-4.95784827006071
H	3.81532938214768	-9.78764745114678	-4.14493907104484
H	3.86443631393215	-7.44929632931296	-3.30434959517256
H	4.12203783218704	-4.91163959252220	-5.37828956410265

D; E_CEPA = -1031.128986181348; E_M06-2X = -1032.65893636; ZPVE_corr = 0.32750606; Q_corr = 0.01834176; H_corr = 0.00094421; G_corr = 0.28283585

C	1.54781222037027	-4.71598408087908	-4.53411569359806
C	0.76664938759556	-3.69674504110544	-5.07833619920574
C	1.12231424041820	-6.03798747063753	-4.66100186527459
C	-0.40838561569572	-3.99191593550406	-5.75255809779617
C	-0.06381267426733	-6.33321199977058	-5.32068718078127
C	-0.82721860054190	-5.31268704296214	-5.87328076794470
H	1.09660242365573	-2.67242491491569	-4.96989109890554
H	1.69857586994315	-6.84415079490580	-4.22672025507225
H	-0.99971265302435	-3.19404883077299	-6.18192166840527
H	-0.39138580618183	-7.36108216023719	-5.40176601731714
H	-1.74700261636533	-5.54508862370476	-6.39368669351172
C	2.80607405487048	-4.32833638706561	-3.80244337010983
O	2.88376035076312	-3.19651266283201	-3.32666051285710
C	3.84650858501812	-5.31729597215624	-3.72243527595220
C	5.06706547176631	-5.12485939454795	-3.13627715325466
C	5.65811335286384	-3.94664649045383	-2.52092035644022
C	5.44274283710302	-2.63732945059449	-2.12164210410708
H	4.51879063535691	-2.09924690745748	-2.20231765994831
C	6.66784425912221	-2.16963183069029	-1.59601856901641
H	6.85785483179097	-1.18885548379539	-1.19302824700361

C	7.59811794786749	-3.19073278765663	-1.68565272603497
H	8.63499678528607	-3.23568579916297	-1.39788750717138
N	6.96759088698044	-4.24643102176590	-2.24185870142168
C	7.20339516057958	-7.65489693756789	-4.49889492048331
C	8.30029562984808	-6.68662086406513	-4.56034891090152
C	8.37983115276199	-5.68961320894736	-3.68407765012793
C	7.33490070621431	-5.59122315652469	-2.60417514229186
N	6.04823392305639	-6.09744047523106	-3.08290727398469
C	6.06178067101738	-7.34439759212970	-3.74156724933859
C	7.25507657232420	-8.87427325888778	-5.16856252424848
C	6.20436356684630	-9.77596934835231	-5.08158728790961
C	5.08991928965117	-9.46535591105386	-4.31179660216514
C	5.01627142589630	-8.25345620872910	-3.63736417151647
H	9.05451009452285	-6.82042441425716	-5.32564141474800
H	9.18630590371914	-4.96790877655108	-3.67687159282337
H	7.65114416931400	-6.14664959140099	-1.71421009219124
H	8.13098744745130	-9.10883800292249	-5.76048271649340
H	6.25707718929964	-10.72064656403492	-5.60513354799924
H	4.27563417220193	-10.17174675889513	-4.22404943544679
H	4.16129307414861	-8.02336647229035	-3.01709314218710
H	3.67076667645129	-6.26265037458484	-4.20438560401325

E; E_CEPA = -1432.453123448534; E_M06-2X = -1434.58569932; ZPVE_corr = 0.46549840; Q_corr = 0.02692453; H_corr = 0.00094421; G_corr = 0.41214890

H	2.68705673712373	0.52297106821178	-0.62686073162147
C	2.09541091191312	-0.39625362609080	1.96306783966230
C	0.76267889061550	-0.54934853927783	2.41390712216227
C	0.12185261981603	0.51850670791521	2.96773159494952
C	0.81745975206919	1.74572852810575	3.07792433028986
N	2.05165815946390	1.92833644472393	2.68542218121425
C	2.70506676922502	0.87278767834335	2.12103311297260
C	2.82964270497797	-1.44990586730871	1.36567956265993
C	4.11720456292270	-1.24815613636327	0.94965881542527
C	4.72734397860519	0.01791607626841	1.11145995101999
C	4.03916749454114	1.05459235687079	1.68041712941301
H	0.27177262742664	-1.50955619993501	2.30757086112938
H	-0.89962696832698	0.45015593798850	3.31514494991841
H	0.31432950238367	2.60224138106105	3.51448546054593
H	2.35140763105245	-2.41465724562677	1.24722451627354
H	4.67499963820494	-2.05544710138694	0.49442420981673
H	5.74596798019541	0.16384582444691	0.77733529108742
H	4.48991534143506	2.03027451072351	1.80815333436711
C	-4.00488759282462	-0.29206782813306	0.42655239846686
C	-5.24939475935266	0.33613281628666	0.46361262890903
C	-3.94097803072896	-1.67917778349437	0.55610008593528
C	-6.41098232016968	-0.40723575896216	0.60742857420490
C	-5.10277472689118	-2.42290229168591	0.71883591512313
C	-6.33924192748598	-1.79009574758011	0.73762642611966
H	-5.29307436749023	1.41310461578037	0.37303908423961
H	-2.98457915798731	-2.18589325659192	0.55619095500059
H	-7.37212017074724	0.08943597785482	0.62106615094088
H	-5.04103733990042	-3.49700809989194	0.83250361371573

