Silver-Catalyzed Regioselective Hydroamination of Alkenyl Diazoacetates to Synthesize γ-Amino Acid Equivalents

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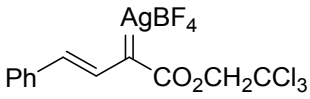
1. Computational Details

All DFT calculations were performed with Gaussian 16 program.[1] The molecular structure optimizations were carried out at the M06 level[2] using the LANL2DZ basis set for Rh and Ag, and the 6-31G* basis set for H, B, C, N, O, F and Cl. The vibrational frequencies were computed at the same level to check whether each optimized structure is an energy minimum (no imaginary frequency) or a transition state (one imaginary frequency) and to evaluate its zero-point vibrational energy (ZPVE) and thermal corrections at 298.15 K. The intrinsic reaction coordinate (IRC) method was used to track minimum energy paths from transition structures to the corresponding local minima.[3]

SM_{Ag}



Energy (RM06) : -2563.250004 A.U.

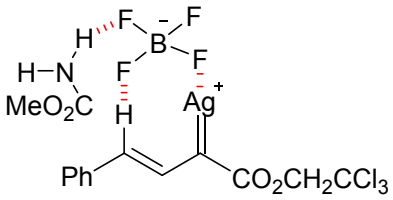
Gibbs Free Energy : -2563.113804 A.U.

Cartesian Coordinates

Atom	X	Y	Z
C	−1.30687400	−1.13030900	−1.13097800
O	−1.49281700	−1.82726200	−2.10229000
C	0.00628400	−0.58826900	−0.73790600
O	−2.28487400	−0.70657600	−0.30957400
C	−3.58538800	−1.14553100	−0.64479800
H	−3.84199900	−0.84721900	−1.66986100
H	−3.66552300	−2.23821700	−0.56499300
C	1.03103200	−1.50756300	−0.62084600
C	2.29395000	−1.06483900	−0.22180900

H	2.41942200	0.01259500	−0.08543900
B	2.87563500	2.70583600	0.18921500
F	3.10205400	1.68342600	1.12478800
F	3.77948300	3.70609300	0.26341200
F	1.53557100	3.21414100	0.44148300
F	2.81646900	2.10617000	−1.08240700
Ag	0.34467700	1.47566400	−0.33702300
H	0.84955600	−2.57084200	−0.80889700
C	3.45677900	−1.83168800	0.05216700
C	4.58882400	−1.12281200	0.51454800
C	3.53025900	−3.23194900	−0.12139800
C	5.76445900	−1.80040300	0.79033500
H	4.50084400	−0.04538700	0.66214900
C	4.70863900	−3.89608900	0.15029200
H	2.66191000	−3.78351100	−0.47700800
C	5.82263300	−3.18017000	0.60523900
H	6.63606500	−1.25809700	1.14875000
H	4.77459900	−4.97296600	0.01284400
H	6.74794500	−3.71275800	0.81890800
C	−4.56281900	−0.50184400	0.32141300
Cl	−4.48134700	1.27332800	0.19318900
Cl	−6.19334000	−1.06728800	−0.14598600
Cl	−4.20932300	−1.00474200	1.99335200

CP$_{\gamma\text{-Ag}}$



Energy (RM06) : -2847.549944 A.U.

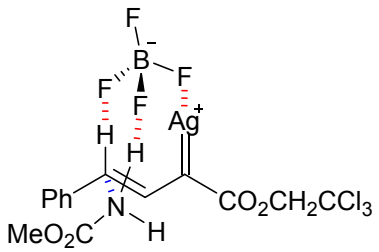
Gibbs Free Energy : -2847.338233 A.U.

Cartesian Coordinates

Atom	X	Y	Z
C	1.74410800	−1.25548400	0.82599300
O	1.74550700	−2.03111100	1.75483900
C	0.54078400	−0.60200900	0.27860600
O	2.86032300	−0.84095900	0.19546200
C	4.06590000	−1.39121500	0.68341200

H	4.17225600	−1.19989900	1.75939700
H	4.10119400	−2.47606800	0.51379500
C	−0.51325800	−1.43130600	−0.02218800
C	−1.69002900	−0.88253000	−0.55734700
H	−1.70206200	0.19910900	−0.70944200
B	−1.75161000	3.30343200	−0.39438600
F	−2.23721800	2.19173000	−1.10502500
F	−2.44060600	4.43378400	−0.63610300
F	−0.35963100	3.45840400	−0.76005100
F	−1.72967900	2.94801100	0.97770400
Ag	0.42159500	1.49845000	−0.00400400
H	−0.43843000	−2.50983000	0.15014000
C	−2.85475600	−1.56481100	−0.99902700
C	−3.90601900	−0.77072600	−1.50905400
C	−3.00696300	−2.96894200	−0.93621400
C	−5.07444500	−1.36812300	−1.95593300
H	−3.78403200	0.31238700	−1.52305000
C	−4.17309800	−3.55339300	−1.38369700
H	−2.20336600	−3.58703400	−0.54057300
C	−5.20347100	−2.75191000	−1.89547900
H	−5.88666400	−0.75435800	−2.33670700
H	−4.29464900	−4.63358000	−1.34345000
H	−6.12022900	−3.22247100	−2.24749500
H	−2.70484100	1.39100200	1.34848800
H	−2.21715700	0.07000900	2.35579400
N	−2.83183300	0.41838600	1.63123700
C	−4.07908000	−0.12133400	1.54503100
O	−5.00442400	0.33520100	0.90880500
O	−4.12169900	−1.29959000	2.20688400
C	−5.36443500	−1.97892800	2.11177300
H	−5.59031500	−2.23321700	1.06804400
H	−5.25564600	−2.88814900	2.70746500
H	−6.18019300	−1.36203500	2.50434200
C	5.21731400	−0.73455300	−0.05557600
Cl	5.21479900	1.02423900	0.23015900
Cl	6.72059900	−1.44933200	0.59817500
Cl	5.10703100	−1.06449500	−1.80267100

$TS_{\gamma\text{-Ag}}$



Energy (RM06) : -2847.543745 A.U.

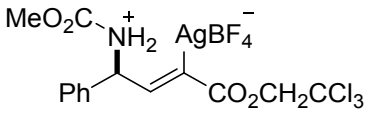
Gibbs Free Energy : -2847.329534 A.U.

Cartesian Coordinates

Atom	X	Y	Z
C	−1.69544500	−1.32246600	−0.73769400
O	−1.70315900	−2.21964900	−1.55120900
C	−0.50721900	−0.58056500	−0.26446500
O	−2.82567000	−0.84939400	−0.16386000
C	−4.01412600	−1.48451500	−0.57409200
H	−4.11602500	−1.45578700	−1.66731100
H	−4.03551200	−2.53413400	−0.24937100
C	0.61938600	−1.32003300	−0.12321100
C	1.84778000	−0.71231700	0.33607500
H	1.74333400	0.28775700	0.76006700
B	1.78406000	3.26213100	0.24356600
F	2.29188600	2.24150100	1.05929400
F	2.50688600	4.39626900	0.28716000
F	0.42137200	3.49827100	0.64078900
F	1.69960800	2.72542600	−1.08011200
Ag	−0.52351200	1.50846000	0.11320600
H	0.61611000	−2.39099400	−0.35337800
C	2.97475600	−1.46079200	0.87625300
C	3.91577600	−0.74969300	1.63762000
C	3.16472000	−2.83100500	0.64226600
C	5.01576500	−1.40341200	2.17524200
H	3.77323200	0.32247500	1.77784500
C	4.26590000	−3.47909000	1.17975900
H	2.45120200	−3.38699200	0.03653300
C	5.18769700	−2.76646600	1.94899300
H	5.74068400	−0.84909600	2.76686600
H	4.40834900	−4.54373900	1.00553200
H	6.04814900	−3.28136000	2.37324600
H	2.39027400	1.12614700	−1.21376400
H	2.01340300	−0.30534000	−2.06765300
N	2.58850100	0.11584200	−1.33839700
C	3.96388000	−0.16723100	−1.45957600
O	4.83015300	0.51640600	−0.98611900
O	4.11822800	−1.33976500	−2.07552900
C	5.46011300	−1.83137200	−2.08199200
H	5.78995600	−2.02103900	−1.05306000
H	5.43280000	−2.76019000	−2.65380100
H	6.13225900	−1.10631200	−2.55093800

C	−5.18482600	−0.74946900	0.05250600
Cl	−5.20949000	0.95079600	−0.48329800
Cl	−6.67134100	−1.57587700	−0.50427600
Cl	−5.09223300	−0.82103600	1.83009800

IN$_{\gamma\text{-Ag}}$



Energy (RM06) : -2847.550041 A.U.

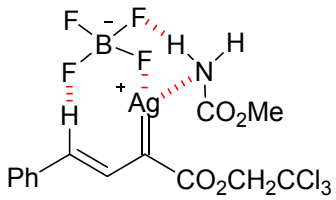
Gibbs Free Energy : -2847.334188 A.U.

Cartesian Coordinates

Atom	X	Y	Z
C	−1.61739200	−1.47676100	−0.55043200
O	−1.61244400	−2.50809700	−1.18634200
C	−0.44715900	−0.66385100	−0.14978300
O	−2.77343700	−0.90486800	−0.12580600
C	−3.94608600	−1.59252500	−0.48434800
H	−3.99790400	−1.74271800	−1.57145000
H	−3.99806100	−2.57550500	0.00448900
C	0.70283100	−1.34924000	−0.05028100
C	2.01380100	−0.70943800	0.29111100
H	1.90230400	0.08683800	1.03521000
B	1.60180500	3.26206500	0.29270200
F	2.01723600	2.25428700	1.16752600
F	2.32954900	4.39053000	0.37018800
F	0.21404800	3.51228700	0.53769400
F	1.66094100	2.68554400	−1.03062600
Ag	−0.62036100	1.40978900	0.23940000
H	0.72393200	−2.43104900	−0.22997200
C	3.12392600	−1.64088500	0.67895800
C	3.94461600	−1.30013700	1.75581300
C	3.38530100	−2.81297300	−0.03729700
C	5.00009600	−2.12635700	2.12593000
H	3.75745700	−0.36973100	2.29259300
C	4.44605700	−3.63398100	0.32615400
H	2.76198200	−3.08233300	−0.89091600

C	5.25084000	−3.29379400	1.41168100
H	5.62916600	−1.85450600	2.97106100
H	4.64099100	−4.54636500	−0.23441700
H	6.07608500	−3.94245200	1.70031100
H	2.04436300	1.10105900	−0.91125500
H	2.07648000	−0.32836900	−1.82148800
N	2.45747300	0.13183900	−0.98753500
C	3.91399800	0.28000900	−1.09133200
O	4.53237400	1.00601700	−0.37821800
O	4.34816200	−0.53996100	−2.02939000
C	5.77780200	−0.67162000	−2.08440900
H	6.12894500	−1.11780900	−1.14679600
H	5.97995400	−1.33072100	−2.92879200
H	6.24235200	0.30770200	−2.22900700
C	−5.13580900	−0.75943700	−0.04324100
Cl	−5.10887100	0.83655200	−0.83946500
Cl	−6.60728000	−1.65091900	−0.53832900
Cl	−5.13399900	−0.54857100	1.72613200

CP$_{\alpha\text{-Ag}}$



Energy (RM06) : -2847.559423 A.U.

