

Supporting Information

Asymmetric aza-Morita-Baylis-Hillman reactions of chiral N-phosphonyl imines with acrylates via GAP chemistry/technology

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Guigen Li^{*,a,d}

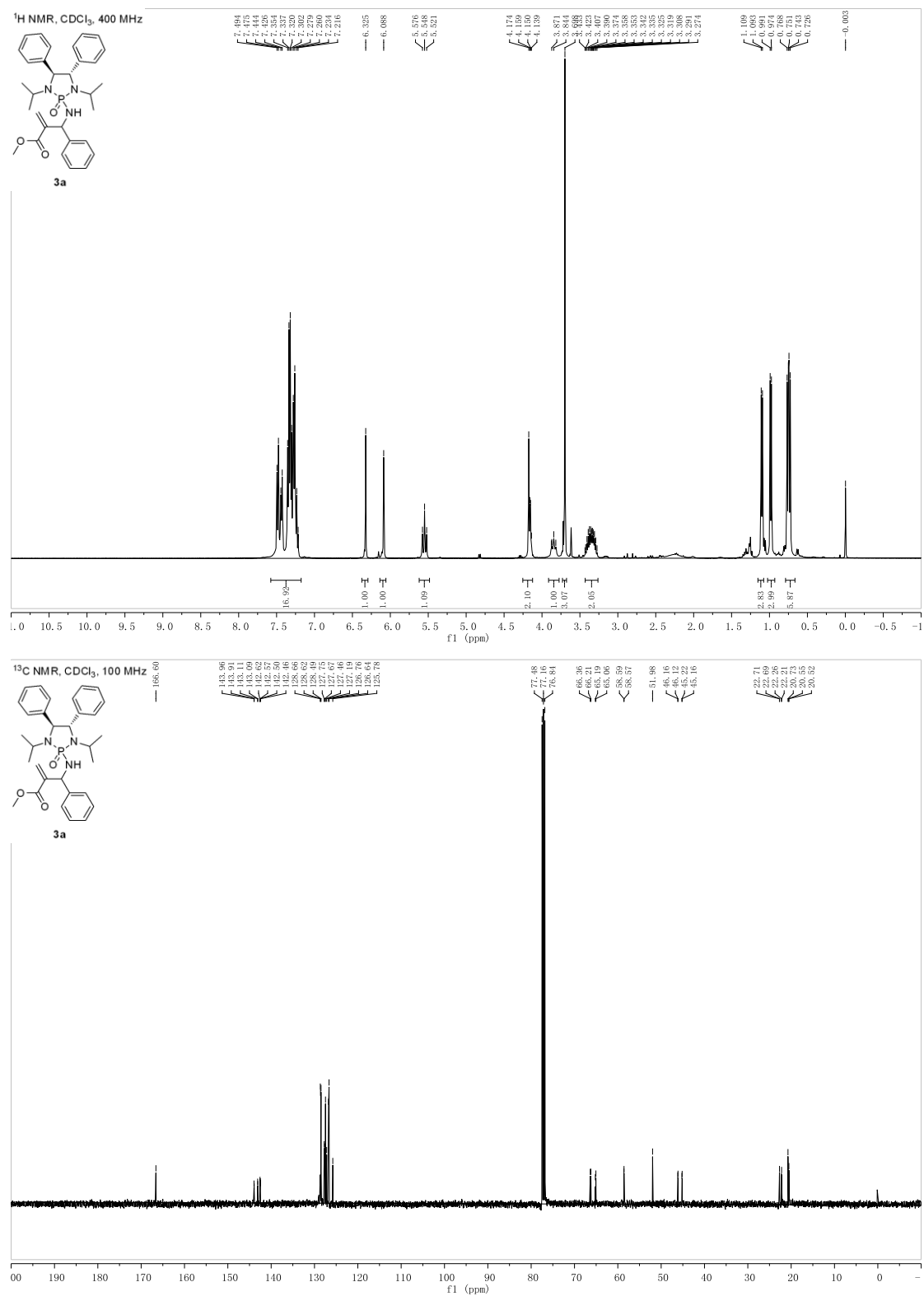
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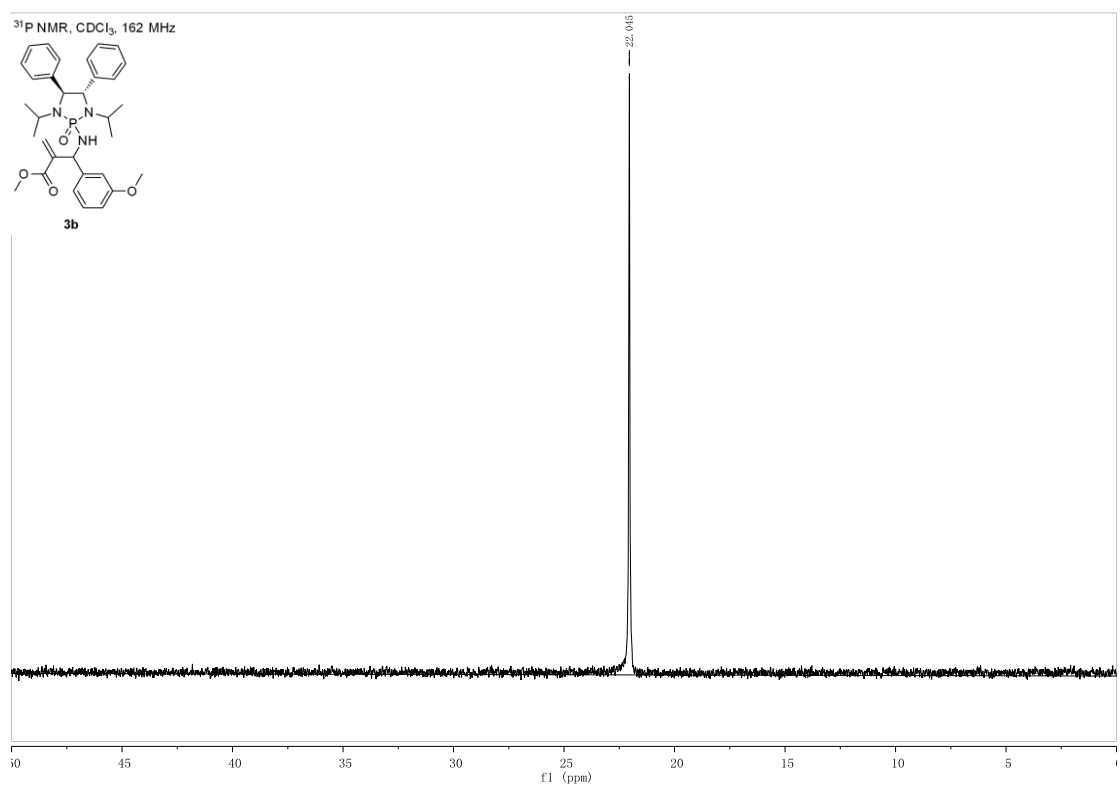
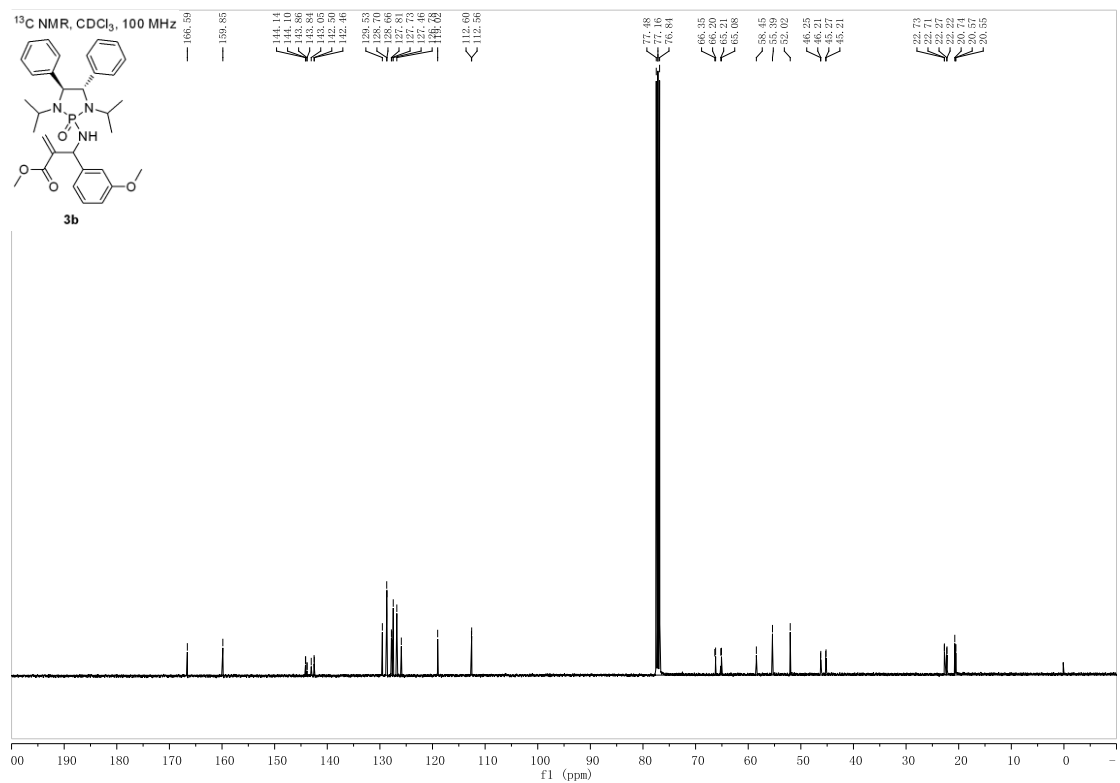
¹These authors have equal contribution to this work

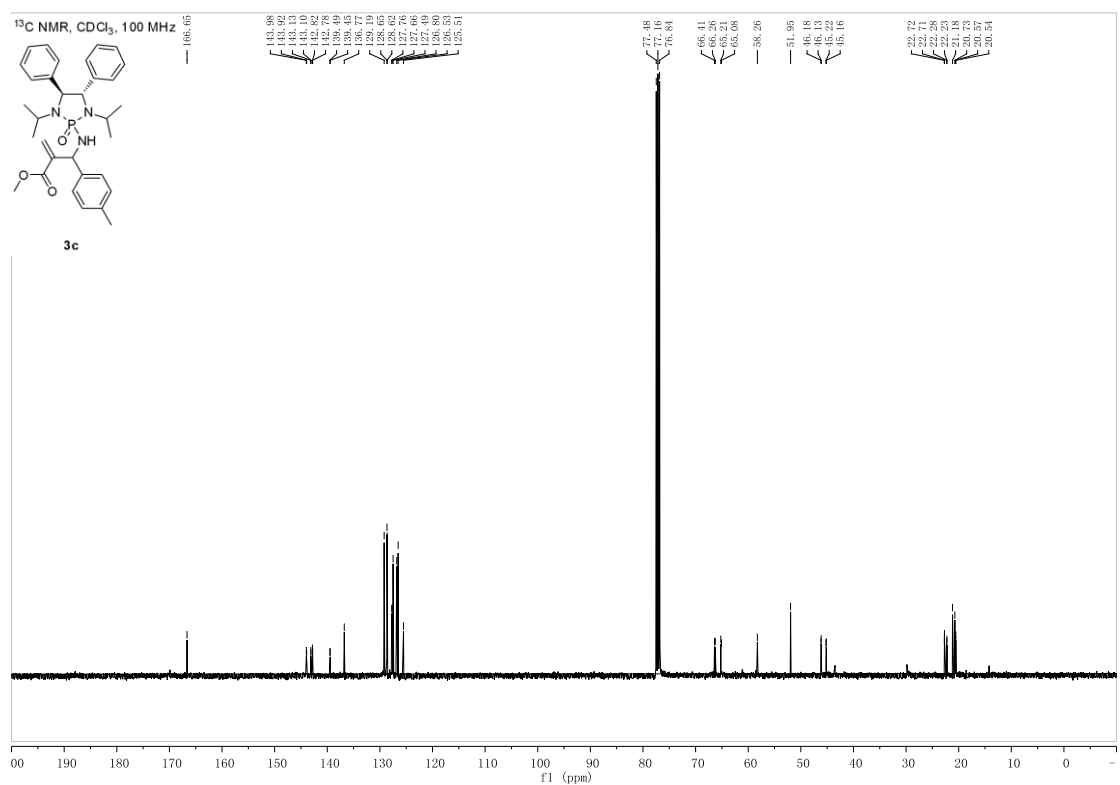
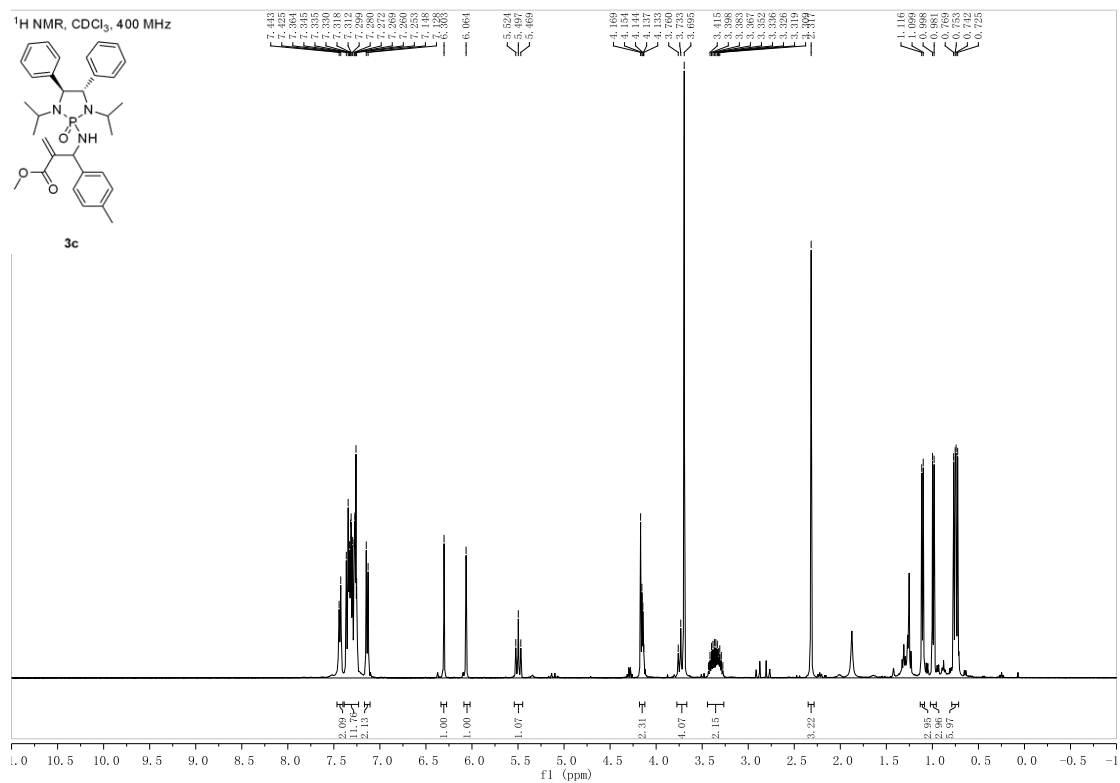
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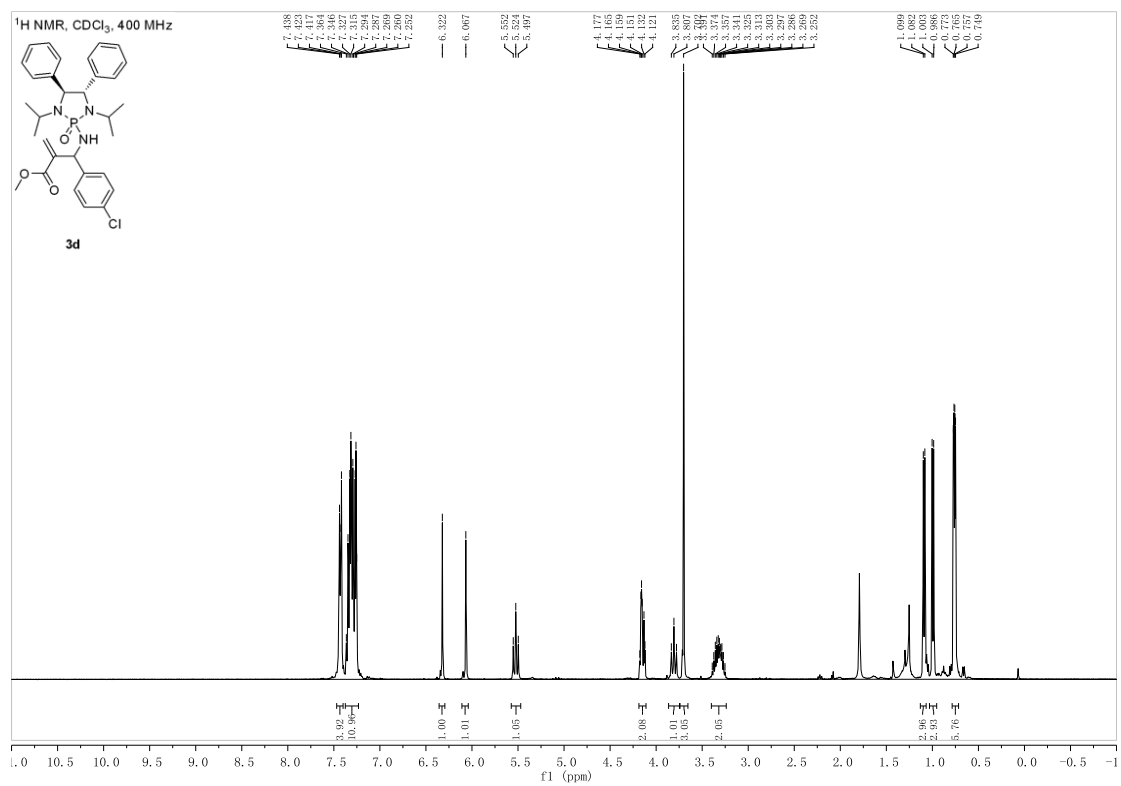
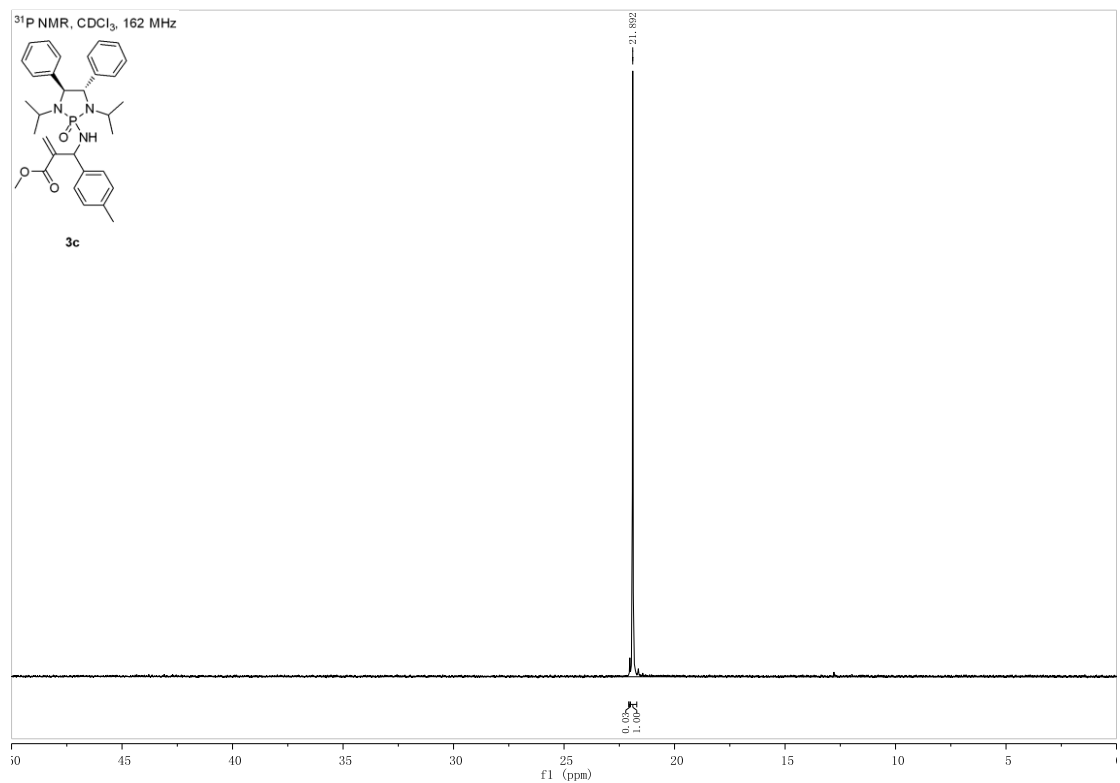
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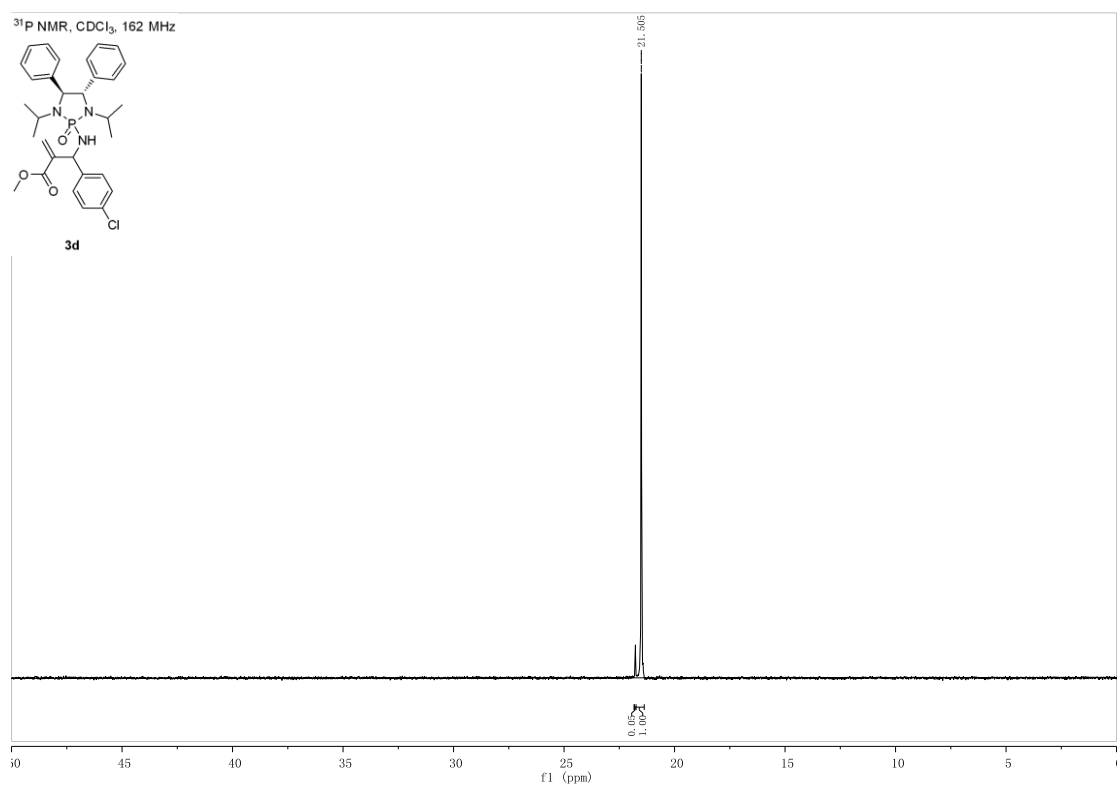
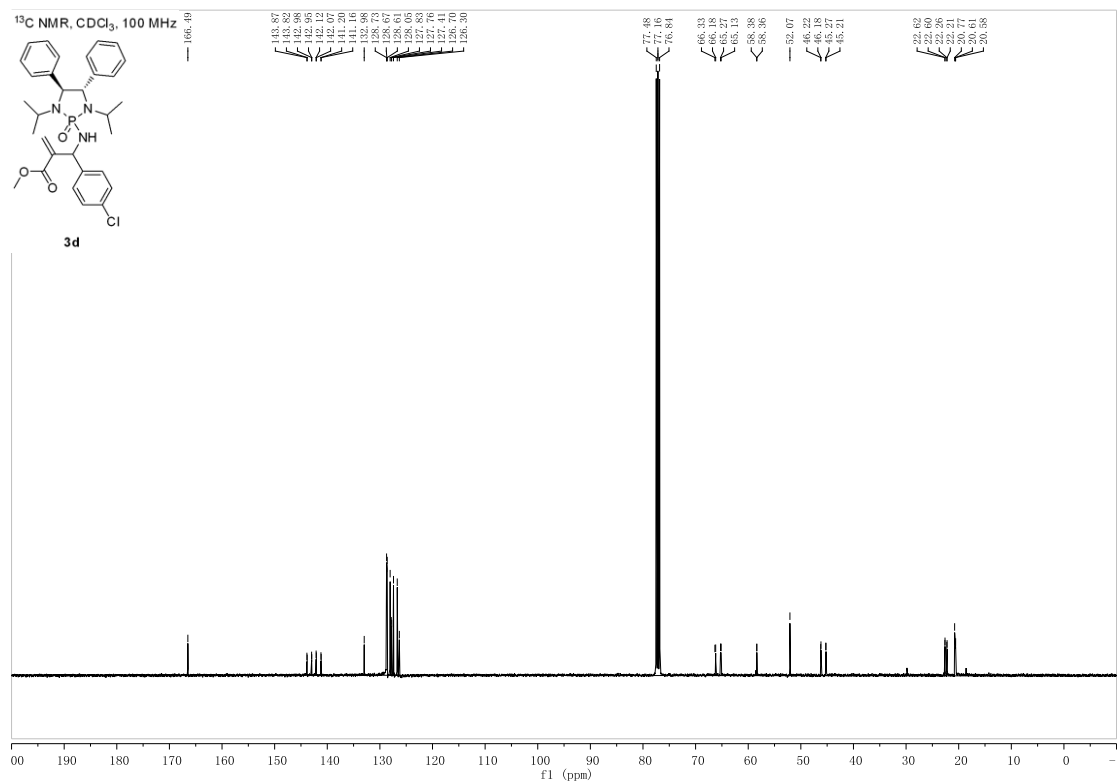
NMR spectra of 3a-j

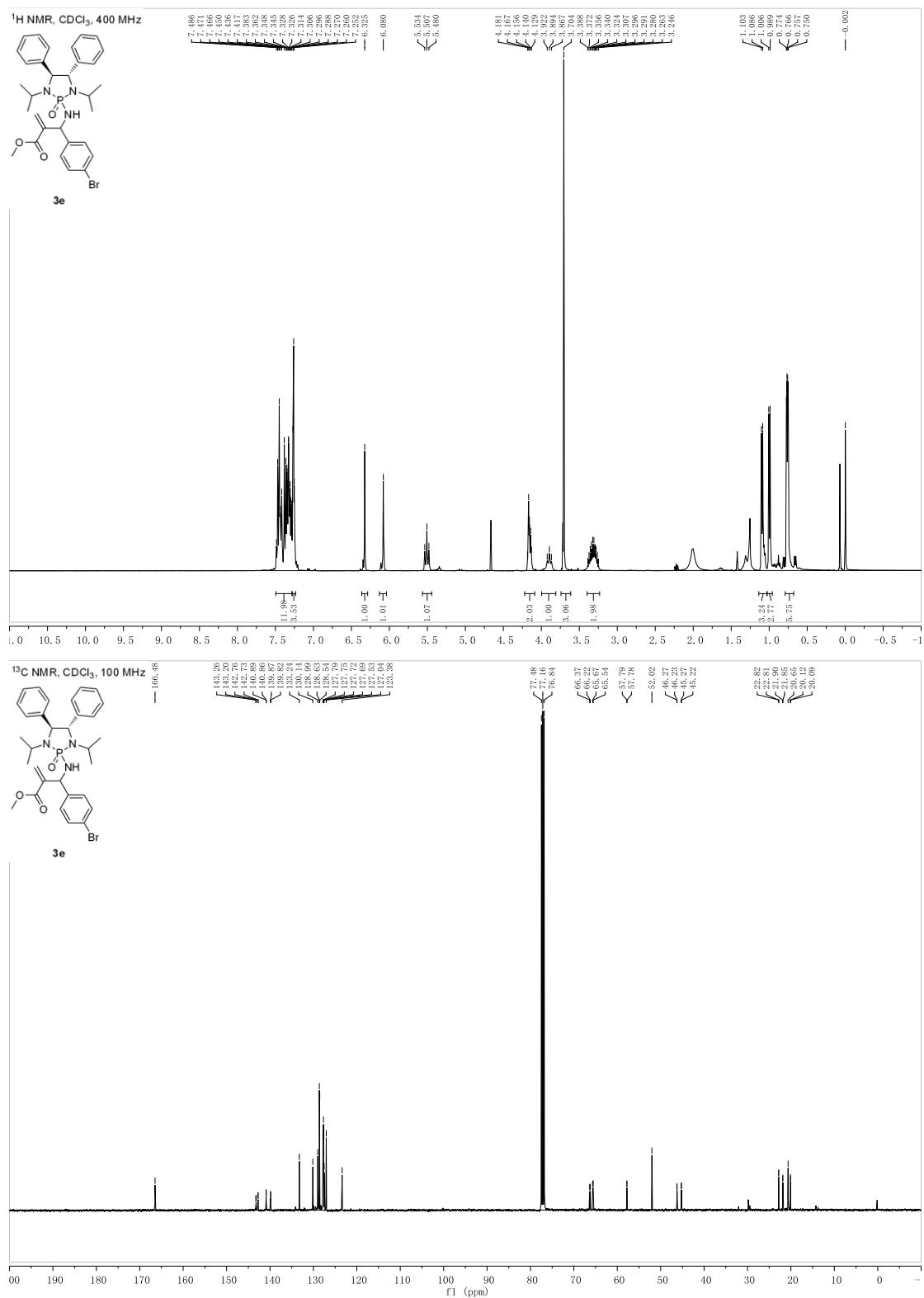


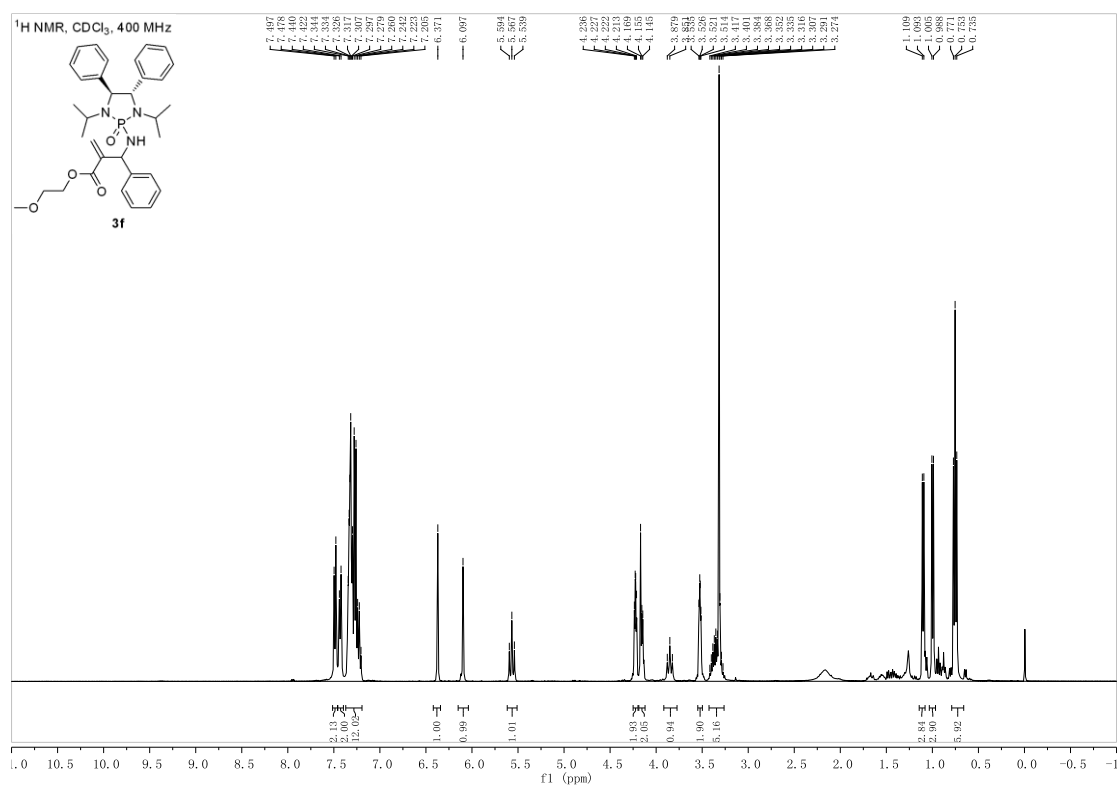
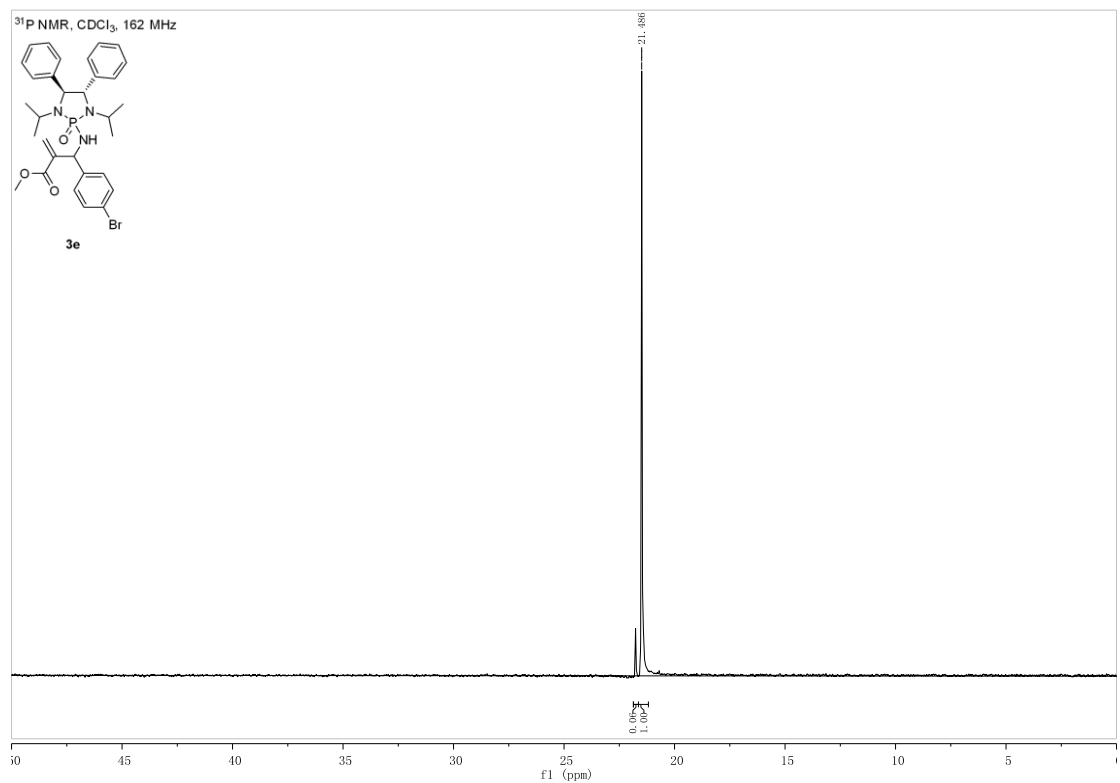