H	-7.24403425823108	-2.37147276054889	0.85659318594998
C	-2.77742397681698	0.56967571334079	0.28604657591669
O	-2.83072103004444	1.73573352870556	0.67822597355886
C	-1.62019583044894	-0.04081812005132	-0.30404149951526
C	-0.41155481074862	0.57680254289599	-0.48146386858484
C	0.00233876573958	1.95078754911449	-0.24787588442784
C	-0.39272419449962	3.20082741253493	0.20241467653629
H	-1.34859337674629	3.44359111824021	0.62354375005634
C	0.70526944270393	4.06577818569330	0.00522744258441
H	0.74600022380530	5.11386827166689	0.25096180409131
C	1.73859587502969	3.33651178506683	-0.55907964507458
H	2.73224818280743	3.62483545606022	-0.85871816207103
N	1.29113493691071	2.07209399564920	-0.70321282011634
C	1.47879994670950	-1.44811223320078	-2.78891685362528
C	2.03556389462295	-0.23879415391592	-3.39953142611973
C	2.19458563482429	0.87296232964144	-2.68704221140742
C	1.82742999990761	0.84386070527550	-1.22742066021161
N	0.69828647080947	-0.05696222007802	-1.00053377813589
C	0.79530281780530	-1.34282905797154	-1.56495225717871
C	1.59842534525641	-2.69949926351573	-3.38745470324557
C	1.06623286802287	-3.82926803389846	-2.78349691015978
C	0.41212822053932	-3.71484213428692	-1.56254441682704
C	0.27739817314513	-2.47636032892570	-0.94930717924816
H	2.33066576173261	-0.28488242712344	-4.44032325987526
H	2.62244799480222	1.78201081064272	-3.08917457352958
H	2.11532347257846	-2.77727507996972	-4.33586866877116
H	1.16715853193087	-4.79560831900638	-3.25807403782543
H	0.01171118903541	-4.59361536542299	-1.07548116763788
H	-0.20745530033843	-2.39511305328947	0.01341947537874
H	-1.71637113091104	-1.05588872757497	-0.64618635542589

TS_{E-F}; E_CEPA = -1432.397359824623; E_M06-2X = -1434.53850405; ZPVE_corr = 0.46018508; Q_corr = 0.02659783; H_corr = 0.00094421; G_corr = 0.40709311; -1124.01 cm^{**}-1 ***imaginary mode***

H	2.43488952792486	1.55830957288877	2.98330367287294
C	-0.04832964521425	1.63907534350908	5.37177641276811
C	-0.70269159377375	2.81788898104982	4.94965085827353
C	-0.20841413223292	3.54779822149466	3.90194580854763
C	0.95089819960376	3.09689952173857	3.25492904515744
N	1.57445567602779	2.00955907869846	3.65177254600227
C	1.12509150364039	1.25076467141180	4.69018332227679
C	-0.51415358190832	0.83164537705433	6.43664758073684
C	0.16695347886993	-0.30057076666978	6.78561224375834
C	1.34558657927063	-0.67226943654185	6.09725143433998
C	1.82776523942880	0.08717832932106	5.06694454486091
H	-1.60310163787450	3.13008608255318	5.46389394788783
H	-0.69174138501573	4.44908227080643	3.55675338431163
H	1.37475221423043	3.61768551941859	2.40287550681703
H	-1.41316996019507	1.12931422152729	6.96066882238215
H	-0.19008774122892	-0.91994548742511	7.59683023709687
H	1.87377357834451	-1.56832576581047	6.39438418683500
H	2.73581417145534	-0.18183552535109	4.54132982866947

C	-1.52624853228177	0.14135333361241	-2.18535138353443
C	-1.90378568563480	0.51055435332527	-3.47603941151139
C	-2.17055630083569	-0.93901535385176	-1.58170481397671
C	-2.88530299234724	-0.19416523969462	-4.15850613755987
C	-3.16457462421395	-1.63621777669805	-2.25648769626159
C	-3.52014601592976	-1.27051495512390	-3.54914537621745
H	-1.41371993294406	1.35654808787679	-3.93871489380555
H	-1.91635265671041	-1.22786325996636	-0.57003368435468
H	-3.15754935484219	0.09667849886378	-5.16475109416305
H	-3.66399970112776	-2.46403113863445	-1.77033964683391
H	-4.29045457260602	-1.81775275483316	-4.07645986259872
C	-0.45790052001039	0.95537170243797	-1.49105132519240
O	-0.32231913765788	2.14351232494798	-1.83769587058143
C	0.30439372846791	0.28834082620106	-0.50669576071750
C	1.37060449840003	0.84281436525581	0.20776719126649
C	2.03385462673809	2.12103508526690	0.07053781267627
C	2.01886310768283	3.36032919618162	-0.56970090678496
H	1.29240169907716	3.68039572191026	-1.29086745526979
C	3.12682511608483	4.07434131553760	-0.07983464079199
H	3.42278449774890	5.06960226947614	-0.36908625607208
C	3.79485028144071	3.28220167016723	0.84843983949614
H	4.66908489352568	3.47026773399395	1.44774011584446
N	3.12069075193172	2.11247589841837	0.92240503108695
C	2.94570927113410	-1.75188074544655	2.28601580233753
C	4.25598377567112	-1.11667739770659	2.24974339660163
C	4.34441381204084	0.20149613334600	1.98953509332559
C	3.14498674460989	0.95994760486958	1.73745192499066
N	2.05154770617077	0.19169718079620	1.18925474930836
C	1.81525334770755	-1.06521819844097	1.79447199316969
C	2.75203948160716	-2.99996324222529	2.88094900443737
C	1.48382796720307	-3.54145406545821	3.02091885098447
C	0.37582002235655	-2.82661031821245	2.58127421155911
C	0.53931989525130	-1.59008938861184	1.97102338969022
H	5.12295651970486	-1.69982467724725	2.52785079588507
H	5.28559568157509	0.73511639216388	2.04316247020587
H	3.61748482728009	-3.53458463977572	3.25270604701944
H	1.35705192148929	-4.50863941058434	3.48841562993343
H	-0.62069650696332	-3.22389175595522	2.71822605926220
H	-0.32652320414911	-1.02501983047402	1.65972241791018
H	0.09649907200173	-0.75325675538187	-0.33929599435861