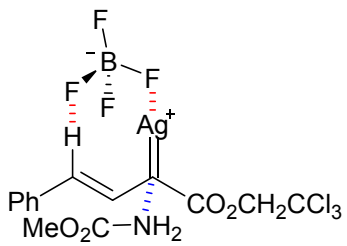
Gibbs Free Energy : -2847.347125 A.U.

Cartesian Coordinates

Atom	X	Y	Z
C	1.30874200	−1.90355800	−0.32327400
O	1.45522800	−2.66485400	0.60693800
C	0.08655100	−1.12912000	−0.53688300
O	2.27992200	−1.57235000	−1.20858900
C	3.60721400	−1.87672100	−0.85399300
H	3.63842600	−2.60809900	−0.03668900
H	4.12099300	−2.27097100	−1.73792000
C	−1.10495800	−1.79547800	−0.73082700
C	−2.28438300	−1.04921500	−0.69436800
H	−2.16949800	0.02942400	−0.57479500

B	−1.66113900	3.36538100	−0.38457100
F	−2.02797900	3.63798100	0.93367600
F	−0.22063100	3.22096700	−0.40845200
F	−2.04872600	4.32288500	−1.25697000
F	−2.18105200	2.09285000	−0.73726600
Ag	0.21972600	0.99254800	−0.21734800
H	−1.13926500	−2.88529300	−0.83520700
C	−3.62979700	−1.49933900	−0.78717300
C	−3.99303600	−2.84180400	−1.01994200
C	−4.63353000	−0.52128200	−0.62626800
C	−5.32757600	−3.18947200	−1.09441600
H	−3.22261700	−3.60012700	−1.14823000
C	−5.96918100	−0.87892100	−0.69660800
H	−4.32689100	0.50839600	−0.44001800
C	−6.31204200	−2.20903800	−0.93156000
H	−5.61487200	−4.22222000	−1.27890700
H	−6.74457100	−0.12719900	−0.56986500
H	−7.36198500	−2.49142500	−0.99015700
H	−1.39574900	2.22349500	1.89467500
H	0.00888300	1.76558700	2.80213800
N	−0.74702500	1.48680900	2.18865500
C	−1.25257200	0.22494800	2.35636700
O	−2.31582300	−0.16514900	1.91624000
O	−0.36889200	−0.54427000	3.01519300
C	−0.72363700	−1.91829100	3.13471500
H	−0.00867300	−2.34853600	3.83870400
H	−1.74676700	−2.02295200	3.50983400
H	−0.62681500	−2.42177200	2.16510000
C	4.32146800	−0.60174300	−0.41286500
Cl	6.00554600	−1.05061200	−0.02291100
Cl	3.52679200	0.07838900	1.03987600
Cl	4.29940400	0.60883500	−1.71670700

TS$_{\alpha\text{-Ag}}$



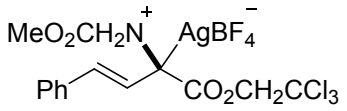
Energy (RM06) : -2847.539158 A.U.

Gibbs Free Energy : -2847.327560 A.U.

Cartesian Coordinates

Atom	X	Y	Z
C	−1.28414100	−1.93656900	0.06451100
O	−1.80190700	−2.85742700	−0.52668600
C	−0.06818700	−1.17886500	−0.26591800
O	−1.82814500	−1.34427300	1.16396800
C	−3.20379800	−1.53597000	1.39147000
H	−3.58214200	−2.38918200	0.81478600
H	−3.35141300	−1.70688200	2.46392700
C	1.05502200	−1.20806200	0.60772400
C	2.01669100	−0.24070100	0.51231700
H	1.88081700	0.53613800	−0.24512000
B	0.92059200	3.19802100	−0.85029800
F	2.08070200	2.49709300	−1.20507900
F	−0.08893900	2.85888800	−1.84740400
F	1.09492600	4.53615300	−0.79787800
F	0.44050400	2.65433600	0.35660000
Ag	−0.47291400	0.76168600	−1.14623800
H	1.14366900	−2.00218900	1.35642300
C	3.20810800	−0.08423900	1.30838200
C	3.67726700	−1.05821600	2.20809500
C	3.91457500	1.12283700	1.16599600
C	4.82293000	−0.82411000	2.94890000
H	3.14517100	−2.00388800	2.31228100
C	5.05646200	1.35467300	1.91961900
H	3.53758000	1.86683000	0.46303600
C	5.51011200	0.38381900	2.80781900
H	5.18801500	−1.58024700	3.64129900
H	5.59499800	2.29382200	1.81275700
H	6.40892100	0.56383200	3.39536700
H	0.00341600	−1.98805800	−2.63846800
H	0.06683500	−3.34307800	−1.61458800
N	0.47841100	−2.44551900	−1.86577100
C	1.87131300	−2.35292200	−1.94389300
O	2.44735800	−1.47654100	−2.53330000
O	2.42505900	−3.30097700	−1.18788700
C	3.84556800	−3.20049300	−1.05901500
H	4.14745900	−4.05155500	−0.44641500
H	4.32331300	−3.24313200	−2.04272800
H	4.11467700	−2.25714800	−0.56931800
C	−3.97329000	−0.27884200	0.99759200
Cl	−5.69214300	−0.57491300	1.37976100
Cl	−3.79734700	0.01753200	−0.76449200
Cl	−3.37649000	1.13241100	1.89151600

$IN_{\alpha\text{-Ag}}$



Energy (RM06) : -2847.564301 A.U.

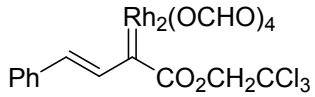
Gibbs Free Energy : -2847.344981 A.U.

Cartesian Coordinates

Atom	X	Y	Z
C	−1.37565900	0.34678200	1.72946800
O	−1.96767700	−0.35344100	2.53811900
C	−0.03725000	0.09968200	1.26065900
O	−1.93283600	1.44791100	1.14327200
C	−3.33230300	1.51532800	1.12353500
H	−3.77152400	0.84893900	1.87713400
H	−3.63408600	2.55202200	1.31399500
C	0.92421400	1.18370100	1.01237500
C	2.23484200	1.04569300	0.72742100
H	2.64067000	0.04762400	0.54905900
B	2.38772500	−2.13594500	−1.40849500
F	2.00959200	−1.87864500	−0.03923500
F	1.27695900	−1.70052200	−2.21062400
F	2.55798500	−3.48625400	−1.55327700
F	3.48946500	−1.38392800	−1.69441400
Ag	−0.27837600	−0.56707700	−0.93943100
H	0.48215700	2.18323200	1.04387700
C	3.17518200	2.14073200	0.51043600
C	2.98396400	3.43088400	1.02226300
C	4.32006600	1.88637400	−0.25844400
C	3.89750000	4.44133800	0.75251800
H	2.12167300	3.63635800	1.65736100
C	5.23245000	2.89834900	−0.52582200
H	4.46436400	0.88562200	−0.66767100
C	5.02475000	4.17990600	−0.02277300
H	3.73612100	5.43807100	1.16091700
H	6.11098100	2.68534700	−1.13285200
H	5.74308700	4.97211300	−0.22735900
H	−0.05728900	−1.06703200	2.93429400
H	1.48849100	−0.93556600	2.24795800
N	0.48576500	−1.06034100	2.04827900

C	0.29359400	−2.44685600	1.47363800
O	−0.56575000	−2.69352700	0.68553900
O	1.13889700	−3.23038900	2.08236100
C	1.30402900	−4.52790900	1.46260800
H	2.01252900	−5.05961300	2.09741000
H	0.34170500	−5.04551800	1.42638300
H	1.70766300	−4.37410300	0.45521100
C	−3.85698200	1.11922000	−0.25546900
Cl	−5.62883000	1.30461200	−0.23122200
Cl	−3.44263100	−0.59387900	−0.60721100
Cl	−3.14967600	2.15912500	−1.51855400

SM_{Rh}



Energy (RM06) : -2968.554963 A.U.

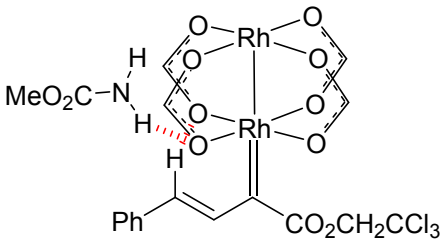
Gibbs Free Energy : -2968.338590 A.U.

Cartesian Coordinates

Atom	X	Y	Z
C	1.50627600	−1.00604600	−0.83896800
O	1.53782700	−1.61135600	−1.87741800
C	0.65654500	0.17256500	−0.56334200
O	2.25553000	−1.29090500	0.25817100
C	3.14309400	−2.37907600	0.16011100
H	2.98133100	−2.92942700	−0.77520000
C	1.32600300	1.39966200	−0.50816300
C	0.66519200	2.57800700	−0.24558400
H	−0.41654700	2.51829800	−0.12542100
H	2.41299300	1.40686000	−0.64544500
C	1.25168000	3.88256900	−0.11691600
C	2.63441700	4.12332100	−0.23569100
C	0.39493900	4.96818100	0.14232700
C	3.13342800	5.40623700	−0.10064300
H	3.31649100	3.29797900	−0.43099900
C	0.89722600	6.25232100	0.27619100
H	−0.67460000	4.78195800	0.23509300
C	2.26732100	6.47143000	0.15453000
H	4.20264300	5.58483800	−0.19262200

H	0.22502700	7.08401500	0.47565600
H	2.66662200	7.47862300	0.25968400
Rh	−1.26911400	−0.23843300	−0.20149400
Rh	−3.62286200	−0.81566500	0.34174500
O	−2.01417400	1.44439500	−1.17896400
C	−3.27308200	1.60734700	−1.20945400
O	−4.17220200	0.90239000	−0.70544500
H	−3.60383900	2.50522800	−1.76171800
O	−0.71714200	−1.97154800	0.79569900
C	−1.63321100	−2.67772500	1.31509600
O	−2.86887200	−2.48731600	1.32527800
H	−1.27201500	−3.58555000	1.82973500
O	−1.51482900	−1.34177800	−1.93090900
C	−2.62966300	−1.90418000	−2.13682100
O	−3.66560100	−1.89334600	−1.43209100
H	−2.68072500	−2.48216800	−3.07594300
O	−1.23133400	0.84875700	1.57490700
C	−2.27898200	0.85947000	2.28998500
O	−3.38165500	0.30845800	2.08337100
H	−2.18931000	1.44467500	3.22276700
C	4.58263400	−1.88309600	0.20042000
Cl	5.63932000	−3.31926300	0.10719400
Cl	4.90545000	−0.80468100	−1.18737700
Cl	4.89678500	−1.00089600	1.71851200
H	2.98114900	−3.03658100	1.02229600

CP$_{\gamma\text{-Rh}}$



Energy (RM06) : -3252.854793 A.U.