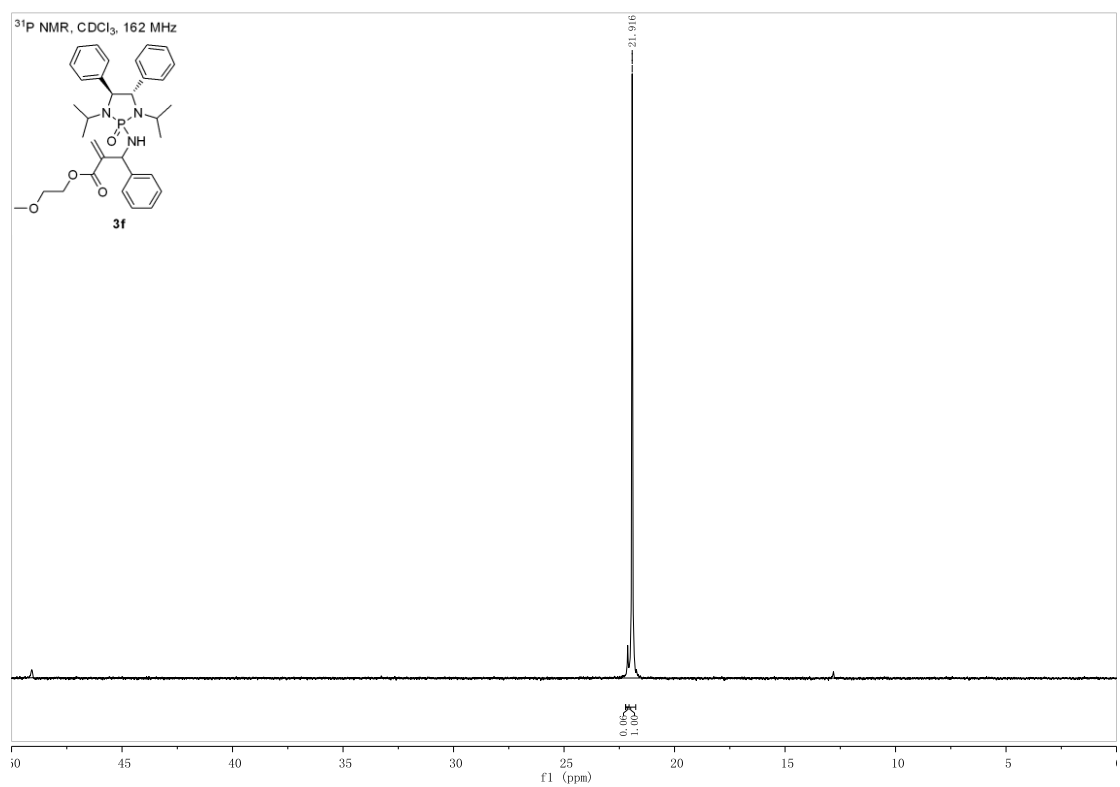
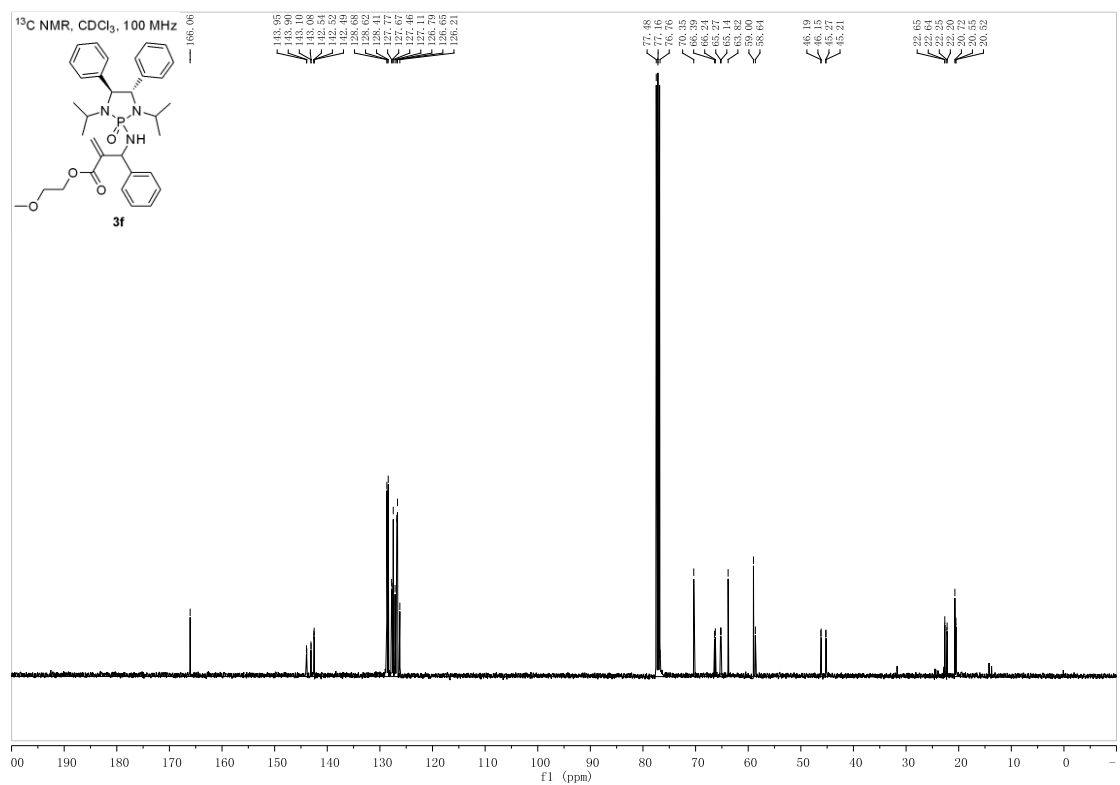


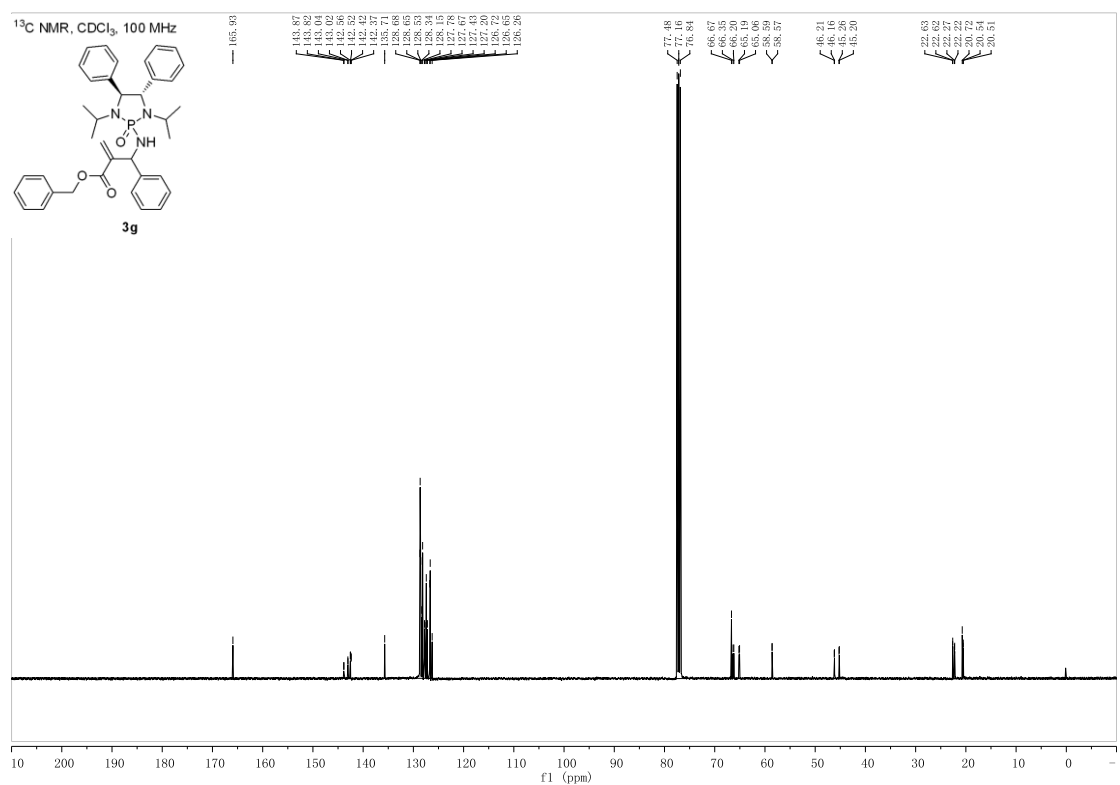
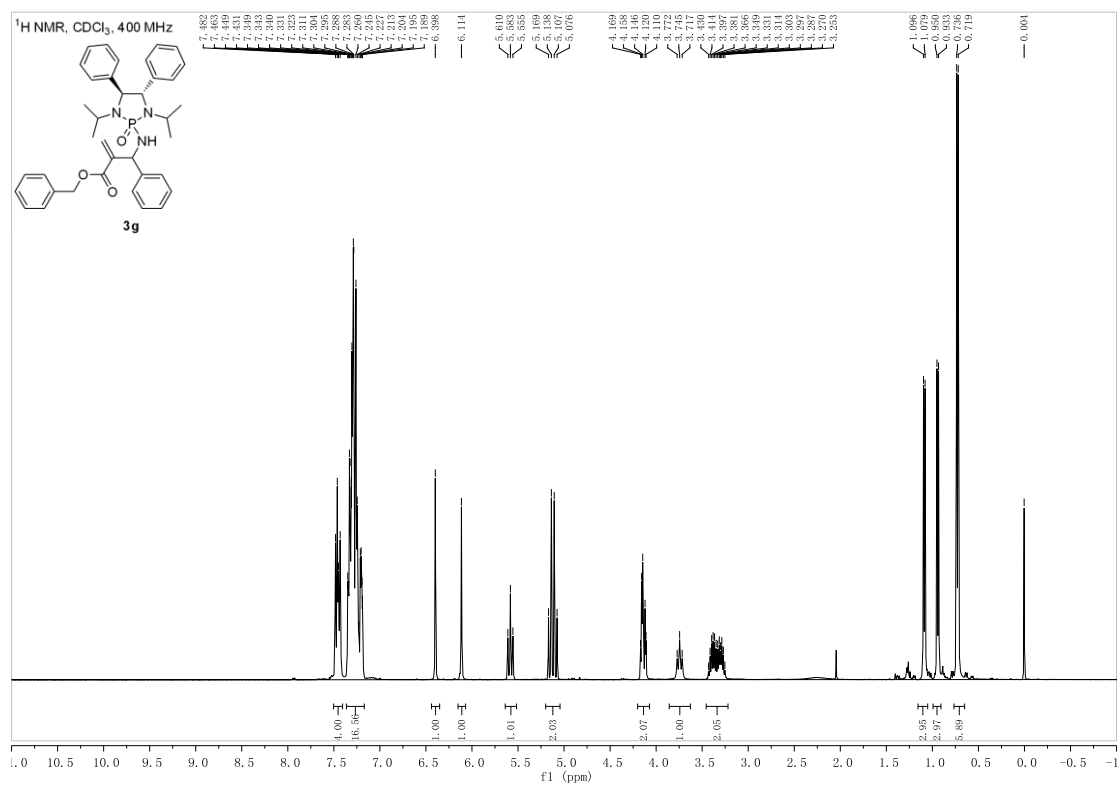


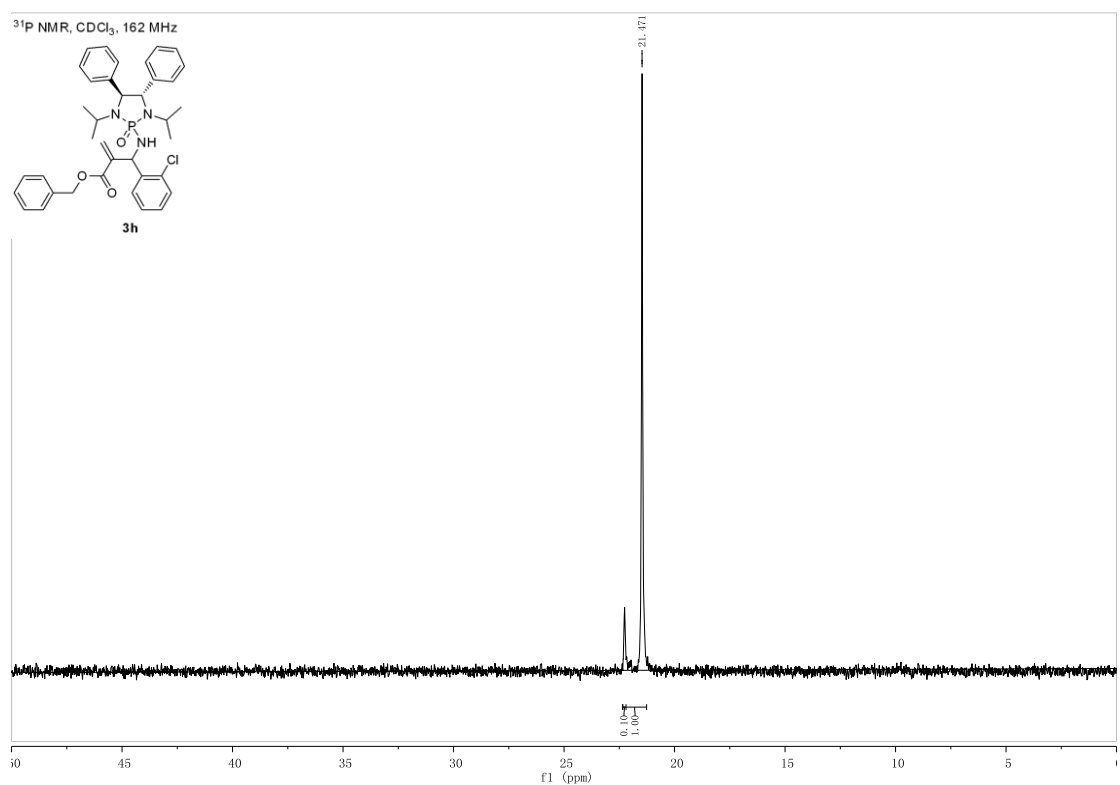
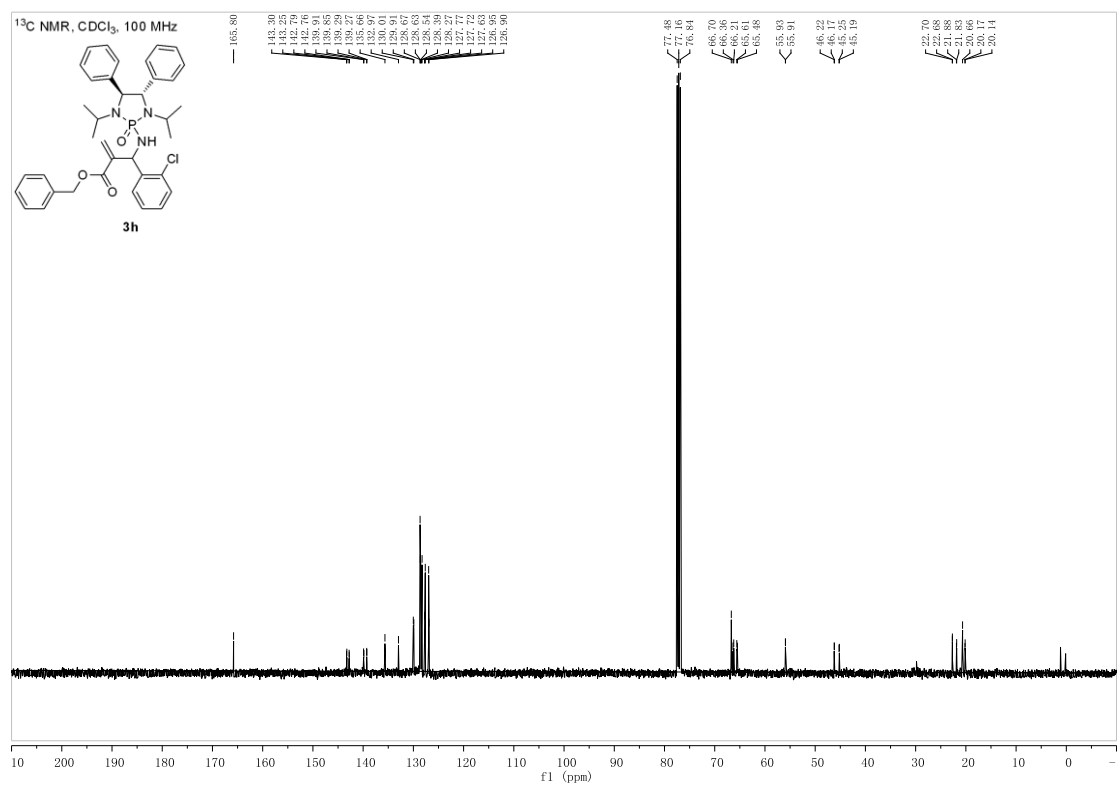


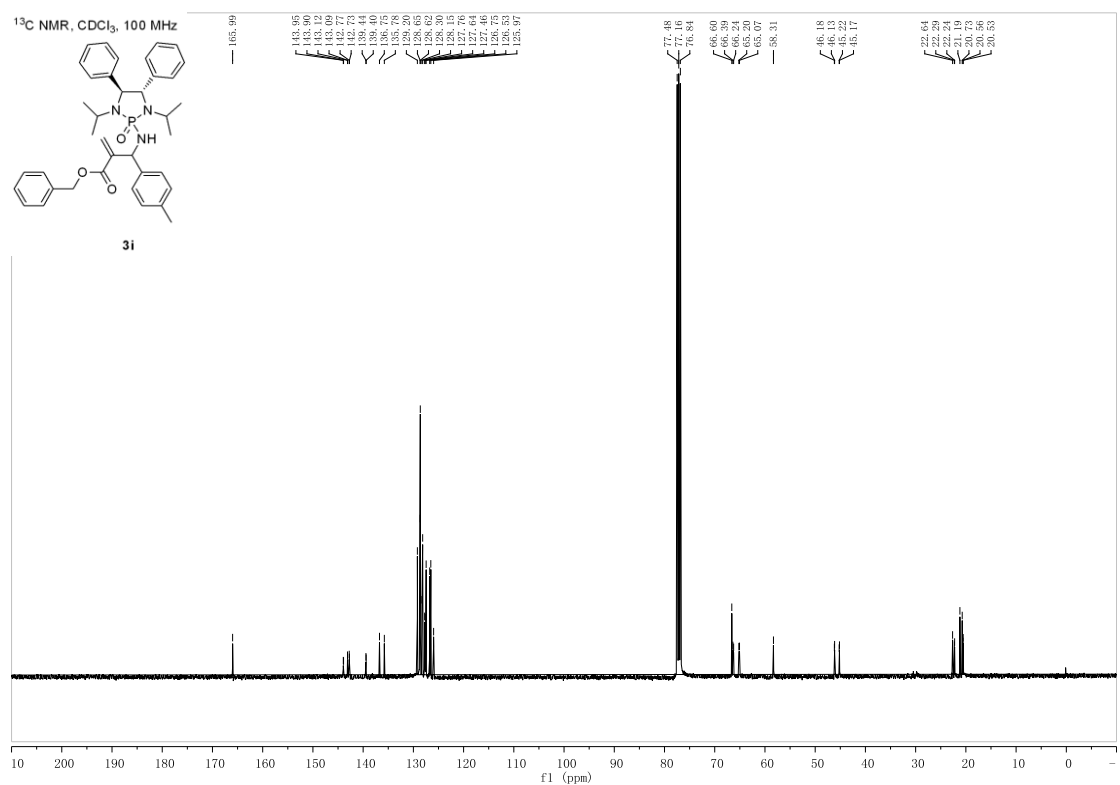
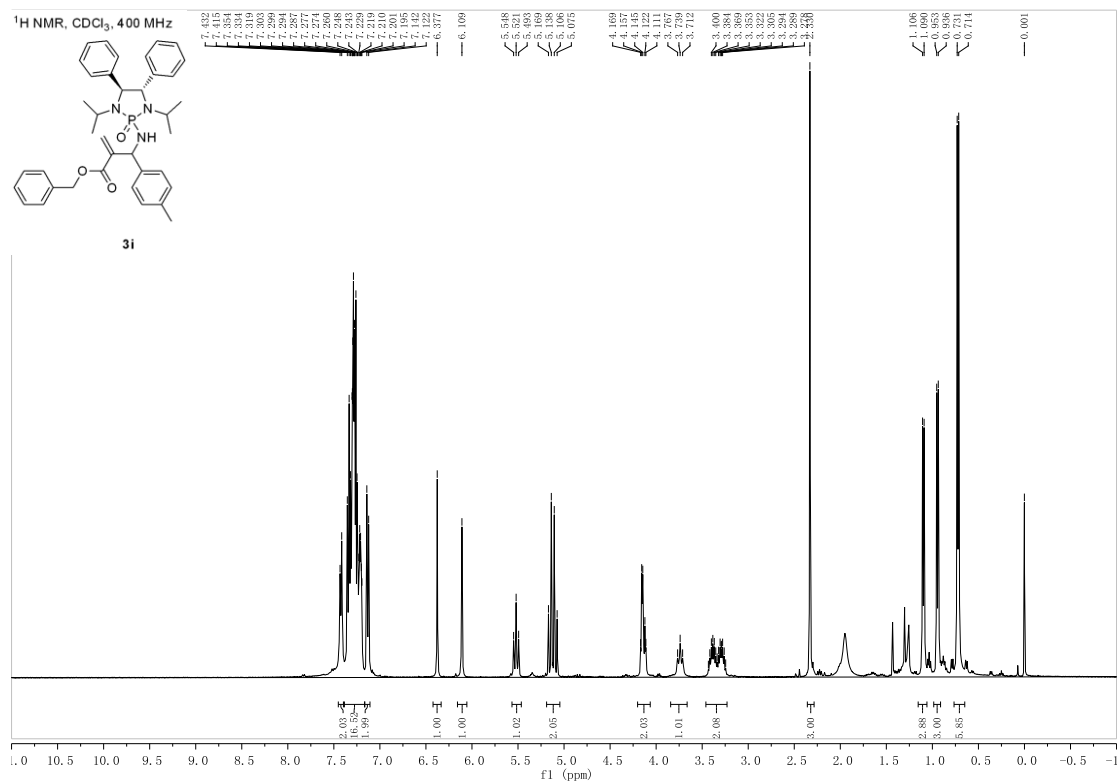


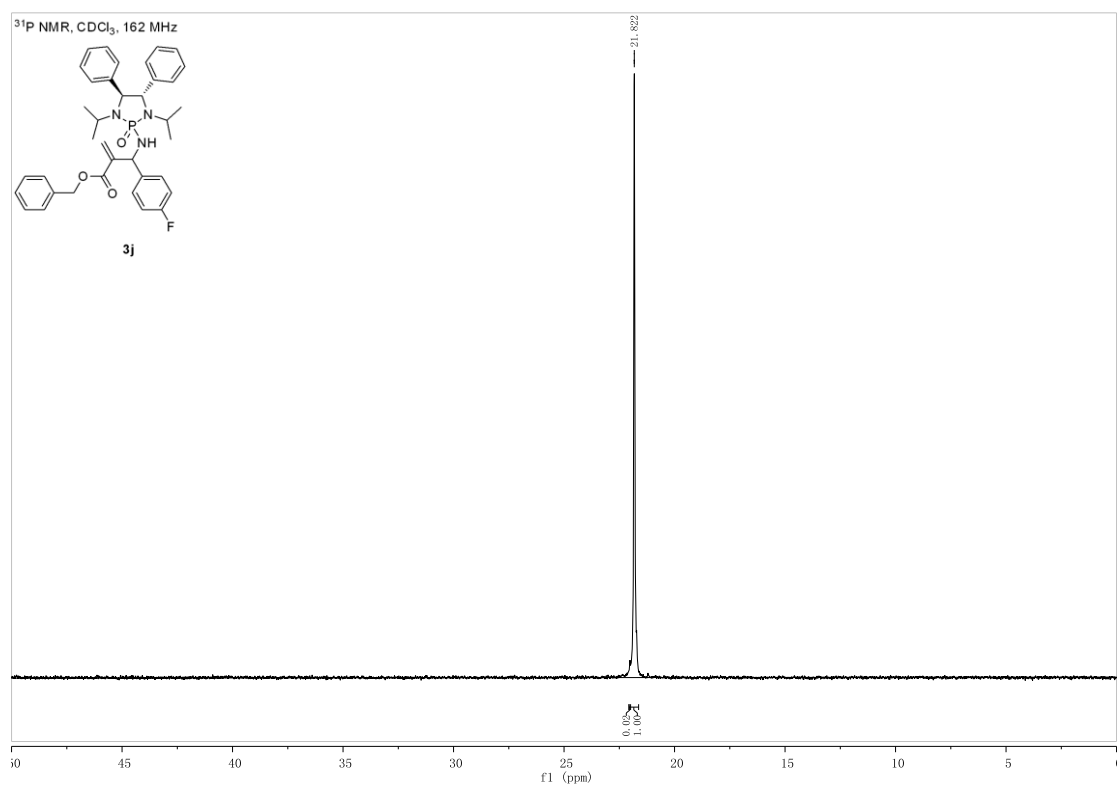
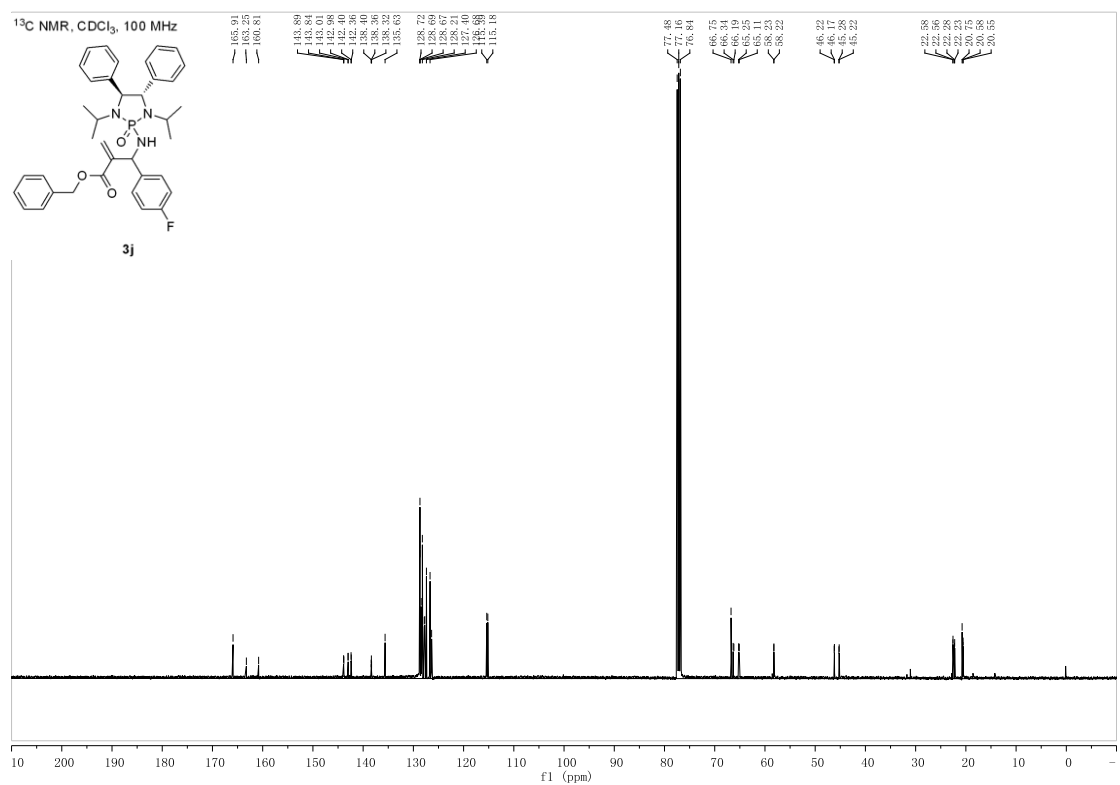


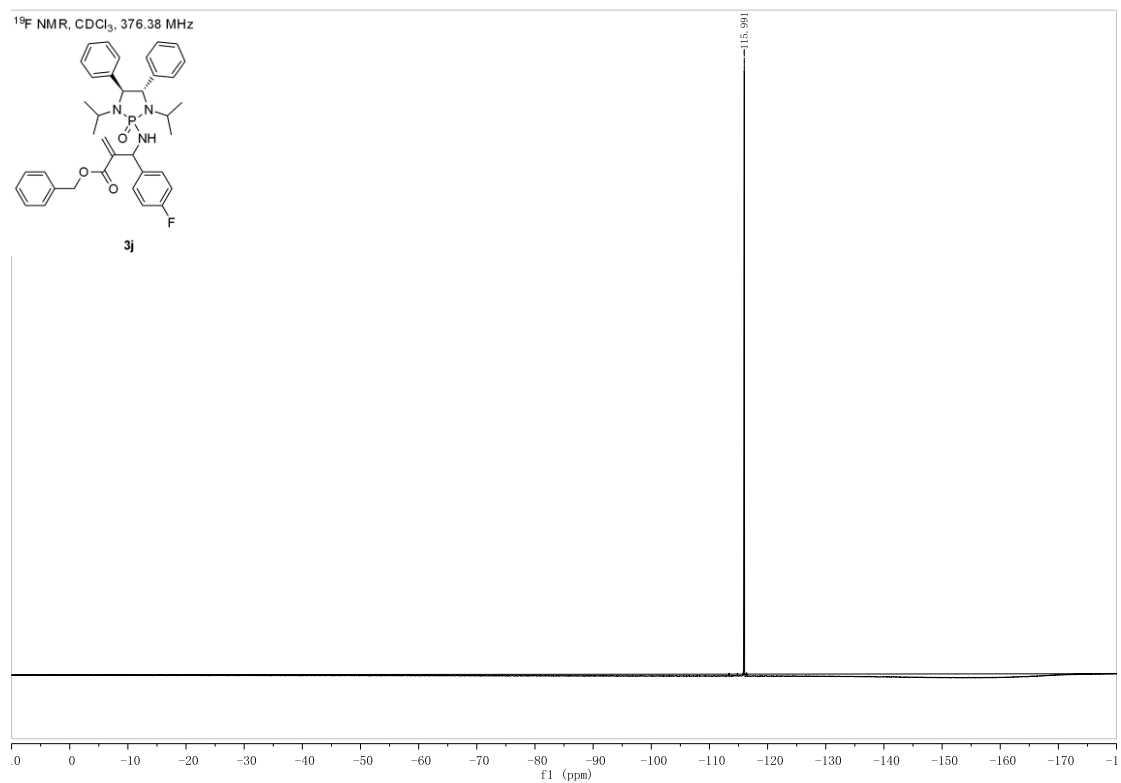




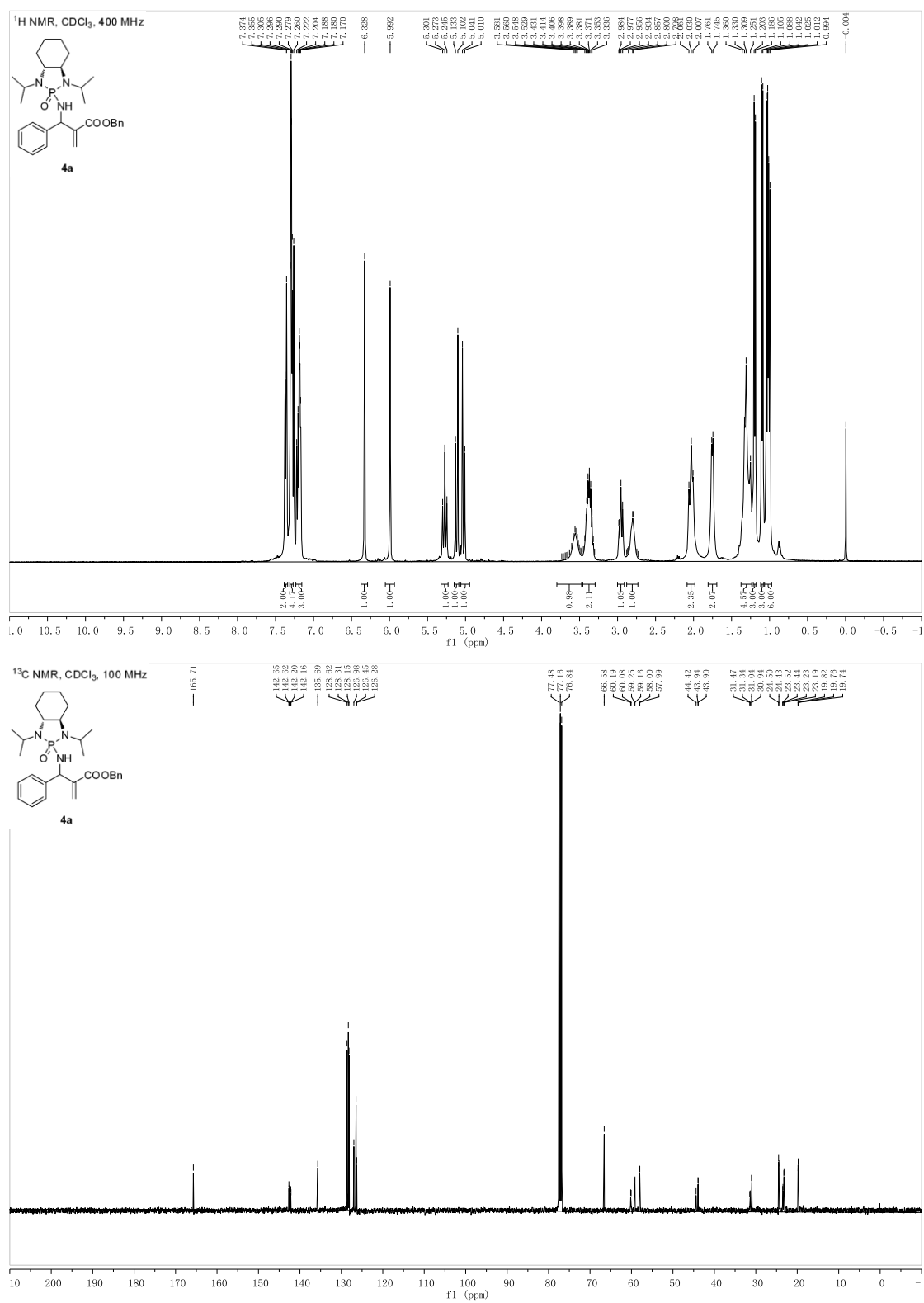


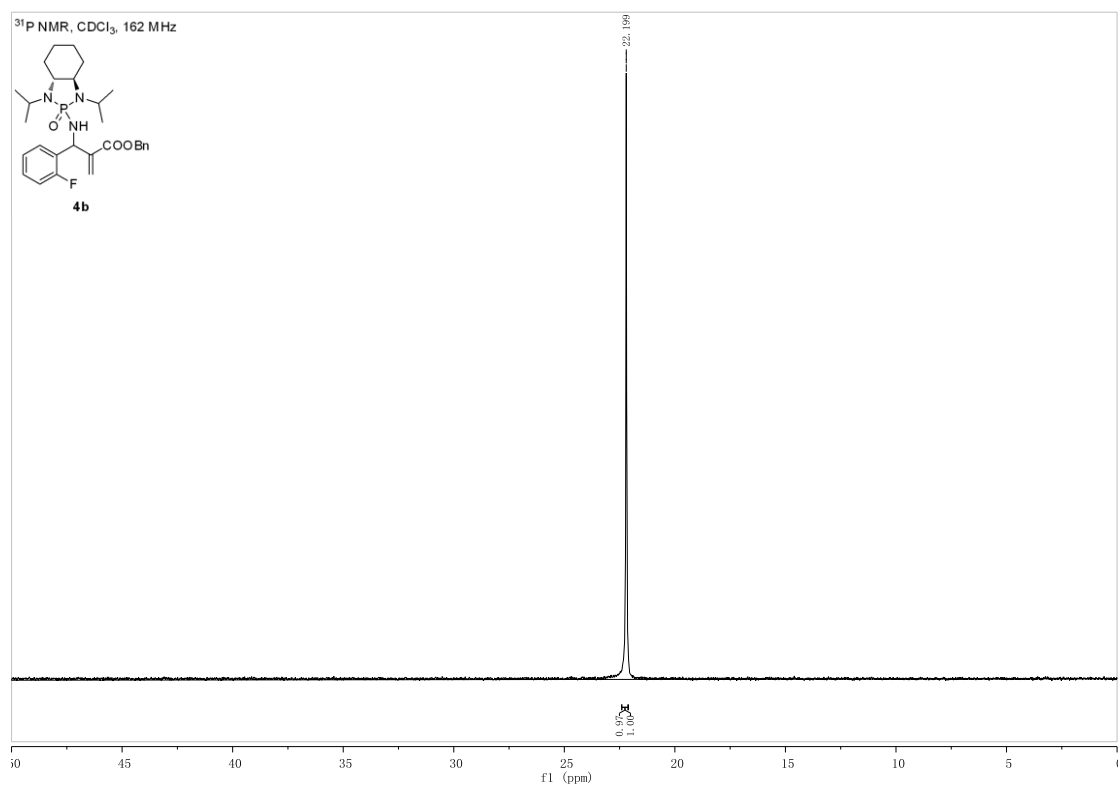
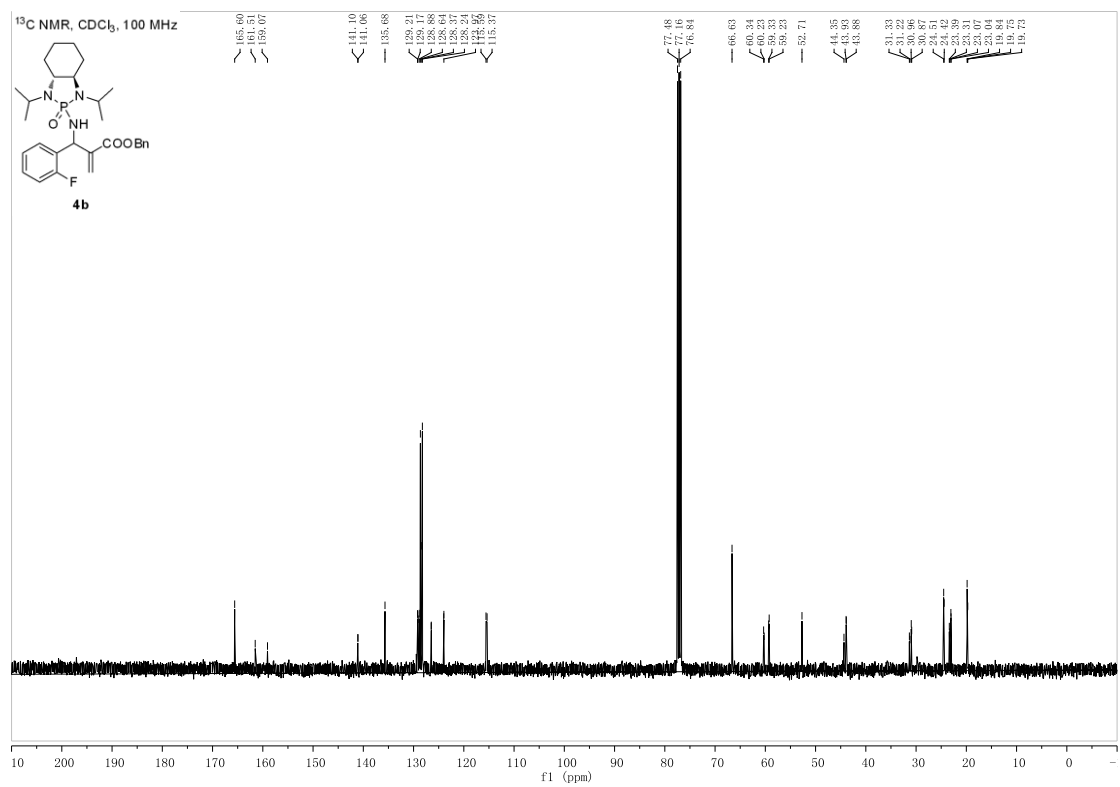