TS_{E1-F}; E_M06-2X = -2065.25358914; ZPVE_corr = 0.64892507; Q_corr = 0.03871066;
H_corr = 0.00094421; G_corr = 0.58434219; -1385.67 cm⁻¹ ***imaginary mode***

C	10.50537369938316	-8.52816165125372	4.90918563097931
C	10.06512301739776	-9.14159035513981	6.08283682759845
C	10.41002098522750	-9.21898510043678	3.70112722847074
C	9.52464496907917	-10.41676493960115	6.04930193762428
C	9.88318580414692	-10.50367599705165	3.67080020739882
C	9.43438955227759	-11.10104788928024	4.84135640263103
H	10.14820303811976	-8.60296094579747	7.01680363540323
H	10.76683965353232	-8.77882948091409	2.77969211186403
H	9.17522174240628	-10.87966523432452	6.96242163853685

H	9.82430835502795	-11.03708999512443	2.73170268498802
H	9.01720341875042	-12.09901340165998	4.81412807278454
C	11.09777722476226	-7.15486192670067	5.01791267048809
O	11.52408751612587	-6.76340096699623	6.09531940816269
C	11.12882340178307	-6.33806618314687	3.81399070697462
C	11.59067723538140	-5.06723641242294	3.77978729319028
C	12.06847901082170	-4.18287560500035	4.82812326916117
C	12.44509900465644	-4.06633301328125	6.15025717266984
H	12.44679567166377	-4.85234980999907	6.87940440396061
C	12.82439344255548	-2.71202720967010	6.35116949438116
H	13.16693451364938	-2.28062077943906	7.27650974903020
C	12.67204762899372	-2.02946984694988	5.16734474276026
H	12.84170278351513	-0.99911616359820	4.90343467192552
N	12.20752338723251	-2.93391503871247	4.25737488661944
C	10.41235361079183	-3.52369083066191	0.64888633572477
C	10.46577831284252	-2.17783717521224	1.17007592473464
C	11.24720105367418	-1.87248229667189	2.21766289935810
C	11.93557803622187	-2.94942842725500	2.89370813565169
N	11.57652106228878	-4.25942298334170	2.61384586918970
C	11.05556181193736	-4.56495156549895	1.34193146186004
C	9.81085977645232	-3.80327240276475	-0.58007489105811
C	9.89707613201313	-5.06511658338148	-1.13628125494335
C	10.61539688155104	-6.06118144823864	-0.47845558517852
C	11.19584989255993	-5.81877128625779	0.75625742720316
H	9.90678559108069	-1.40503390292475	0.65722587468903
H	11.37739749499240	-0.86881508439898	2.59696827089294
H	13.33133158401862	-2.84015786506148	2.36445103668689
H	9.30295876339486	-3.00222889438795	-1.10179391964849
H	9.43604560008412	-5.27060154648378	-2.09233929577937
H	10.73363761084172	-7.03486682350542	-0.93384978493304
H	11.78361782408236	-6.58631409124538	1.23718339100534
H	10.70270745648040	-6.75329422297152	2.92018903734082
C	12.23450040295376	-0.69183457180501	-1.08305941365376
C	11.53030870288787	-1.31893695568084	-2.10972056584701
C	11.90124399753033	0.61495567255771	-0.72702489061657
C	10.51558206726318	-0.65057886960931	-2.77802840380698
C	10.87290453683075	1.27840869592999	-1.38337157000273
C	10.18177325768726	0.64905907645275	-2.41193562276868
H	11.78601062211289	-2.33727590540677	-2.37002111873873
H	12.42113662651510	1.10943353384337	0.08293745865551
H	9.98020273366286	-1.14304531538483	-3.57917883868119
H	10.60923839783170	2.28571376767206	-1.08975838718708
H	9.38414175177626	1.16927765968488	-2.92577028735191
C	13.27866942268579	-1.48547732722224	-0.35084281499229
O	13.17959367370021	-2.71302724763031	-0.34194950862348
C	14.34513355357011	-0.74198181549911	0.28239351307365
C	15.33742044402191	-1.27867105640791	1.05097086720751
C	16.43595134565552	-0.58424516571159	1.61118124563728
C	17.46907781585016	-1.13702973773709	2.41155850490897
H	17.56407621223682	-2.17048317970845	2.71002187276389
C	18.31359194758087	-0.08338450114576	2.71710353108771
H	19.21485315578133	-0.11109842072797	3.30943536657207