Gibbs Free Energy : -3252.563697 A.U.

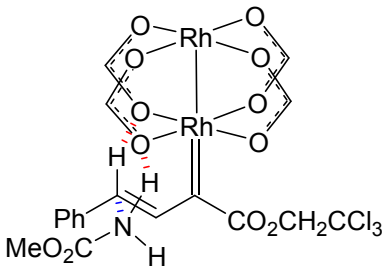
Cartesian Coordinates

Atom	X	Y	Z
C	1.11334000	2.04759700	−1.02470100

O	1.05545700	2.54237500	−2.12752500
C	−0.05941600	1.39980500	−0.38536000
O	2.22542300	1.97725100	−0.28437600
C	3.40208900	2.41496400	−0.92444500
H	3.49402100	1.95650200	−1.91835000
H	3.40578300	3.50823300	−1.03460300
C	−1.18743500	2.21177800	−0.25571500
C	−2.38065700	1.74708400	0.25889200
H	−2.43590500	0.68987300	0.52996800
H	−1.10352700	3.25846000	−0.56659900
C	−3.55783200	2.52964300	0.51508300
C	−4.64924600	1.88981900	1.13381000
C	−3.66252100	3.89750500	0.19624200
C	−5.80640000	2.59491000	1.42560200
H	−4.56558600	0.82724000	1.36406200
C	−4.82163000	4.59522100	0.48415400
H	−2.83097600	4.41073500	−0.28303300
C	−5.89377400	3.94629100	1.10038500
H	−6.64301400	2.09392800	1.90919000
H	−4.89714800	5.65102300	0.23240300
H	−6.80214200	4.50164500	1.32776900
H	−2.76110000	−0.18440100	−1.98280100
H	−4.16221000	0.29009400	−2.92886800
N	−3.75832500	0.01876900	−2.04444300
C	−4.55439800	−0.54278400	−1.10326600
O	−4.16923200	−1.04739600	−0.06327300
O	−5.85472300	−0.43235500	−1.44786400
C	−6.76823700	−0.96994800	−0.50493000
H	−6.72622400	−0.41738700	0.44211900
H	−7.75838200	−0.86483800	−0.95386400
H	−6.55095800	−2.02440300	−0.30321000
C	4.59130300	2.00451800	−0.07316700
Cl	4.74067400	0.23074800	0.00694000
Cl	6.04483600	2.68348800	−0.87293600
Cl	4.44687600	2.66941100	1.57208900
Rh	0.21154700	−0.55713900	−0.01456100
Rh	0.64771000	−2.97301500	0.37333200
O	−1.22478000	−0.69345900	1.48162900
C	−1.46139500	−1.83244900	1.98867800
O	−0.88092500	−2.92005800	1.78397200
H	−2.29071500	−1.84495800	2.71668900
O	−1.19237900	−1.15176700	−1.44060100
C	−1.38768400	−2.39804400	−1.61083800
O	−0.79725000	−3.36037700	−1.08460400
H	−2.18830800	−2.64041800	−2.33343300
O	2.12722200	−2.81865200	−1.08897300
C	2.30240800	−1.71652800	−1.65243100
O	1.69294700	−0.61935300	−1.47192100

H	3.09603200	−1.67608200	−2.41987400
O	1.60943300	−0.18209900	1.45986300
C	2.19059300	−1.16489400	2.00621000
O	2.03610100	−2.39114600	1.80264300
H	2.93853300	−0.88229800	2.76824900

$TS_{\gamma\text{-Rh}}$



Energy (RM06) : -3252.839493 A.U.

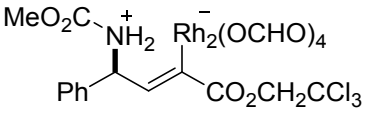
Gibbs Free Energy : -3252.545156 A.U.

Cartesian Coordinates

Atom	X	Y	Z
C	0.86424000	2.03101000	−1.09603900
O	0.82816900	2.49057300	−2.21503700
C	−0.24412700	1.27347600	−0.46980500
O	1.93512600	2.12933800	−0.28728800
C	3.08160900	2.67804100	−0.88793400
H	3.28933800	2.18523600	−1.84779800
H	2.96175600	3.75652300	−1.06260600
C	−1.42965700	1.93241600	−0.37642300
C	−2.60614000	1.32387500	0.17615600
H	−2.42297400	0.47276700	0.83640500
H	−1.50947100	2.96108300	−0.74521600
C	−3.80759900	2.10997500	0.49532900
C	−4.60792300	1.71270300	1.57245900
C	−4.20466900	3.20110100	−0.28686800
C	−5.77703500	2.40315200	1.87195800
H	−4.30167200	0.85692300	2.17465100
C	−5.37927600	3.87937700	0.00326100
H	−3.59715000	3.51029700	−1.13765300
C	−6.16568200	3.48239500	1.08375100
H	−6.38519900	2.09790100	2.72148900

H	−5.68485400	4.72302300	−0.61242500
H	−7.08380600	4.02041700	1.31306000
H	−2.45770800	−0.48505100	−1.37439100
H	−3.39506600	0.77510000	−2.04499500
N	−3.25096900	0.17268000	−1.23399400
C	−4.42897300	−0.46432500	−0.78079200
O	−4.42035300	−1.36534300	0.01551100
O	−5.49524900	0.14673300	−1.28949200
C	−6.74898200	−0.29015300	−0.75933100
H	−6.79248500	−0.07407900	0.31404400
H	−7.51014200	0.27824900	−1.29553300
H	−6.87906500	−1.36465700	−0.92111800
C	4.26173500	2.46382200	0.04341600
Cl	4.61130500	0.72835000	0.24516200
Cl	5.67112500	3.26384100	−0.72653200
Cl	3.95406200	3.20317600	1.63445300
Rh	0.24916700	−0.69490500	−0.07993000
Rh	1.01189900	−3.04150100	0.29815100
O	−1.27894200	−1.09614700	1.29498900
C	−1.37079400	−2.27123200	1.76682300
O	−0.62586300	−3.25500100	1.57642900
H	−2.23366900	−2.42972300	2.43784900
O	−1.00386600	−1.47149600	−1.59443000
C	−0.93419000	−2.72039300	−1.85011500
O	−0.21554100	−3.58284600	−1.31729700
H	−1.60480900	−3.06271400	−2.65888200
O	2.57050800	−2.62427100	−1.01958300
C	2.60311800	−1.50141900	−1.57032800
O	1.81233200	−0.52048300	−1.43857200
H	3.43443400	−1.32577100	−2.27683800
O	1.47845400	−0.15085800	1.47709600
C	2.13388200	−1.05624000	2.07006200
O	2.15927900	−2.29085800	1.85626700
H	2.77133900	−0.68752300	2.89337400

$IN_{\gamma\text{-Rh}}$



Energy (RM06) : -3252.843641 A.U.

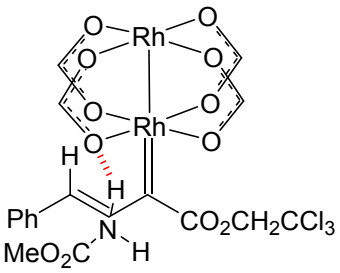
Gibbs Free Energy : -3252.545822 A.U.

Cartesian Coordinates

Atom	X	Y	Z
C	0.81493500	2.11095800	−1.04532800
O	0.76049300	2.66501200	−2.12082700
C	−0.27647800	1.30878700	−0.44659800
O	1.91119200	2.14452200	−0.26047900
C	3.03834700	2.75043200	−0.83531100
H	3.21713700	2.36498800	−1.84891000
H	2.92051200	3.84215300	−0.89036600
C	−1.46972100	1.91760500	−0.34162700
C	−2.69228500	1.21889200	0.13033700
H	−2.46536500	0.48572000	0.91236800
H	−1.58504200	2.96584800	−0.63984800
C	−3.88329300	2.05824900	0.48076700
C	−4.64713900	1.72885900	1.60228500
C	−4.29424900	3.11319700	−0.33881300
C	−5.80049600	2.44685000	1.90523200
H	−4.32795200	0.90481800	2.24124300
C	−5.44902600	3.82535400	−0.04098800
H	−3.70784300	3.38203300	−1.21886200
C	−6.20418800	3.49244800	1.08122600
H	−6.38119700	2.19068300	2.78955200
H	−5.76000600	4.64630600	−0.68431600
H	−7.10610600	4.05477500	1.31621800
H	−2.36130000	−0.41195600	−1.26801900
H	−3.31335900	0.84187900	−1.89814700
N	−3.15316300	0.26048500	−1.06847800
C	−4.35054100	−0.48910900	−0.70347200
O	−4.31775200	−1.36631700	0.10756700
O	−5.38521500	0.00284200	−1.35414300
C	−6.66025300	−0.51257300	−0.93874800
H	−6.84352000	−0.21594500	0.09952100
H	−7.39170000	−0.05791800	−1.60676700
H	−6.67340400	−1.60291600	−1.02320000
C	4.24430600	2.43615800	0.03320300
Cl	4.59950100	0.68972200	0.03165200
Cl	5.63478200	3.31969300	−0.67903100
Cl	3.98043400	2.98946000	1.70596700
Rh	0.25131300	−0.66855700	−0.06780100
Rh	1.03163000	−3.02060100	0.27843200
O	−1.21231300	−1.06049100	1.38165900
C	−1.25029900	−2.22049200	1.89530000
O	−0.51089900	−3.20361900	1.68047700
H	−2.05811300	−2.36784300	2.63513100
O	−1.08010400	−1.44809700	−1.52679600
C	−1.05841400	−2.70842400	−1.74950900
O	−0.32357100	−3.56810000	−1.24237400

H	−1.79063400	−3.05599500	−2.50141400
O	2.48987200	−2.61395700	−1.15496700
C	2.50415200	−1.48495900	−1.69533600
O	1.74323800	−0.49136700	−1.50138500
H	3.28968000	−1.31661500	−2.45434900
O	1.53989700	−0.12620500	1.43703800
C	2.24931400	−1.02569200	1.97274900
O	2.28602400	−2.25755300	1.74116800
H	2.93277000	−0.65473200	2.75738400

CP$_{\alpha\text{-Rh}}$



Energy (RM06) : -3252.858923 A.U.