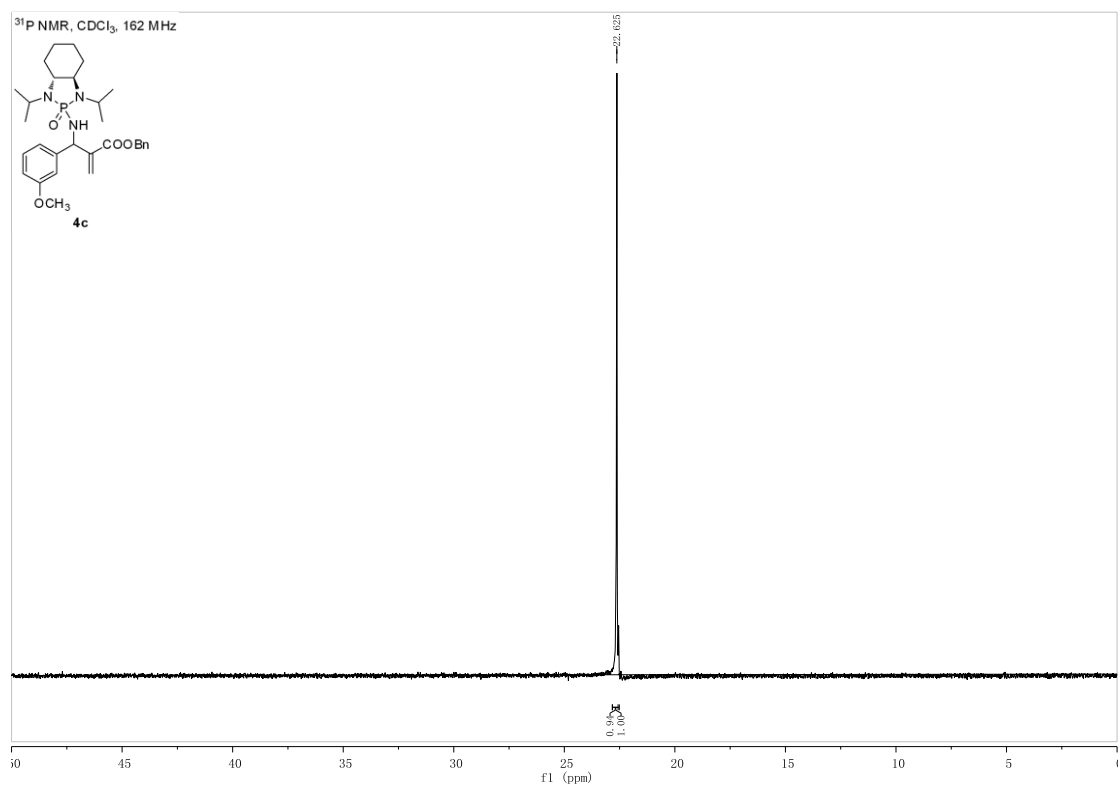
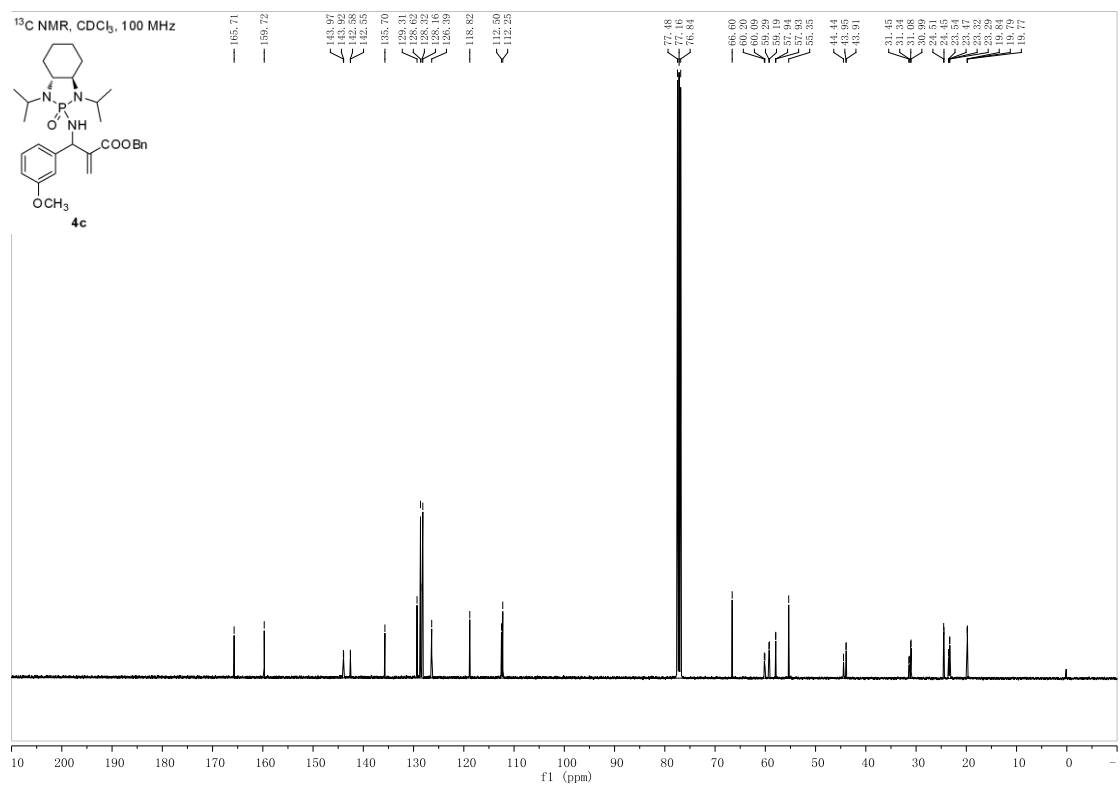


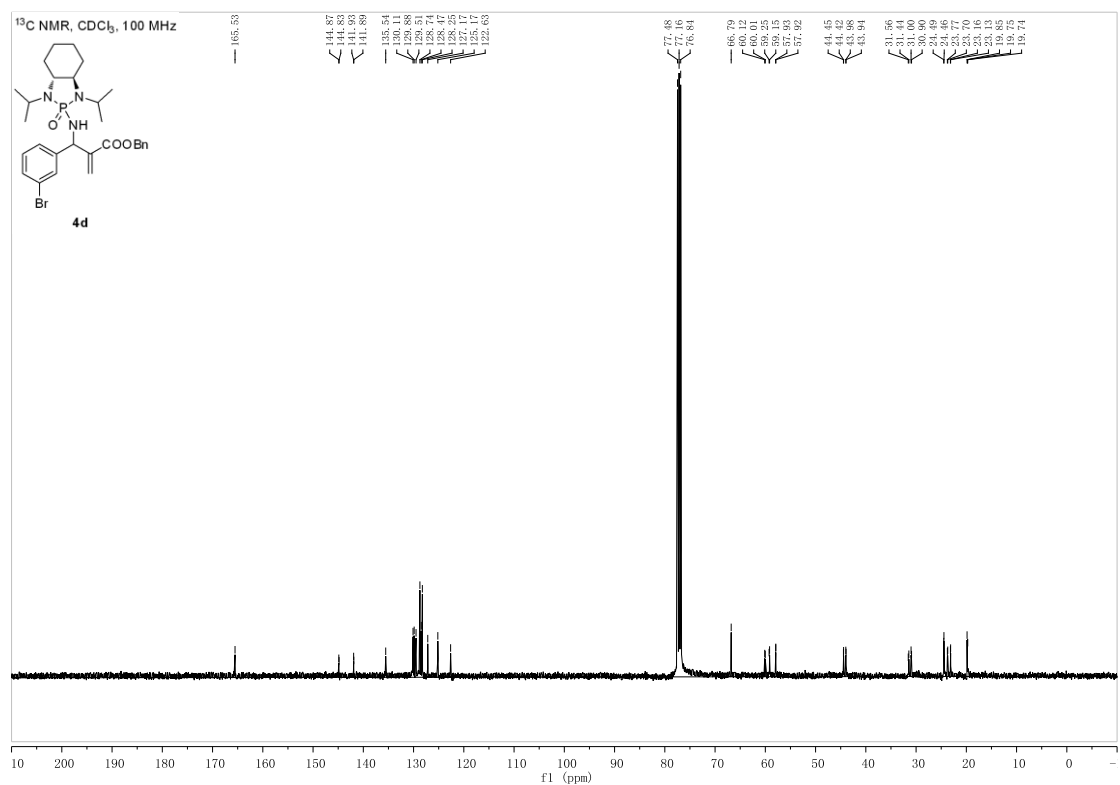
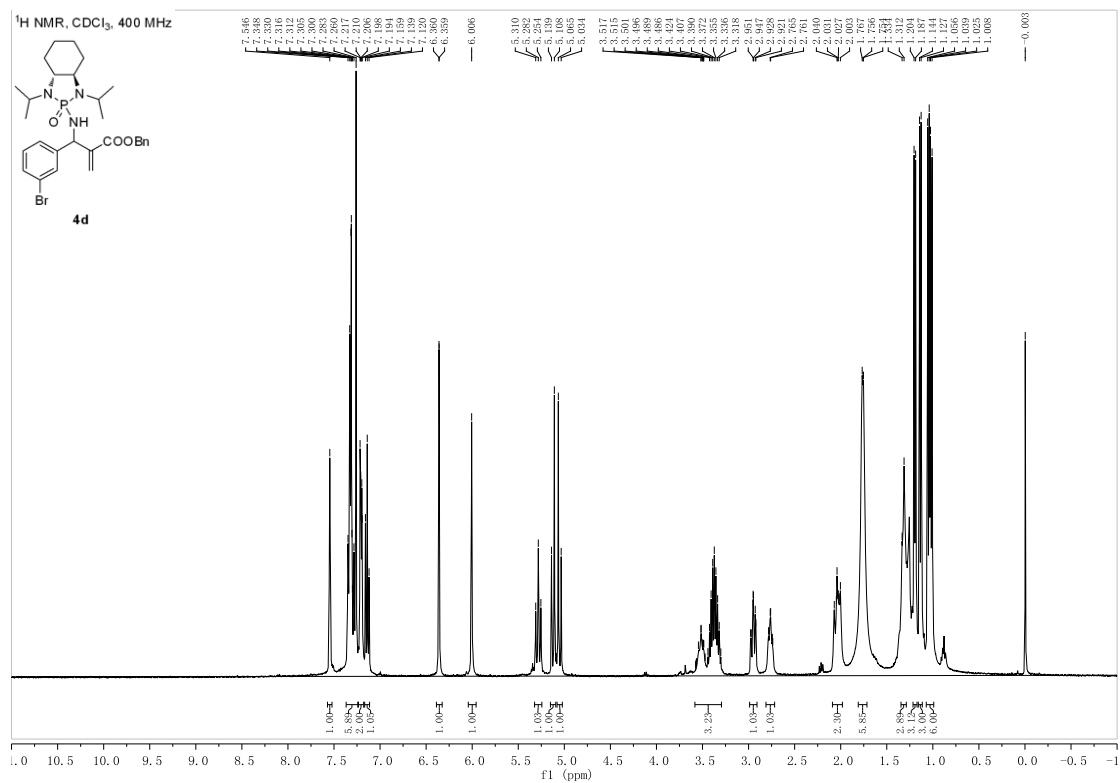


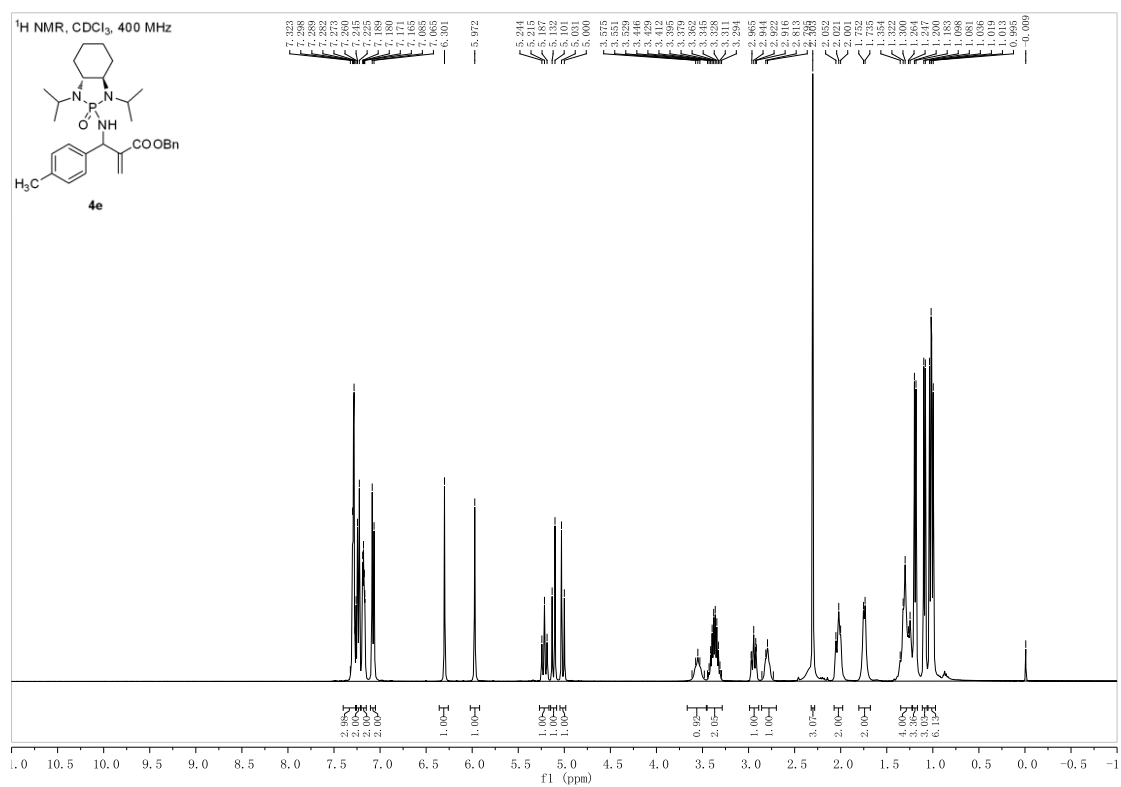
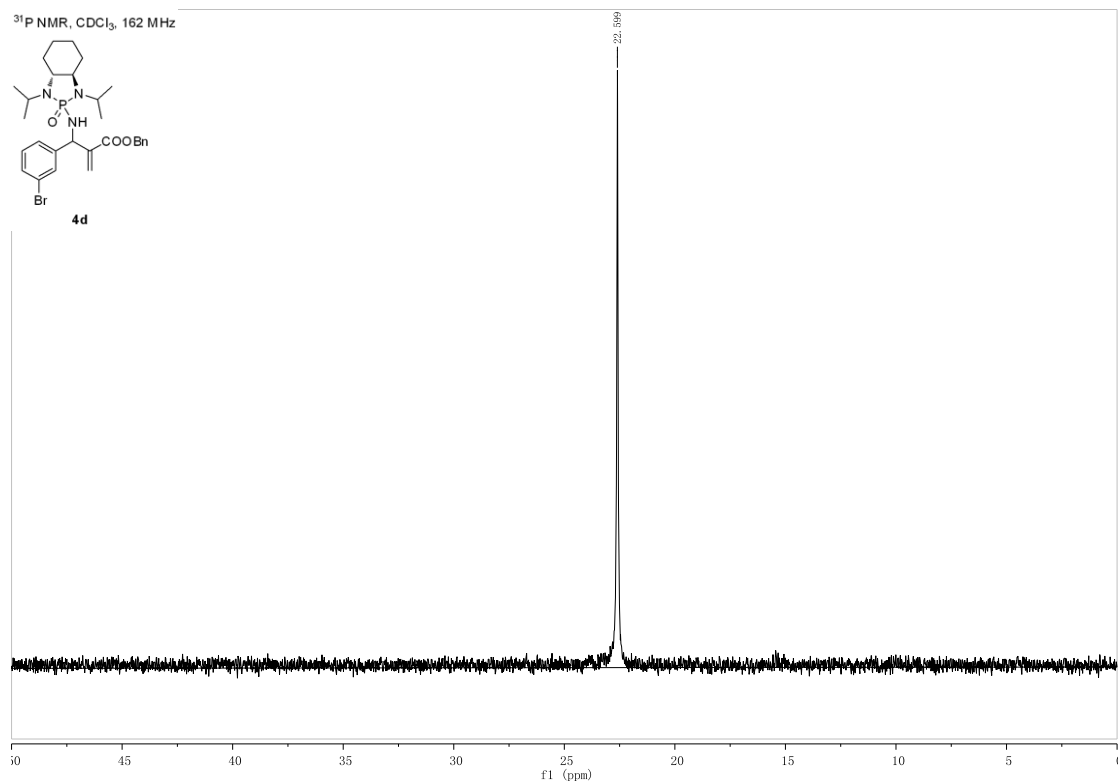
NMR spectra of 4a-t

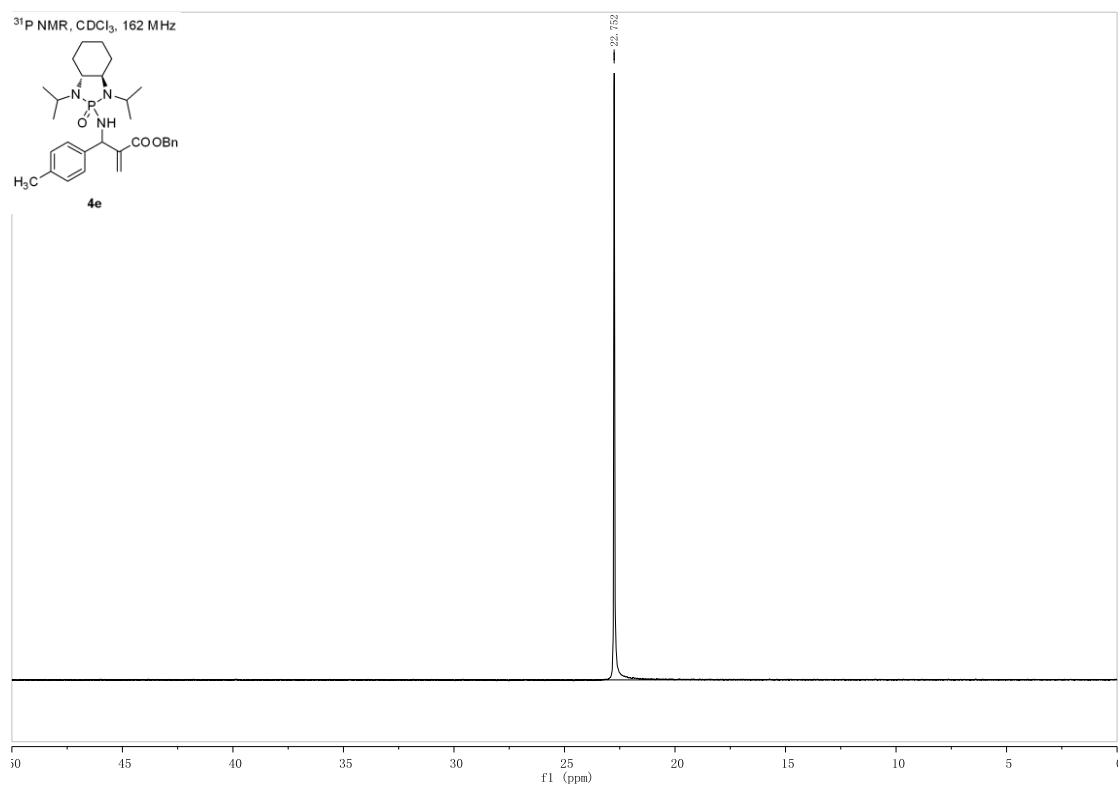
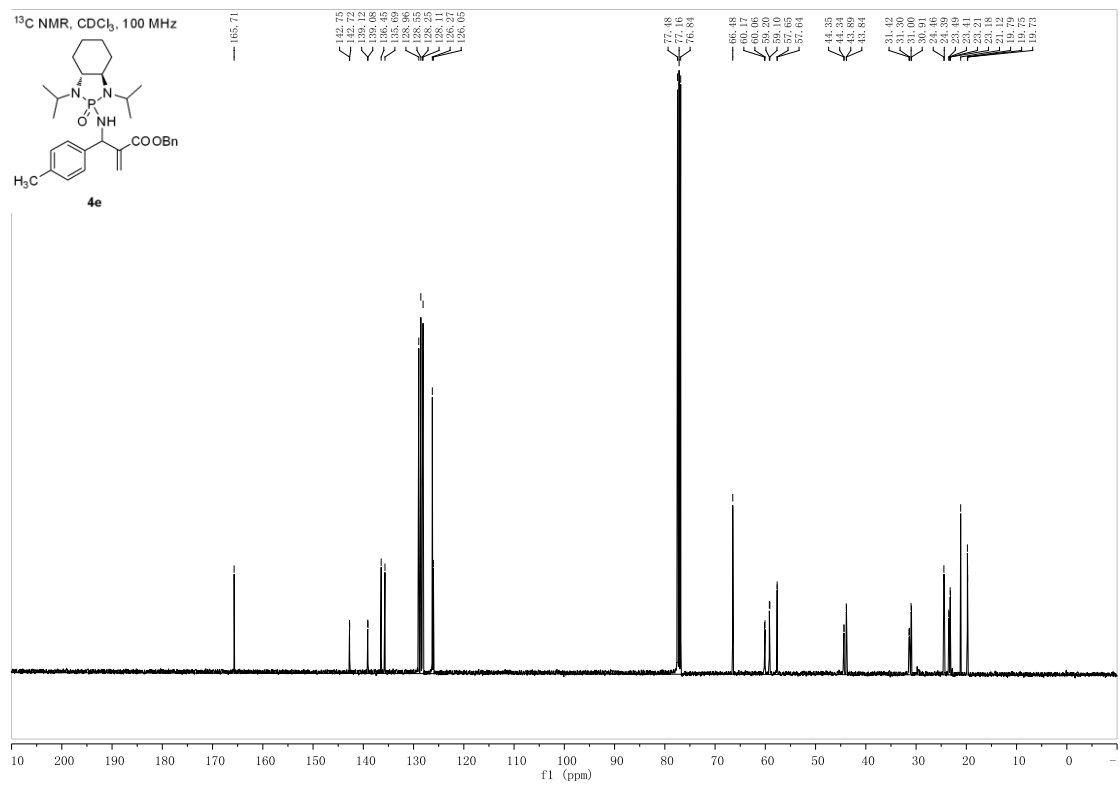


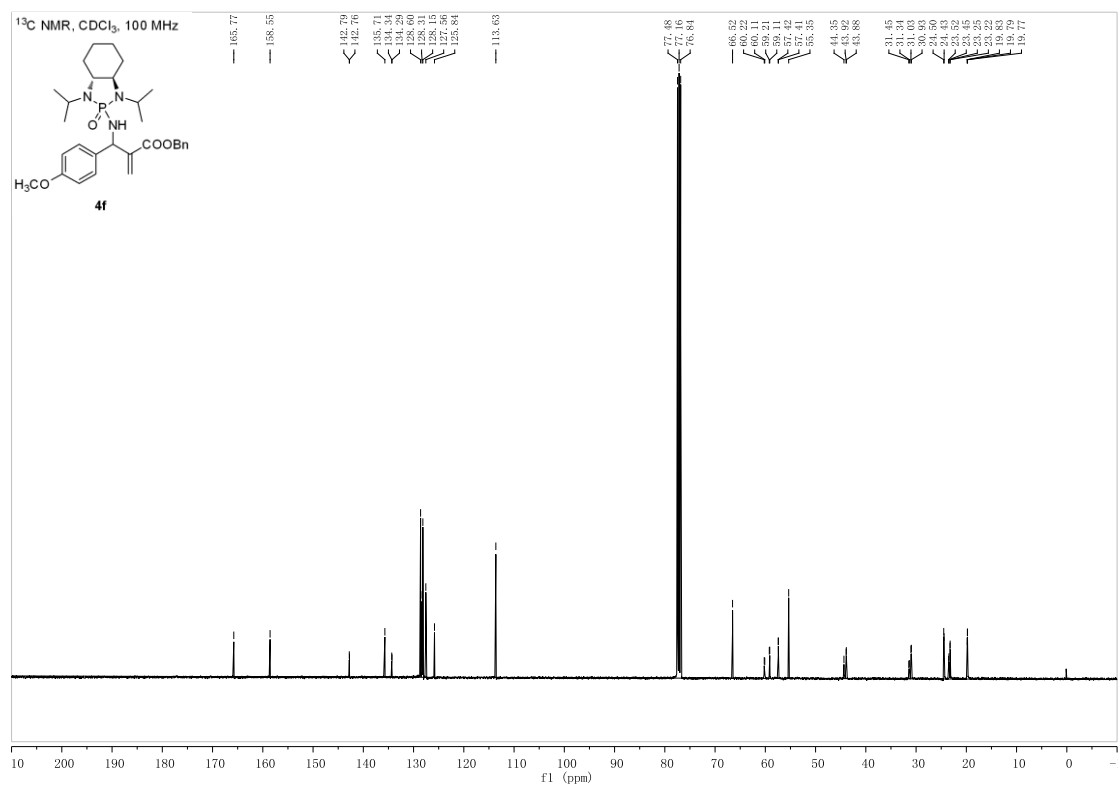
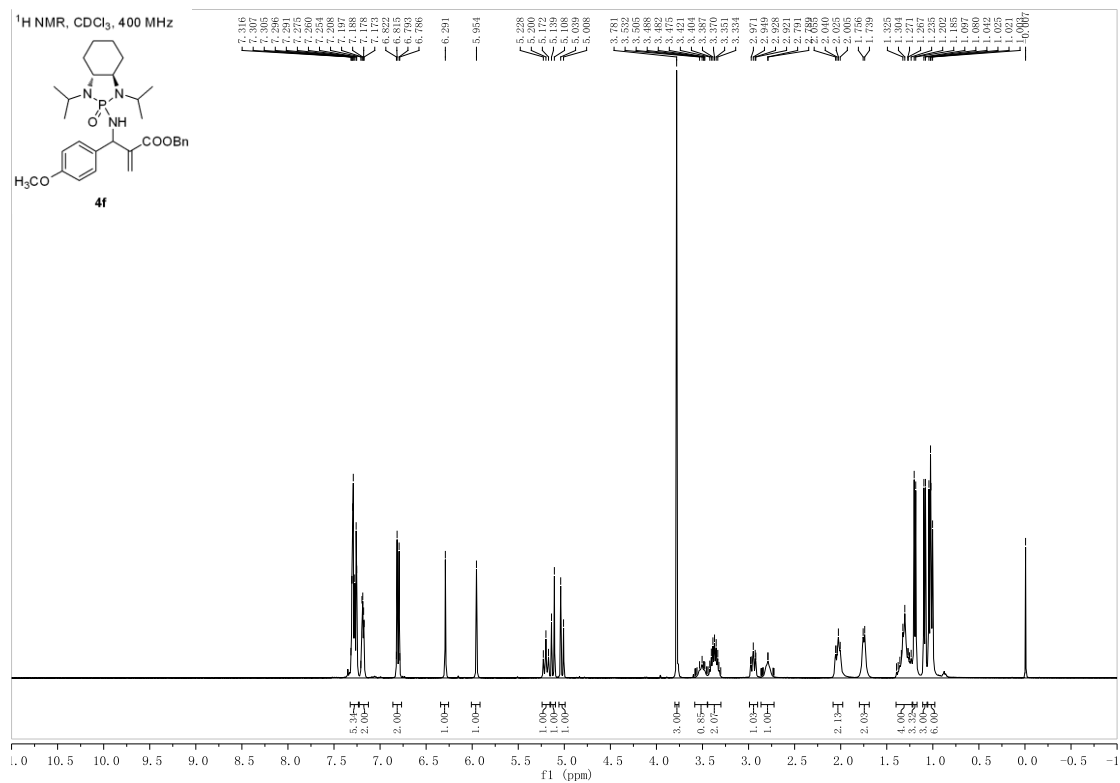


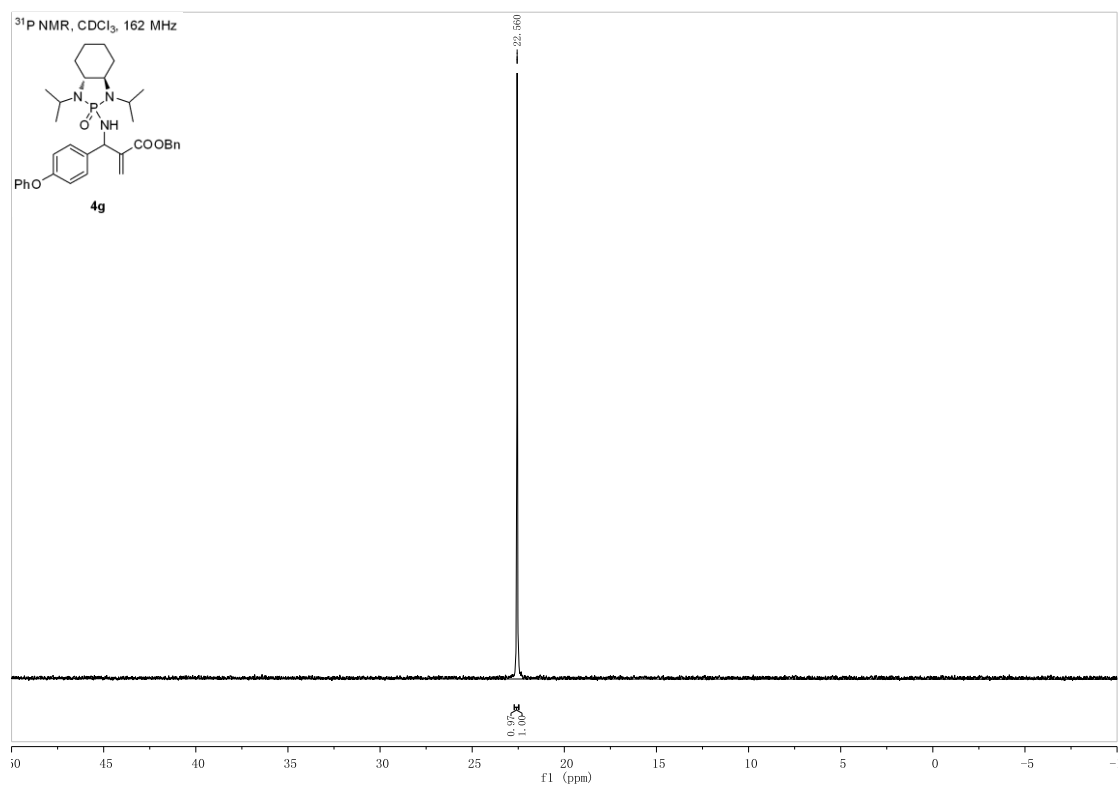
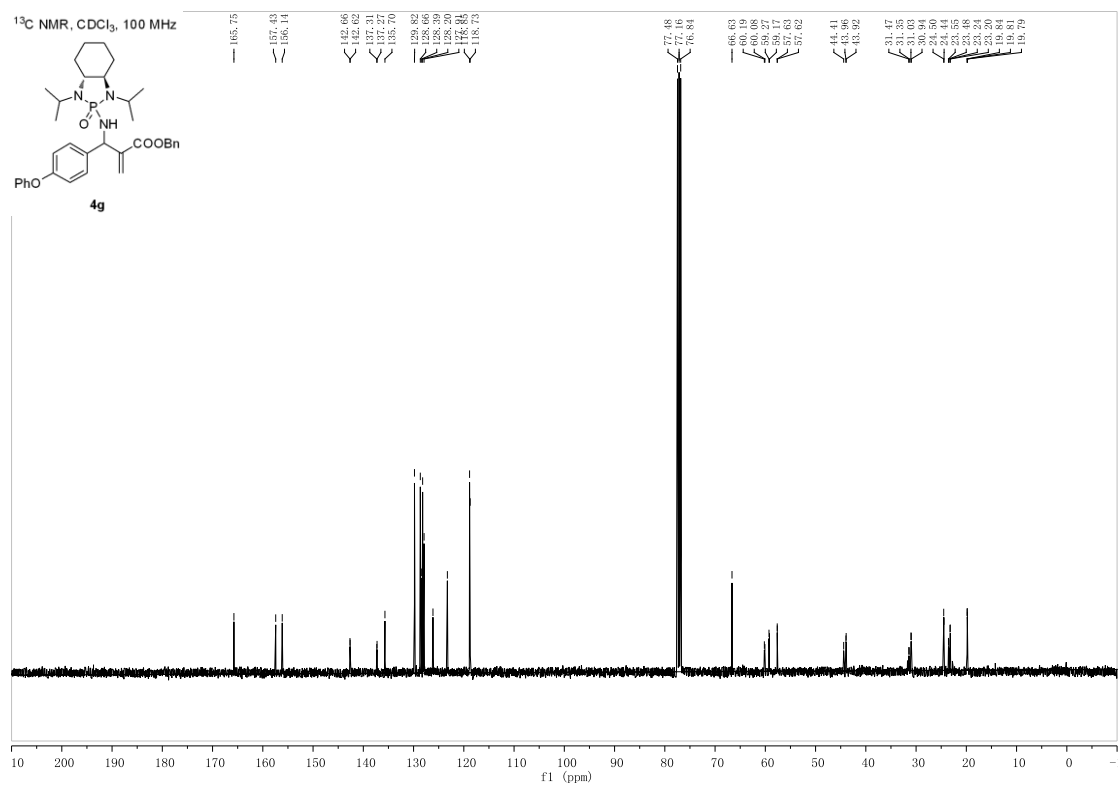


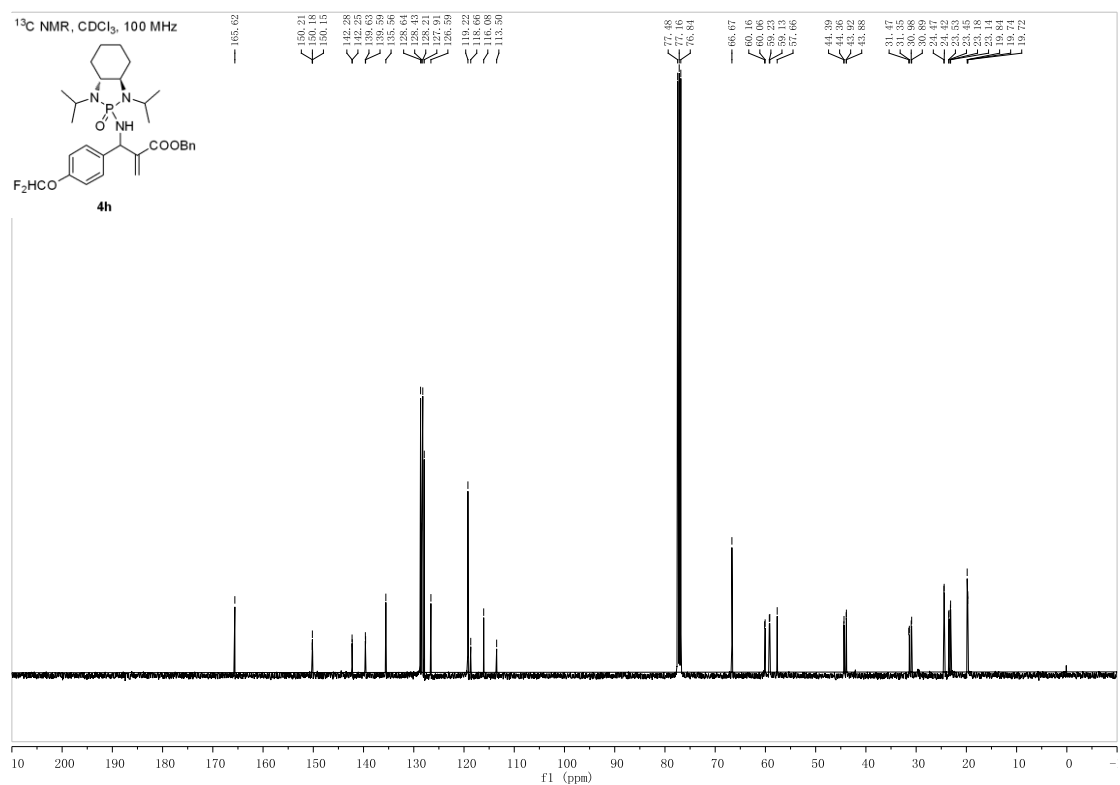
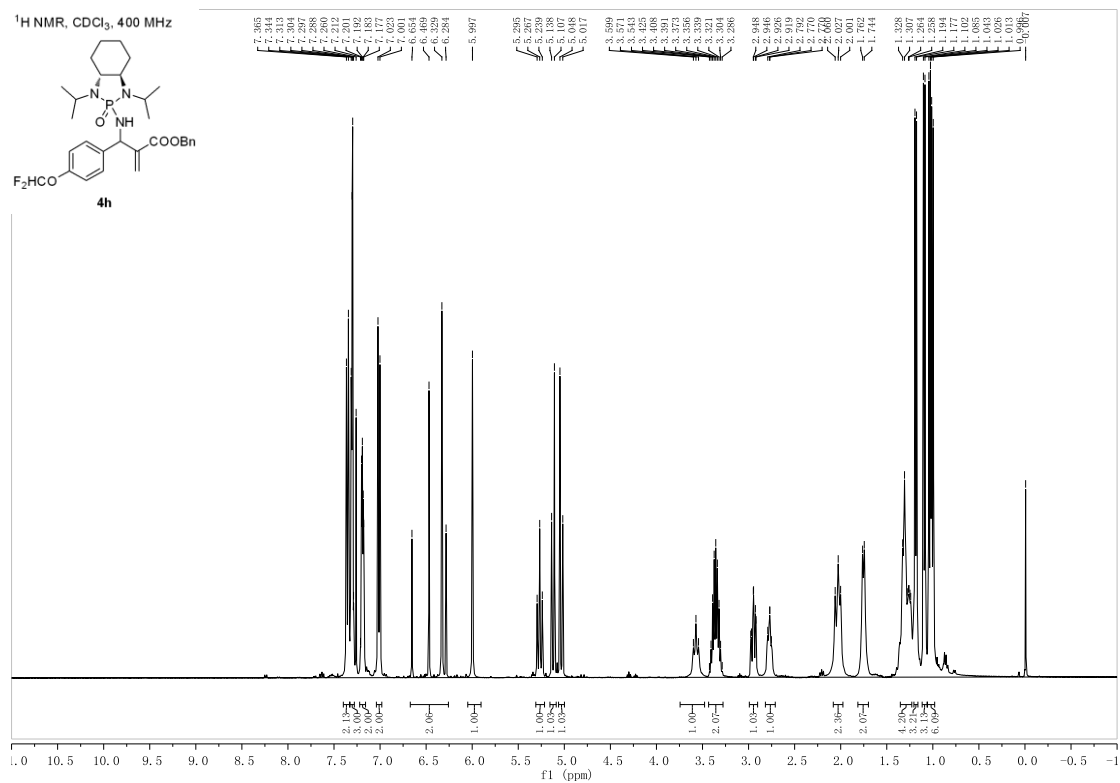