C	17.74762527283488	1.05303024659425	2.08655014909324
H	18.13573000750468	2.06330858654833	2.10627497220614
N	16.62990084879530	0.76439999726993	1.42592449773645
C	15.68386050711727	-4.99481763985646	0.90397402271691
C	15.21075050935138	-5.31403561198811	2.22120869815548
C	14.74137654652360	-4.35529191162883	3.03953199937712
C	14.60640140603200	-2.98711093752089	2.55838985209479
N	15.28684081704280	-2.67990451825063	1.39116256134284
C	15.74251716378442	-3.63930433529640	0.51884634497600
C	16.15868272239221	-5.97925282245260	0.02523333048836
C	16.68155703909146	-5.63738109485747	-1.20097249693728
C	16.75305817292634	-4.28571776873913	-1.56465835328455
C	16.29647404742236	-3.29526994730540	-0.72373283049122
H	15.28701818732004	-6.33980035282322	2.56098724758465
H	14.45275126131274	-4.57039394573325	4.05786324537161
H	16.10981792587939	-7.01470479642600	0.33860455972953
H	17.04292943107762	-6.40092441599612	-1.87535600493067
H	17.17186283385343	-4.01007172724359	-2.52337749270742
H	16.35107660082554	-2.25730796969921	-1.01977061696296
H	14.41043754801367	0.31885187334264	0.09525887752484
H	14.69162647696091	-2.19910929463525	3.30865885387969

F; E_CEPA = -1432.411872961265; E_M06-2X = -1434.55698981; ZPVE_corr = 0.46520701; Q_corr = 0.02668205; H_corr = 0.00094421; G_corr = 0.41287675

H	2.63781507480620	2.19782998919796	1.00504062538909
C	2.19822552750545	-0.99747524955501	1.69342063299497
C	0.85514830817962	-0.89283801535441	2.13641413767032
C	0.21519327715178	0.31522981811422	2.15246691783853
C	0.90674516886253	1.45193508771397	1.72176007586379
N	2.15878687334508	1.35308557501057	1.30162690056273
C	2.85697187868058	0.17067694609260	1.26010999751945
C	2.89921779494179	-2.21971137441522	1.64453935634704
C	4.19333909631044	-2.25299574227159	1.19381176731400
C	4.83554582606954	-1.07243291600458	0.77397412532797
C	4.18077370769254	0.13342822559481	0.79862817954815
H	0.34226084396889	-1.79225972178380	2.45400252958716
H	-0.81897535030392	0.42914227954799	2.44328082011104
H	0.46878310828382	2.43976392960956	1.71510240565267
H	2.39349031267064	-3.12052779161855	1.96649171425067
H	4.72932670701642	-3.19137285933466	1.15543601890139
H	5.85668356943329	-1.11688213934284	0.42060134934917
H	4.65872524463331	1.04808788997932	0.47303910376059
C	-4.08480424170925	-0.37627855172726	0.66090860798314
C	-5.22399629368328	0.19704053133738	1.22733897836416
C	-4.15194399491477	-1.71089194914380	0.25291350269588
C	-6.40246133313398	-0.52599953055811	1.35810855154202
C	-5.32448403586680	-2.44127563747705	0.39400762557132
C	-6.45806528956108	-1.85041714174355	0.94132226645223
H	-5.17218020611711	1.22419210055956	1.56186836533394
H	-3.27838129965931	-2.19687387369054	-0.16205055694658
H	-7.27761780050399	-0.05627119737520	1.78862039688197
H	-5.35152429032497	-3.47701057104055	0.08064254382964

H	-7.37236394802970	-2.41930207355784	1.04764598649822
C	-2.83669226317869	0.47074778865129	0.54375685306502
O	-2.71494239114551	1.43226252852631	1.35849794651792
C	-1.91837010037715	0.11976316329476	-0.43974217137667
C	-0.76207751725426	0.90165789537465	-0.74418278532318
C	-0.63582743938257	2.31493625724550	-0.72377475860995
C	-1.28311359322279	3.52032556769420	-0.44075806841846
H	-2.26414292791413	3.62501116435433	-0.01631489904516
C	-0.36584288797025	4.54174536438794	-0.76445034705803
H	-0.53686901513875	5.60134508673229	-0.65500633105338
C	0.81183601672055	3.98903026319517	-1.24155425033190
H	1.72666425363655	4.43201238568964	-1.59168488846545
N	0.62715502283315	2.62606558568104	-1.21747366946309
C	2.21250770241598	-1.05470114586295	-1.98080655364357
C	3.00488650038534	0.06775303654282	-2.36600074666939
C	2.54069046606715	1.33023836047952	-2.13425736941266
C	1.28808017913404	1.49364852138026	-1.56223691733616
N	0.44048534463454	0.43323915297317	-1.24016617927942
C	0.93293495860910	-0.88516305303408	-1.38999779260817
C	2.70585739032761	-2.36526204632324	-2.14065718877468
C	1.99705386074184	-3.46043606656999	-1.70929842662655
C	0.76178320187296	-3.27499219570887	-1.08414345974345
C	0.23496954145595	-2.00684728045519	-0.92967802917747
H	3.97864800322252	-0.10117876484670	-2.80288092572184
H	3.11851045791710	2.21350773341406	-2.37064726989968
H	3.67729882815240	-2.48587365813554	-2.60407345245207
H	2.40033480454527	-4.45606987229527	-1.83744720391592
H	0.20358081873597	-4.12456948134848	-0.71472549677731
H	-0.70264146737230	-1.88843842376096	-0.41668795788885
H	-2.11540201919538	-0.74397377503906	-1.05239775470514