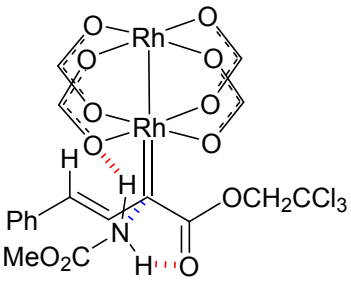
Gibbs Free Energy : -3252.564737 A.U.

Cartesian Coordinates

Atom	X	Y	Z
C	−1.14925300	−1.43866100	0.53738400
O	−1.17122800	−1.85488000	1.66931000
C	−0.46353100	−0.20170400	0.09778100
O	−1.78785600	−2.01521900	−0.51061800
C	−2.67815800	−3.06846200	−0.22631300
H	−2.54516000	−3.42867700	0.80130100
C	−1.31996000	0.81825000	−0.31322800
C	−0.88937600	2.11880200	−0.48063500
H	0.15517900	2.33301000	−0.24890200
H	−2.38535300	0.58684400	−0.42586400
C	−1.71108000	3.22613900	−0.88373600
C	−3.00317100	3.05877700	−1.41758200
C	−1.19770100	4.52592300	−0.73500300
C	−3.75138100	4.16210400	−1.78987700
H	−3.40947500	2.05759800	−1.55792300

C	−1.95360700	5.62851000	−1.09864600
H	−0.20745700	4.64931600	−0.29872900
C	−3.22928100	5.44668800	−1.62813500
H	−4.74549800	4.02730300	−2.21095600
H	−1.55294300	6.63150700	−0.96897000
H	−3.82341700	6.31132000	−1.91895300
H	0.66297800	1.03411700	2.58568600
H	−0.54503300	−0.13948600	2.97855600
N	−0.27184700	0.83756800	2.92745800
C	−1.20359100	1.76638300	2.61047800
O	−0.97580200	2.89687100	2.21802000
O	−2.45118300	1.27194400	2.78024600
C	−3.49347900	2.19066600	2.49929600
H	−4.42431000	1.67849200	2.75649200
H	−3.38627500	3.10305200	3.09624200
H	−3.49878800	2.47069100	1.43695300
Rh	1.54121100	−0.27983600	−0.02881600
Rh	4.00285800	−0.45551200	−0.32900600
O	1.89515100	1.54625800	0.92598300
C	3.09990000	1.94669500	1.02868300
O	4.14450800	1.39386300	0.63176400
H	3.21470800	2.91670800	1.54337700
O	1.39520700	−2.12609100	−0.95534200
C	2.46498600	−2.68564800	−1.34336600
O	3.64539700	−2.28278400	−1.25517900
H	2.31530300	−3.66684800	−1.82708400
O	1.80284900	−1.22446800	1.80104800
C	2.97536700	−1.57426300	2.13321200
O	4.05217300	−1.41755600	1.51582000
H	3.03903100	−2.08578200	3.10969600
O	1.48628000	0.68405700	−1.86877400
C	2.57991500	0.84883400	−2.48958000
O	3.73736800	0.51575700	−2.15371900
H	2.47964100	1.36234100	−3.46233800
C	−4.11374800	−2.58494700	−0.40346200
Cl	−5.18579100	−3.97336300	−0.08021300
Cl	−4.46614000	−1.26374100	0.74820200
Cl	−4.37094900	−1.99479700	−2.06853500
H	−2.49434600	−3.87805500	−0.94161800

$TS_{\alpha\text{-Rh}}$



Energy (RM06) : -3252.852249 A.U.

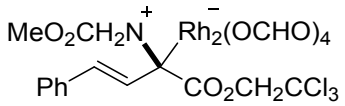
Gibbs Free Energy : -3252.557661 A.U.

Cartesian Coordinates

Atom	X	Y	Z
C	−1.15103100	−1.30384900	0.75208100
O	−1.16541600	−1.89809400	1.80412700
C	−0.49382200	−0.00632200	0.43538300
O	−1.72513900	−1.76035600	−0.38667900
C	−2.44854700	−2.96425300	−0.31496000
H	−2.29791000	−3.45435900	0.65464800
C	−1.33844100	0.98263400	−0.15361100
C	−0.93259400	2.26371400	−0.35225100
H	0.08946700	2.51961700	−0.06525100
H	−2.37658900	0.69962000	−0.35768400
C	−1.75727500	3.35414200	−0.83416700
C	−3.01041100	3.15358900	−1.43647500
C	−1.28420000	4.66538800	−0.68227300
C	−3.76074200	4.23476000	−1.87076200
H	−3.38662400	2.14161300	−1.58415300
C	−2.04061800	5.74747700	−1.10939200
H	−0.31719300	4.82233000	−0.20477600
C	−3.27992300	5.53377200	−1.70574100
H	−4.72596600	4.06758800	−2.34523300
H	−1.66364900	6.75989500	−0.97807800
H	−3.87374000	6.38011700	−2.04663900
H	0.62761500	0.96892500	2.48057100
H	−0.48814700	−0.30893800	2.86376800
N	−0.32968100	0.61873000	2.46553500
C	−1.28963500	1.60275400	2.64027000
O	−1.06478100	2.78570000	2.54570400
O	−2.49465000	1.04596900	2.79516200
C	−3.57677500	1.97446400	2.77605500
H	−4.47911000	1.38434100	2.94496800

H	−3.45634400	2.72631100	3.56265500
H	−3.62269100	2.48035800	1.80342000
Rh	1.52509500	−0.20847400	0.04983700
Rh	3.94763500	−0.46266900	−0.43061000
O	2.00362100	1.58244800	1.02294800
C	3.22596400	1.93802400	1.04584400
O	4.21795000	1.36061300	0.55922500
H	3.41599700	2.88978800	1.57300700
O	1.24877200	−2.03123800	−0.89831500
C	2.26651200	−2.61347800	−1.37817100
O	3.46437500	−2.25166900	−1.36972700
H	2.05155800	−3.57739900	−1.87262500
O	1.86752900	−1.19574900	1.85073700
C	3.04600800	−1.60241600	2.08507600
O	4.07814800	−1.47430900	1.39121700
H	3.16289200	−2.14155700	3.04215700
O	1.37607200	0.77945200	−1.77058400
C	2.42769200	0.92395000	−2.46102200
O	3.59794500	0.55555200	−2.20993900
H	2.27867200	1.45452900	−3.41828600
C	−3.93307100	−2.67656500	−0.50453600
Cl	−4.78957400	−4.24040300	−0.44748500
Cl	−4.52384300	−1.61114600	0.80313600
Cl	−4.21831100	−1.88721500	−2.07952300
H	−2.11391600	−3.61675800	−1.12968600

IN$_{\alpha\text{-Rh}}$



Energy (RM06) : -3252.875258 A.U.

Gibbs Free Energy : -3252.579497 A.U.

Cartesian Coordinates

Atom	X	Y	Z
C	−1.31609800	−0.99375800	0.78297900
O	−1.31294000	−1.77102000	1.71753200
C	−0.62959400	0.30208600	0.79823400
O	−1.88559900	−1.23604400	−0.41584200
C	−2.39953500	−2.52639700	−0.62748500

H	−2.14712300	−3.18680500	0.21098500
C	−1.07289800	1.41464700	−0.01834700
C	−0.96631200	2.72539900	0.27120300
H	−0.56777200	3.04700500	1.23799400
H	−1.47478400	1.10411700	−0.98255300
C	−1.33844600	3.81587800	−0.62575200
C	−1.48288600	3.63555200	−2.00923400
C	−1.55089300	5.09671600	−0.09891900
C	−1.85580900	4.69311800	−2.82599500
H	−1.27012600	2.66158200	−2.44918000
C	−1.92244100	6.15593500	−0.91711900
H	−1.42721500	5.25450700	0.97359600
C	−2.08217100	5.95725000	−2.28494300
H	−1.95862500	4.53379800	−3.89836500
H	−2.08619900	7.14186900	−0.48471900
H	−2.36955800	6.78581100	−2.92988500
H	0.53406200	1.20632100	2.26840700
H	−0.12541900	−0.28844600	2.65702400
N	−0.33389100	0.63795400	2.22921800
C	−1.37982100	1.34285400	3.01728400
O	−1.08927200	2.23807600	3.75478700
O	−2.54790200	0.81781500	2.76182600
C	−3.66002800	1.46275700	3.40298700
H	−4.53945100	0.90158900	3.08862200
H	−3.53688800	1.42730800	4.48927300
H	−3.71961400	2.50274100	3.06750000
Rh	1.39490500	−0.27333100	0.11547300
Rh	3.74574400	−0.74721000	−0.46421500
O	2.05115400	1.47155900	1.06453900
C	3.29886800	1.72587400	1.02586600
O	4.20824000	1.06567100	0.48669200
H	3.59765900	2.65641000	1.53917800
O	0.89359700	−2.07545200	−0.78973800
C	1.83436400	−2.75243700	−1.29919600
O	3.06021400	−2.49754300	−1.34594500
H	1.52055900	−3.70206300	−1.76787200
O	1.72499600	−1.23460000	1.94050700
C	2.86991200	−1.75138800	2.12884700
O	3.86551600	−1.74220300	1.37477600
H	2.98848800	−2.27469600	3.09402300
O	1.23224500	0.67975300	−1.72405400
C	2.26409400	0.73403100	−2.45291900
O	3.41168500	0.27451600	−2.23898100
H	2.12745700	1.26414100	−3.41199900
C	−3.91389000	−2.47062400	−0.77731400
Cl	−4.47383600	−4.13986000	−1.08084100
Cl	−4.66557300	−1.84588900	0.71874100
Cl	−4.36884400	−1.42545800	−2.14872300

H	−1.97108400	−2.91517800	−1.55901000

1d

NH_2CO_2Me

Energy (RM06) : -284.283804 A.U.