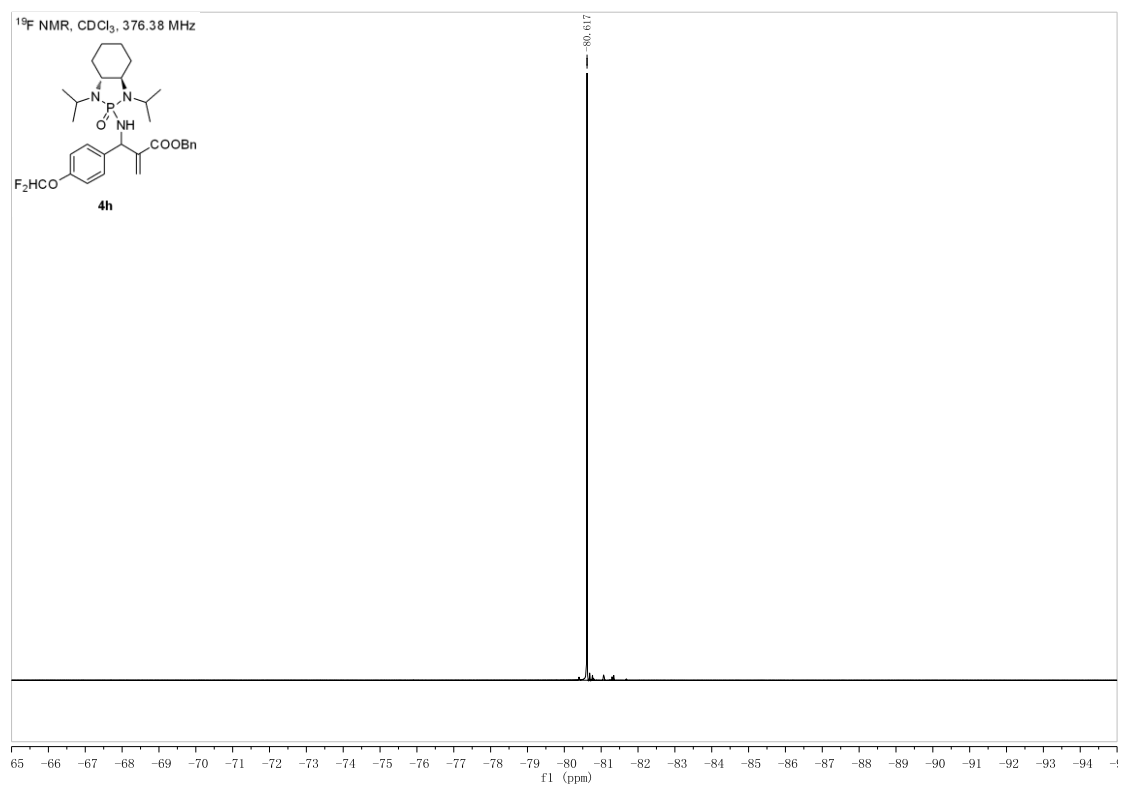
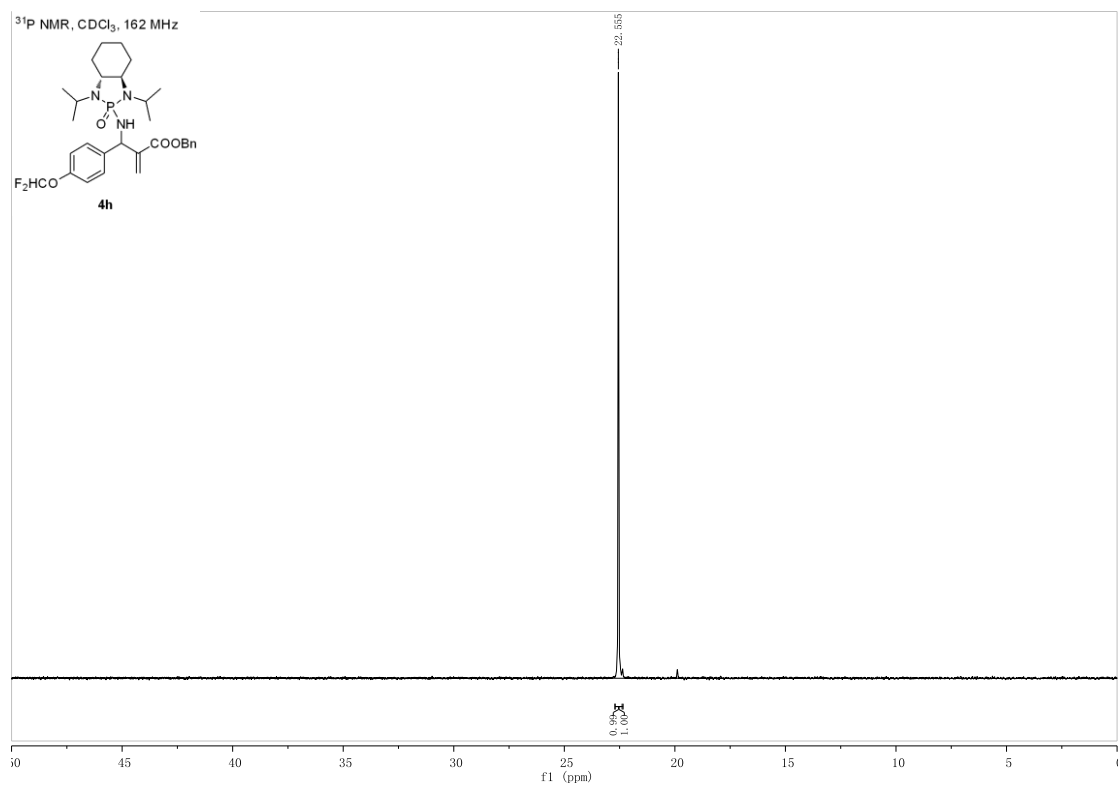


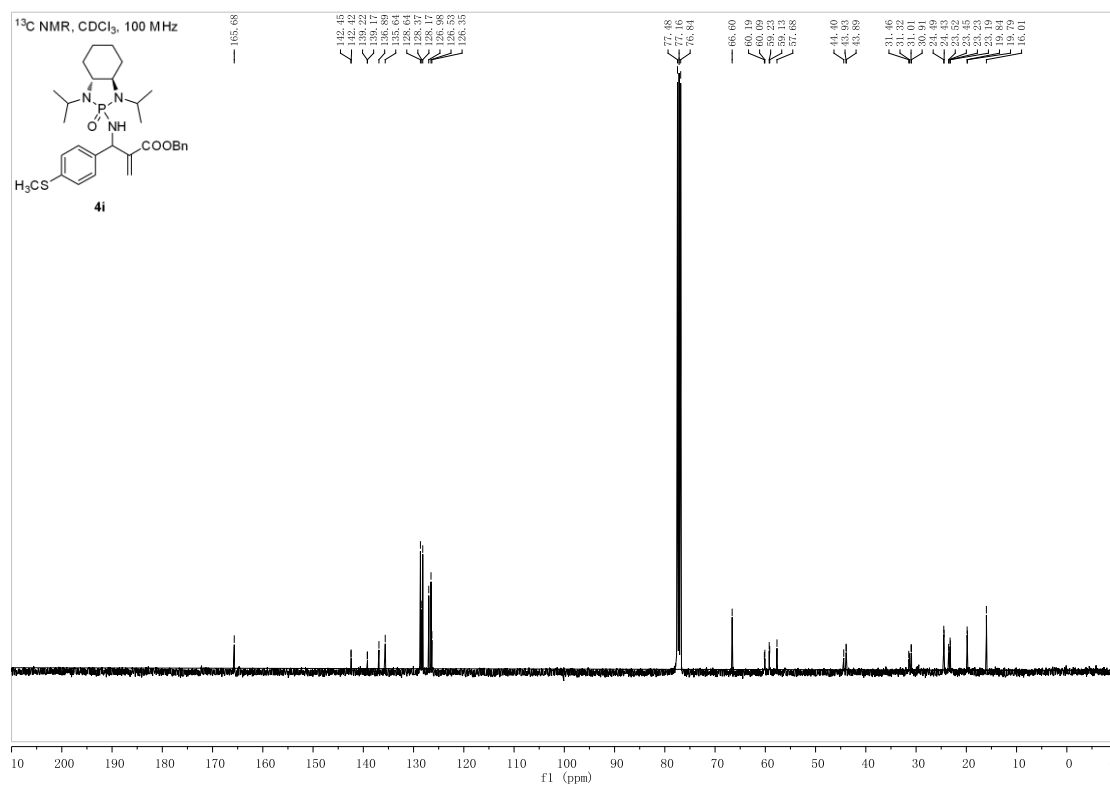
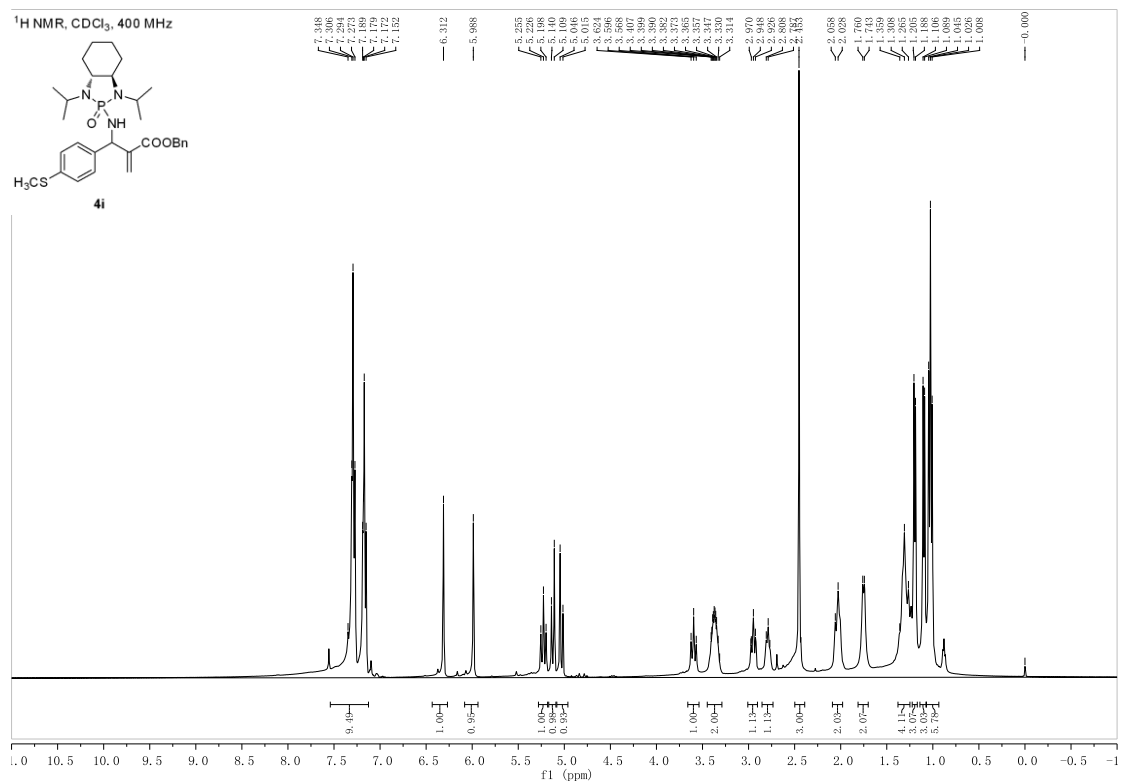


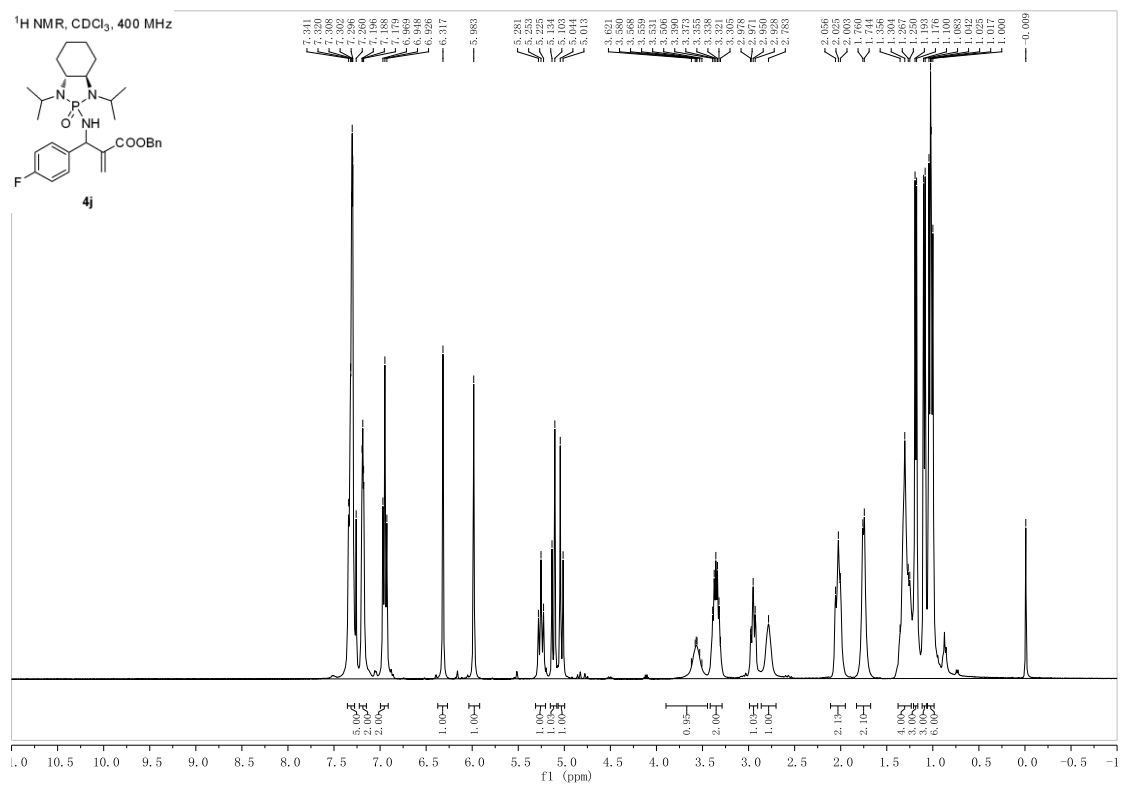
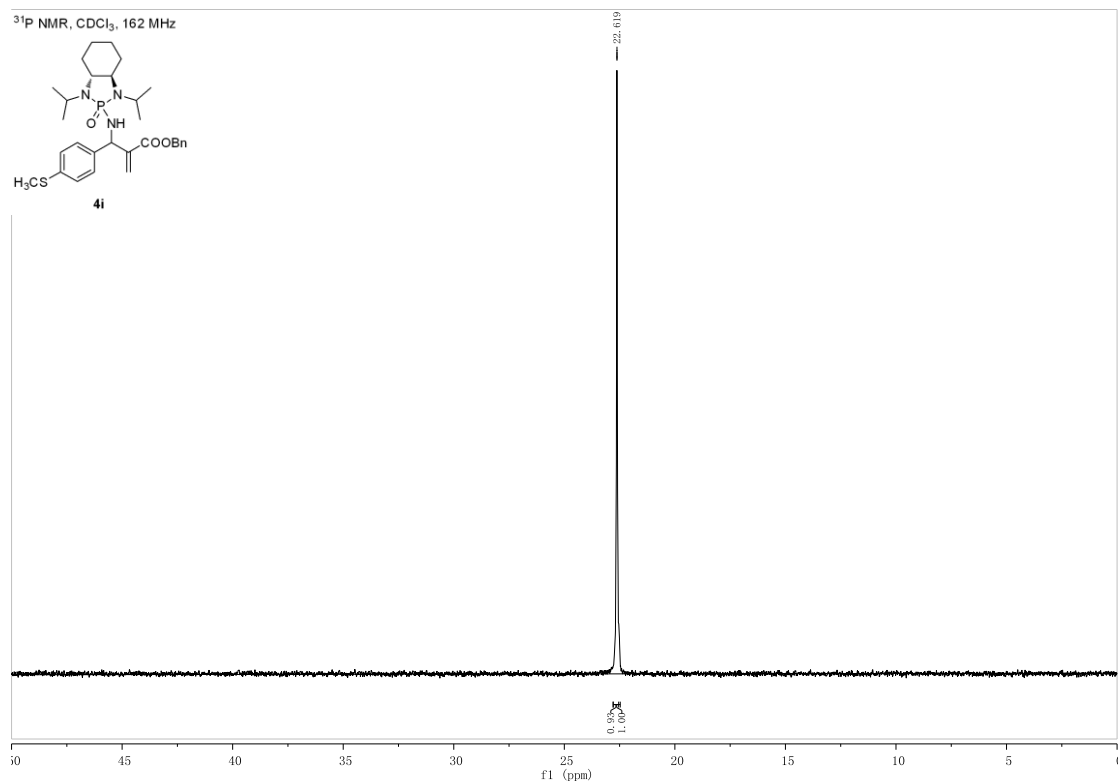


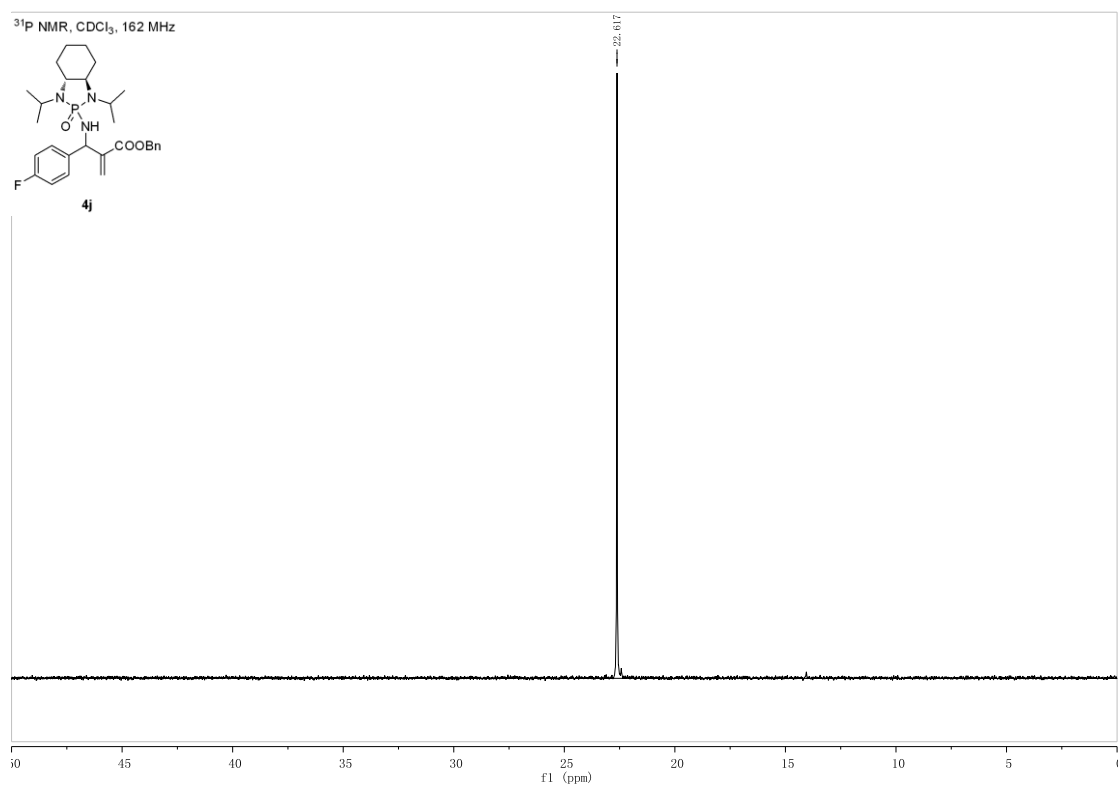
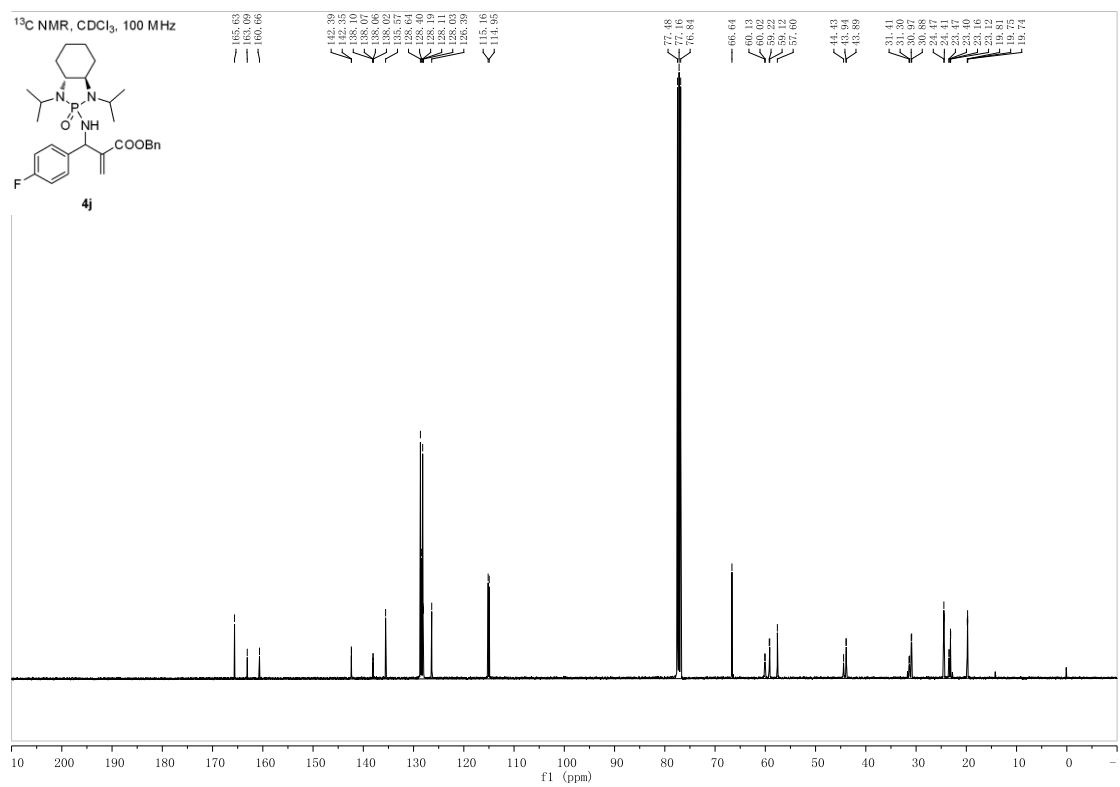


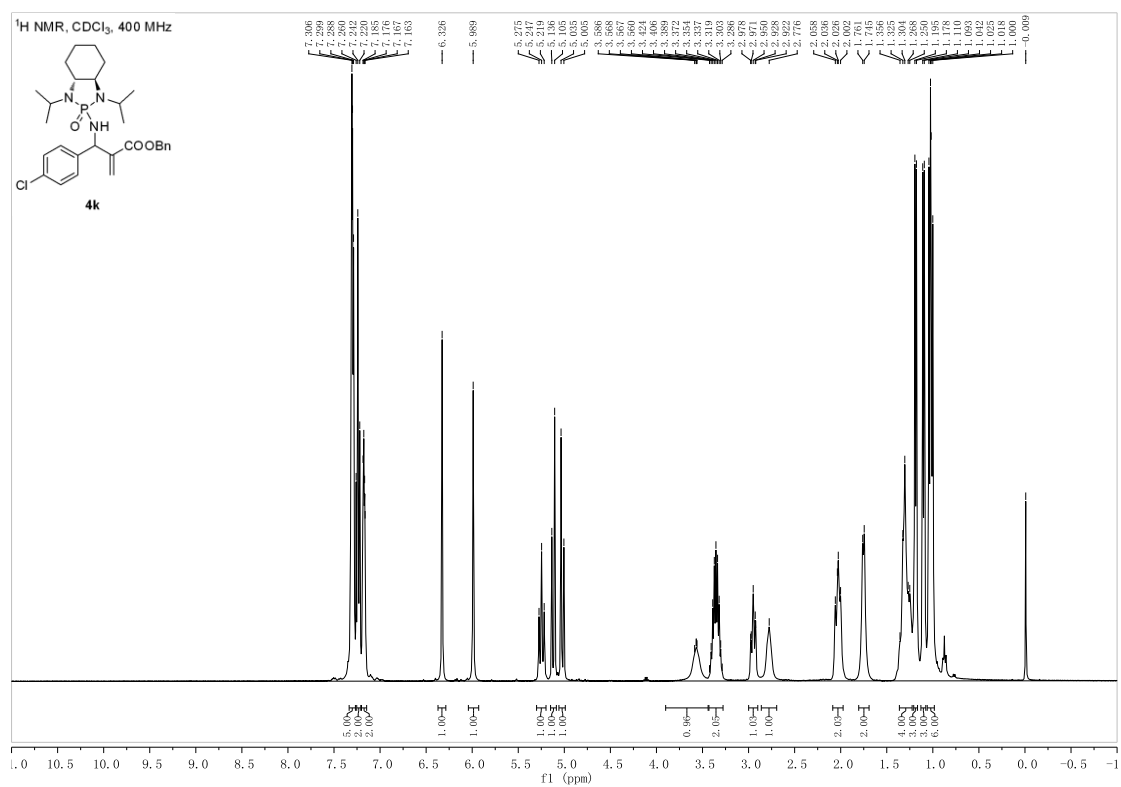
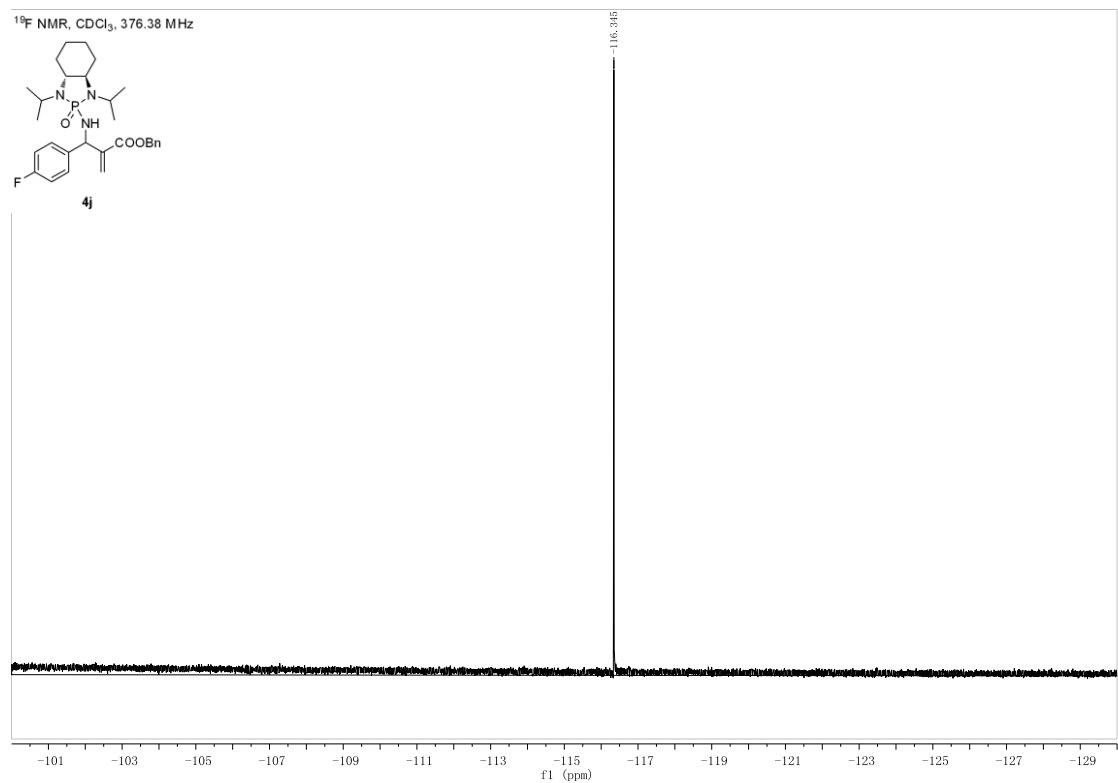


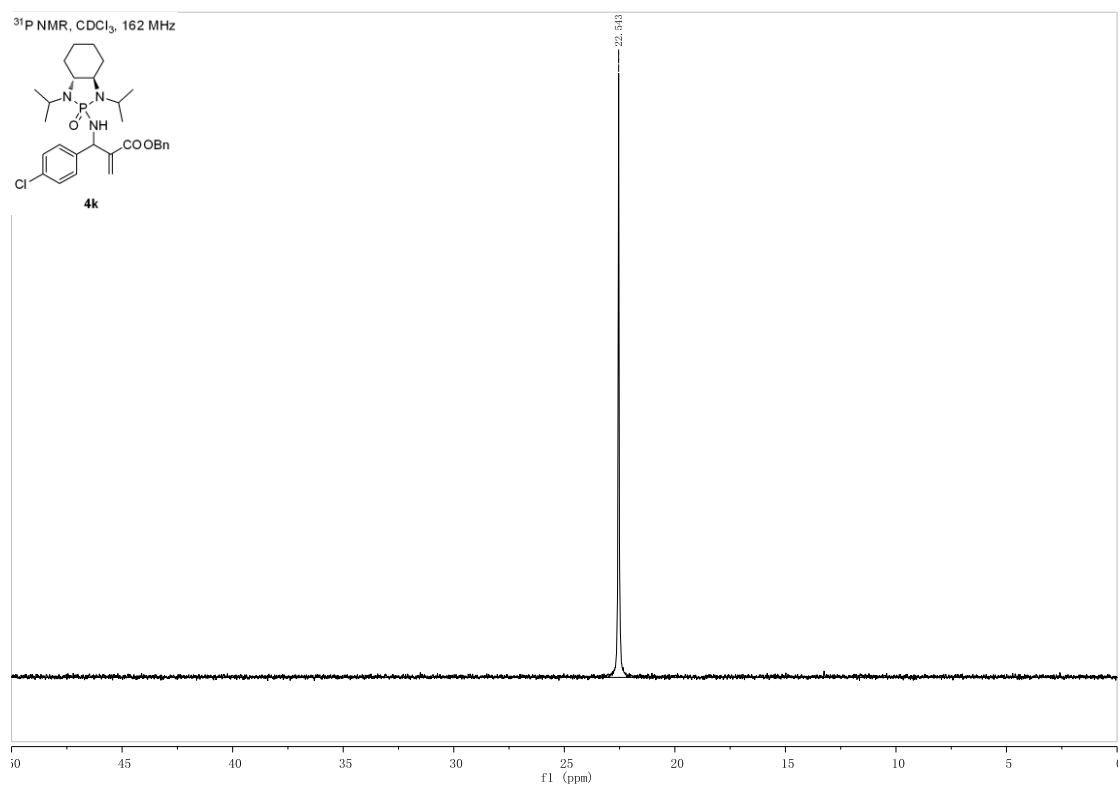
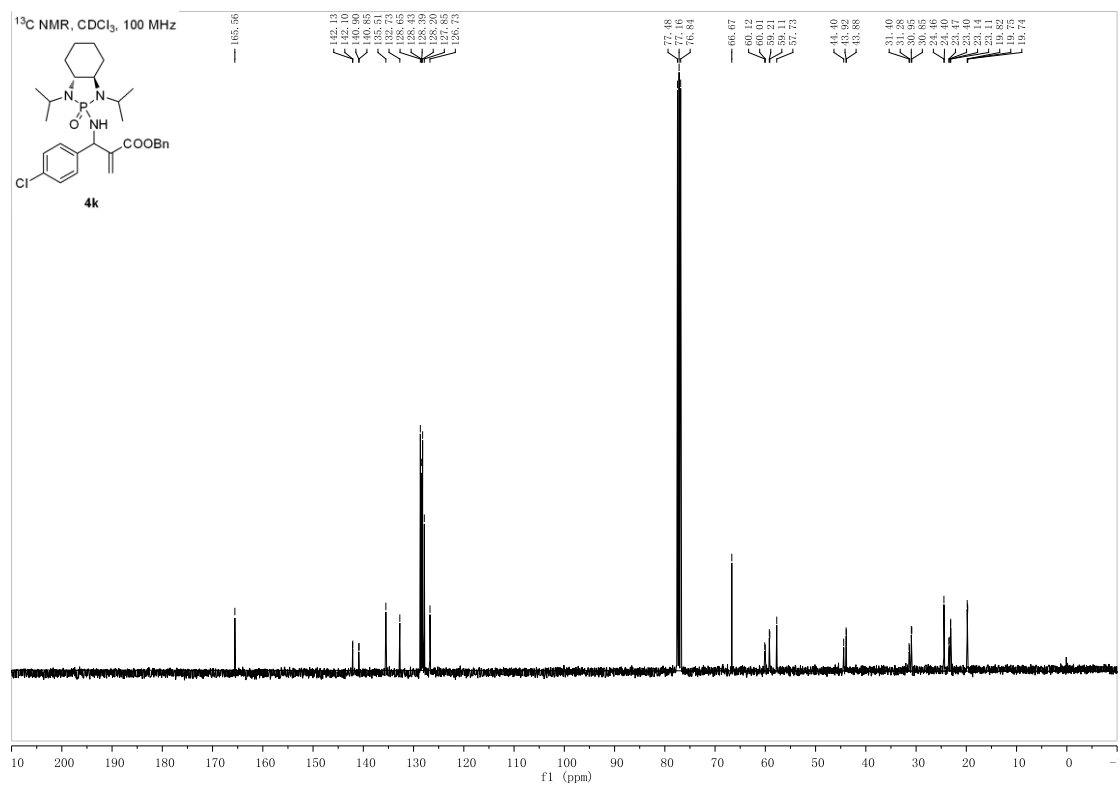


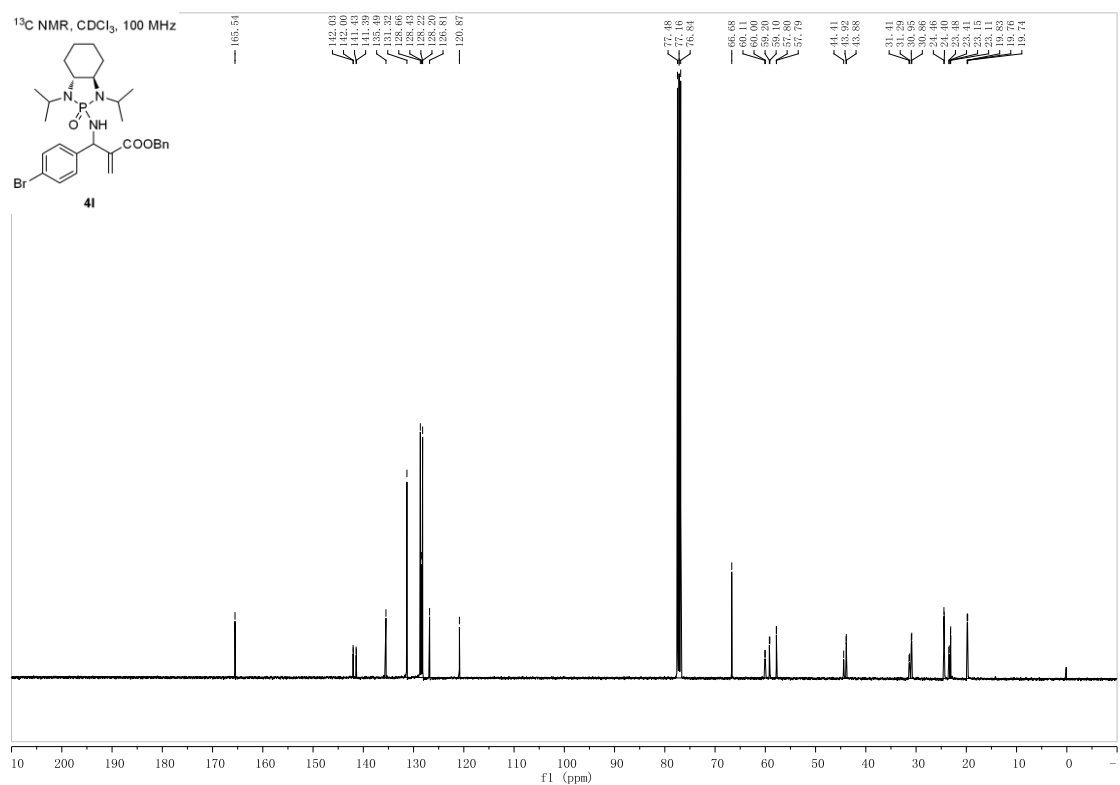
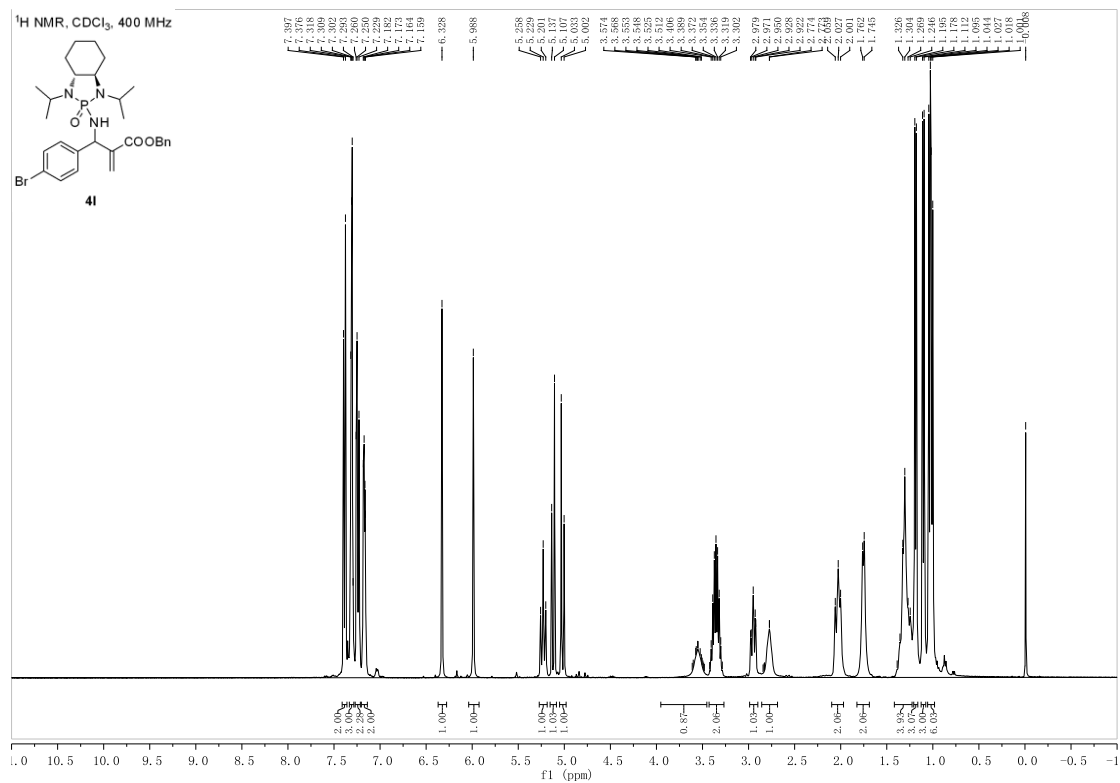