F' (cation); E_CEPA = -1030.366825954475; E_M06-2X = -1031.89765697;
 ZPVE_corr = 0.31759304; Q_corr = 0.01794846; H_corr = 0.00094421; G_corr =
 0.27332794

C	1.39332130520564	-4.69559217262080	-4.43705196950404
C	0.48606846795231	-3.64558650609649	-4.59202254128896
C	1.09069087465789	-5.94908484480306	-4.96970104229610
C	-0.69872330487251	-3.84106988611849	-5.28059873703487
C	-0.10542174681297	-6.14671692808855	-5.64627585343495
C	-0.99651541837789	-5.09437770228029	-5.80767490400505
H	0.72717381402246	-2.67862854333105	-4.17211225392266
H	1.76243326504229	-6.78710556438712	-4.84338987121404
H	-1.39219361384410	-3.02074781838304	-5.40694639277474
H	-0.33972508329017	-7.12371642338119	-6.04636937738003
H	-1.92423652687781	-5.24916790066591	-6.34245255232999
C	2.64282800962860	-4.42458076743820	-3.66858213873866
O	2.72234837520744	-3.46561780596853	-2.92255121708146
C	3.77881429818285	-5.34353922099454	-3.84869670967130
C	4.98874930822140	-5.10357192725389	-3.32183096133107
C	5.55215607694490	-3.94019930192055	-2.66330880693532
C	5.31624966927545	-2.71260982440925	-2.09731655384587
H	4.35697736932596	-2.27427279410709	-1.90307064727714

C	6.59328634543134	-2.13835416930853	-1.80403673496583
H	6.76019936896890	-1.17905523744164	-1.34429655864379
C	7.57241427681603	-3.00554704071514	-2.19446075654662
H	8.64642896818647	-2.95059850485470	-2.14936782160939
N	6.92928787278377	-4.10582296825664	-2.71105636180116
C	7.44480125828842	-7.80997852662020	-4.31675337759671
C	8.60944593837187	-7.02909450320643	-4.10144369513821
C	8.54079685458135	-5.79931173481271	-3.51975631248043
C	7.26653609930695	-5.30030369207006	-3.25220067897146
N	6.12987211032439	-5.96984489538883	-3.54332549237053
C	6.17370727523087	-7.29654140863487	-3.96771878730104
C	7.54702894662810	-9.12962592066345	-4.79894887843419
C	6.43660802582045	-9.92693532008187	-4.88374208646181
C	5.20017617931519	-9.43317259698143	-4.44474625038597
C	5.05773655311889	-8.14142280908329	-3.98933069459149
H	9.56921749342193	-7.44963931208505	-4.37351859879809
H	9.40800921205314	-5.19919346901981	-3.29071388057180
H	8.52598705399099	-9.49878906973287	-5.07472724064013
H	6.51511086608951	-10.94127868008862	-5.24796863191963
H	4.33489065050894	-10.08180805743616	-4.44412045612910
H	4.10286209198773	-7.82375119938042	-3.60654873275401
H	3.64914025018290	-6.18946436388910	-4.49731234682219

B-H⁺; E_CEPA = -1031.843878156291; E_M06-2X = -1033.37426584; ZPVE_corr = 0.33490660; Q_corr = 0.01968606; H_corr = 0.00094421; G_corr = 0.28857693

C	1.61867091738181	-5.37927654324160	-4.02193666921000
C	0.59102561920199	-6.01703150699785	-3.32662732593086
C	1.29466070302438	-4.56162942035363	-5.10459603841873
C	-0.73346298739177	-5.82935977195228	-3.69141350365274
C	-0.03079380301919	-4.38640625177610	-5.48206052414167
C	-1.04743437722459	-5.01401600657157	-4.77359044488658
H	0.84604216237452	-6.65850704110184	-2.49406256427607
H	2.07413715558996	-4.07473618345088	-5.67443116317691
H	-1.52159301311347	-6.31987743980331	-3.13542054956909
H	-0.26812020346627	-3.76014584536249	-6.33179659098062
H	-2.07984390443344	-4.87110667719465	-5.06449255216915
C	3.03969398834225	-5.64172159809808	-3.58632594588545
O	3.26829713082050	-6.68317147315750	-2.96721378338174
C	4.02060047831526	-4.63765713039831	-3.91952701774251
C	5.37058633086761	-4.71697718309547	-3.70267917668947
C	6.29803187078869	-3.71063790667508	-4.08991277898184
C	7.70172251622788	-3.74812514289881	-3.90333476042098
H	8.25743107243284	-4.54545964184297	-3.43395490672491
C	8.19040866316387	-2.56622808917912	-4.44117650149675
H	9.21658833314748	-2.23529500452998	-4.48702780003198
C	7.05463935940393	-1.87424778188378	-4.92619013127486
H	7.04551320111140	-0.90803196726070	-5.41480359612630
N	5.92338773407524	-2.54757282324017	-4.72137605549004
C	6.67496582733468	-8.13739538185582	-3.03970322276630
C	6.84727774134868	-8.04424130062130	-1.59382512348799
C	6.46709101069232	-6.96371156130740	-0.91833049550594
C	5.81752388957308	-5.79087600544759	-1.58153688202872