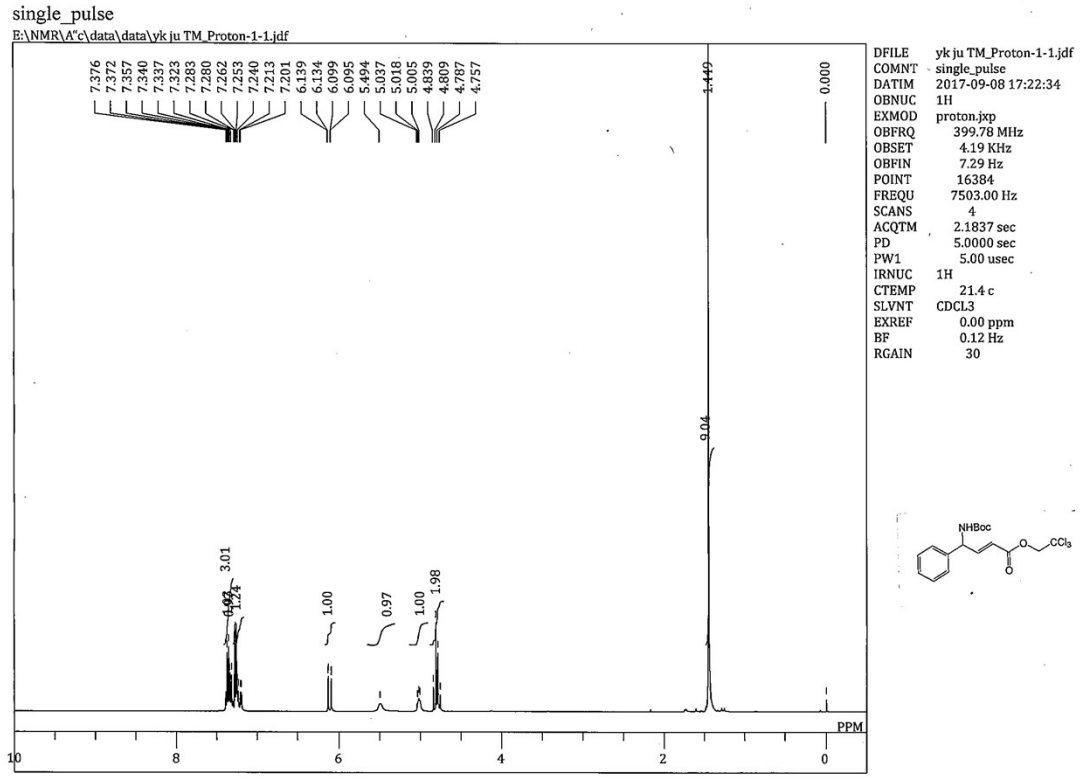
Gibbs Free Energy : -284.232961 A.U.

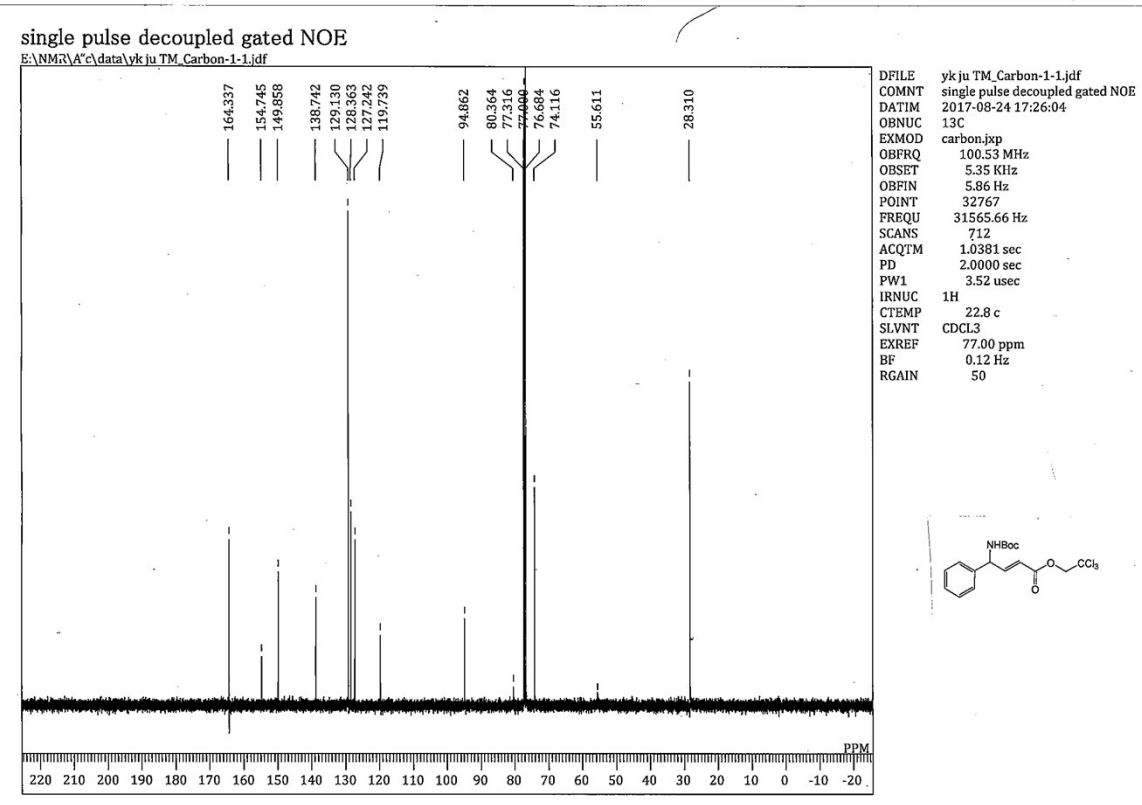
Cartesian Coordinates

Atom	X	Y	Z
H	−2.50358700	−0.02206000	−0.13302200
H	−1.66447400	−1.54006500	−0.14784600
N	−1.66396700	−0.55021800	0.04752900
C	−0.48953400	0.14078400	0.00294200
O	−0.38398900	1.34560600	−0.00547300
O	0.55071000	−0.72154700	−0.00147200
C	1.82582600	−0.09620900	−0.00159600
H	1.95419700	0.52837200	0.88927300
H	2.55721100	−0.90742300	−0.00393900
H	1.95289500	0.53277200	−0.88967800

2. Charts of ^{1}H- and ^{13}C-NMR Spectra

3bc





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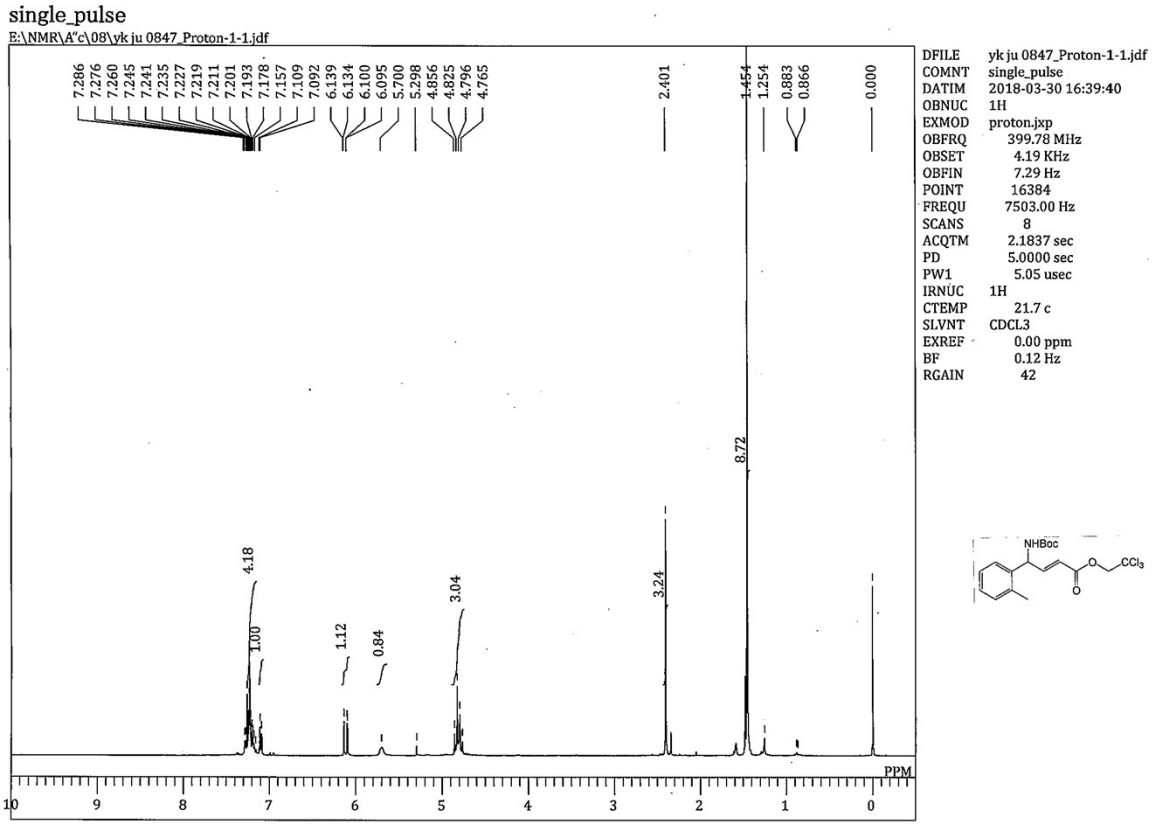
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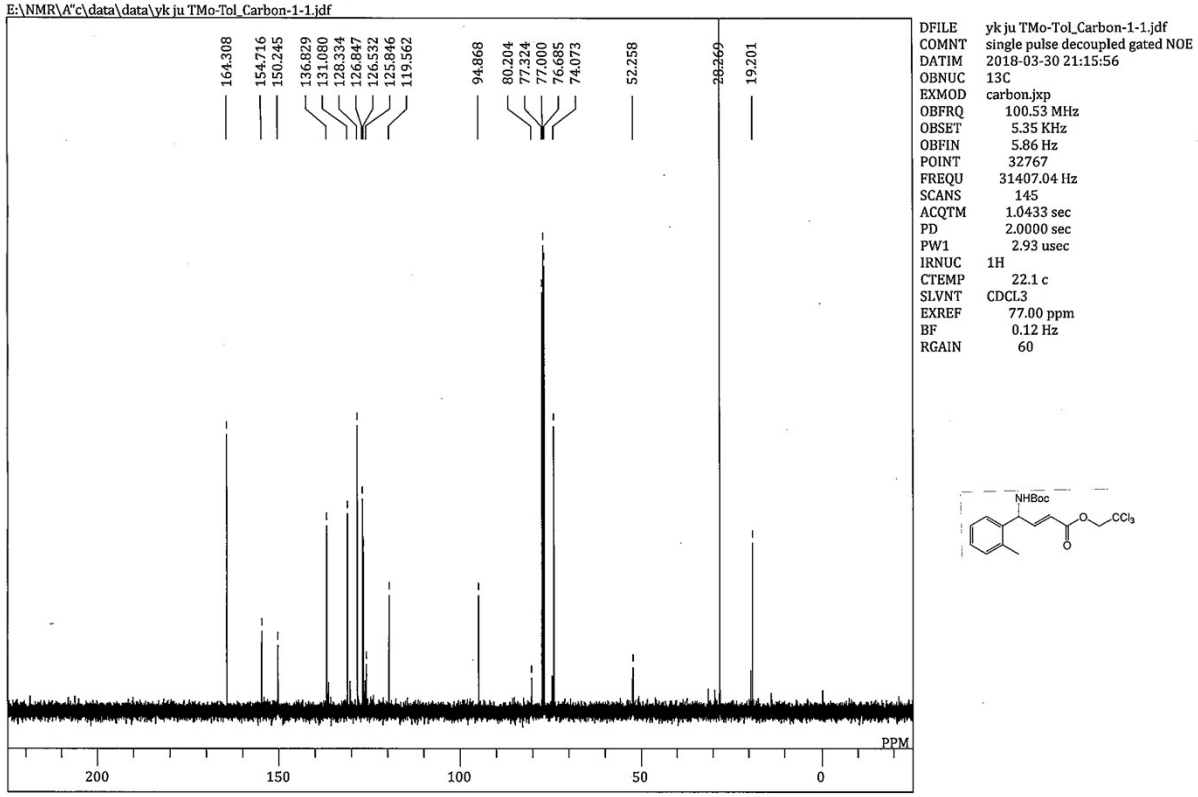
7.286 7.276 7.260 7.245 7.241 7.235 7.227 7.219 7.211 7.201 7.193 7.178 7.157 7.109 7.092 6.139 6.134 6.100 6.095 5.700 5.298 4.856 4.825 4.796 4.765
2.401
1.454 1.254 0.883 0.866
0.000
8.72
4.18 1.00 1.12 0.84 3.04 3.24
PPM
10 9 8 7 6 5 4 3 2 1 0
DFILE yk ju 0847_Proton-1-1.jdf
COMNT single_pulse
DATIM 2018-03-30 16:39:40
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 7503.00 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.05 usec
IRNUC 1H
CTEMP 21.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 42
NHBoc
CCl3
O
O