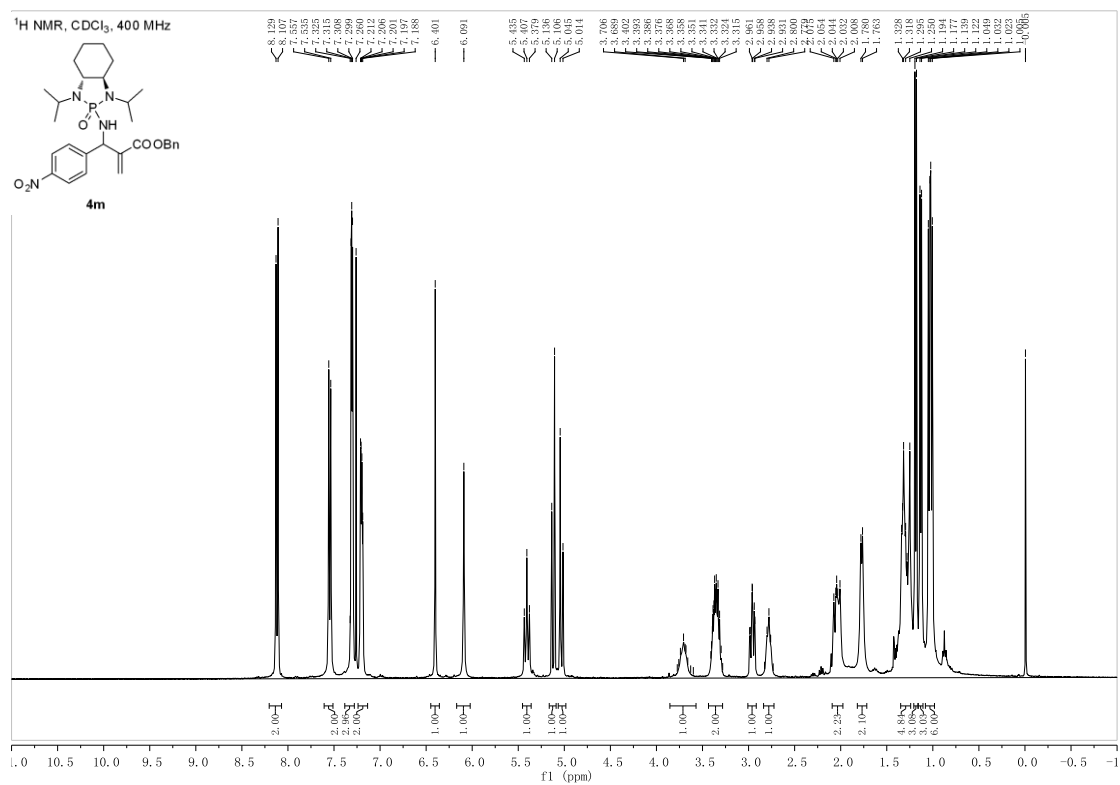
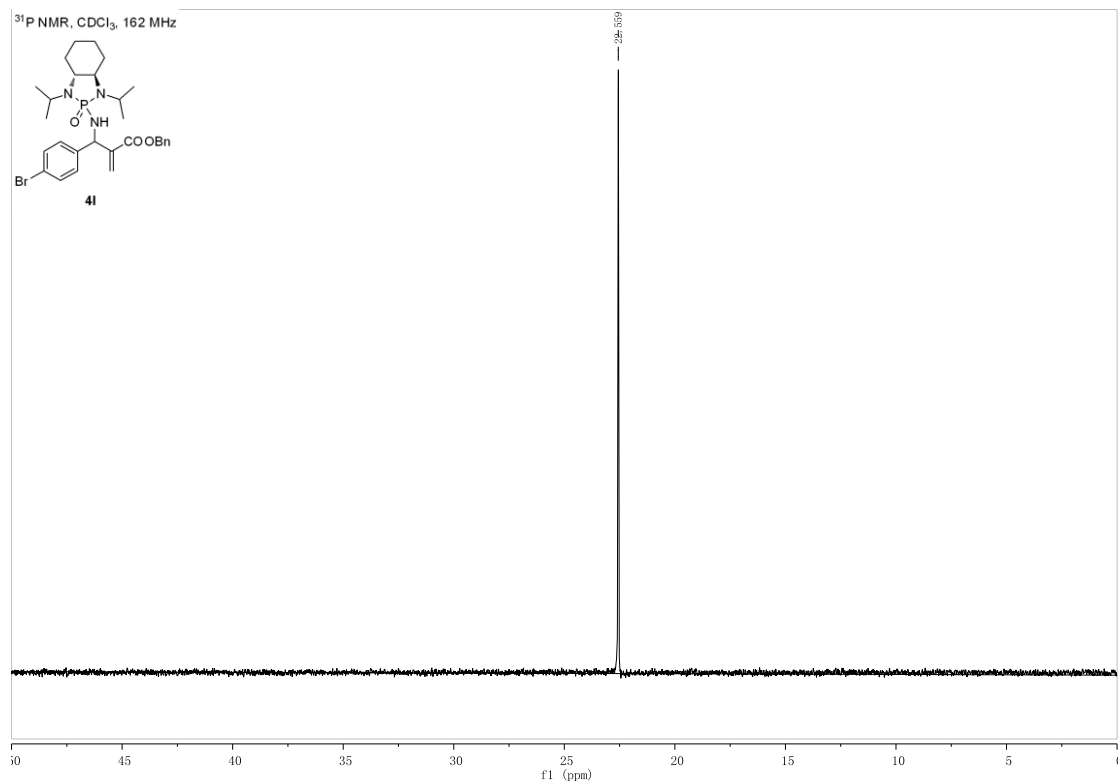


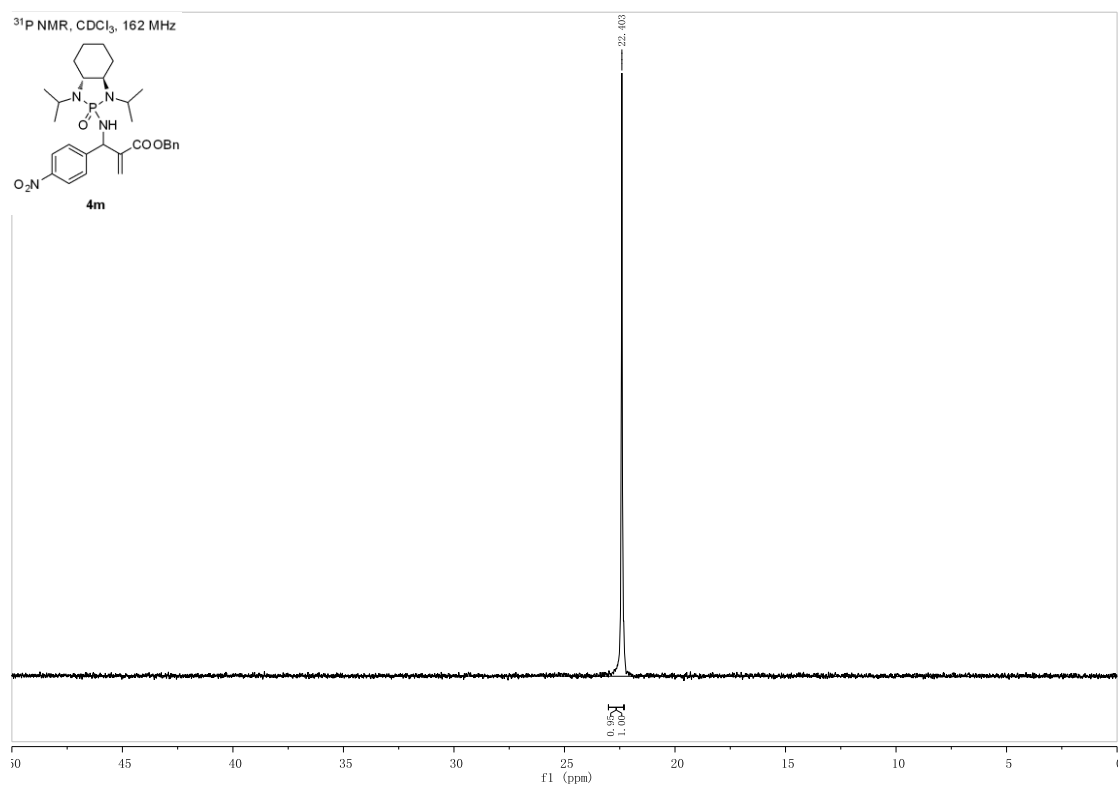
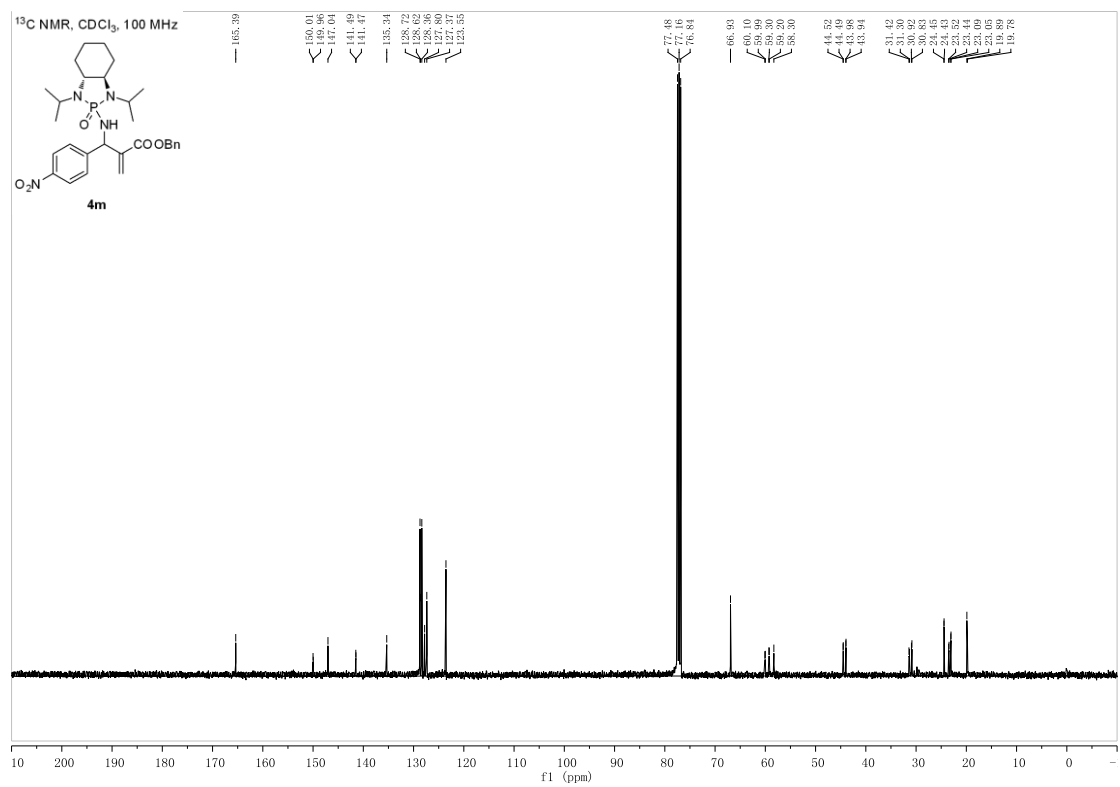


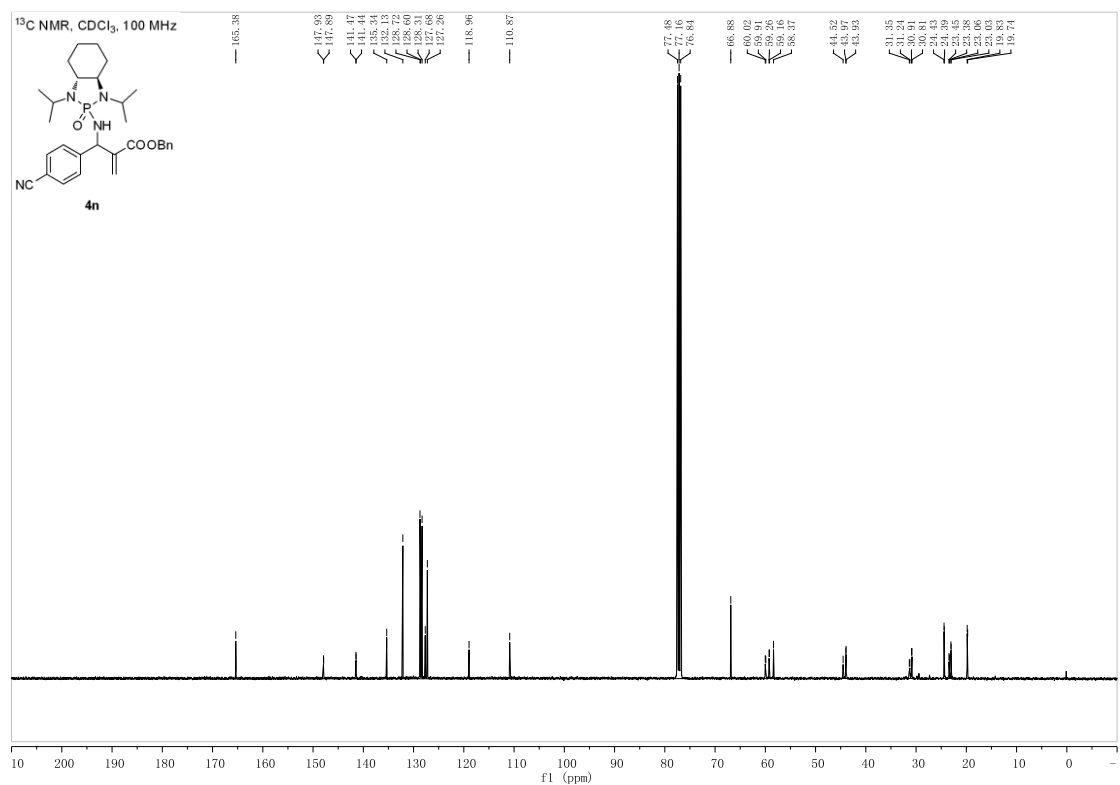
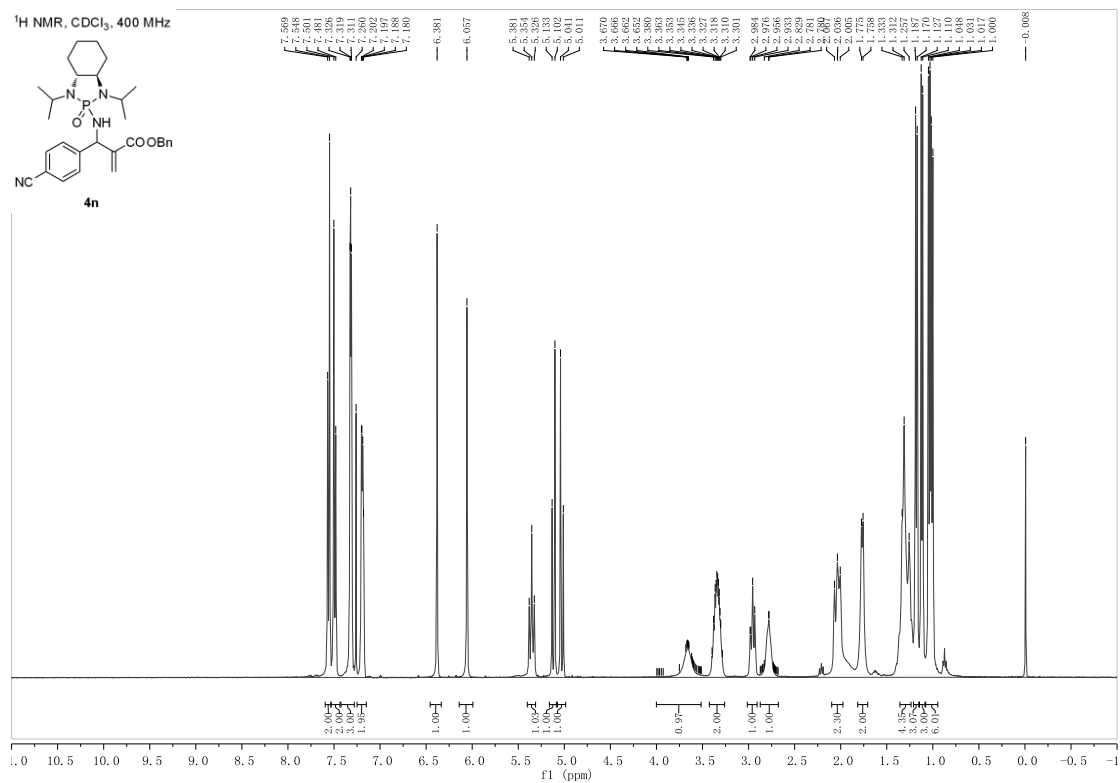


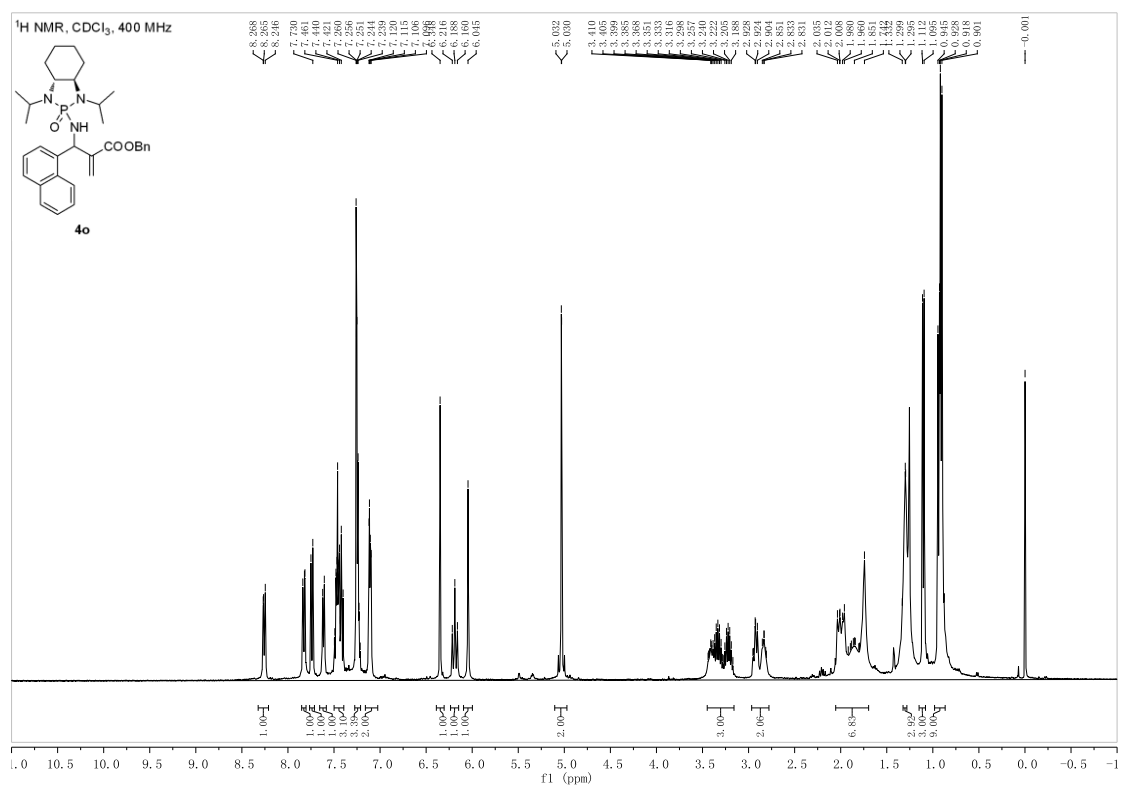
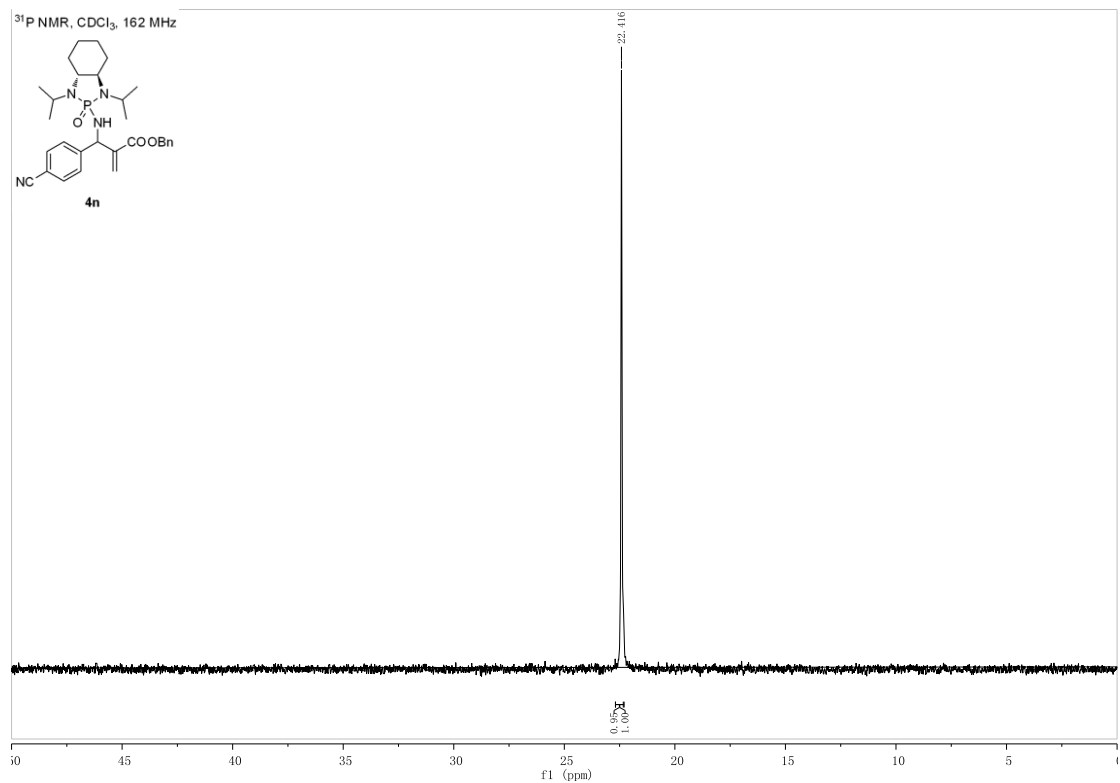


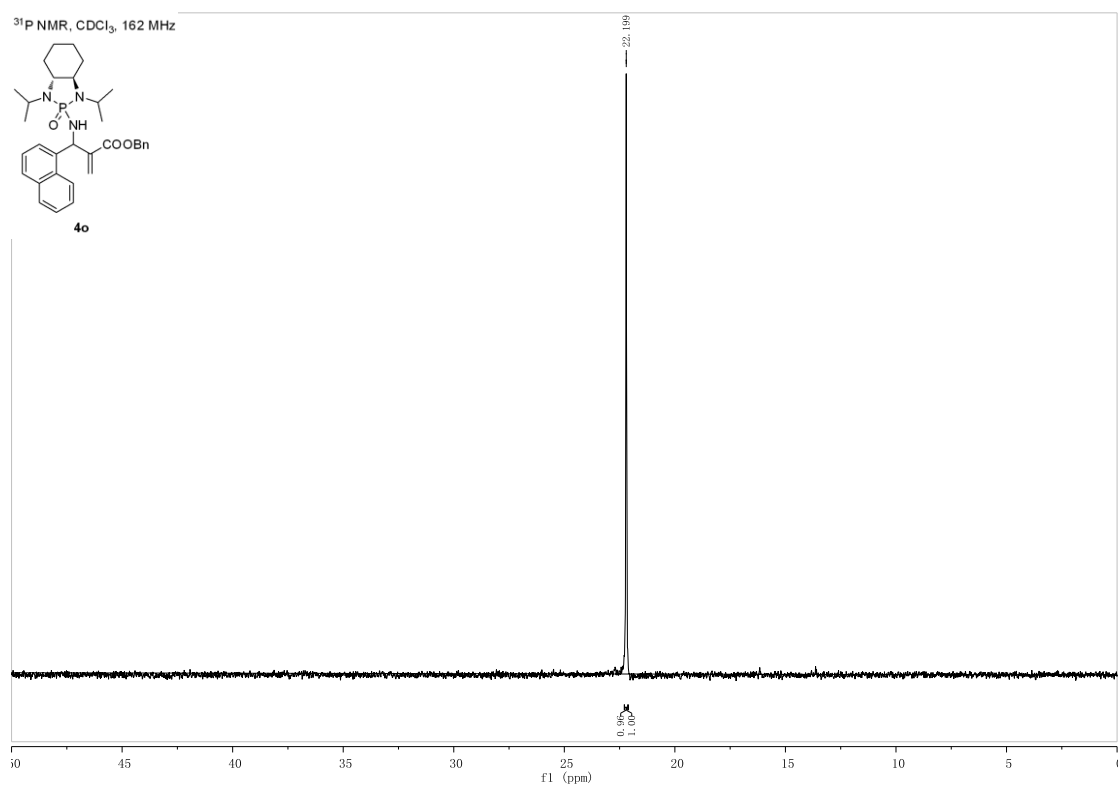
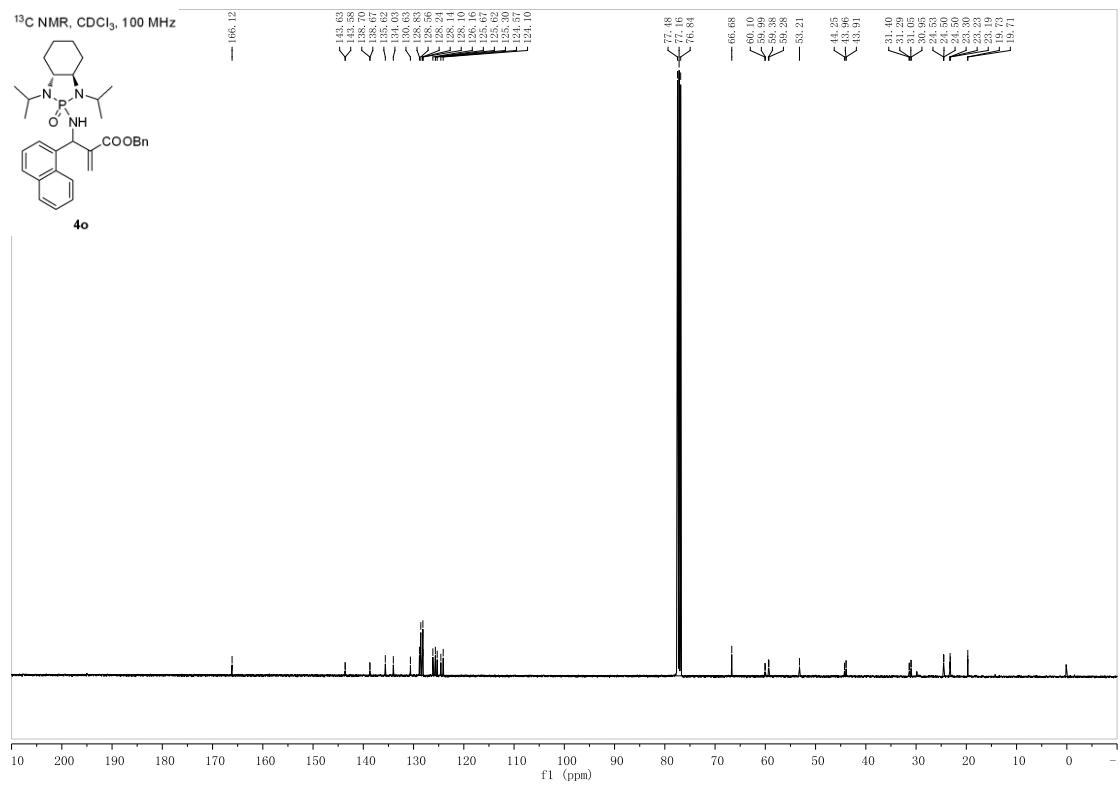


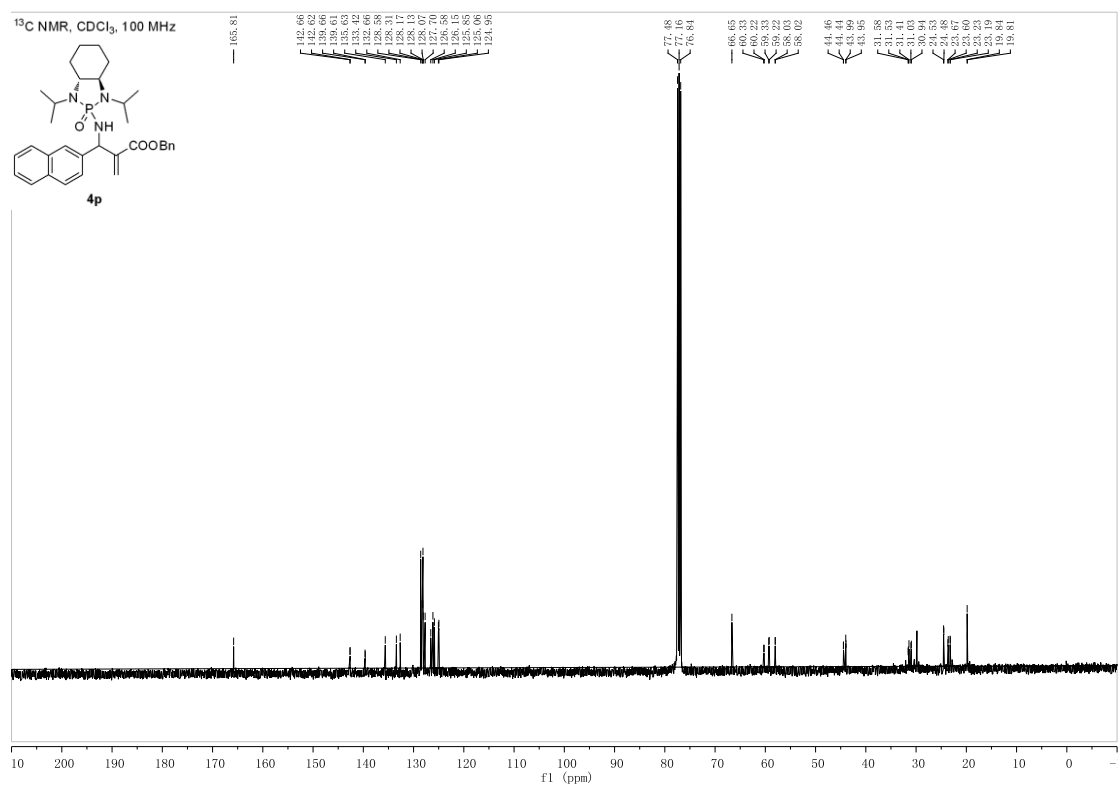
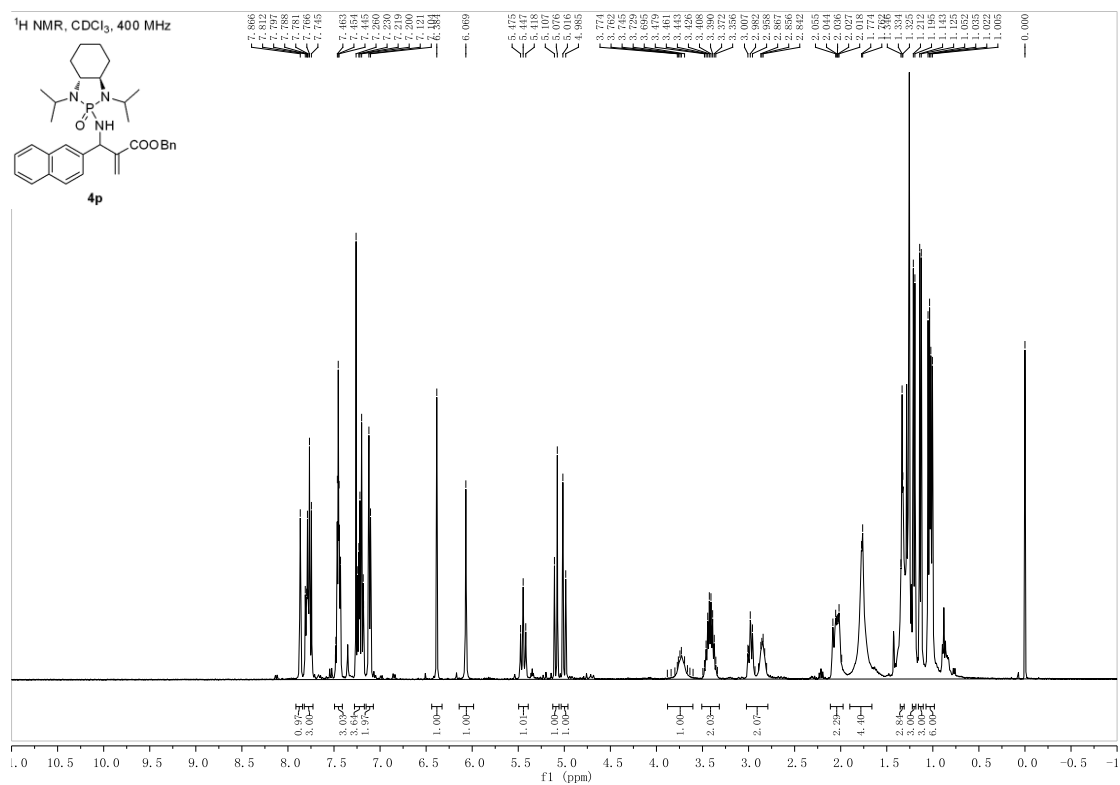


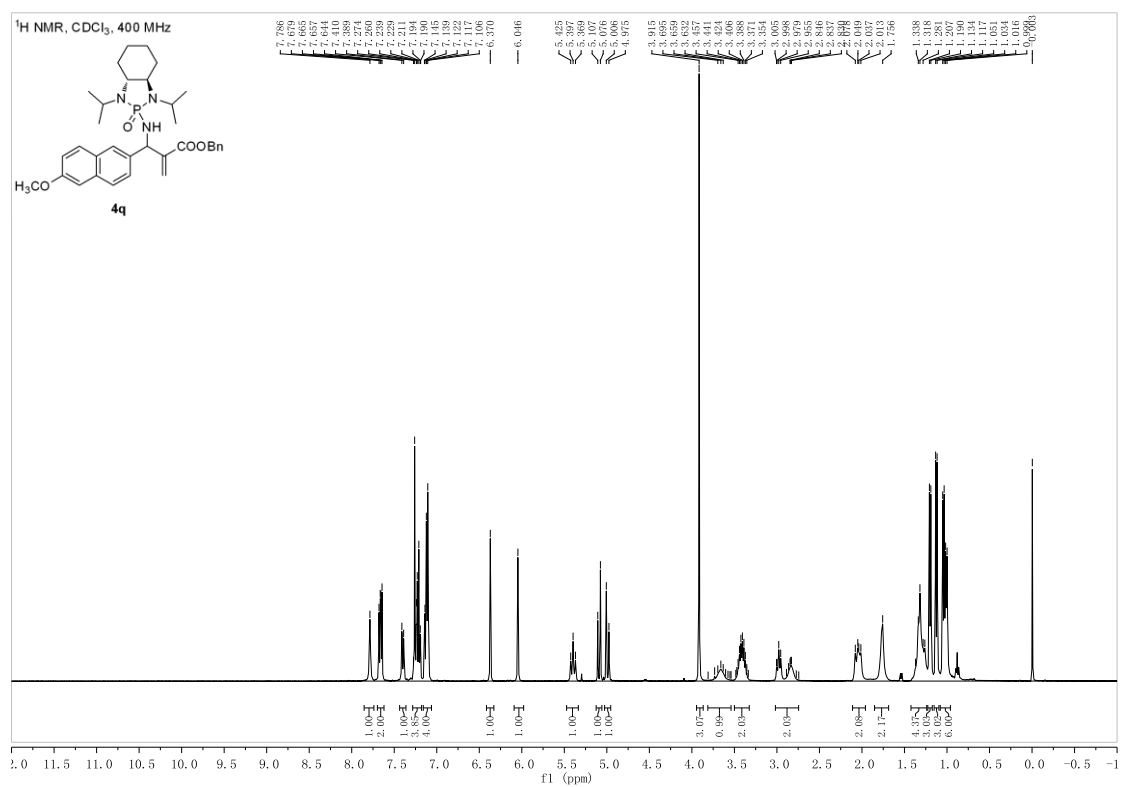
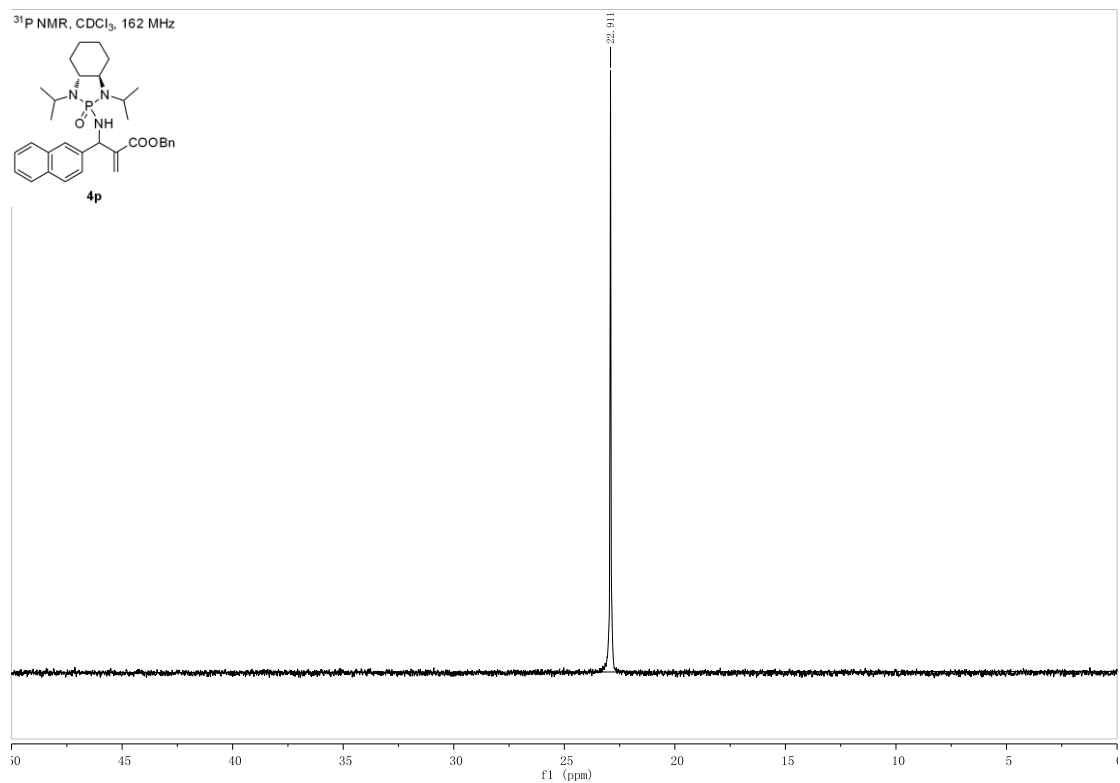