N	5.94447438846320	-5.84263481808209	-3.03522565015813
C	6.20025901559576	-6.99949535878426	-3.73086719052533
C	6.98606085179966	-9.29339955522156	-3.74412419590737
C	6.83964267710996	-9.36458754983008	-5.12502483962267
C	6.37683163806898	-8.24375818740826	-5.80225706919456
C	6.05859740523027	-7.07436526880851	-5.12264874305326
H	7.29562396063722	-8.88817863014743	-1.08255162755898
H	6.58852548199251	-6.90491392613125	0.15596148596787
H	4.75744961869716	-5.74398916291123	-1.29721595014056
H	7.35160003540110	-10.14975403911525	-3.18892426779070
H	7.08450122058606	-10.27227227348548	-5.65878200385879
H	6.25653145944244	-8.27245299988610	-6.87787282340593
H	5.69971888700861	-6.21469653258271	-5.67152596634445
H	3.67369973822716	-3.73667859797085	-4.40109413615109
H	6.28098668317020	-4.86137879833658	-1.23590131880779

G; E_CEPA = -1031.115806370100; E_M06-2X = -1032.65347960; ZPVE_corr = 0.32700462; Q_corr = 0.01841129; H_corr = 0.00094421; G_corr = 0.28259982

C	5.33867138472579	-0.67307078922505	-1.03029657627108
C	5.89943586983280	-1.55197167497377	-0.09930069353843
C	6.13301638944627	0.35946926154812	-1.53990827057060
C	7.21036872435838	-1.38793523248491	0.32664067044444
C	7.43965432444999	0.52307931261668	-1.10849862401206
C	7.98503460092179	-0.34845093187901	-0.17151704510316
H	5.30070792486211	-2.35942107344156	0.29701215135136
H	5.73626749330255	1.02635731552501	-2.29336153073811
H	7.62652378720697	-2.07484201477708	1.05181324940975
H	8.03945163663716	1.32642967939925	-1.51540606756132
H	9.00731121217505	-0.22239656523423	0.15915784850561
C	3.93574449700618	-0.84272423548100	-1.44587718576669
O	3.45400157687340	-2.08652406524875	-1.17836380888817
C	3.18856252311015	0.13657723594120	-1.99190541964061
C	1.86099842466005	-0.06515790644705	-2.51401006973561
C	1.39239624531364	-1.17569958462190	-3.24823264103180
C	1.71200141295310	-2.44080238564099	-3.74995416767112
H	2.62392564493832	-2.98749747181094	-3.58785135478997
C	0.59356379352464	-2.84547365324576	-4.51676504980892
H	0.49998109600834	-3.78296845316848	-5.04198931184636
C	-0.37903764341598	-1.86668831641149	-4.49892228916291
H	-1.35108587011419	-1.80736840998657	-4.95355046246815
N	0.12102778204161	-0.84800570796258	-3.71548384776329
C	-0.38020375216970	2.93825380439807	-2.29052888992694
C	-1.39341119523523	2.45360007148334	-3.17282677983710
C	-1.31908761568877	1.18429058473581	-3.65259607977809
C	-0.20434598831610	0.40686862024858	-3.32719893847019
N	0.84396352293490	0.87280652541399	-2.56431358159790
C	0.72303212085880	2.12583358629576	-1.93965478361887
C	-0.48209081905815	4.21500702271056	-1.70396250314149
C	0.43692722424930	4.65340142442826	-0.78316700216620
C	1.48359118307988	3.80809294114041	-0.39517724001087
C	1.62629830557728	2.56014480325627	-0.96110928287774
H	-2.22667768030333	3.09720443149601	-3.41709390001782

H	-2.07935615634397	0.75556656221742	-4.29004436859555
H	2.50554381688090	-2.12642106039860	-1.35625729337099
H	-1.31995304975940	4.83900112520338	-1.98809198361201
H	0.33979009139368	5.63522356955042	-0.34047023807755
H	2.18557435067759	4.12667218638414	0.36312039729520
H	2.41755953885461	1.91349420987905	-0.62173918719935
H	3.63275134454953	1.11657227156800	-2.08201707233931

TS_{G-H}; E_CEPA = -1031.084064970887; E_M06-2X = -1032.61746417; ZPVE_corr = 0.32211378; Q_corr = 0.01796397; H_corr = 0.00094421; G_corr = 0.27788801; -1639.91 cm⁻¹ ***imaginary mode***