single pulse decoupled gated NOE
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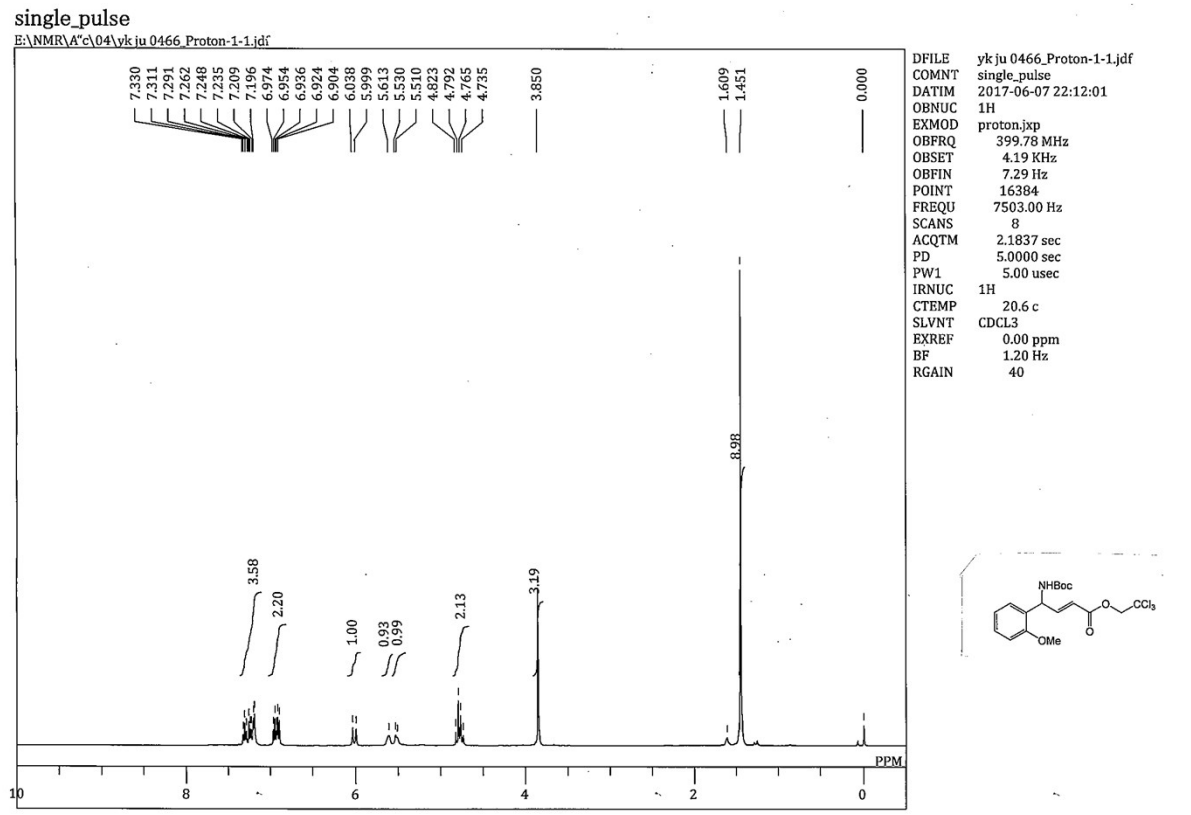
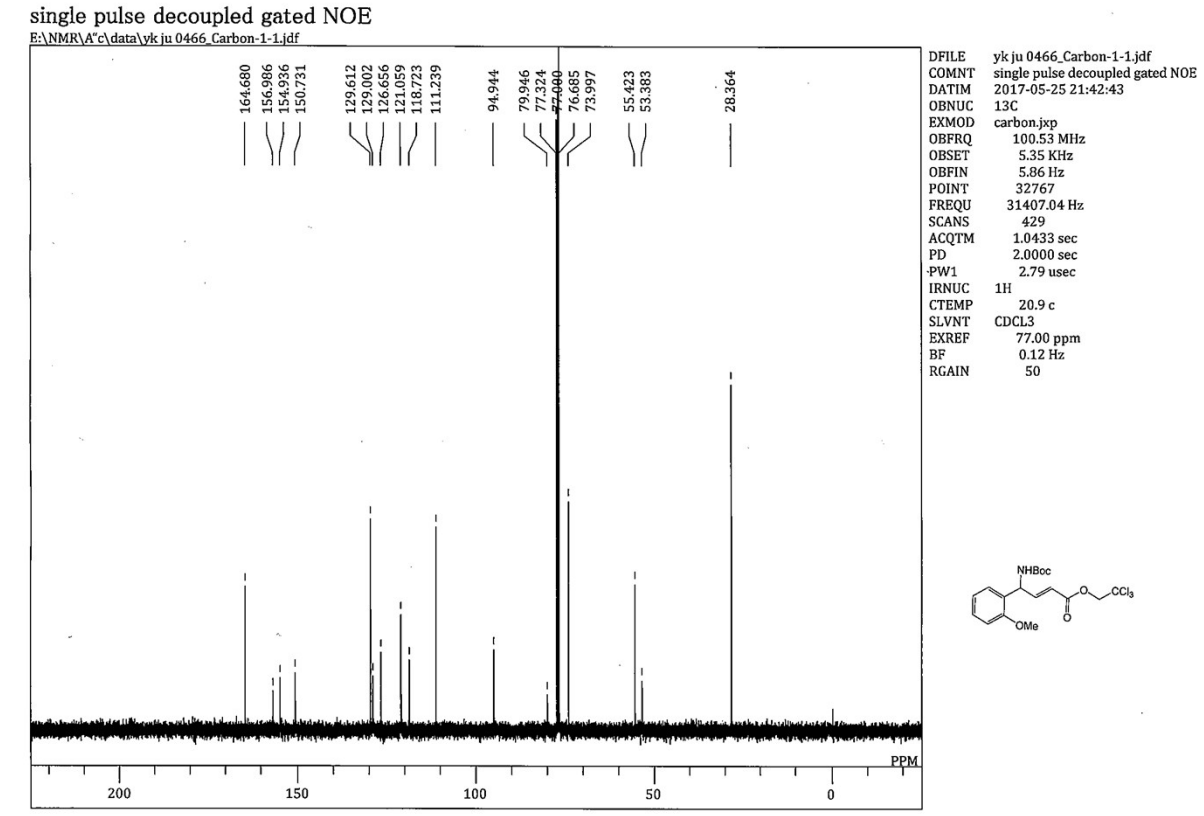
164.308 154.716 150.245 136.829 131.080 128.334 126.847 126.532 125.846 119.562
94.868 80.204 77.324 77.000 76.685 74.073
52.258
28.269
19.201
PPM
200 150 100 50 0
DFILE yk ju TMo-Tol_Carbon-1-1.jdf
COMNT single pulse decoupled gated NOE
DATIM 2018-03-30 21:15:56
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 32767
FREQU 31407.04 Hz
SCANS 145
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 2.93 usec
IRNUC 1H
CTEMP 22.1 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 60
NHBoc
CCl3
O
O