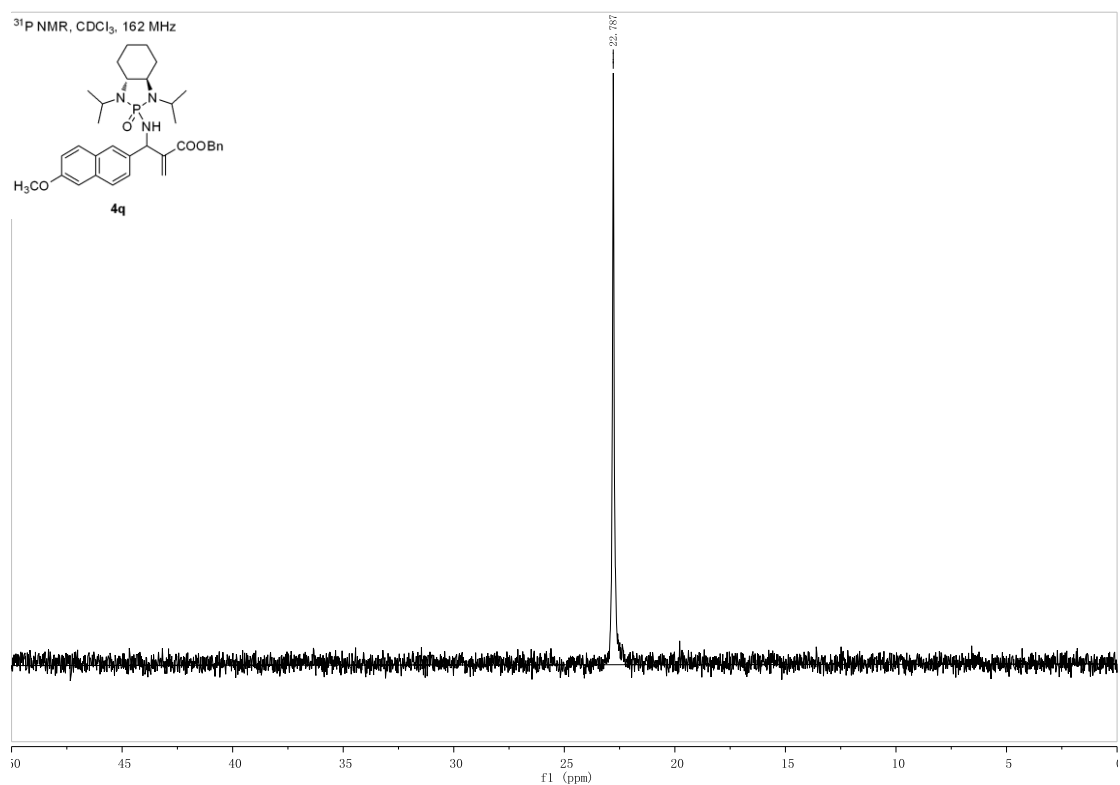
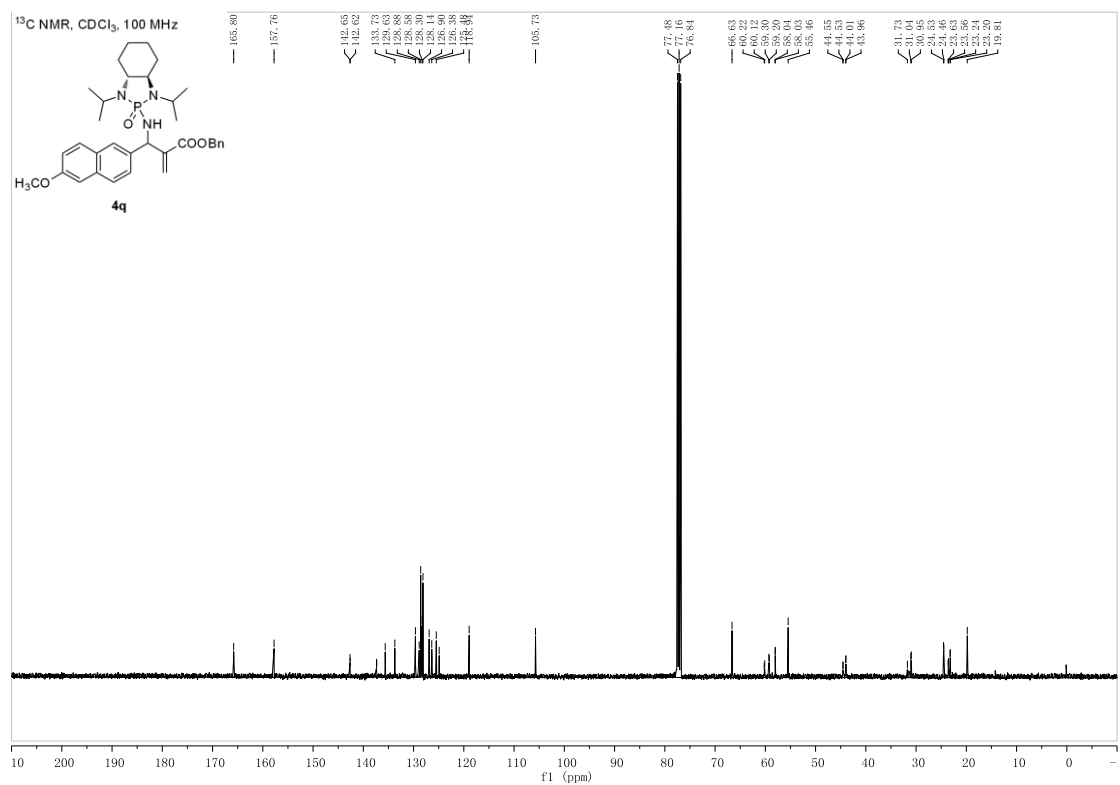


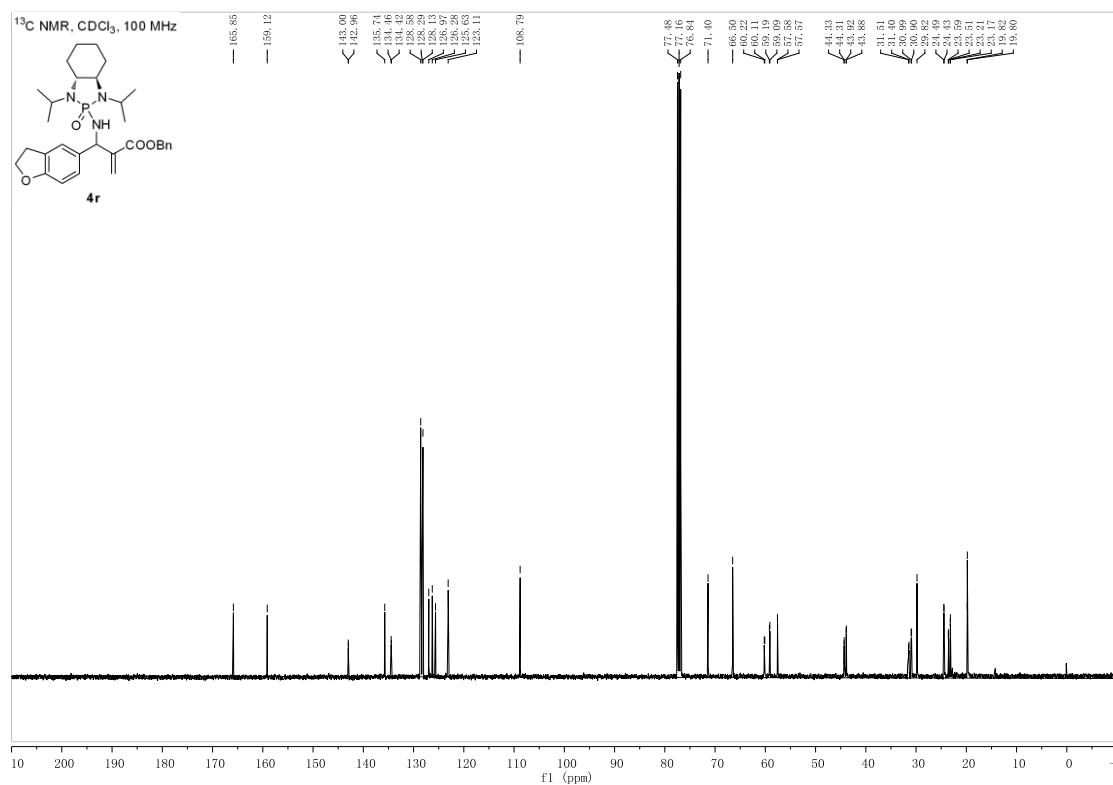
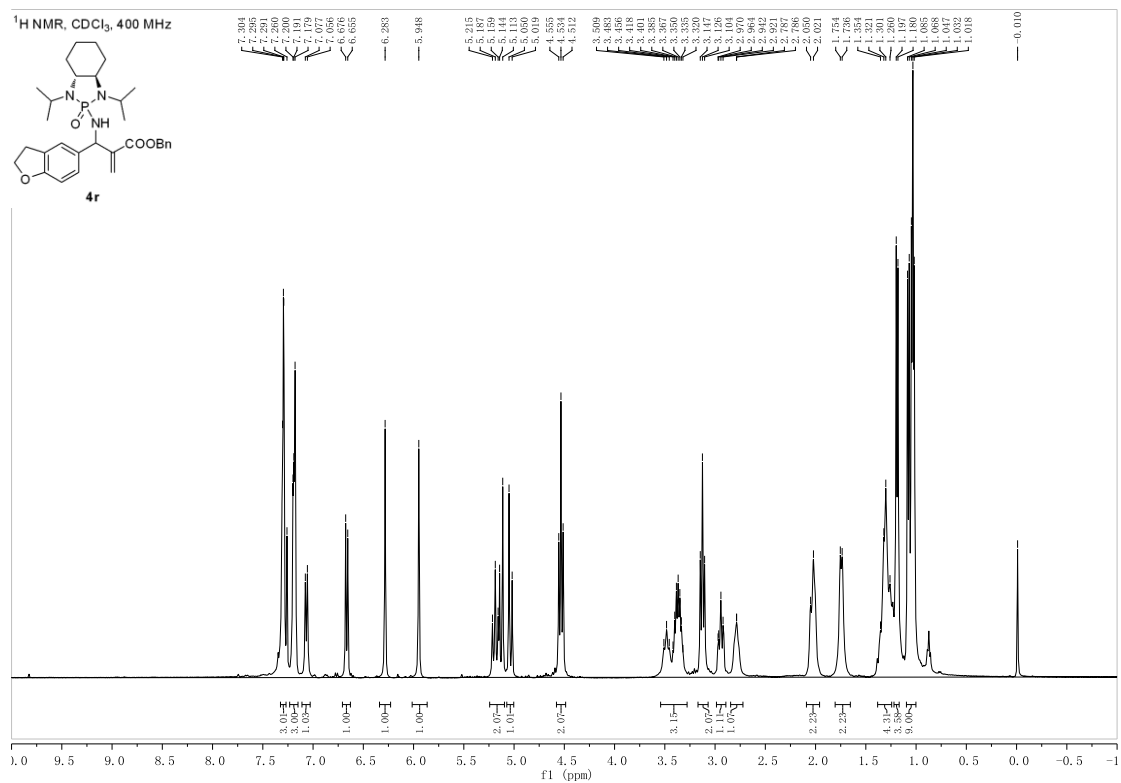


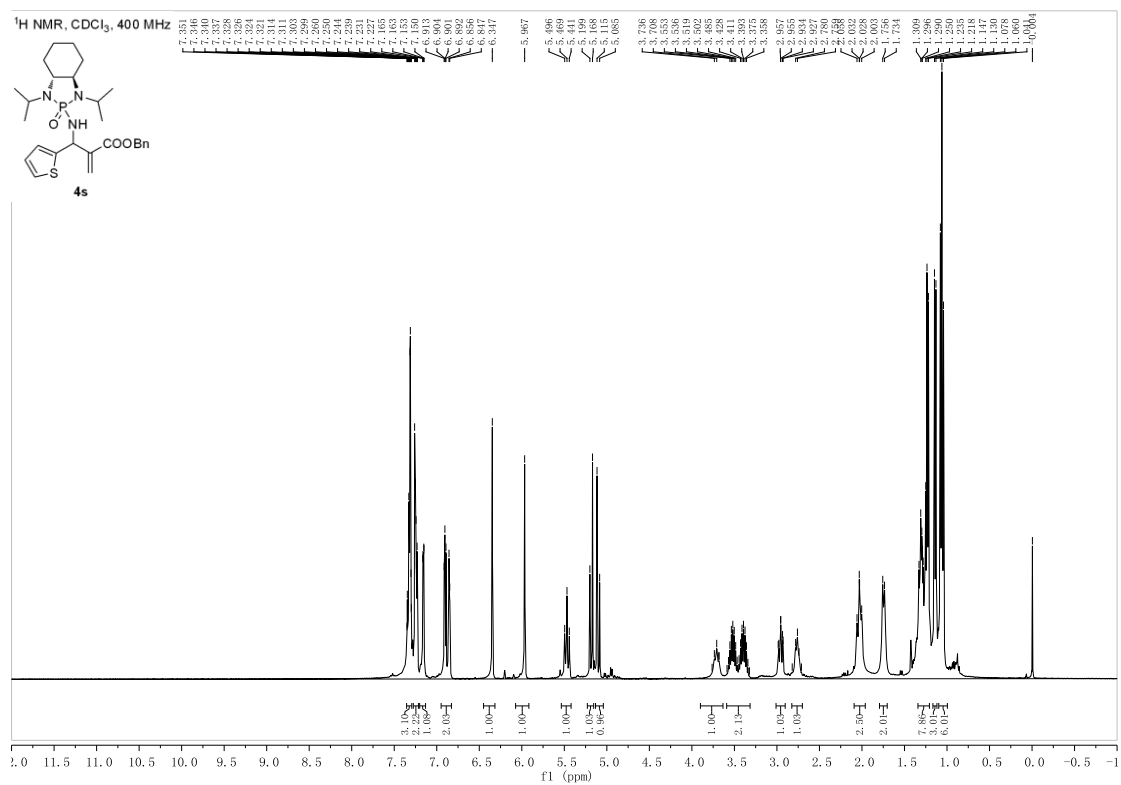
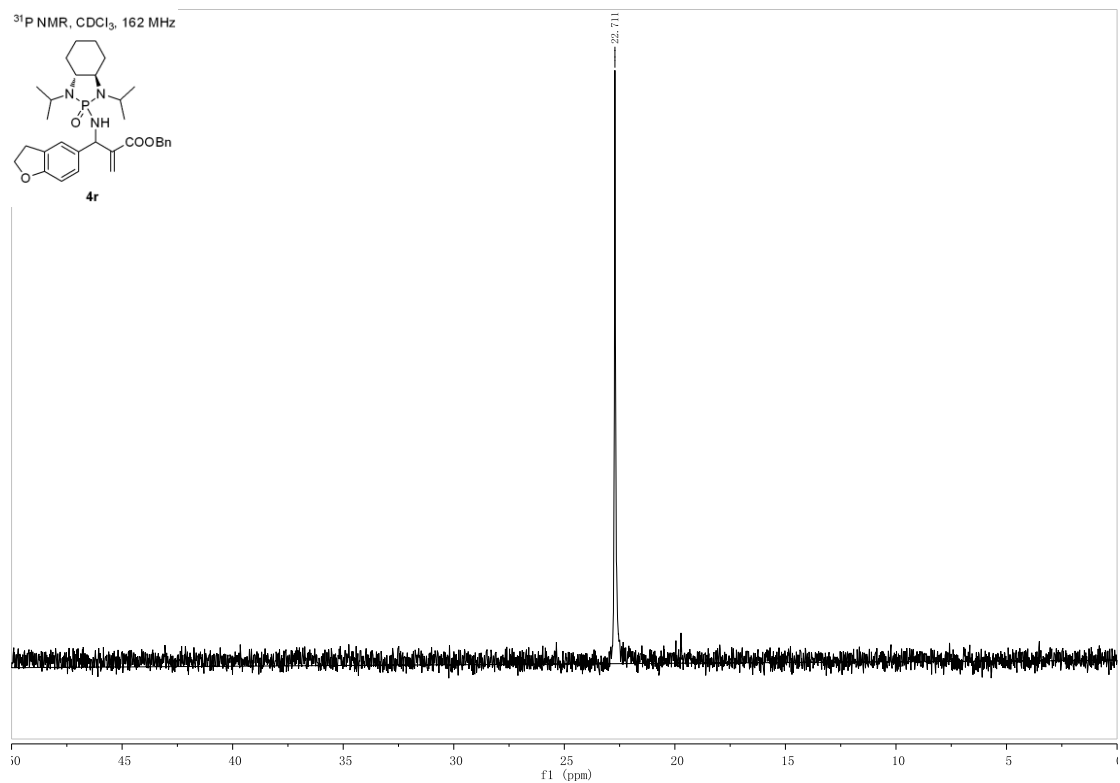


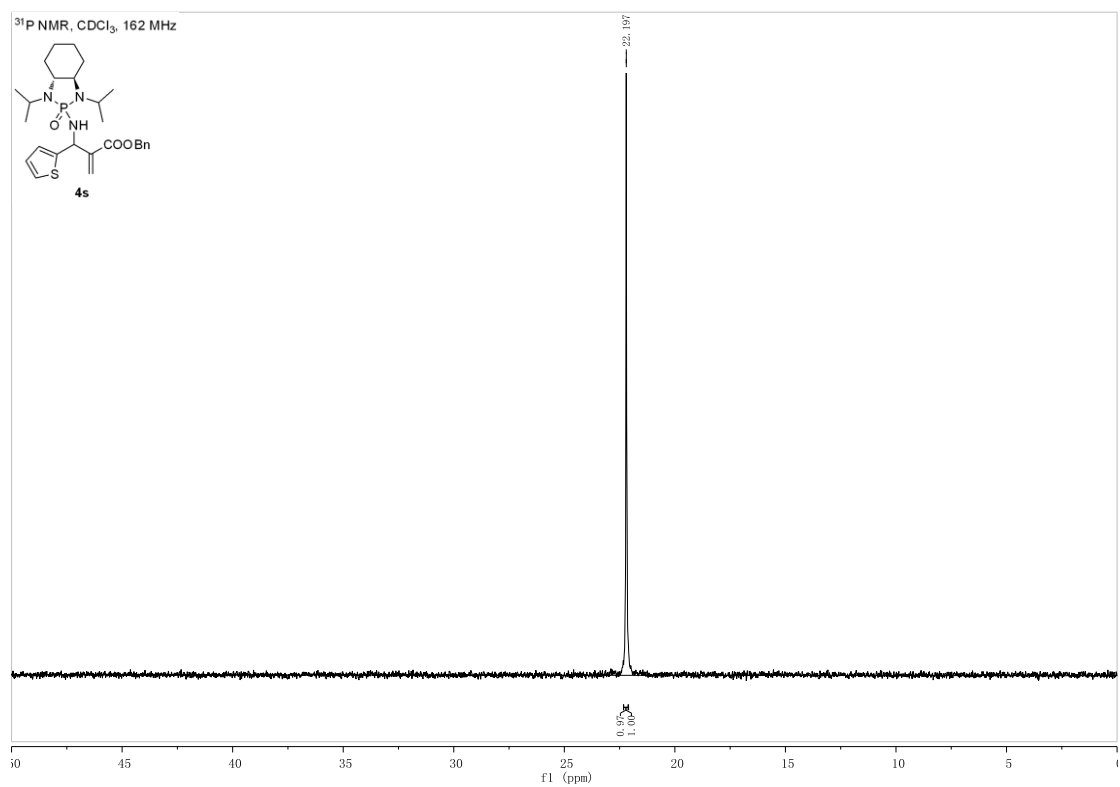
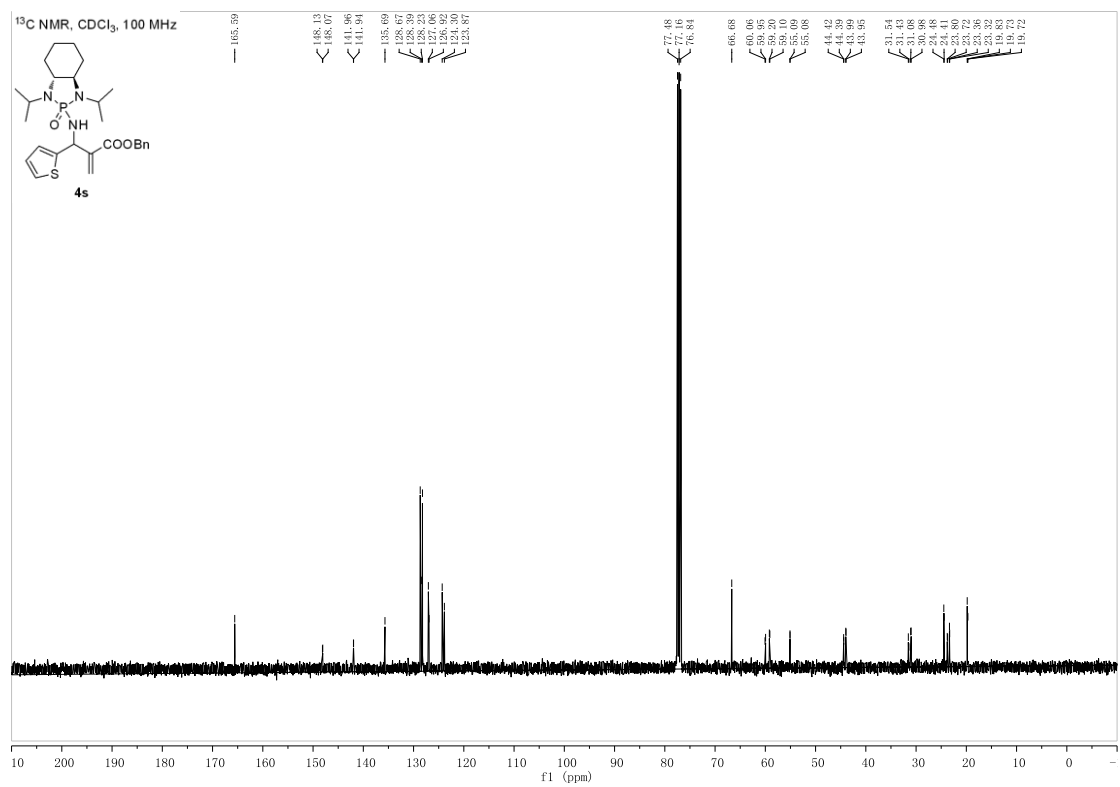


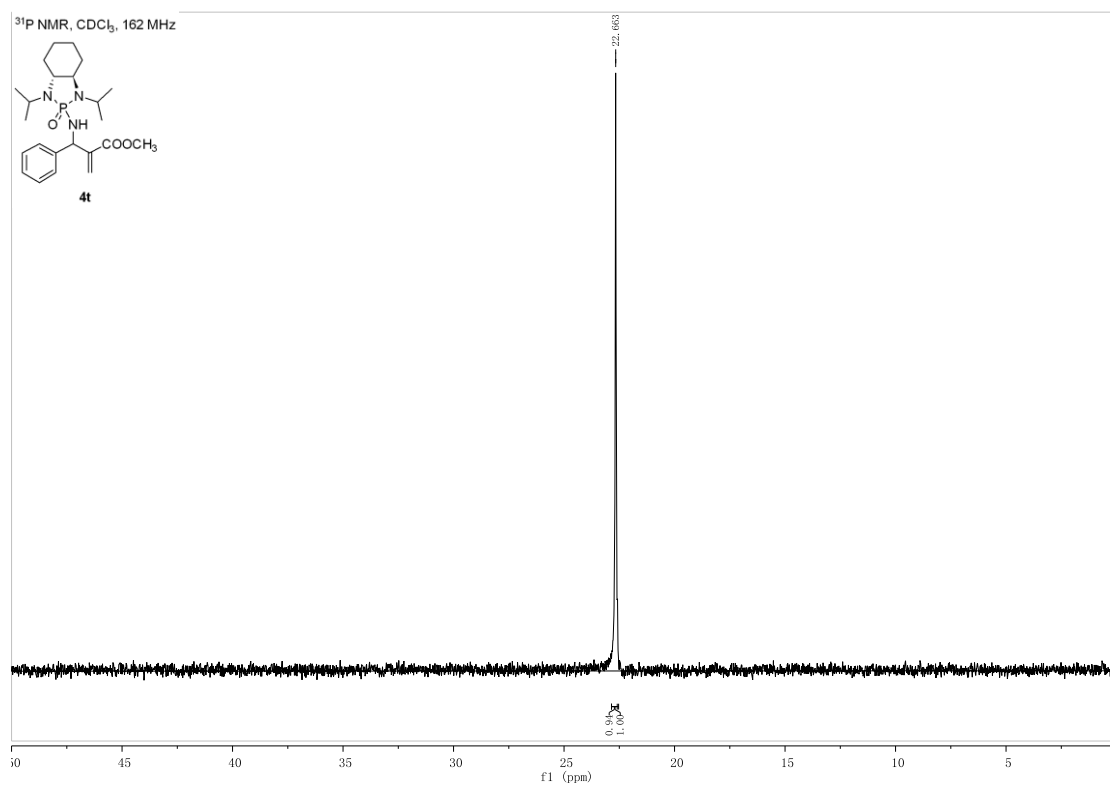




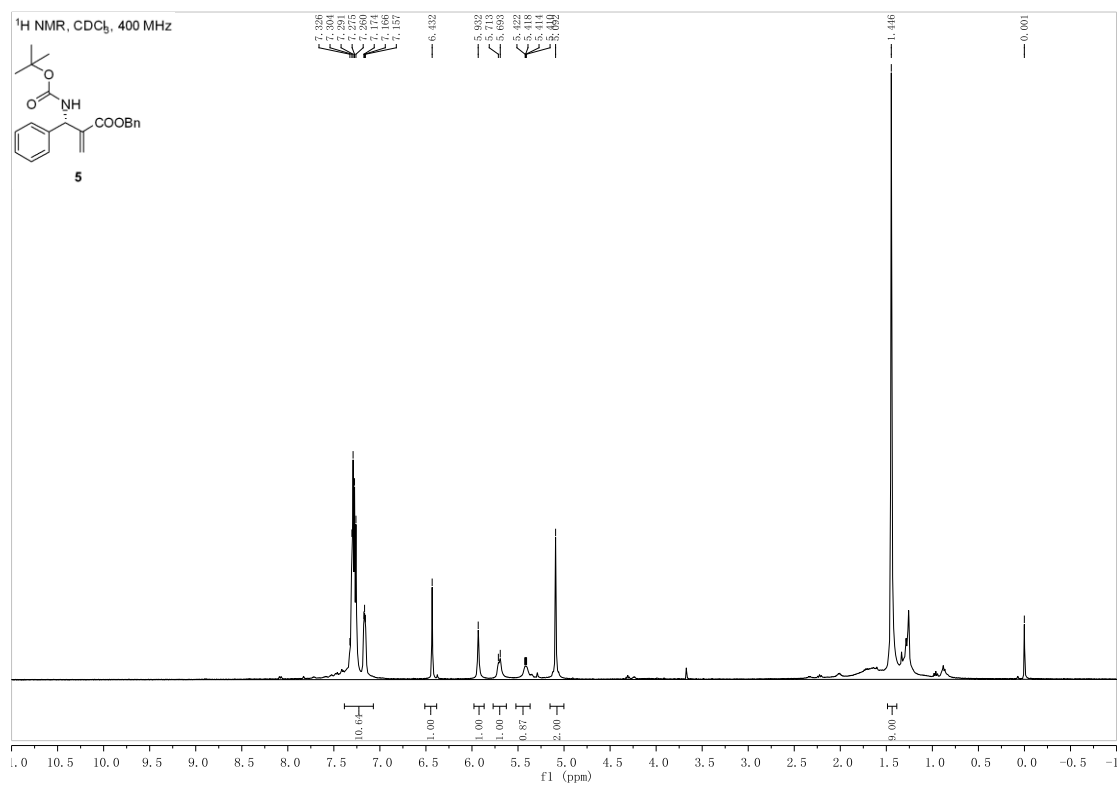


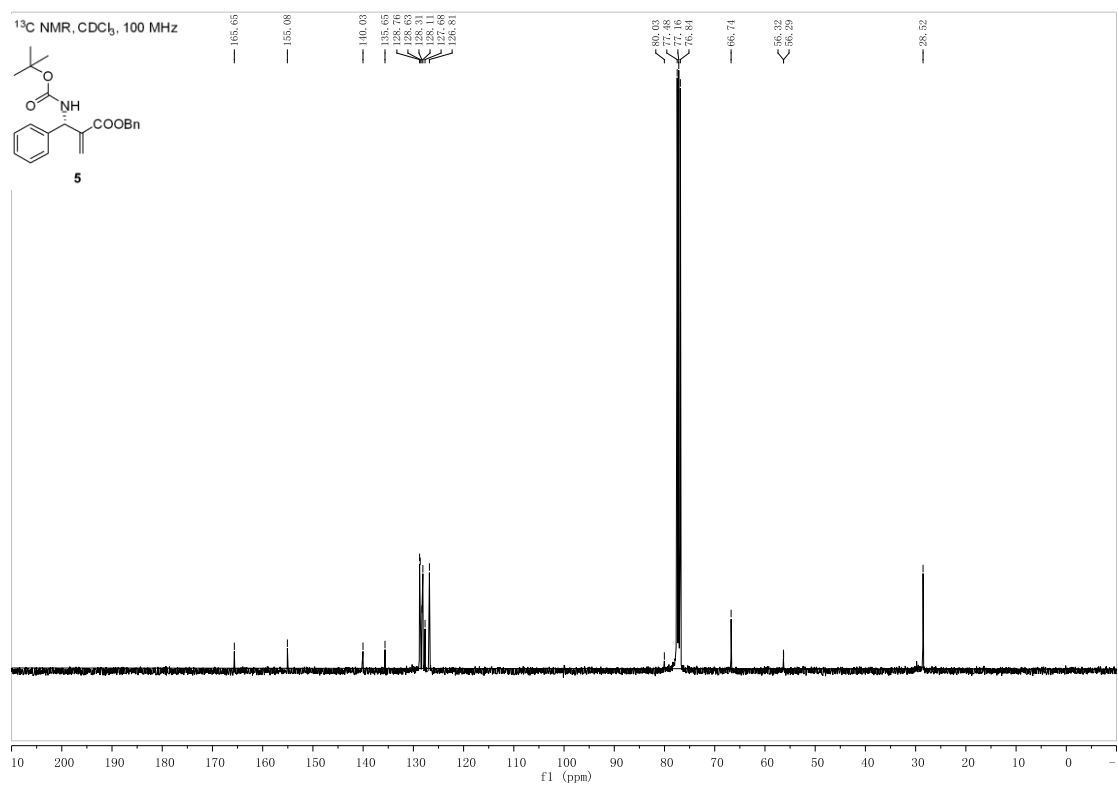






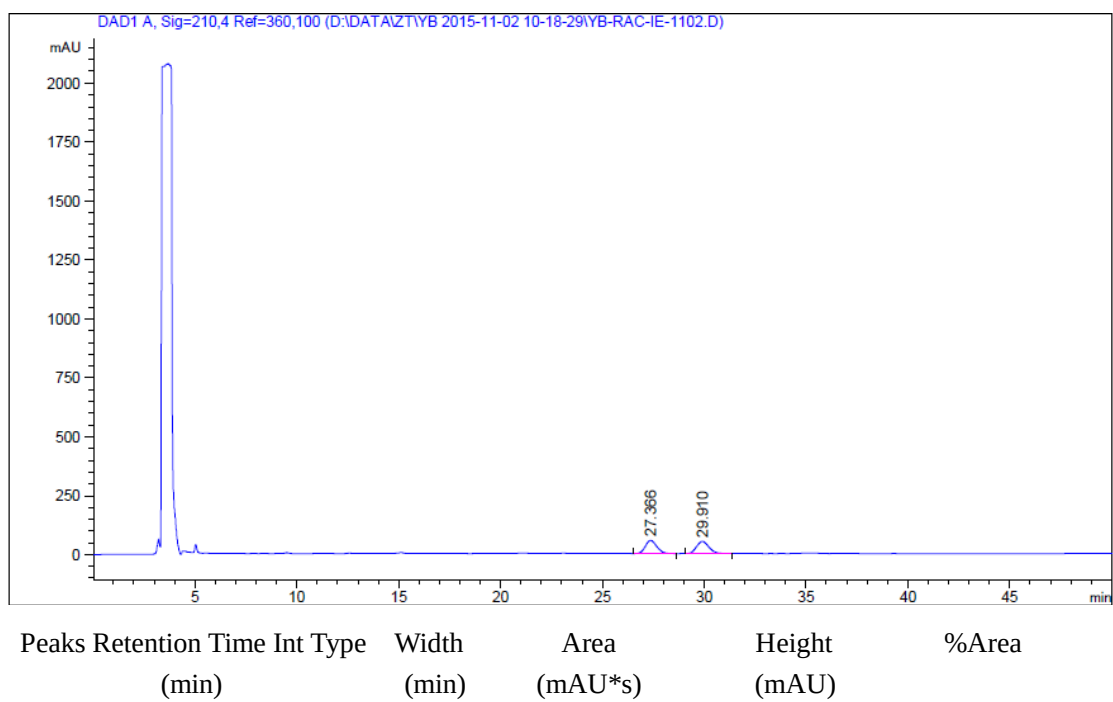
NMR spectra of 5





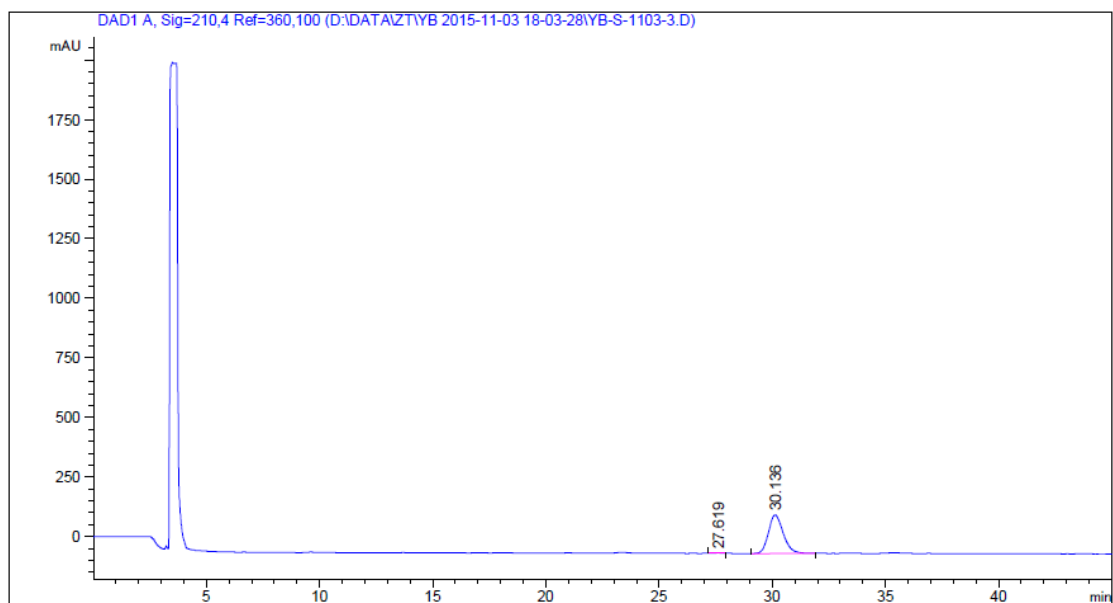
HPLC data

Racemic mixture:



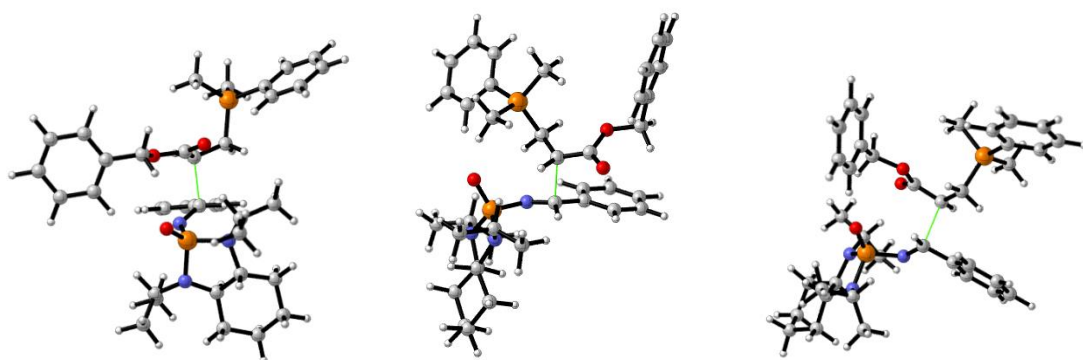
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1	27.366	BB	0.6094	2230.42480	56.15083	50.4877
2	29.910	BB	0.6607	2187.33374	51.38039	49.5123

5:



Peaks #	Retention Time (min)	Int Type	Width (min)	Area (mAU*s)	Height (mAU)	%Area
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	27.619	BB	0.3224	37.18357	1.70514	0.5059
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Computational details



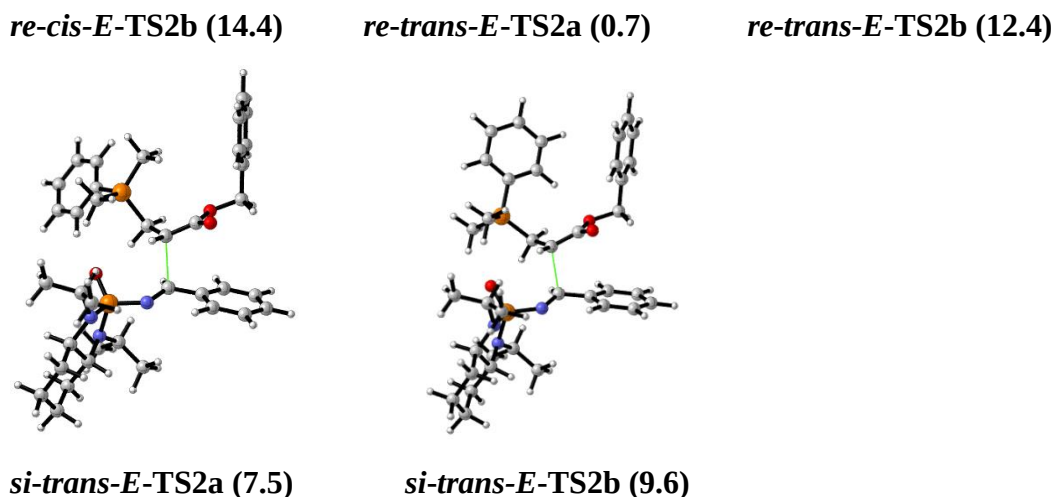


Figure S1 The optimized structure and the relative free energy barriers (in kcal/mol) for less stable TS2s. The key bond lengths are given in angstroms (grey: carbon, white: hydrogen, blue: nitrogen, red: oxygen, orange: phosphorus).