H	-1.10593849819752	0.54985011324252	0.82711291316277
C	-4.26964238329647	-0.16854974059016	0.25603496952303
C	-4.85899096097902	-0.61349048191149	1.43868859874191
C	-5.05564040673201	-0.07316614425232	-0.89527041259673
C	-6.20413553692323	-0.96084176474516	1.47162570151571
C	-6.39706754275885	-0.41845834784036	-0.86198953064389
C	-6.97669684381685	-0.86499767392685	0.32246443376650
H	-4.25265389773319	-0.68538597585728	2.33065504540748
H	-4.61884045472980	0.27839632943054	-1.82038542750136
H	-6.64767479217037	-1.30559503480116	2.39649951609995
H	-6.99468996860480	-0.33755817388414	-1.76038667764314
H	-8.02466952531019	-1.13316949479665	0.34664296065729
C	-2.83208660648487	0.18723916695227	0.24466293327713
O	-2.17919172328687	0.15867731794891	1.39315170086806
C	-2.10486635243715	0.51890126127808	-0.85503288069165
C	-0.71516195312395	0.88734117434992	-0.45852344319188
C	-0.25798528102009	2.25183873265836	-0.70583590901031
C	-0.61122497078368	3.57321211548598	-0.62098883676356
H	-1.54065761517563	3.96703338456625	-0.24757267336197
C	0.50205312992343	4.32364229749637	-1.12251708891841
H	0.55886834512720	5.39816792846628	-1.18931275213027
C	1.49738739033441	3.46699919627723	-1.50708212421754
H	2.47560865291190	3.63149332664950	-1.92211831125540
N	1.01862959603710	2.19687810692630	-1.24795552443379
C	1.73449191587857	-1.80525155262460	-1.55522638725754
C	2.74189297949123	-0.93324018526952	-2.05424427212829
C	2.59913431998068	0.41445014759780	-1.96668923037525
C	1.40129212105229	0.90543267037852	-1.42012255119934
N	0.41537557143960	0.10972408441053	-0.97879554531598
C	0.56718308625456	-1.26367982684168	-0.97385077355435
C	1.89113043798425	-3.20609361535440	-1.58430786282337
C	0.94033190866416	-4.02554582636573	-1.03518592416625
C	-0.19098220278834	-3.46616648073664	-0.41624741744339
C	-0.38479083482688	-2.10625219400405	-0.37896527602510
H	3.63517647858587	-1.36516110666419	-2.48628688998617
H	3.34906613906536	1.11175333475495	-2.30872035388182
H	2.78478475434473	-3.61432085381269	-2.03845367466526
H	1.06650657167823	-5.09902069694904	-1.05680703005108
H	-0.92059676187741	-4.11520773102552	0.04892500388041
H	-1.24004958615527	-1.68620335831896	0.12539267425896
H	-2.48584169954115	0.60473057170229	-1.86162566992612

H; E_CEPA = -1031.120289686410; E_M06-2X = -1032.65133070; ZPVE_corr = 0.32725131; Q_corr = 0.01817296; H_corr = 0.00094421; G_corr = 0.28284685

C	1.91138075494129	-0.28839904982904	-0.39464471334008
C	2.90024907562729	-0.94683655675537	0.33554672116685
C	2.26352465418722	0.85988043999654	-1.10572545081800
C	4.21081487328446	-0.48744765463448	0.33907399980641
C	3.57071569699462	1.32904510800307	-1.09519904592002
C	4.55140395106175	0.65370137634372	-0.37742601575150
H	2.62495002157277	-1.82758684377317	0.89997636232836
H	1.50852596628757	1.40428140566168	-1.65757322034956
H	4.96695430424682	-1.01830807895136	0.90315357503046
H	3.82333114551235	2.22711534121622	-1.64409298681753
H	5.57014840875635	1.01854168534210	-0.37123744007139
C	0.50470491708221	-0.84060653137207	-0.36744516148365
O	0.17377888813206	-1.52879466633362	0.65032434350922
C	-0.31450035679115	-0.57809709741610	-1.44622846061772
C	-1.65989165618120	-1.18440094625288	-1.52188156100384
C	-2.03387539578145	-1.73981434776985	-2.86480104288403
C	-1.63220459814589	-2.61977957716499	-3.81859049672532
H	-0.77845017961936	-3.27402625147229	-3.77247413050501
C	-2.57062225373573	-2.50515075797245	-4.90342744814044
H	-2.54750123755012	-3.06873114264163	-5.82133088156472
C	-3.50275048900716	-1.56030396693005	-4.58603465853430
H	-4.35662880596301	-1.17771037551431	-5.11707175120059
N	-3.16296019730273	-1.09807408090266	-3.33167436571951
C	-4.15882296614677	1.49394230793681	-0.33519273649770
C	-4.96741908197543	1.51434020878706	-1.50120921468742
C	-4.71967011687102	0.68015425693519	-2.54950408071698
C	-3.61739503899524	-0.17850376452059	-2.43195015320067
N	-2.82895203339922	-0.19632514021991	-1.36067177226125
C	-3.06826052109070	0.59807621125407	-0.26848301590259
C	-4.42328987787243	2.32674020856288	0.77232714612411
C	-3.63856170365843	2.25473209023212	1.89173554834311
C	-2.56973654024487	1.33958902347959	1.94464961952987
C	-2.27395883259604	0.51475561431734	0.88652784760016
H	-5.80121589323721	2.20368331049707	-1.54099697862074
H	-5.32295130754060	0.65902935691499	-3.44435940242558
H	-5.25945917086475	3.01158431809852	0.71624622619801
H	-3.84181628384929	2.89114252387445	2.74160157841933
H	-1.96806249754979	1.27999883000978	2.84181805468217
H	-1.46007568937835	-0.19841407343454	0.94363844421774
H	0.03707121289579	-0.03146201733484	-2.30805575859166
H	-1.78109014523459	-1.91155769626701	-0.71610652260395

TS_{H-3a}; E_CEPA = -1031.112694169845; E_M06-2X = -1032.64477892; ZPVE_corr = 0.32548791; Q_corr = 0.01812058; H_corr = 0.00094421; G_corr = 0.28093165; -323.74 cm⁻¹ ***imaginary mode***

C	3.87549361642472	0.36797501900867	1.47028993660308
C	4.67561203997894	0.53707748958758	2.59972591537090
C	4.46337590384130	0.46557146358617	0.20929256958167
C	6.03603106114840	0.77964694071370	2.47606169686841