3be


single_pulse
E:\NMR\A"c\04\yk ju 0466_Proton-1-1.jdf
7.330
7.311
7.291
7.262
7.248
7.235
7.209
7.196
6.974
6.954
6.936
6.924
6.904
6.038
5.999
5.613
5.530
5.510
4.823
4.792
4.765
4.735
3.850
1.609
1.451
0.000
8.98
3.58
2.20
1.00
0.93
0.99
2.13
3.19
PPM
10
8
6
4
2
0
DFILE yk ju 0466_Proton-1-1.jdf
COMNT single_pulse
DATIM 2017-06-07 22:12:01
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 7503.00 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.00 usec
IRNUC 1H
CTEMP 20.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 40
NHBoc
CCl3
OMe


single pulse decoupled gated NOE
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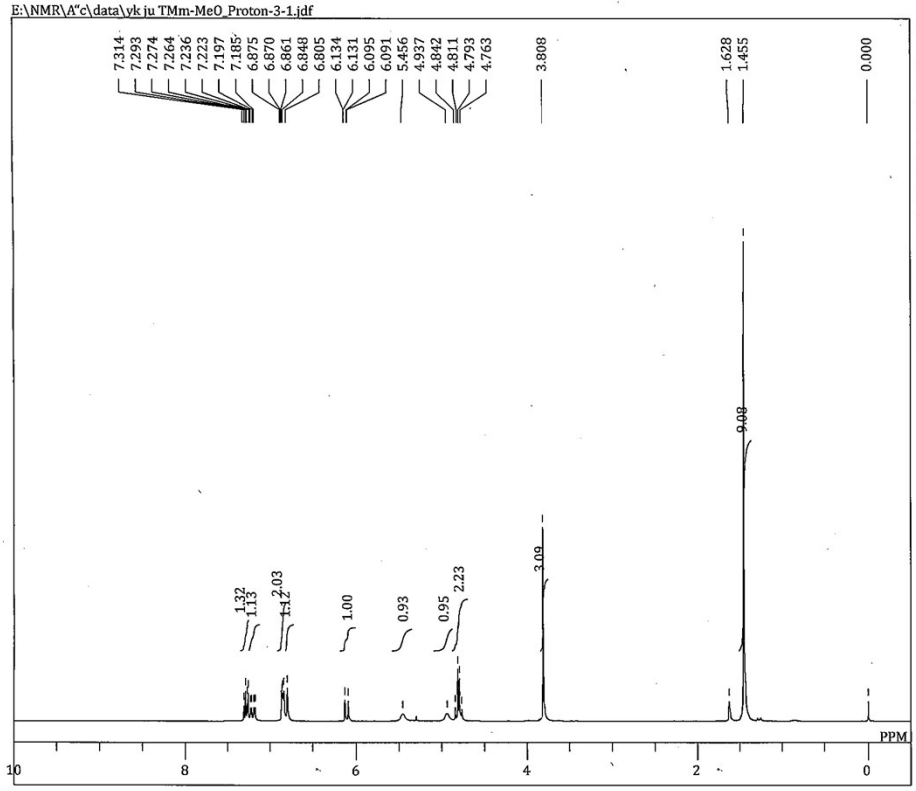
164.680
156.986
154.936
150.731
129.612
129.002
126.656
121.059
118.723
111.239
94.944
79.946
77.324
77.000
76.685
73.997
55.423
53.383
28.364
PPM
200
150
100
50
0
DFILE yk ju 0466_Carbon-1-1.jdf
COMNT single pulse decoupled gated NOE
DATIM 2017-05-25 21:42:43
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 32767
FREQU 31407.04 Hz
SCANS 429
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 2.79 usec
IRNUC 1H
CTEMP 20.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50
NHBoc
CCl3
OMe

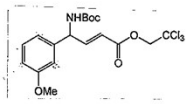
3bf

single_pulse

E:\NMR\A"c\data\yk ju TMm-MeO_Proton-3-1.jdf



DFILE	yk ju TMm-MeO_Proton-3-1.jdf
COMNT	single_pulse
DATIM	2017-08-22 22:06:33
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	16384
FREQU	7503.00 Hz
SCANS	8
ACQTM	2.1837 sec
PD	5.0000 sec
PW1	5.00 usec
IRNUC	1H
CTEMP	23.3 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	1.20 Hz
RGAIN	38



single pulse decoupled gated NOE

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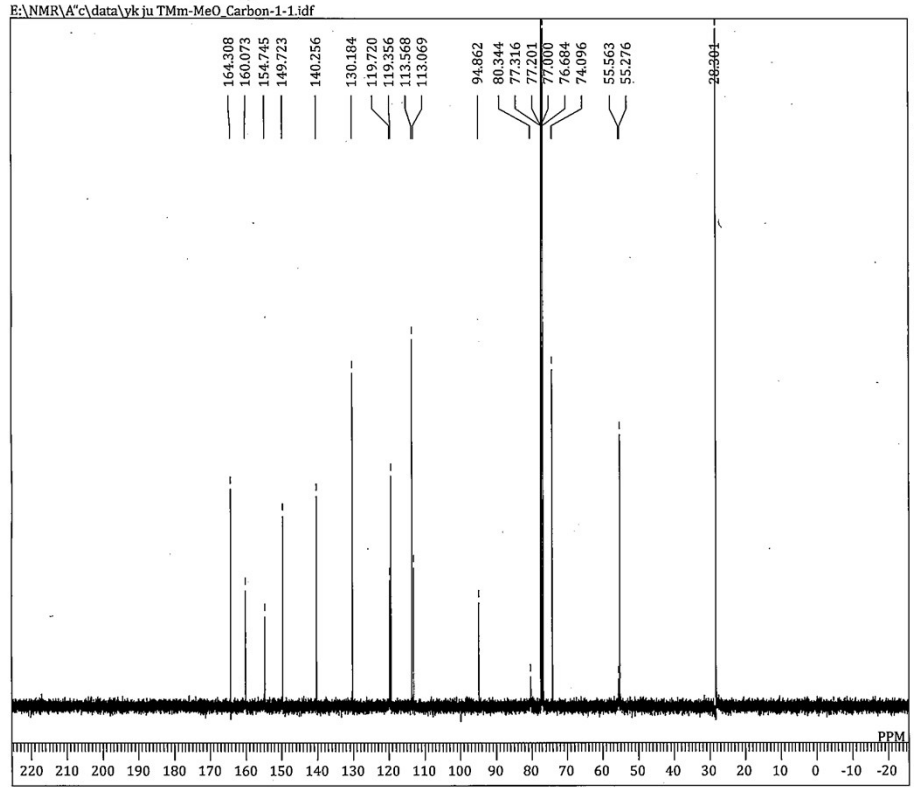
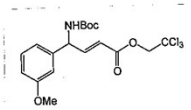


DFILE	yk ju TMm-MeO_Carbon-1-1.jdf
COMNT	single pulse decoupled gated NOE
DATIM	2017-08-25 01:01:51
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	32767
FREQU	31565.66 Hz
SCANS	1070
ACQTM	1.0381 sec
PD	2.0000 sec
PW1	3.52 usec
IRNUC	1H
CTEMP	22.7 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	50



3bg

single_pulse

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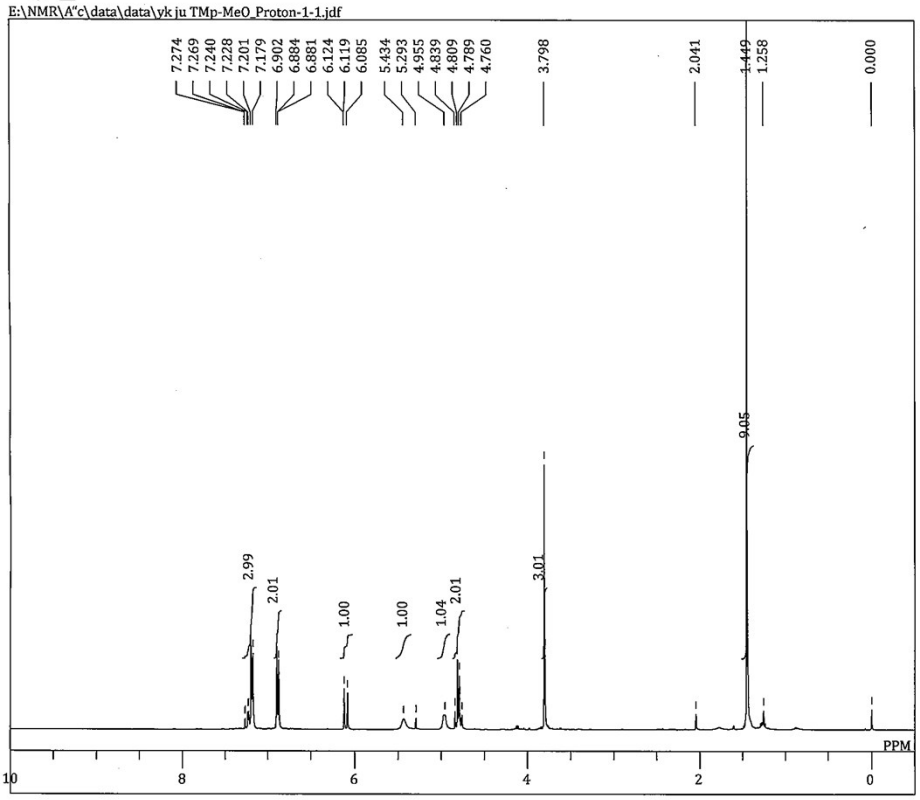
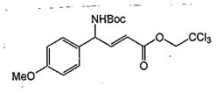


DFILE	yk ju TMp-MeO_Proton-1-1.jdf
COMNT	single_pulse
DATIM	2018-03-23 22:37:45
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	16384
FREQU	7503.00 Hz
SCANS	8
ACQTM	2.1837 sec
PD	5.0000 sec
PW1	5.05 usec
IRNUC	1H
CTEMP	21.4 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	30



single pulse decoupled gated NOE

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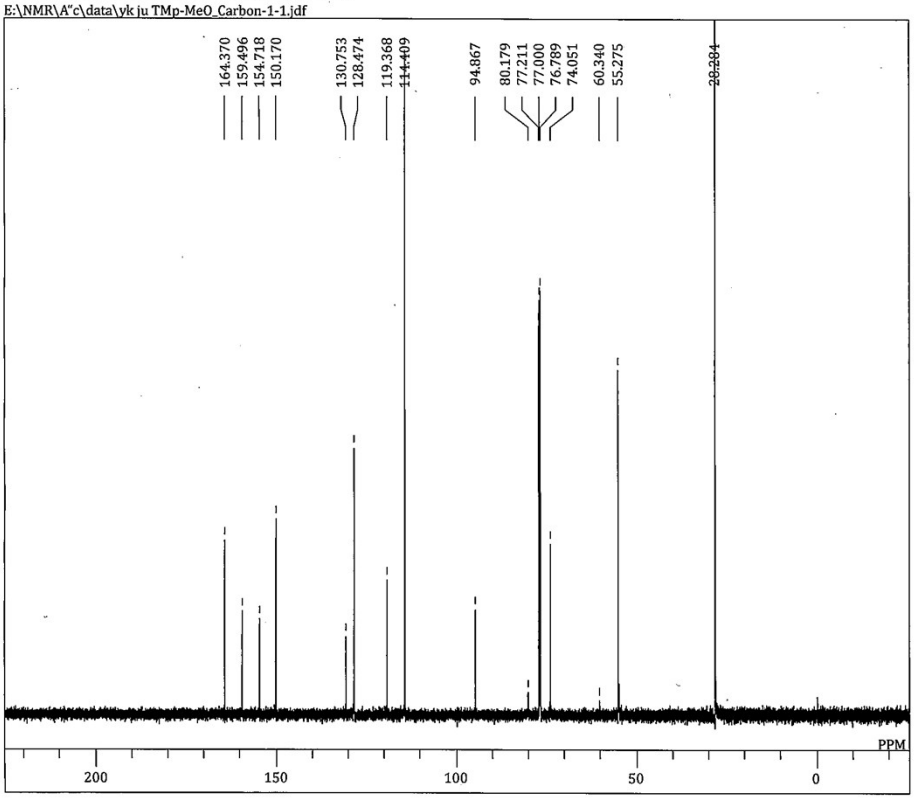
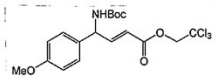