The optimized coordinates of the key stationary points in PES at the SMD-B3LYP-631G(d) level.

Catalyst

P	1.64218500	-0.65282800	-0.00031300
C	-0.16500900	-0.22471500	-0.00018800
C	-1.09162400	-1.27859200	-0.00043400
C	-0.65262800	1.09262900	0.00021300
C	-2.46652500	-1.02691300	-0.00026300
H	-0.73251700	-2.30517000	-0.00074500
C	-2.02424300	1.34824900	0.00037200
H	0.04132800	1.92950700	0.00042400
C	-2.93484600	0.28737900	0.00013600
H	-3.16896800	-1.85651400	-0.00044300
H	-2.38360200	2.37438000	0.00068800
H	-4.00334500	0.48693400	0.00026900
C	2.26515900	0.37710500	1.42422400
H	3.35886400	0.30897800	1.45873500
H	1.98494200	1.43469500	1.35279000
H	1.87563400	-0.02569900	2.36564700
C	2.26544800	0.37854300	-1.42368900
H	3.35915900	0.31043200	-1.45804500
H	1.87610900	-0.02329800	-2.36560000

H	1.98523700	1.43606500	-1.35125600
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Imine-E

N	-1.16994000	-1.16485500	-0.71402000
P	-0.23761200	0.19590000	-1.06347000
N	-1.18721000	1.28042800	-0.18311000
C	-0.58392600	-2.50343700	-0.97262500
C	-1.14411700	2.71057200	-0.57578900
N	1.20018900	0.03765400	-0.12584300
O	0.04249200	0.48898600	-2.50560300
C	2.33493000	0.23672000	-0.69297800
C	-2.35868400	3.14624600	-1.40612100
C	-0.90127600	3.62461700	0.63363100
C	-0.04924900	-3.19376500	0.29017500
C	-1.54596300	-3.39854600	-1.76566000
C	-2.42955700	0.61138400	0.24834600
C	-3.10742000	1.13731900	1.51821500
C	-4.36417400	0.29279200	1.80318300
C	-4.06380800	-1.21382800	1.86245700
H	0.27577500	-2.31717000	-1.62879700
H	-0.26779700	2.80454000	-1.22762800
H	-2.22390600	4.17947400	-1.74668700
H	-2.47348300	2.51171400	-2.29131300
H	-3.29000000	3.11015900	-0.82923600
H	-0.71992900	4.65344100	0.29837400
H	-0.02328100	3.28828200	1.19546800
H	-1.75570800	3.64470900	1.31809900
H	0.47272200	-4.11788500	0.01531100
H	0.65890100	-2.54739600	0.81824600
H	-0.85296600	-3.46605200	0.98363400
H	-1.03146900	-4.31549500	-2.07863100
H	-1.89772300	-2.88034500	-2.66376700
H	-2.41986200	-3.69370200	-1.17616300
H	-3.17310900	0.64568100	-0.56552800
H	-2.40354800	1.08679400	2.35946100
H	-3.39438800	2.18700200	1.39928400
H	-4.82516300	0.62015400	2.74317400
H	-5.10406300	0.48199600	1.01223800
H	-3.46469000	-1.42704200	2.75924800
H	-4.99811000	-1.77849200	1.97134800
C	3.61765200	0.12374200	0.01569000
C	4.80698200	0.36599400	-0.69034600
C	3.68404100	-0.21408500	1.37927500
C	6.04169300	0.27246000	-0.04913700

H	4.75673100	0.62812900	-1.74464900
C	4.91635200	-0.30811700	2.01702100
H	2.76025700	-0.39463900	1.92005700
C	6.09739600	-0.06479900	1.30482600
H	6.95695600	0.46174600	-0.60313400
H	4.96257200	-0.56947600	3.07080400
H	7.05836800	-0.13827700	1.80713800
H	2.40106800	0.50876600	-1.75508400
C	-2.03152600	-0.86653400	0.44497800
H	-1.44562900	-0.93499600	1.37749700
C	-3.29519300	-1.71544800	0.62427900
H	-3.91898800	-1.64276800	-0.27629800
H	-3.04149600	-2.77155900	0.75868000

Imine-Z

N	1.58906900	-1.15225900	0.46966400
P	0.02809400	-0.51830700	0.56843900
N	0.46439500	1.05800000	0.14798200
C	1.73147500	-2.62956200	0.40955400
C	-0.40234600	2.17713300	0.59401400
N	-0.77783200	-1.11910500	-0.80913000
O	-0.67794400	-0.77291600	1.86667200
C	-1.99116800	-1.14795600	-1.21599700
C	0.18455800	2.95493700	1.77981500
C	-0.79605500	3.09547800	-0.57140600
C	1.98110500	-3.17264900	-1.00521300
C	2.77423200	-3.12967800	1.41856400
C	1.93471500	1.16934600	0.08011200
C	2.51812600	2.21767800	-0.87349100
C	4.05683900	2.15560000	-0.80650600
C	4.60411300	0.74093800	-1.05833200
H	0.76324400	-3.02601800	0.74110300
H	-1.32474800	1.70666900	0.95213100
H	-0.54020300	3.69902000	2.13035400
H	0.40864800	2.28374700	2.61589100
H	1.10115000	3.49156200	1.51045600
H	-1.55456700	3.81645500	-0.24215500
H	-1.21807300	2.50985100	-1.39506300
H	0.05596100	3.66336000	-0.95844900
H	1.96293500	-4.26881200	-0.98754500
H	1.20584200	-2.83004600	-1.69700100
H	2.95811700	-2.86949900	-1.39834800
H	2.76638200	-4.22612200	1.45655500
H	2.54842000	-2.75011300	2.42055900

H	3.78878100	-2.81438400	1.15376300
H	2.33512800	1.37370800	1.08683600
H	2.16397200	2.02566700	-1.89510300
H	2.18475500	3.22360800	-0.59884500
H	4.48784100	2.85864300	-1.52995800
H	4.38055800	2.49576900	0.18779000
H	4.43572700	0.47078900	-2.11068500
H	5.69014600	0.72665700	-0.90401500
C	-3.27626000	-0.67088900	-0.66040500
C	-4.35430600	-0.60782800	-1.56459500
C	-3.49447500	-0.30547000	0.68244200
C	-5.60811900	-0.16133900	-1.15520600
H	-4.19782900	-0.90417300	-2.59929500
C	-4.75506200	0.12743800	1.08964900
H	-2.68362600	-0.39053900	1.39897100
C	-5.81051300	0.20888600	0.17642200
H	-6.42531900	-0.10844600	-1.86932600
H	-4.91637200	0.39825700	2.12972400
H	-6.78907900	0.55029200	0.50363400
H	-2.12714500	-1.59906400	-2.20939200
C	2.41725600	-0.23660400	-0.33359900
H	2.19130200	-0.36568200	-1.40683600
C	3.93797600	-0.32149900	-0.16221800
H	4.19983800	-0.16006800	0.89183200
H	4.30837300	-1.31336300	-0.43877800

Alkene-trans

C	-3.46620100	0.75032400	0.00015200
C	-3.09553900	2.03341900	0.00025900
C	-2.53095600	-0.40076300	-0.00002500
O	-2.90209600	-1.56108800	-0.00016200
O	-1.23295300	-0.03084700	-0.00002200
C	-0.26896700	-1.12053700	-0.00024900
C	1.11180000	-0.52395100	-0.00011800
C	1.76119900	-0.23423900	-1.20717900
C	3.03530300	0.33509500	-1.20882700
C	3.67493000	0.61940000	0.00013800
C	3.03530600	0.33454800	1.20897500
C	1.76120100	-0.23478400	1.20707200
H	-4.51280100	0.45898700	0.00017600
H	-3.83560200	2.82942800	0.00037800
H	-2.05027800	2.32757700	0.00022600
H	-0.44419800	-1.73875400	0.88490500
H	-0.44419500	-1.73837200	-0.88567000

H	1.26435100	-0.45775500	-2.14846700
H	3.53069600	0.55204500	-2.15152400
H	4.66890800	1.05890400	0.00023600
H	3.53070000	0.55107300	2.15177000
H	1.26435400	-0.45872300	2.14825900

Alkene-cis

C	-3.23198500	-0.16176900	-1.02074900
C	-4.56452800	-0.14741500	-0.94408300
C	-2.39366900	0.03164400	0.18965300
O	-2.80855300	0.22117300	1.31823200
O	-1.08202600	-0.03118600	-0.12717200
C	-0.15642900	0.14651900	0.98093500
C	1.24478300	0.06512200	0.43975600
C	1.90478200	-1.16760900	0.35512300
C	3.19940800	-1.24570100	-0.16014100
C	3.84892900	-0.08836100	-0.59616100
C	3.19918800	1.14554700	-0.51523500
C	1.90447600	1.21997200	0.00026900
H	-2.70869500	-0.31490200	-1.96012600
H	-5.18556700	-0.28895000	-1.82399700
H	-5.06685600	0.00605200	0.00744300
H	-0.35605900	1.11564100	1.44710000
H	-0.35185900	-0.63251300	1.72353200
H	1.40146700	-2.06906200	0.69700700
H	3.70207200	-2.20756700	-0.21744400
H	4.85863600	-0.14716600	-0.99393900
H	3.70143900	2.04943600	-0.84961400
H	1.40032700	2.18144500	0.06534700

TS1-trans

C	-0.11392200	2.79498600	-0.84903700
C	0.70497500	1.70649600	-1.28383100
C	-1.43571700	2.65308700	-0.34752300
O	-2.20139100	3.55024400	0.01372700
O	-1.85029100	1.31503400	-0.29949300
C	-3.19792400	1.11038600	0.14070500
C	-3.51002400	-0.36275400	0.03622600
C	-3.50055900	-1.00463100	-1.21150800
C	-3.79792100	-2.36271100	-1.31562700
C	-4.11319100	-3.10235400	-0.17103200
C	-4.12553400	-2.47445700	1.07481100
C	-3.82209200	-1.11349000	1.17531900
H	0.28550700	3.80389400	-0.84564500

H	1.51214400	1.95674300	-1.97649600
H	0.18384000	0.80490400	-1.60658300
H	-3.31833300	1.46089100	1.17227600
H	-3.87842600	1.70545900	-0.48020500
H	-3.25654300	-0.43158700	-2.10264300
H	-3.78882300	-2.84540500	-2.28973700
H	-4.34943200	-4.16025100	-0.25269800
H	-4.36890400	-3.04180200	1.96965700
H	-3.83105100	-0.62770000	2.14850900
P	1.83535900	0.93496600	0.29963100
C	3.00710300	-0.45492200	0.12697300
C	4.25950300	-0.24768000	-0.48337100
C	2.62981900	-1.76809900	0.46489500
C	5.11462300	-1.32048800	-0.72836000
H	4.57333700	0.75342200	-0.76613600
C	3.48977300	-2.83771300	0.21559800
H	1.66839500	-1.95980200	0.93141800
C	4.73391100	-2.61918000	-0.37966800
H	6.08074500	-1.14129600	-1.19250900
H	3.18640500	-3.84404000	0.49170600
H	5.40178200	-3.45417300	-0.57199600
C	2.78592000	2.36150800	0.94156700
H	2.09973000	3.21081200	1.02289200
H	3.21250900	2.14599600	1.92557500
H	3.59043000	2.63211200	0.25138400
C	0.66415400	0.50552100	1.63639000
H	0.01442600	1.36978800	1.79665600
H	0.03382300	-0.33832300	1.34611300
H	1.19413500	0.27262700	2.56496900

TS1-cis

C	0.37315000	0.61926900	0.97037400
C	-0.77987300	-0.19589300	1.14559500
C	1.33478900	0.30914800	-0.02616600
O	1.28781700	-0.62204500	-0.84644600
O	2.40725200	1.18845900	0.00241500
C	3.45889600	0.96252600	-0.95113700
C	4.62132700	0.20019900	-0.35278500
C	5.82621200	0.84959200	-0.05951900
C	6.90047700	0.14952300	0.49573200
C	6.77810500	-1.21375100	0.76811700
C	5.57825000	-1.87188700	0.48051100
C	4.50880800	-1.17158200	-0.07725400
H	0.50539100	1.51942600	1.56067600

H	-1.29346100	-0.12703200	2.10526400
H	-0.69096900	-1.22951800	0.80815600
H	3.04744700	0.42707900	-1.81091200
H	3.78544400	1.95745400	-1.27003000
H	5.92493400	1.91276700	-0.26856100
H	7.82969400	0.66941700	0.71555200
H	7.61163300	-1.76151100	1.20055000
H	5.47849500	-2.93453800	0.68799300
H	3.57437200	-1.67735500	-0.30423200
P	-2.35138300	0.41479400	-0.16031600
C	-4.10601200	-0.07405900	0.01112200
C	-4.69672900	-1.02435300	-0.84055800
C	-4.85482700	0.41746000	1.09810800
C	-6.00657100	-1.45373700	-0.62157100
H	-4.14291100	-1.42645100	-1.68296200
C	-6.16274500	-0.01309900	1.31060400
H	-4.41740000	1.14161900	1.78082500
C	-6.74414600	-0.94967700	0.45086700
H	-6.45094800	-2.18128200	-1.29550800
H	-6.72938500	0.38307500	2.14895800
H	-7.76409300	-1.28447500	0.61805700
C	-2.32111000	2.24449900	-0.11713000
H	-1.27383800	2.56232500	-0.15265200
H	-2.86182000	2.67024700	-0.96753900
H	-2.76436800	2.61411200	0.81260400
C	-1.81105300	-0.04286700	-1.84809900
H	-0.76199000	0.24569200	-1.95535100
H	-1.85923300	-1.12792600	-1.97816500
H	-2.41847400	0.44578000	-2.61658400

IM1-trans

C	-0.03206700	-2.72879900	-0.86258600
C	-0.85836000	-1.55655400	-1.16948300
C	1.30498100	-2.65615000	-0.43306700
O	2.08893800	-3.58072800	-0.18291100
O	1.74990900	-1.31516000	-0.29910600
C	3.11469600	-1.16772200	0.09428400
C	3.46783600	0.29870700	0.02209200
C	3.46810700	0.96823600	-1.21123200
C	3.79404000	2.32152900	-1.28795200
C	4.12655900	3.03078100	-0.12895600
C	4.12925100	2.37612200	1.10309200
C	3.79857700	1.01951000	1.17542000
H	-0.46231300	-3.72038800	-0.95321800

H	-1.64971400	-1.73851500	-1.90774300
H	-0.29240700	-0.67362900	-1.48187800
H	3.26654900	-1.55058700	1.11139200
H	3.75670400	-1.76257800	-0.56652800
H	3.20935500	0.41924700	-2.11335500
H	3.79306000	2.82445600	-2.25190700
H	4.38432200	4.08514300	-0.18895900
H	4.38656400	2.91926300	2.00911000
H	3.80109500	0.51300100	2.13821500
P	-1.83169600	-0.95432400	0.37729300
C	-2.92336500	0.48340100	0.15022400
C	-4.15814200	0.33181400	-0.50932200
C	-2.49457500	1.77610100	0.50294700
C	-4.94587700	1.44531800	-0.79577600
H	-4.50981100	-0.65397300	-0.80055600
C	-3.28830400	2.88564900	0.21321000
H	-1.54480500	1.92186600	1.00799400
C	-4.51471000	2.72454800	-0.43482100
H	-5.89900100	1.31274200	-1.30022700
H	-2.94785900	3.87713700	0.49865000
H	-5.13077700	3.59086800	-0.65871600
C	-2.84494700	-2.35714200	0.94731000
H	-2.18681600	-3.22735200	1.03417600
H	-3.29880900	-2.14163400	1.91862500
H	-3.63199700	-2.58521200	0.22255200
C	-0.65371200	-0.58600500	1.71448700
H	-0.05160600	-1.48263300	1.87987600
H	0.01947600	0.22408900	1.42636600
H	-1.18645900	-0.32540800	2.63364000

IM1-cis

C	-0.25736800	0.69773400	-0.99944700
C	0.97255100	-0.11238400	-1.00169000
C	-1.24559800	0.46556200	-0.03927800
O	-1.20579100	-0.34926900	0.91138700
O	-2.37786700	1.26989300	-0.23201600
C	-3.42922800	1.13778500	0.72945300
C	-4.53335200	0.20768800	0.26906200
C	-5.80619000	0.70320000	-0.03667700
C	-6.82842700	-0.15416300	-0.45351000
C	-6.58486900	-1.52299800	-0.57380000
C	-5.31579700	-2.02808800	-0.27279600
C	-4.29885200	-1.17104700	0.14679200
H	-0.38588500	1.48269800	-1.73574400

H	1.47281500	-0.16995700	-1.97593600
H	0.82275700	-1.13243600	-0.62764100
H	-3.00428300	0.78297100	1.67309700
H	-3.83188600	2.14646600	0.87516800
H	-5.99926100	1.77054400	0.05159800
H	-7.81141400	0.24804600	-0.68669600
H	-7.37706900	-2.19281900	-0.89912700
H	-5.12064900	-3.09424900	-0.36133400
H	-3.31051000	-1.55268800	0.38757900
P	2.28920800	0.60579500	0.17280400
C	3.96129800	-0.10072500	0.01684200
C	4.48913000	-0.96858100	0.98793700
C	4.70137100	0.14406000	-1.15554100
C	5.73485300	-1.56711900	0.79466600
H	3.93817700	-1.17598800	1.89962100
C	5.94464800	-0.45680500	-1.34231800
H	4.31092400	0.80598800	-1.92407600
C	6.46460500	-1.31319400	-0.36778600
H	6.13479100	-2.23058800	1.55642100
H	6.50809100	-0.25586400	-2.24928100
H	7.43371100	-1.78146000	-0.51574400
C	2.41134700	2.39097300	-0.16422200
H	1.40153700	2.80914000	-0.11900000
H	3.05217600	2.87810800	0.57603300
H	2.81841600	2.56272100	-1.16539700
C	1.71163600	0.40936000	1.88570200
H	0.66878400	0.73360800	1.92567800
H	1.72946900	-0.64555800	2.17199400
H	2.32987800	0.99185000	2.57541300

TS2a-re-trans-E

C	-1.19720400	-0.51971800	-0.37546600
C	-1.32433300	0.81725500	0.28249300
C	-2.25867100	-1.48635400	-0.36207700
O	-2.29197500	-2.52152600	-1.03221200
O	-3.25066000	-1.18715400	0.55736500
C	-4.28385000	-2.17423100	0.74954800
C	-5.52930500	-1.84532800	-0.04368600
C	-5.57133400	-2.07253400	-1.42869900
C	-6.71390300	-1.75683900	-2.16449300
C	-7.83298300	-1.21155400	-1.52766600
C	-7.80183800	-0.98418900	-0.15074700
C	-6.65511100	-1.29791800	0.58369500
H	-0.62850200	-0.54358500	-1.29940600

H	-0.33495700	1.15316000	0.63356500
H	-2.00144400	0.79160300	1.14200400
H	-3.89072700	-3.15336000	0.46833400
H	-4.49922500	-2.16594200	1.82180400
H	-4.69879100	-2.49837900	-1.91616900
H	-6.73475100	-1.94299100	-3.23552200
H	-8.72447300	-0.97060700	-2.10120200
H	-8.66887300	-0.56332800	0.35236300
H	-6.63518200	-1.12007900	1.65693300
P	-1.93569400	2.15475200	-0.81510700
C	-1.56632100	3.78303400	-0.10112800
C	-0.21609400	4.14623200	0.05897800
C	-2.58112900	4.65793400	0.31501100
C	0.10216300	5.38006400	0.62555900
H	0.57683000	3.46781500	-0.25210000
C	-2.24977200	5.88939400	0.88199000
H	-3.62646300	4.38895700	0.19858800
C	-0.91036900	6.25093500	1.03684200
H	1.14475000	5.66020400	0.74672500
H	-3.03917500	6.56402800	1.20129100
H	-0.65515800	7.21043900	1.47835100
C	-1.12580300	2.05722600	-2.43957200
H	-1.45365200	1.14971100	-2.95433100
H	-1.39747900	2.93178800	-3.03851900
H	-0.04145400	2.01743300	-2.28548300
C	-3.72800600	1.98082500	-1.06563300
H	-3.91962900	0.98456500	-1.47443000
H	-4.26085700	2.06787800	-0.11477800
H	-4.09769900	2.73359900	-1.76790600
N	1.37918700	-0.28130000	0.87066100
C	0.55107700	-1.31110700	0.71282300
C	-0.08038700	-1.90671700	1.92226300
C	-0.63061300	-3.19833200	1.86593900
C	-1.20593000	-3.77826600	2.99661700
C	-1.23988600	-3.07816700	4.20593600
C	-0.68972600	-1.79489300	4.27402000
C	-0.11130300	-1.21615400	3.14464400
H	0.70367200	-2.02871600	-0.09860200
H	-0.61434400	-3.74147900	0.92510900
H	-1.62312300	-4.78047700	2.93539800
H	-1.68451800	-3.53125900	5.08845400
H	-0.70542000	-1.24656400	5.21308300
H	0.33244500	-0.22685100	3.19565100
N	3.86257200	0.62972700	0.35679500

P	2.33450100	0.33128000	-0.33458900
N	2.88479000	-0.88898800	-1.40820200
C	3.89689100	1.39966400	1.62508700
C	2.22365900	-0.98409600	-2.73512500
O	1.71370100	1.53995500	-1.00540800
C	3.01070200	-0.30834200	-3.86806100
C	1.83698200	-2.42780900	-3.08856200
C	4.01870600	0.53103500	2.88587800
C	4.96233600	2.50479000	1.57595800
C	4.35069800	-1.01182400	-1.29241600
C	4.95506900	-2.39410300	-1.56830000
C	6.48429500	-2.33064400	-1.38873200
C	6.89587200	-1.75009300	-0.02585300
H	2.92542800	1.90570000	1.67986200
H	1.28896300	-0.42224800	-2.63153600
H	2.41186800	-0.30926300	-4.78676300
H	3.24099600	0.73269000	-3.61715500
H	3.94972000	-0.82782500	-4.09204000
H	1.23752600	-2.44311300	-4.00772200
H	1.23829900	-2.87816700	-2.28957600
H	2.71273900	-3.06308500	-3.25614500
H	3.91169600	1.15701200	3.78017800
H	3.23311300	-0.22963400	2.90695100
H	4.99140400	0.03081500	2.95349700
H	4.87173700	3.15835900	2.45289600
H	4.83439500	3.11673100	0.67672100
H	5.97971200	2.09993800	1.56887300
H	4.83718800	-0.29191200	-1.97128400
H	4.51129700	-3.12986700	-0.88402300
H	4.72405400	-2.72267300	-2.58678100
H	6.91627600	-3.33104400	-1.51706600
H	6.90828000	-1.70497300	-2.18758700
H	6.62788900	-2.46298900	0.76712000
H	7.98602400	-1.63284200	0.01792800
C	4.69461300	-0.56582400	0.14343500
H	4.39056900	-1.37408000	0.83278000
C	6.21431500	-0.40058100	0.26993600
H	6.56053000	0.36884800	-0.43332600
H	6.49097600	-0.06730000	1.27509200
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C	1.35316900	0.79502500	0.99823100
C	2.64468600	0.81708800	0.22921500
C	0.89904100	-0.46891000	1.53861700
O	0.13432300	-0.60994600	2.48935700

O	1.37740900	-1.54793900	0.83315200
C	0.77314500	-2.82283600	1.15303600
C	1.19516000	-3.80440200	0.09141700
C	2.20353900	-4.74585800	0.32806800
C	2.59446700	-5.63837500	-0.67410100
C	1.97702000	-5.59345200	-1.92540100
C	0.96708200	-4.65646400	-2.16864500
C	0.57575800	-3.76766400	-1.16744200
H	1.20072500	1.61857100	1.69126600
H	2.79403900	1.76340100	-0.30519100
H	2.69194900	0.00898600	-0.50849100
H	1.10402900	-3.14211800	2.14824600
H	-0.30971200	-2.69025400	1.16170200
H	2.68052700	-4.78575200	1.30564400
H	3.37515400	-6.36897300	-0.47644000
H	2.27635000	-6.28806700	-2.70641700
H	0.47901100	-4.62517100	-3.13976100
H	-0.21494200	-3.03976700	-1.33529700
P	4.16598000	0.64450000	1.27028400
C	5.66163800	0.61253000	0.24046900
C	6.50112800	1.73274100	0.13490000
C	5.94389300	-0.53915200	-0.51562900
C	7.61139600	1.69665900	-0.70951500
H	6.29698800	2.63239300	0.70662400
C	7.05484600	-0.56692100	-1.35667000
H	5.30112500	-1.41298200	-0.45309600
C	7.89055100	0.54870400	-1.45299500
H	8.25822200	2.56620100	-0.78270600
H	7.26783500	-1.46088100	-1.93558800
H	8.75592200	0.52353800	-2.10922600
C	4.24637400	2.05551800	2.41379200
H	3.36004700	2.02628900	3.05466600
H	5.14148100	1.99564800	3.03907700
H	4.24279000	2.99977300	1.86173200
C	4.13447900	-0.86621900	2.28355800
H	3.28972800	-0.82080300	2.97638800
H	4.02095000	-1.74862900	1.65051900
H	5.06676500	-0.93561900	2.85234200
N	-3.52443800	-0.17351200	1.21455400
P	-2.40496600	-0.09184000	-0.07065500
N	-3.60221400	0.33369500	-1.23944000
C	-3.05565700	0.09762800	2.59408400
C	-3.21815100	0.12978200	-2.65453100
N	-1.44244700	1.23632000	0.15802500

O	-1.67555900	-1.37433000	-0.40802400
C	-0.22319300	1.29855300	-0.38917100
C	-3.63682900	-1.23343600	-3.22669000
C	-3.67101900	1.30048700	-3.54076100
C	-3.49013600	1.47102100	3.12812800
C	-3.42077500	-1.04144800	3.55879100
C	-4.91176500	-0.09501300	-0.73115800
C	-6.15930600	0.53652600	-1.36242800
C	-7.41772400	-0.00191900	-0.65493100
C	-7.36371400	0.18709000	0.86968200
H	-1.96516500	0.11256400	2.53644400
H	-2.12137700	0.14725000	-2.66081100
H	-3.23397200	-1.35816700	-4.23954600
H	-3.24628700	-2.04157500	-2.60086100
H	-4.72624000	-1.33748700	-3.29359200
H	-3.22831100	1.21294000	-4.54161100
H	-3.34843600	2.25258300	-3.10577700
H	-4.75836100	1.33480800	-3.66386500
H	-3.02189200	1.65295200	4.10337800
H	-3.17200200	2.26800600	2.44752000
H	-4.57485700	1.54851400	3.26917900
H	-2.92321200	-0.88969500	4.52552900
H	-3.08582000	-2.00260700	3.15411200
H	-4.49789700	-1.10907700	3.74780700
H	-5.02424200	-1.19201900	-0.81368900
H	-6.10307000	1.63006200	-1.27412800
H	-6.21760900	0.30158300	-2.43019000
H	-8.31209200	0.48603400	-1.06344300
H	-7.51843700	-1.07347400	-0.88121700
H	-7.43585700	1.25955800	1.10293500
H	-8.23344700	-0.29097900	1.33844200
C	0.28468000	2.66157400	-0.74245500
C	1.10698600	2.84511700	-1.86503500
C	-0.08531100	3.79160600	0.00600400
C	1.55931500	4.11854500	-2.22455800
H	1.37650500	1.98435100	-2.47367200
C	0.37136600	5.05960000	-0.34572900
H	-0.74934700	3.65638800	0.85419200
C	1.19830000	5.23021200	-1.46245300
H	2.18532900	4.24011600	-3.10539800
H	0.07563100	5.92231700	0.24666800
H	1.54584300	6.22203400	-1.74039600
H	0.11051200	0.51324900	-1.07676400
C	-4.85825200	0.25218300	0.76759400

H	-4.95237600	1.34961200	0.84808600
C	-6.06498600	-0.36712000	1.48567900
H	-6.02681900	-1.46100800	1.39109100
H	-6.04380200	-0.13631800	2.55546100

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C	-1.43513000	0.01455200	0.32418800
C	-1.18089800	1.46533100	0.57067700
C	-2.65726300	-0.54689100	0.82650800
O	-3.43955200	-0.02998400	1.62912900
O	-2.85343400	-1.82930500	0.34464500
C	-4.04272700	-2.51391800	0.78810200
C	-5.18102200	-2.35019400	-0.19438600
C	-5.38851000	-3.29735800	-1.20541000
C	-6.42181700	-3.14011500	-2.13139900
C	-7.26395000	-2.02878700	-2.05590300
C	-7.06722000	-1.07810900	-1.05030600
C	-6.03319400	-1.23787700	-0.12624500
H	-1.10226600	-0.38825900	-0.62613700
H	-0.09996400	1.65370700	0.66616200
H	-1.67959300	1.80001200	1.48749700
H	-3.75509000	-3.56636500	0.86477500
H	-4.31950700	-2.14255200	1.77693000
H	-4.73556300	-4.16545900	-1.26572900
H	-6.57063300	-3.88596100	-2.90810800
H	-8.07107400	-1.90632500	-2.77362000
H	-7.72456700	-0.21473300	-0.98262300
H	-5.87228700	-0.50069800	0.65522200
P	-1.77183600	2.58284500	-0.76081900
C	-0.95605900	4.20162600	-0.64964000
C	0.43764800	4.25499200	-0.83830000
C	-1.66859500	5.37348800	-0.35423700
C	1.09893500	5.47860400	-0.73732800
H	0.99832700	3.34706700	-1.05649800
C	-0.99504700	6.59176900	-0.25467900
H	-2.74324900	5.34505000	-0.20324900
C	0.38659100	6.64520200	-0.44667400
H	2.17451000	5.51906400	-0.88480700
H	-1.55159800	7.49680100	-0.02782500
H	0.90853200	7.59505500	-0.36845300
C	-1.40241200	1.88019900	-2.39596200
H	-1.99553300	0.97301500	-2.54220300
H	-1.65601400	2.60839000	-3.17224400
H	-0.33652800	1.63005700	-2.43526400

C	-3.57496500	2.78302100	-0.63274500
H	-4.02779700	1.78853300	-0.67952000
H	-3.84518600	3.23612400	0.32498000
H	-3.95940900	3.39379400	-1.45478500
N	1.36786600	-0.03276000	0.98983200
C	0.36619600	-0.85356800	1.29070500
C	-0.06798900	-0.95640700	2.71030000
C	-0.82791800	-2.05840700	3.13576200
C	-1.21865000	-2.18536900	4.46818000
C	-0.85497200	-1.21142700	5.40207200
C	-0.09446600	-0.11331300	4.99082900
C	0.29949200	0.01152600	3.65875700
H	0.20626600	-1.76954600	0.71487700
H	-1.11472400	-2.81596100	2.41085500
H	-1.80438800	-3.04699900	4.77908400
H	-1.15726400	-1.30989100	6.44160000
H	0.19838900	0.64551700	5.71263300
H	0.90440000	0.85361400	3.33761400
N	3.78909900	0.14414800	-0.18124400
P	2.11792100	0.02093500	-0.48490600
N	2.20843500	-1.52543700	-1.22571900
C	4.23264300	1.18335600	0.77994100
C	1.25323200	-1.80463700	-2.32888800
O	1.56820300	1.12040500	-1.37106400
C	1.84435800	-1.59378800	-3.73080400
C	0.59317200	-3.18453500	-2.19140500
C	4.50202000	0.65734100	2.19750100
C	5.41670000	1.98768600	0.22298900
C	3.62395300	-1.92289100	-1.34496600
C	3.92701300	-3.42534200	-1.31385600
C	5.44705000	-3.64298400	-1.44012200
C	6.24577300	-2.84559900	-0.39672500
H	3.39097800	1.88198900	0.85795600
H	0.45810200	-1.06026800	-2.21393200
H	1.05263500	-1.68746600	-4.48397400
H	2.28147300	-0.59399200	-3.82384700
H	2.61437900	-2.33510900	-3.97382400
H	-0.21847200	-3.28718800	-2.92283500
H	0.16422800	-3.31420200	-1.19193900
H	1.29876400	-4.00315800	-2.36659100
H	4.70212100	1.49871200	2.87216500
H	3.63201000	0.11503100	2.57915400
H	5.37340800	-0.00617900	2.23726000
H	5.63083200	2.84588700	0.87283700

H	5.18294300	2.36508400	-0.77840800
H	6.33035600	1.38786100	0.15514700
H	4.04596900	-1.51689200	-2.27942300
H	3.54709600	-3.85620000	-0.37762700
H	3.41881600	-3.94124000	-2.13488200
H	5.67891000	-4.71220400	-1.35454800
H	5.76509200	-3.33619900	-2.44708200
H	6.06026000	-3.26876900	0.60089000
H	7.32137500	-2.95406200	-0.58448400
C	4.35310500	-1.21585100	-0.18408200
H	4.09083400	-1.74183700	0.75177300
C	5.86861700	-1.35177100	-0.37985300
H	6.16296200	-0.86852800	-1.32128700
H	6.41377100	-0.84875900	0.42486900

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C	-1.49731100	0.60850200	0.93625500
C	-2.52987600	-0.48124800	0.98090800
C	-1.38109200	1.26275800	-0.35370300
O	-1.77991900	0.79206200	-1.42977800
O	-0.75208200	2.45496500	-0.27501400
C	-0.45543800	3.11026700	-1.53716100
C	0.25394600	4.40419500	-1.23358100
C	1.64254100	4.40814500	-1.03782400
C	2.30911700	5.60047300	-0.75212500
C	1.59838600	6.80076200	-0.66144500
C	0.21560900	6.80476400	-0.85755700
C	-0.45090800	5.61077900	-1.14208700
H	-1.48682500	1.29225700	1.78076600
H	-2.49270400	-1.03292900	1.92724200
H	-2.36884000	-1.19813300	0.16948700
H	0.17842000	2.44201300	-2.12183300
H	-1.39472000	3.28485200	-2.07290800
H	2.18065800	3.46656500	-1.12037200
H	3.38638900	5.59492800	-0.60500600
H	2.12056500	7.72924300	-0.44352400
H	-0.34197100	7.73599800	-0.79294800
H	-1.52771200	5.61569300	-1.29917800
P	-4.31149100	0.04332900	0.81134900
C	-5.19129500	-1.03704200	-0.34898300
C	-6.35924100	-1.72598500	0.01016300
C	-4.65985500	-1.17924600	-1.64385300
C	-6.99465400	-2.54712800	-0.92237300
H	-6.77711600	-1.62822000	1.00729500