C	5.82269557615144	0.72205885436618	0.08259585588839
C	6.61377018341577	0.87349732981208	1.21490972994446
H	4.21396875897404	0.47241042866877	3.57565265217268
H	3.85913849764183	0.36297117106796	-0.68185411874245
H	6.64623814004653	0.89802810366988	3.36196717024181
H	6.26356095888371	0.80682331460790	-0.90197306116365
H	7.67343729439194	1.06856572192167	1.11503113502992
C	2.40228246969137	0.11018659542231	1.66874283372315
O	1.89046794150797	0.47963859011469	2.74720738043642
C	1.69753497531244	-0.55636630041225	0.64301624747962
C	0.34552738672320	-0.90572913537464	0.81723802324784
C	-0.19634261037152	-2.06444616898593	0.05757469244225
C	0.10443782008681	-3.38370405666563	-0.10115577735037
H	0.90805790653390	-3.91381351944459	0.38156362550454
C	-0.85744358849693	-3.92364525576376	-1.01865053768546
H	-0.91006337604171	-4.94409347005732	-1.35965681774327
C	-1.70145525992441	-2.91955927667234	-1.39788267071463
H	-2.53798504687685	-2.90248926211895	-2.07437423758594
N	-1.29200079625164	-1.78797108771180	-0.72940441238833
C	-2.05302466688356	2.23478471361150	-0.54959475916215
C	-2.86104841355529	1.45753933220832	-1.41904998195269
C	-2.68676273031935	0.10963729991062	-1.52371841318077
C	-1.66106122172705	-0.45983957758445	-0.74481071372293
N	-0.90187053783972	0.23561158264850	0.06704215590105
C	-1.06016955854704	1.57742273986260	0.21594274095465
C	-2.21306920169899	3.63038946837286	-0.40716534296666
C	-1.42045788673214	4.32904855035611	0.46279229487768
C	-0.44668002628991	3.65688528068324	1.23112674944785
C	-0.25970592258700	2.30298609810462	1.12041486721675
H	-3.62632842343810	1.95558096136895	-2.00111825143515
H	-3.28838296238221	-0.50863017471377	-2.17286646413662
H	-0.02514292022653	-0.79857064345733	1.83397891745167
H	-2.97435682934607	4.12852028011892	-0.99393973507565
H	-1.54298204906328	5.39769586148813	0.57231626905724
H	0.16103534567750	4.22163399845707	1.92559809858014
H	0.47232781315785	1.78048668294829	1.72372052906832
H	2.19749833900959	-0.85719894372455	-0.26443579208375

3a; E_CEPA = -1031.148774212946; E_M06-2X = -1032.67805946; ZPVE_corr = 0.32579399; Q_corr = 0.01917863; H_corr = 0.00094421; G_corr = 0.27974005

C	-3.70638072430328	1.05423853934751	-1.06939515034912
C	-4.72382894895673	0.11828847415559	-1.26276541965317
C	-4.02339471825777	2.41218651890693	-1.04699024804521
C	-6.03689301643525	0.53030300938498	-1.41871110359180
C	-5.33818693661808	2.82560437846011	-1.21919956525965
C	-6.34562953093632	1.88705893988856	-1.39888429604171
H	-4.46961341705153	-0.93263331160313	-1.28270711302060
H	-3.25111643515552	3.15763139347960	-0.91875550308458
H	-6.82086323283923	-0.20223141470568	-1.55642152183835
H	-5.57414188097325	3.88117358218580	-1.21236432291097
H	-7.37039366190744	2.21083418420923	-1.52480160873363
C	-2.30385070916500	0.55112295967994	-0.92161527601872

O	-2.02622513078594	-0.58035028450462	-1.29120292551421
C	-1.30069004571128	1.43756177554332	-0.30885549132539
C	-0.02075905610062	1.04302581074069	-0.22914505979649
C	1.04647504859626	1.82998716134920	0.33138394601990
C	1.09304517834336	3.18510827275189	0.59604762282009
H	0.27378789105447	3.87042745279429	0.45213938010397
C	2.40038306655724	3.50490853343268	1.02014945334253
H	2.77212539352319	4.47347787531449	1.30845046756994
C	3.12814501318163	2.34211969070665	1.00223712969361
H	4.14735424440338	2.14898497861405	1.29033864510070
N	2.31539945847948	1.32293947791902	0.58592282155778
C	3.50210646328949	-2.64856102603829	0.48300884940661
C	4.41565555364764	-1.64095401252019	0.09025035083043
C	4.03179903163106	-0.33557991299516	0.10798173471619
C	2.71583584938316	-0.03488030655467	0.54501463779462
N	1.84684975098380	-0.92542984153487	0.92454492058106
C	2.20919678222139	-2.23856779159546	0.88618603554878
C	3.82519552108440	-4.02472124334230	0.47789651549445
C	2.89378169520010	-4.95216526318361	0.85805740154390
C	1.60244566805459	-4.54136510806467	1.25806055072808
C	1.26370863485936	-3.21557441699149	1.27364266256079
H	5.40855944825057	-1.92241069015347	-0.23786464251978
H	4.69046023878746	0.45612344516312	-0.21734143147350
H	0.23228977991578	0.06947488036657	-0.62814429286666
H	4.81790001330135	-4.32583564704647	0.16732621592420
H	3.14075287766484	-6.00511898682451	0.85363002937334
H	0.87634457742522	-5.28665477449395	1.55435493357038
H	0.27916281963100	-2.88524485425219	1.57744762039753
H	-1.61679455427298	2.38569855501049	0.10109704736467