C	-5.30546300	-1.99901000	-2.56796500
H	-3.74597200	-0.65670800	-1.91826100
C	-6.47048200	-2.68248800	-2.20930000
H	-7.89835500	-3.08041300	-0.64168100
H	-4.89450000	-2.10676900	-3.56752600
H	-6.96760300	-3.32323100	-2.93221400
C	-5.09764600	-0.02704500	2.45174100
H	-4.51793000	0.60752200	3.13056800
H	-6.12672900	0.34136000	2.41669500
H	-5.08652100	-1.05022200	2.83803100
C	-4.47429300	1.75872700	0.22707800
H	-3.91661100	2.42895800	0.88743300
H	-4.07599900	1.84231100	-0.78617500
H	-5.53322400	2.03506600	0.23136000
N	1.38870000	0.26586500	0.79603600
C	0.31222000	-0.36773800	1.27494000
C	0.19199500	-0.44342700	2.77141400
C	-0.33694800	-1.58652100	3.38857800
C	-0.43810800	-1.67051000	4.78116500
C	-0.00889800	-0.60969100	5.57897700
C	0.53253400	0.53081600	4.97395700
C	0.63673700	0.61072200	3.58693100
H	-0.02207400	-1.28963400	0.77849900
H	-0.64816700	-2.42893000	2.77406400
H	-0.84228500	-2.57009500	5.23961800
H	-0.08382700	-0.67190800	6.66168400
H	0.87884600	1.35811200	5.58900200
H	1.06803900	1.48715200	3.11192200
N	3.71442000	-0.56463000	-0.32120200
P	2.11615400	-0.03074400	-0.64916300
N	1.60199000	-1.54571600	-1.31074000
C	4.56376400	0.30753100	0.52245100
C	0.72026900	-1.45659500	-2.50463900
O	2.08638800	1.13245800	-1.60855900
C	1.47657300	-1.34845100	-3.83826200
C	-0.33162500	-2.57630300	-2.55325400
C	4.60114300	-0.08085700	2.00844400
C	5.97494500	0.45334200	-0.06882300
C	2.73088300	-2.49401600	-1.29132300
C	2.38855500	-3.97719400	-1.08935500
C	3.68393200	-4.81090200	-1.10067500
C	4.72367600	-4.29760700	-0.09234800
H	4.09996400	1.29964000	0.46152100
H	0.16671500	-0.52296600	-2.37190600

H	0.76750500	-1.16228100	-4.65484200
H	2.18618100	-0.51613100	-3.80929800
H	2.02112500	-2.26808800	-4.08529100
H	-1.12184700	-2.31005100	-3.26671800
H	-0.79619200	-2.72289700	-1.57181900
H	0.08653400	-3.53550000	-2.87776900
H	5.16516700	0.66979500	2.57577100
H	3.58930500	-0.12816000	2.42011600
H	5.08996700	-1.04821600	2.17244700
H	6.53128700	1.23479300	0.46478800
H	5.91759600	0.73474500	-1.12570900
H	6.55316400	-0.47358100	0.00654000
H	3.30573400	-2.40772700	-2.22824700
H	1.85394400	-4.10134800	-0.13718900
H	1.72166300	-4.33658700	-1.87866500
H	3.45277000	-5.86487000	-0.89954900
H	4.11621100	-4.77552500	-2.11132400
H	4.36474700	-4.49380100	0.92838400
H	5.66264900	-4.85504700	-0.20345900
C	3.66722400	-2.02113500	-0.15637700
H	3.19422200	-2.28932700	0.80779100
C	4.99336600	-2.78857200	-0.24180700
H	5.47778700	-2.57793400	-1.20489900
H	5.68405100	-2.46551500	0.54356300

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C	1.34533600	-0.48402100	0.34980700
C	1.44028700	0.78420400	-0.45037300
C	2.47560000	-1.36369400	0.47098500
O	2.63660000	-2.22593700	1.33403400
O	3.38525100	-1.20703200	-0.57076000
C	4.50328000	-2.11514000	-0.59349600
C	5.73312200	-1.50792900	0.04487800
C	5.92810500	-1.57767000	1.43301200
C	7.05521700	-1.00104300	2.02090400
C	8.00345700	-0.34537900	1.23036100
C	7.81847500	-0.26961200	-0.15169900
C	6.68985600	-0.84790100	-0.73749600
H	0.74961300	-0.44356500	1.25407100
H	0.45650300	1.09567300	-0.82052500
H	2.12819700	0.68865200	-1.29603600
H	4.21711300	-3.04075800	-0.09030400
H	4.68704800	-2.32136200	-1.65203100
H	5.18523200	-2.08337600	2.04334700

H	7.19713600	-1.06808800	3.09676900
H	8.88326400	0.09925400	1.68865100
H	8.55422700	0.23396800	-0.77394000
H	6.55195500	-0.79293200	-1.81544000
P	1.98851800	2.25012900	0.51752500
C	1.73428000	3.76148800	-0.45472500
C	0.42566300	4.06720700	-0.87445000
C	2.80000600	4.59819500	-0.81897000
C	0.19739700	5.20900400	-1.64147900
H	-0.40522700	3.41498500	-0.61169800
C	2.55887900	5.73711500	-1.58856300
H	3.81426100	4.37068000	-0.50540800
C	1.25999200	6.04361300	-1.99820900
H	-0.81321100	5.44475800	-1.96260000
H	3.38675900	6.38337500	-1.86642000
H	1.07535000	6.93204500	-2.59590100
C	0.97711500	2.37516300	2.02317100
H	1.20965500	1.53891100	2.68850700
H	1.18588000	3.31822700	2.53694700
H	-0.07742400	2.32194200	1.73445400
C	3.72858400	2.10426500	1.01929300
H	3.83269300	1.19661400	1.62114000
H	4.38008300	2.01691400	0.14587700
H	4.02974500	2.96536300	1.62283100
N	-3.65456800	0.08136000	-1.03521500
P	-2.36489400	0.08932600	0.09272300
N	-3.38617700	-0.08901500	1.44707500
C	-3.33219900	-0.27843100	-2.43486700
C	-2.84299400	0.33059300	2.75778800
N	-1.48254100	-1.30832000	0.03809900
O	-1.54618500	1.36899800	0.03889100
C	-0.38339700	-1.48378500	-0.69436800
C	-3.29803100	1.73278700	3.19010900
C	-3.09067400	-0.72517800	3.84569900
C	-3.67315100	-1.73206100	-2.79596900
C	-3.93339400	0.72373900	-3.43245500
C	-4.77913500	0.17575900	1.05626800
C	-5.88017700	-0.43446900	1.93288300
C	-7.25854100	-0.09500700	1.33305900
C	-7.37627900	-0.50665200	-0.14269100
H	-2.24337700	-0.17477000	-2.52125500
H	-1.75616500	0.37751700	2.61837300
H	-2.78033700	2.03138600	4.10976900
H	-3.06883400	2.47081800	2.41421300

H	-4.37423700	1.77201900	3.39442500
H	-2.53542500	-0.46860700	4.75707500
H	-2.74964600	-1.70745100	3.50234100
H	-4.14856100	-0.80584500	4.11512700
H	-3.29592100	-1.96751300	-3.79827800
H	-3.21361500	-2.42905700	-2.08809900
H	-4.75444200	-1.91116700	-2.80345500
H	-3.55713400	0.52470200	-4.44397700
H	-3.65556800	1.74708000	-3.15800400
H	-5.02594000	0.66719100	-3.46889800
H	-4.96656100	1.26328200	0.99923700
H	-5.74015700	-1.52198400	1.99301700
H	-5.82539400	-0.04533600	2.95483800
H	-8.04851100	-0.57784800	1.92206500
H	-7.42521300	0.98850400	1.41915500
H	-7.38088600	-1.60390400	-0.21138500
H	-8.33539700	-0.16557000	-0.55232100
C	0.13528200	-2.86564100	-0.86850500
C	0.97080600	-3.16761400	-1.95598300
C	-0.22808600	-3.89865500	0.00880100
C	1.42946400	-4.46819000	-2.16398200
H	1.25746000	-2.37515500	-2.64357700
C	0.23448500	-5.19748400	-0.19524300
H	-0.88528000	-3.66545900	0.84052600
C	1.06214000	-5.48961900	-1.28337600
H	2.06630600	-4.68705500	-3.01771900
H	-0.05519300	-5.98716200	0.49380300
H	1.41632200	-6.50456500	-1.44500400
H	-0.15343400	-0.82882400	-1.54114800
C	-4.88353900	-0.38483800	-0.37544500
H	-4.88480300	-1.48649000	-0.30004300
C	-6.21864200	0.03799800	-1.00106300
H	-6.26481000	1.13357800	-1.06454900
H	-6.31231300	-0.34852500	-2.02098400

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C	-1.01083300	0.20563800	0.15394600
C	-1.13894900	-0.74497000	-1.00705400
C	-2.09384300	1.05996200	0.55327500
O	-2.19877300	1.63020100	1.63848200
O	-3.02217600	1.27994500	-0.46495500
C	-3.98809200	2.32849200	-0.24070400
C	-5.32199500	1.80918700	0.24838000
C	-5.46904500	1.32712000	1.55880000
C	-6.70538300	0.86383500	2.00842300

C	-7.81600100	0.87873500	1.15852000
C	-7.68086100	1.35682600	-0.14629700
C	-6.43952800	1.81669200	-0.59612400
H	-0.43167100	-0.14357300	0.99912100
H	-0.19299400	-0.82939800	-1.55536600
H	-1.91219100	-0.43195700	-1.71425800
H	-3.56485900	3.03923300	0.47201500
H	-4.10973100	2.82141600	-1.20957100
H	-4.60280400	1.32208300	2.21378700
H	-6.80562000	0.49716000	3.02699000
H	-8.78035600	0.52367000	1.51301000
H	-8.53948400	1.37693600	-0.81289100
H	-6.33870900	2.19225000	-1.61234100
P	-1.44609400	-2.51675800	-0.58436400
C	-3.20723900	-2.97012300	-0.60133000
C	-3.56763100	-4.32497700	-0.49345800
C	-4.20640800	-1.99228500	-0.71336600
C	-4.91122800	-4.69369400	-0.50560200
H	-2.80536100	-5.09404500	-0.40062200
C	-5.55090200	-2.37033100	-0.72219800
H	-3.94757300	-0.94022600	-0.78231900
C	-5.90362100	-3.71628100	-0.62217400
H	-5.18296000	-5.74249400	-0.42541800
H	-6.31881600	-1.60697500	-0.80396600
H	-6.95090400	-4.00562700	-0.63188700
C	-0.56552100	-3.53423600	-1.81238000
H	0.49405200	-3.26326700	-1.75384500
H	-0.68643400	-4.60120300	-1.60514700
H	-0.94805200	-3.31565600	-2.81425400
C	-0.75363100	-2.92687500	1.04324400
H	0.30748500	-2.66018200	1.02185100
H	-1.27066200	-2.36161400	1.82308000
H	-0.87254900	-3.99783700	1.23429100
N	3.95110400	-0.12186300	-1.18112000
P	2.64419600	-0.34622600	-0.09436300
N	3.65275400	-0.54853100	1.26546200
C	3.67026700	0.60553700	-2.43948300
C	3.05911300	-1.20712600	2.44845600
N	1.81320300	1.04988600	0.20112000
O	1.77616600	-1.53750300	-0.46770600
C	0.73401200	1.44654200	-0.47736700
C	3.40943700	-2.69849300	2.56693300
C	3.35266300	-0.43563800	3.74370900
C	4.09687000	2.08092100	-2.41010300

C	4.22789200	-0.13623200	-3.66430300
C	5.03100000	-0.80497200	0.82582700
C	6.15431200	-0.50038900	1.82458600
C	7.51551100	-0.78416000	1.16141700
C	7.68913400	-0.03569800	-0.16976100
H	2.57863500	0.59081100	-2.54872900
H	1.97471500	-1.14432700	2.29717000
H	2.84738300	-3.15349700	3.39171300
H	3.15642800	-3.23327600	1.64522000
H	4.47453400	-2.85609800	2.77317000
H	2.76143000	-0.84721000	4.57176300
H	3.08391100	0.61887200	3.62252300
H	4.40737100	-0.48908000	4.03221900
H	3.75884800	2.58818600	-3.32158500
H	3.65686900	2.59769800	-1.55109300
H	5.18616300	2.19169400	-2.35903100
H	3.87029600	0.33507200	-4.58866400
H	3.89620000	-1.18011100	-3.66029000
H	5.32212700	-0.12835100	-3.69089400
H	5.14886800	-1.85675500	0.50723700
H	6.08809700	0.54855600	2.14277000
H	6.05527300	-1.11703100	2.72372000
H	8.32726400	-0.51853800	1.85016600
H	7.60208600	-1.86540500	0.98076100
H	7.77276700	1.04189900	0.03167500
H	8.62904600	-0.33554300	-0.64997400
C	0.24969100	2.83621100	-0.26087200
C	-0.53309500	3.46591300	-1.24138300
C	0.59142600	3.55695900	0.89351700
C	-0.96064600	4.78346800	-1.07650000
H	-0.80176900	2.91735100	-2.14133900
C	0.15938200	4.87138000	1.06233300
H	1.20829300	3.07237600	1.64347400
C	-0.61698500	5.49132400	0.07872300
H	-1.55629800	5.26002200	-1.85139800
H	0.43036400	5.41671300	1.96313900
H	-0.94758400	6.51871700	0.20902900
H	0.53634700	1.08090300	-1.49120700
C	5.19738700	0.07965000	-0.42656100
H	5.27275700	1.12587000	-0.08180200
C	6.51192100	-0.26889500	-1.13612800
H	6.48553100	-1.31540200	-1.46915900
H	6.65006400	0.35026000	-2.02840700

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C	1.50964200	0.05098200	-0.35258200
C	1.21196600	1.41839600	-0.89502200
C	2.79469600	-0.50173000	-0.67824600
O	3.53581400	-0.14219600	-1.60129700
O	3.11224900	-1.56593700	0.13616100
C	4.31057500	-2.30099400	-0.18168100
C	5.47952300	-1.86965900	0.67605400
C	5.82164900	-2.59019800	1.82703600
C	6.89361500	-2.19151400	2.62887600
C	7.63834300	-1.06114800	2.28704400
C	7.30610800	-0.33416500	1.14004400
C	6.23517700	-0.73569900	0.34027000
H	1.12821200	-0.19449100	0.63094900
H	0.13708800	1.57431400	-1.03852800
H	1.73758700	1.58546500	-1.84179700
H	4.06464000	-3.34920100	0.00968800
H	4.53583000	-2.17188200	-1.24216100
H	5.24493800	-3.47296500	2.09460900
H	7.14726500	-2.76427300	3.51744000
H	8.47518200	-0.75043600	2.90749400
H	7.88750900	0.54283000	0.86562800
H	5.97104200	-0.17482500	-0.55210600
P	1.69406700	2.79854200	0.21829000
C	0.96381700	4.35114100	-0.37320900
C	-0.43499200	4.41052100	-0.52114700
C	1.75215500	5.46120100	-0.71168800
C	-1.02657900	5.57902700	-0.99985700
H	-1.05388800	3.54972500	-0.27413800
C	1.14798600	6.62447700	-1.19054100
H	2.83207200	5.42535300	-0.60579400
C	-0.23943600	6.68434300	-1.33377600
H	-2.10597100	5.62374500	-1.11404000
H	1.76241600	7.48184800	-1.45052400
H	-0.70722800	7.59084200	-1.70800000
C	1.05234000	2.47405800	1.88816200
H	1.57353900	1.61543000	2.32096200
H	1.20927400	3.35153100	2.52227300
H	-0.01544600	2.24655000	1.81131500
C	3.50207500	2.95050000	0.32702300
H	3.90382900	1.99198200	0.66814600
H	3.92630500	3.17188800	-0.65594000
H	3.78501000	3.73049400	1.03983500
N	-3.70423500	-0.26039600	-0.72109200

P	-2.22245500	-0.11265300	0.12535600
N	-2.86914000	-0.66936000	1.60265500
C	-3.63967600	-0.39107600	-2.19459200
C	-2.11918300	-0.32765600	2.83058600
N	-1.13600300	-1.27305300	-0.32806600
O	-1.68734600	1.30998500	0.13322100
C	-0.18944400	-1.11460600	-1.25281600
C	-2.68085600	0.89200600	3.57730100
C	-1.93971200	-1.54477700	3.75036700
C	-3.82054500	-1.83180400	-2.69542000
C	-4.59087900	0.59029900	-2.89692900
C	-4.33769300	-0.63311900	1.54230800
C	-5.10395500	-1.54869000	2.50572300
C	-6.61697400	-1.40194600	2.25169500
C	-6.99445500	-1.63958900	0.78104700
H	-2.62478800	-0.08074100	-2.47259000
H	-1.11386400	-0.05474400	2.48693200
H	-2.01767700	1.16560700	4.40710500
H	-2.76311400	1.75403900	2.90676800
H	-3.67095000	0.69376900	4.00391200
H	-1.24578400	-1.30466700	4.56623200
H	-1.52580800	-2.38589400	3.18447700
H	-2.88218400	-1.86885300	4.20328900
H	-3.65234300	-1.87740900	-3.77791700
H	-3.10628900	-2.50652300	-2.21292200
H	-4.83271300	-2.20644600	-2.50470100
H	-4.40205100	0.59302100	-3.97806000
H	-4.43606800	1.60682000	-2.51942600
H	-5.64304800	0.32825500	-2.74582500
H	-4.70831900	0.39580700	1.70098400
H	-4.78378200	-2.58874500	2.35668200
H	-4.88659100	-1.29040900	3.54715000
H	-7.17070000	-2.09447200	2.89820100
H	-6.92764800	-0.38838800	2.54480700
H	-6.84493400	-2.70133000	0.53695100
H	-8.06159200	-1.43399900	0.62950900
C	0.50403500	-2.32785600	-1.76242700
C	1.22360300	-2.27279800	-2.96700100
C	0.41448100	-3.55491800	-1.08662200
C	1.83547100	-3.41383900	-3.48537200
H	1.30321200	-1.32743700	-3.49801800
C	1.03037400	-4.69463200	-1.60157400
H	-0.15613300	-3.59719400	-0.16424600
C	1.74259500	-4.63030900	-2.80345800

H	2.38251100	-3.35436000	-4.42302600
H	0.94909600	-5.63885100	-1.06823600
H	2.21584800	-5.52143900	-3.20812200
H	-0.24422200	-0.30908700	-1.99200800
C	-4.66567200	-1.02384900	0.08761600
H	-4.47660000	-2.10703300	-0.01147700
C	-6.15542200	-0.78592000	-0.18884500
H	-6.38600100	0.28116100	-0.06638800
H	-6.40947000	-1.05461600	-1.21926800

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C	-1.31815900	-0.46638100	0.85127600
C	-2.64626900	0.27688100	0.97043700
C	-1.42756100	-1.84638300	1.27884300
O	-2.49699700	-2.47573200	1.28608100
O	-0.25288200	-2.43949800	1.63872400
C	-0.32786200	-3.79123300	2.16395900
C	-0.12811600	-4.86105500	1.11541200
C	1.12359300	-5.47175200	0.96291500
C	1.32025600	-6.47112700	0.00718300
C	0.26199700	-6.87201200	-0.81038500
C	-0.99158400	-6.27112600	-0.66495400
C	-1.18635700	-5.27485200	0.29200800
H	-0.86735300	-0.06008900	-0.38805000
H	-2.48003800	1.34775600	0.84106400
H	-3.15223100	0.14097400	1.93653800
H	0.47519100	-3.83326200	2.90391700
H	-1.28864400	-3.91201200	2.66840900
H	1.94942800	-5.16426500	1.60036600
H	2.29697300	-6.93656200	-0.09619200
H	0.41096300	-7.65060500	-1.55400000
H	-1.82044200	-6.58404400	-1.29503000
H	-2.15769800	-4.80460300	0.40851900
P	-3.90428400	-0.16754900	-0.30740200
C	-4.53442500	1.35883800	-1.07171000
C	-3.60899500	2.26018800	-1.62878500
C	-5.90673800	1.64118000	-1.13563500
C	-4.06109300	3.42667000	-2.24349400
H	-2.54083400	2.06097600	-1.57741900
C	-6.34955400	2.81359400	-1.75065100
H	-6.63390100	0.95730900	-0.70907600
C	-5.42927200	3.70429000	-2.30516900
H	-3.34183900	4.11791800	-2.67279800
H	-7.41345200	3.02881300	-1.79424800

H	-5.77706600	4.61568800	-2.78353500
C	-3.21371300	-1.18734500	-1.64497300
H	-2.83139200	-2.12154800	-1.22798500
H	-4.00795300	-1.39807000	-2.36826300
H	-2.40601400	-0.64871500	-2.14750200
C	-5.28194200	-1.07503600	0.45118800
H	-4.85012400	-1.94961300	0.94427800
H	-5.78150000	-0.45078900	1.19774700
H	-6.00400700	-1.39381100	-0.30553300
N	-0.03361900	1.02311400	-0.26460400
C	-0.04401400	0.40004700	1.09329600
C	-0.10145400	1.34036000	2.28566400
C	0.35103200	0.89357200	3.53764300
C	0.25789900	1.70435700	4.66998500
C	-0.29678800	2.98334400	4.57391200
C	-0.74672600	3.44277100	3.33414500
C	-0.64549300	2.63055700	2.20211200
H	0.79534300	-0.28996600	1.23745800
H	0.77971900	-0.10293200	3.62057300
H	0.62088200	1.33825200	5.62742400
H	-0.36931800	3.61727500	5.45394400
H	-1.16996200	4.44063800	3.24494500
H	-0.96747700	3.00068000	1.23326800
N	2.49597800	2.26211100	-0.56709800
P	1.30225700	1.23465000	-1.22408700
N	2.32546900	-0.16146900	-1.13229700
C	2.15652200	3.62135100	-0.11645100
C	1.91487300	-1.27673200	-2.02369600
O	0.84712100	1.61349700	-2.60987600
C	2.53486500	-1.22264500	-3.42876900
C	2.11161800	-2.64571200	-1.35886900
C	2.56758700	3.91334700	1.33566400
C	2.68136900	4.69969100	-1.08023400
C	3.72244100	0.29887300	-1.12379200
C	4.79462300	-0.68761900	-0.64430400
C	6.17703000	-0.00800000	-0.70226800
C	6.20972900	1.34188100	0.03280900
H	1.06113000	3.67048400	-0.14925800
H	0.83239100	-1.15113400	-2.15349500
H	2.09528800	-2.00502400	-4.05982900
H	2.33664000	-0.25374000	-3.89677300
H	3.61828200	-1.39111800	-3.40896500
H	1.63605800	-3.42909800	-1.96249900
H	1.65418200	-2.65659100	-0.36567700

H	3.16851500	-2.91074600	-1.25243100
H	2.11534500	4.85639600	1.66459900
H	2.22898400	3.12554500	2.01401000
H	3.65203300	4.01980900	1.44645100
H	2.31154100	5.69177300	-0.78848000
H	2.34201000	4.49216300	-2.10029300
H	3.77628900	4.74050700	-1.08614800
H	4.01703800	0.63539700	-2.13419100
H	4.56234100	-1.01518000	0.37826200
H	4.81106100	-1.58342800	-1.27316800
H	6.94016800	-0.67975100	-0.28861900
H	6.44483800	0.15266900	-1.75657300
H	6.12956500	1.16659100	1.11538200
H	7.17716300	1.83385400	-0.13072700
C	3.72555300	1.54787300	-0.21804300
H	3.68277900	1.20635600	0.83258700
C	5.06608200	2.27843700	-0.40232400
H	5.18559400	2.56777100	-1.45504000
H	5.10546100	3.19764500	0.18928800

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C	-1.47945700	-0.31812000	1.08858600
C	-1.89440900	1.05142000	1.61888200
C	-2.57260800	-1.20715000	0.76945000
O	-3.74290500	-0.83840500	0.58732100
O	-2.20604000	-2.50161200	0.54658200
C	-3.20336100	-3.37353500	-0.00451100
C	-3.30329600	-3.27282900	-1.51333300
C	-2.17738400	-2.97527300	-2.29280400
C	-2.27254500	-2.93503600	-3.68521200
C	-3.49038500	-3.19894900	-4.31671500
C	-4.61582900	-3.49862200	-3.54593800
C	-4.52181800	-3.53068700	-2.15314000
H	-0.55500300	-0.27405600	0.02483000
H	-0.98609200	1.64363600	1.76882200
H	-2.41740600	1.00849800	2.58782100
H	-2.87211600	-4.37472800	0.29137800
H	-4.17279100	-3.17568600	0.45934100
H	-1.22960100	-2.76747200	-1.80449200
H	-1.39157800	-2.70176700	-4.27799000
H	-3.56209800	-3.16938900	-5.40093800
H	-5.56941600	-3.69934300	-4.02793900
H	-5.40410800	-3.75385900	-1.55686200
P	-2.98179700	2.09574500	0.56144100

C	-2.42572400	3.82888100	0.69300700
C	-1.05204400	4.13009100	0.66774300
C	-3.36463000	4.87058000	0.77269300
C	-0.63798900	5.46212000	0.72121100
H	-0.29647500	3.34558600	0.62127600
C	-2.93809500	6.19748000	0.82795600
H	-4.42836300	4.65726100	0.79486700
C	-1.57431500	6.49467700	0.80196100
H	0.42454200	5.68797000	0.70610600
H	-3.67231700	6.99557600	0.89396800
H	-1.24286700	7.52857500	0.84727900
C	-2.92261800	1.62825300	-1.19566300
H	-3.32646500	0.62014700	-1.30935600
H	-3.52183700	2.34093900	-1.77082900
H	-1.89107800	1.65836000	-1.55473200
C	-4.71132600	2.02077100	1.12036100
H	-4.99417300	0.96668900	1.13305400
H	-4.80027600	2.44215600	2.12583500
H	-5.36369300	2.56955400	0.43515200
N	3.40438900	0.26143700	0.68312000
P	1.78541600	0.61375300	0.23697700
N	2.13101900	0.66465400	-1.43736600
C	3.66367300	-0.23703500	2.05183800
C	1.25757600	1.51060600	-2.27852300
N	0.70295900	-0.64402500	0.37771100
O	1.30132200	1.90344400	0.87690200
C	-0.09033900	-0.77202300	1.64845100
C	1.88343600	2.85917300	-2.66656400
C	0.72625600	0.74475400	-3.50000700
C	3.95257200	-1.74357300	2.12832000
C	4.74899000	0.59198100	2.75656800
C	3.58349600	0.61539400	-1.65587700
C	4.06737500	0.03806800	-2.99215600
C	5.60794700	0.05128900	-3.02468900
C	6.22958700	-0.64641000	-1.80391200
H	2.73452100	-0.06106300	2.60853600
H	0.39028400	1.74582700	-1.65030300
H	1.14364500	3.47686300	-3.19000200
H	2.21179500	3.40588000	-1.77623600
H	2.74236400	2.74047600	-3.33662100
H	-0.02325000	1.34388700	-4.03369600
H	0.25584100	-0.19219100	-3.18345300
H	1.52185800	0.50073200	-4.21177900
H	3.98149600	-2.06397300	3.17651700

H	3.17245000	-2.32088200	1.62462400
H	4.91868200	-2.00282800	1.68095400
H	4.82658300	0.30009800	3.81191200
H	4.50190300	1.65805200	2.71324400
H	5.73509900	0.45234100	2.30096800
H	4.01822700	1.62535700	-1.55390500
H	3.68415500	-0.98428400	-3.11026300
H	3.68311400	0.62452800	-3.83343400
H	5.96594700	-0.41880600	-3.94944100
H	5.95090700	1.09560200	-3.05407500
H	6.03189900	-1.72620400	-1.86580700
H	7.32058500	-0.52876000	-1.81965000
C	0.00924600	-2.13119400	2.32706200
C	-0.43654500	-2.27184900	3.64952800
C	0.54940400	-3.25210600	1.68605400
C	-0.35646600	-3.49867800	4.31055200
H	-0.84863900	-1.40901300	4.17038400
C	0.63675000	-4.48032100	2.34471200
H	0.90041800	-3.14200400	0.66543000
C	0.18297000	-4.61082100	3.65954600
H	-0.70621400	-3.58334500	5.33688000
H	1.06248300	-5.33833600	1.82928100
H	0.25315000	-5.56651000	4.17311600
H	0.20934500	-0.02871400	2.39893600
C	4.13566700	-0.23018500	-0.49083100
H	3.88377800	-1.28772300	-0.69094200
C	5.66621800	-0.11629900	-0.47138100
H	5.95477600	0.93277000	-0.32037500
H	6.09424600	-0.68983500	0.35630500

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C	1.13010500	-0.24051700	1.94018800
C	1.91962800	-1.38056100	2.12788300
C	1.79241800	1.00159800	2.17747800
O	2.99040500	1.11872900	2.44701600
O	0.97750300	2.10016000	2.07863000
C	1.59805800	3.36339000	2.33648400
C	2.19208200	3.97083600	1.08817000
C	1.46254500	4.89654500	0.34163800
C	1.98597500	5.43766700	-0.83020300
C	3.24987500	5.05227000	-1.26847700
C	3.98908900	4.13361200	-0.52526700
C	3.46642800	3.59909800	0.64888100
H	0.10697000	-2.09538000	0.21898400

H	1.43758200	-2.35841100	2.15362800
H	2.75004200	-1.29228900	2.82584500
H	0.79442900	3.99843500	2.71811600
H	2.36048400	3.23418800	3.10714300
H	0.47113700	5.19112400	0.67878700
H	1.40671400	6.15729500	-1.40139200
H	3.66032900	5.47041000	-2.18282300
H	4.98015200	3.83871400	-0.85805800
H	4.03363800	2.88584300	1.23937600
P	3.27890600	-1.64480600	0.37616200
C	3.10712000	-2.97425400	-0.84799300
C	2.00800300	-2.92883100	-1.71574500
C	3.95464200	-4.08826800	-0.87194100
C	1.75877300	-3.97905600	-2.59185200
H	1.32012600	-2.08759600	-1.71410300
C	3.70979200	-5.13014400	-1.76173300
H	4.81086700	-4.14288900	-0.20465900
C	2.61227300	-5.07977100	-2.61985900
H	0.88512600	-3.92218800	-3.23343400
H	4.37747800	-5.98624500	-1.78254700
H	2.42183700	-5.90086300	-3.30422400
C	3.03056100	-0.09070000	-0.53832100
H	3.55067800	0.71690100	-0.01602300
H	3.37506200	-0.17394100	-1.57170800
H	1.95866900	0.13476500	-0.51025700
C	5.02985700	-1.61968100	0.91312000
H	5.14298300	-0.73923000	1.55334400
H	5.26434600	-2.50827900	1.50475000
H	5.71912900	-1.55402200	0.06675200
N	-0.27025700	-1.15572100	0.14410700
C	-0.26724900	-0.34319100	1.36610000
C	-1.24369300	-0.83899400	2.42515000
C	-1.85167400	0.09131700	3.27234400
C	-2.70448900	-0.32341800	4.29091800
C	-2.95249800	-1.68101600	4.48643800
C	-2.34106400	-2.61614900	3.65597800
C	-1.49724900	-2.19636300	2.63017400
H	-0.58359700	0.65802800	1.05607100
H	-1.63851800	1.14850700	3.12806000
H	-3.17629900	0.41358900	4.93446500
H	-3.61796200	-2.00685600	5.27992800
H	-2.52890800	-3.67645500	3.79979300
H	-1.04800200	-2.93790000	1.97308500
N	-2.94290800	-0.84818900	-0.71782600

P	-1.32966500	-0.95140800	-1.13979200
N	-1.19099400	0.68830100	-1.49265900
C	-3.64406200	-1.99786200	-0.13583600
C	-0.02428100	1.07450300	-2.30690600
O	-0.98198800	-1.98442200	-2.15881900
C	-0.35570100	1.19772300	-3.79360400
C	0.65842700	2.31340300	-1.73314500
C	-4.45026500	-1.64770100	1.11667400
C	-4.49613600	-2.70901900	-1.18704300
C	-2.52033600	1.22945600	-1.76377900
C	-2.70067800	2.73864900	-1.65276900
C	-4.16297300	3.07580800	-1.98041400
C	-5.15953600	2.26731700	-1.14102900
H	-2.85336700	-2.69379800	0.17830000
H	0.68309800	0.23983800	-2.21343900
H	0.55725900	1.39813100	-4.36253500
H	-0.79731700	0.26572300	-4.15988300
H	-1.05380800	2.01960900	-3.98736600
H	1.63620500	2.47271300	-2.20261800
H	0.80749500	2.20059700	-0.65401300
H	0.06506300	3.21889300	-1.89362600
H	-4.67574300	-2.56377900	1.67079700
H	-3.89076500	-0.98407600	1.78066400
H	-5.40545900	-1.17740700	0.86652000
H	-4.94595400	-3.61676600	-0.76974900
H	-3.87618500	-2.98013300	-2.04553800
H	-5.30548200	-2.05683300	-1.53295100
H	-2.85461900	0.92443000	-2.77277100
H	-2.43086800	3.06347000	-0.63907800
H	-2.04123700	3.26522500	-2.34934000
H	-4.34076900	4.14759400	-1.84332600
H	-4.33815700	2.86165700	-3.04344100
H	-5.09792100	2.59482700	-0.09451300
H	-6.18157500	2.47444000	-1.47513000
C	-3.44151700	0.52136600	-0.75606400
H	-3.30563600	0.99930200	0.23227400
C	-4.88631600	0.75629000	-1.19530100
H	-5.02400400	0.37204000	-2.21446900
H	-5.59719000	0.23367500	-0.55119200

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C	-1.61886400	-0.97554500	1.47746000
C	-3.02901500	-0.87559000	1.37197600
C	-1.08522200	-2.29581700	1.56206300

O	-1.72961700	-3.34892700	1.45191100
O	0.28642000	-2.33575700	1.81001500
C	0.83999000	-3.61885500	2.17364200
C	1.48663400	-4.35009200	1.01800000
C	0.70771700	-4.91308900	-0.00559100
C	1.31109700	-5.61623300	-1.04826400
C	2.70084300	-5.76991100	-1.08475300
C	3.48380100	-5.21367100	-0.07226400
C	2.87764400	-4.50706200	0.97036900
H	1.14029500	-0.37975700	1.00692800
H	-3.48616100	0.07353600	1.64904300
H	-3.60217000	-1.73359800	1.71949000
H	1.58813200	-3.39904000	2.94092200
H	0.04447500	-4.22478300	2.61328700
H	-0.37100600	-4.79445000	0.03516400
H	0.69600300	-6.05289100	-1.83141300
H	3.16840200	-6.32208300	-1.89599500
H	4.56456600	-5.32917200	-0.09116100
H	3.49147700	-4.07938800	1.76041500
P	-3.80496600	-0.96265400	-0.71246800
C	-4.66886500	0.47413400	-1.43496100
C	-3.93249600	1.63529100	-1.74449800
C	-6.06618900	0.48896600	-1.59188600
C	-4.58747200	2.77024900	-2.22207300
H	-2.85203000	1.66083800	-1.61628900
C	-6.71169500	1.63090500	-2.06786100
H	-6.65621600	-0.39113600	-1.35364500
C	-5.97521200	2.77344800	-2.38660100
H	-4.00779400	3.65681300	-2.46541800
H	-7.79138500	1.62422000	-2.19280000
H	-6.47911200	3.66129600	-2.75901300
C	-2.33415500	-1.25489400	-1.75527800
H	-1.79481900	-2.11714700	-1.35167000
H	-2.61593300	-1.45242100	-2.79446800
H	-1.68231100	-0.37683100	-1.71241300
C	-4.88125100	-2.43292400	-0.95762300
H	-4.31648800	-3.31320000	-0.63374900
H	-5.77635800	-2.36071900	-0.33219300
H	-5.18064700	-2.56238000	-2.00314900
N	1.79473000	2.60791400	-0.24496900
P	0.77724600	1.28935800	-0.58337600
N	1.95706300	0.43491400	-1.45450500
C	1.45734200	3.48326300	0.90015100
C	1.48314200	-0.65372200	-2.34646500

N	0.43995800	0.28899800	0.71150100
O	-0.52403600	1.70332400	-1.22063500
C	-0.80749600	0.31726700	1.49867100
C	1.20699000	-0.18896400	-3.78335600
C	2.39878900	-1.88489500	-2.29911400
C	2.37896100	3.28589700	2.11180100
C	1.35251100	4.95730600	0.48175200
C	3.02157000	1.37535500	-1.86064500
C	4.38326000	0.78469200	-2.24123100
C	5.35598700	1.93177300	-2.57756300
C	5.44929000	2.98126600	-1.45885000
H	0.45252500	3.17857700	1.21533800
H	0.52875700	-0.97089100	-1.91262400
H	0.77277000	-1.01023800	-4.36613800
H	0.49996600	0.64720300	-3.79501500
H	2.12452000	0.12573000	-4.29437800
H	1.89576000	-2.73825000	-2.76840600
H	2.62835800	-2.15341700	-1.26375700
H	3.34221700	-1.72912100	-2.83074300
H	2.00153800	3.86339800	2.96326400
H	2.41471400	2.23399100	2.41285800
H	3.40218300	3.62329900	1.91139700
H	0.95675000	5.55839700	1.31005000
H	0.67520300	5.06327600	-0.37231500
H	2.32361300	5.37785500	0.20076700
H	2.67948000	1.98958300	-2.71142700
H	4.76934600	0.17599300	-1.41273600
H	4.29408900	0.12825200	-3.11183000
H	6.35037000	1.52092200	-2.79211400
H	5.01644100	2.42129400	-3.50151900
H	5.94939500	2.53706800	-0.58624800
H	6.07812900	3.81972000	-1.78320100
C	-0.57620600	0.84576500	2.92192600
C	-1.27541400	1.97884400	3.36150700
C	0.30492500	0.22241600	3.82104700
C	-1.10674000	2.47710900	4.65718100
H	-1.96135500	2.47949600	2.68091000
C	0.47896500	0.71936000	5.11263700
H	0.84731400	-0.66367400	3.50670300
C	-0.22677000	1.84926900	5.53848200
H	-1.66209800	3.35713300	4.97260500
H	1.16657700	0.22111300	5.79209500
H	-0.09065900	2.23349900	6.54608900
H	-1.42861500	1.06296900	0.99564100

C	3.17633000	2.31271300	-0.64678800
H	3.69611100	1.74689800	0.14706500
C	4.06596400	3.50299800	-1.02635900
H	3.59266400	4.06909300	-1.83978300
H	4.18227600	4.18854800	-0.18111600