DFILE	yk ju TMp-MeO_Carbon-1-1.jdf
COMNT	single pulse decoupled gated NOE
DATIM	2018-03-24 10:10:43
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	150.92 MHz
OBSET	8.52 KHz
OBFIN	1.74 Hz
POINT	32767
FREQU	47348.49 Hz
SCANS	1229
ACQTM	0.6921 sec
PD	2.0000 sec
PW1	3.40 usec
IRNUC	1H
CTEMP	23.0 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	56



3bh

single_pulse

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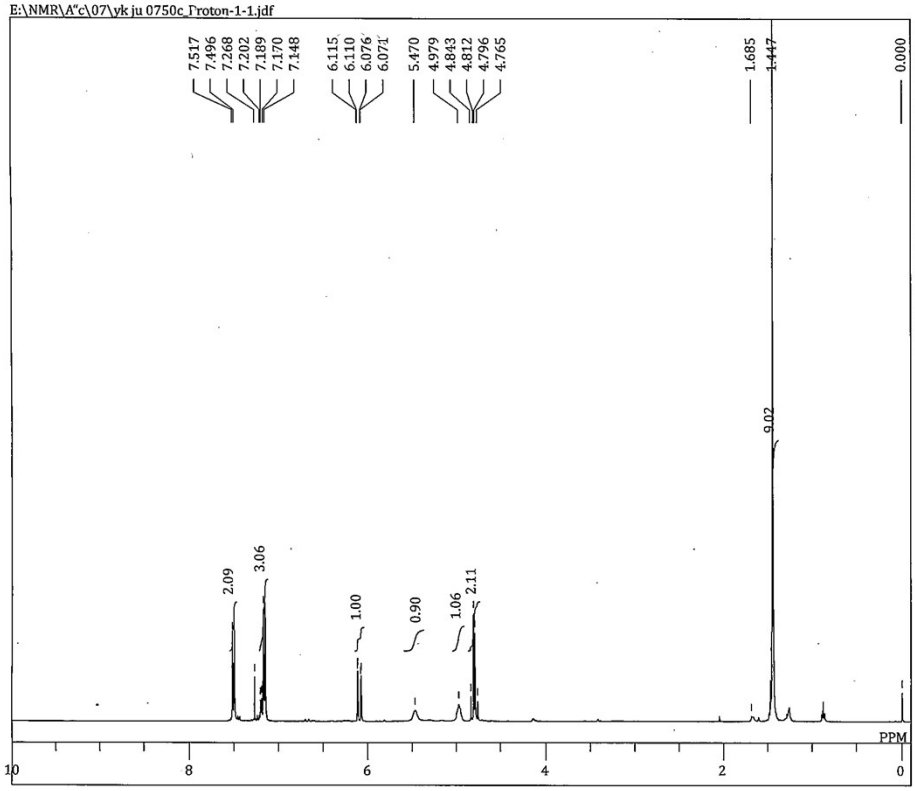
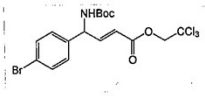


DFILE	yk ju 0750c_Proton-1-1.jdf
COMNT	single_pulse
DATIM	2017-10-16 10:58:49
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	16384
FREQU	7503.00 Hz
SCANS	6
ACQTM	2.1837 sec
PD	5.0000 sec
PW1	5.00 usec
IRNUC	1H
CTEMP	19.1 c
SLVNT	CDCl3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	36



single pulse decoupled gated NOE

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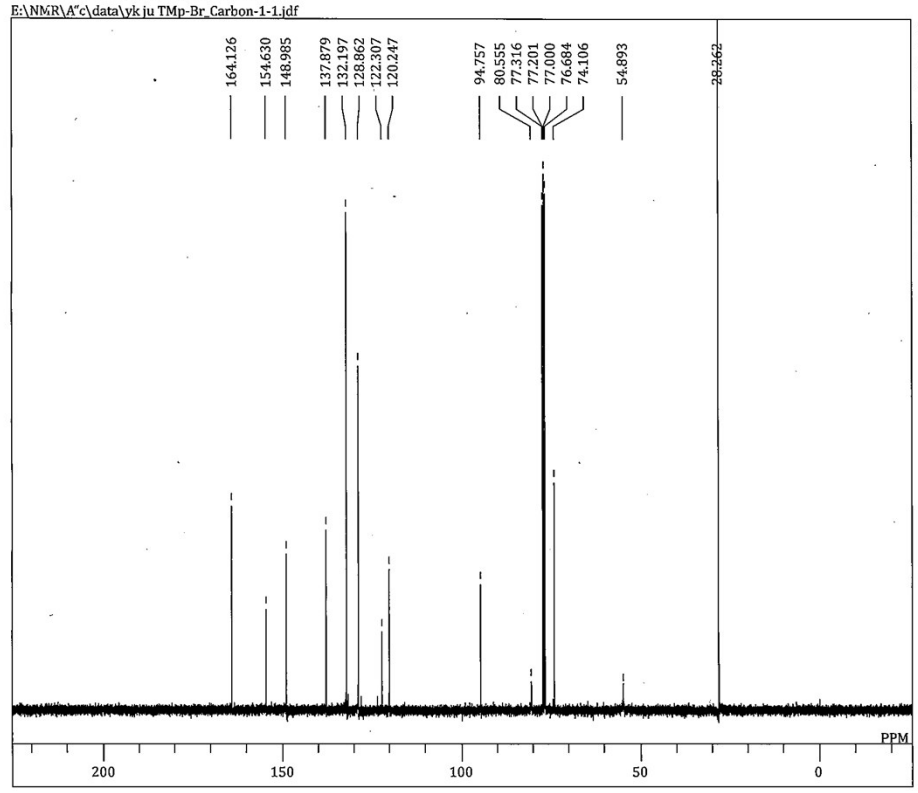
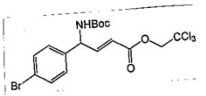
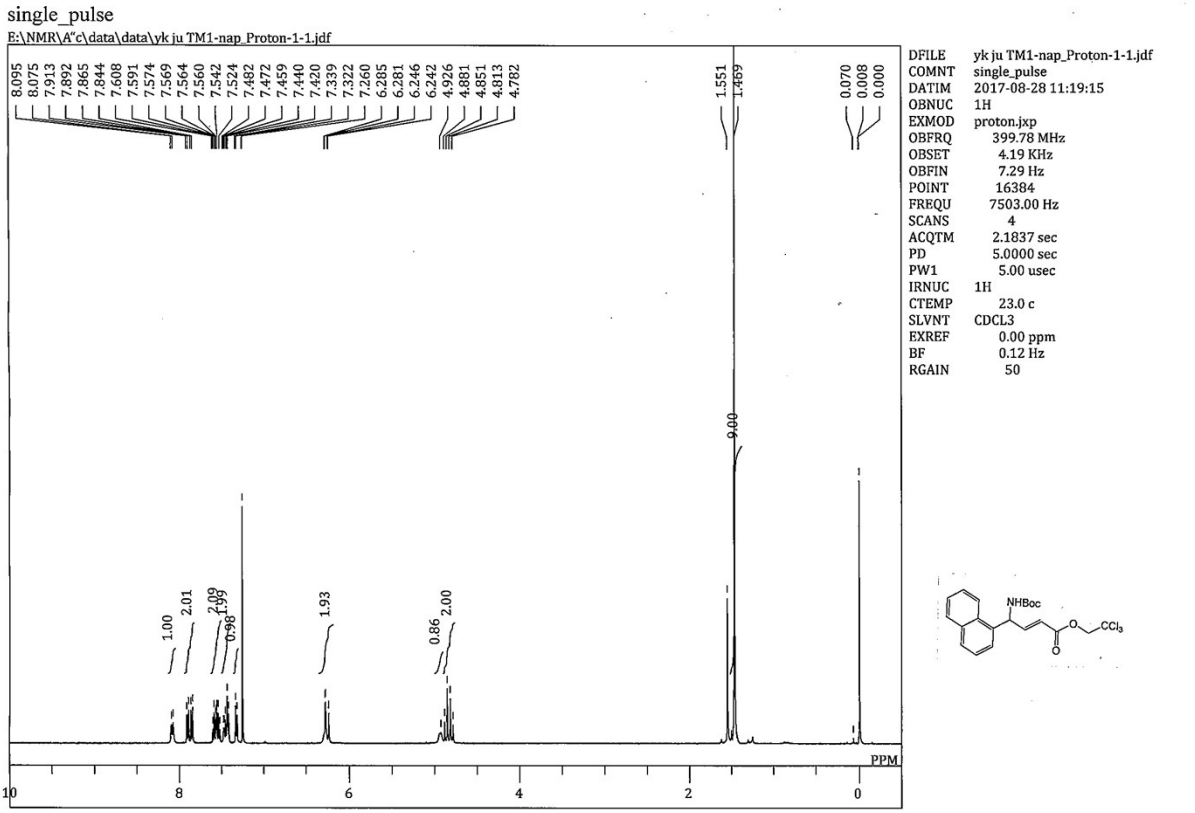


DFILE	yk ju TMp-Br_Carbon-1-1.jdf
COMNT	single pulse decoupled gated NOE
DATIM	2017-10-17 22:51:40
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	32767
FREQU	31565.66 Hz
SCANS	983
ACQTM	1.0381 sec
PD	2.0000 sec
PW1	3.52 usec
IRNUC	1H
CTEMP	19.2 c
SLVNT	CDCl3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	50



3bi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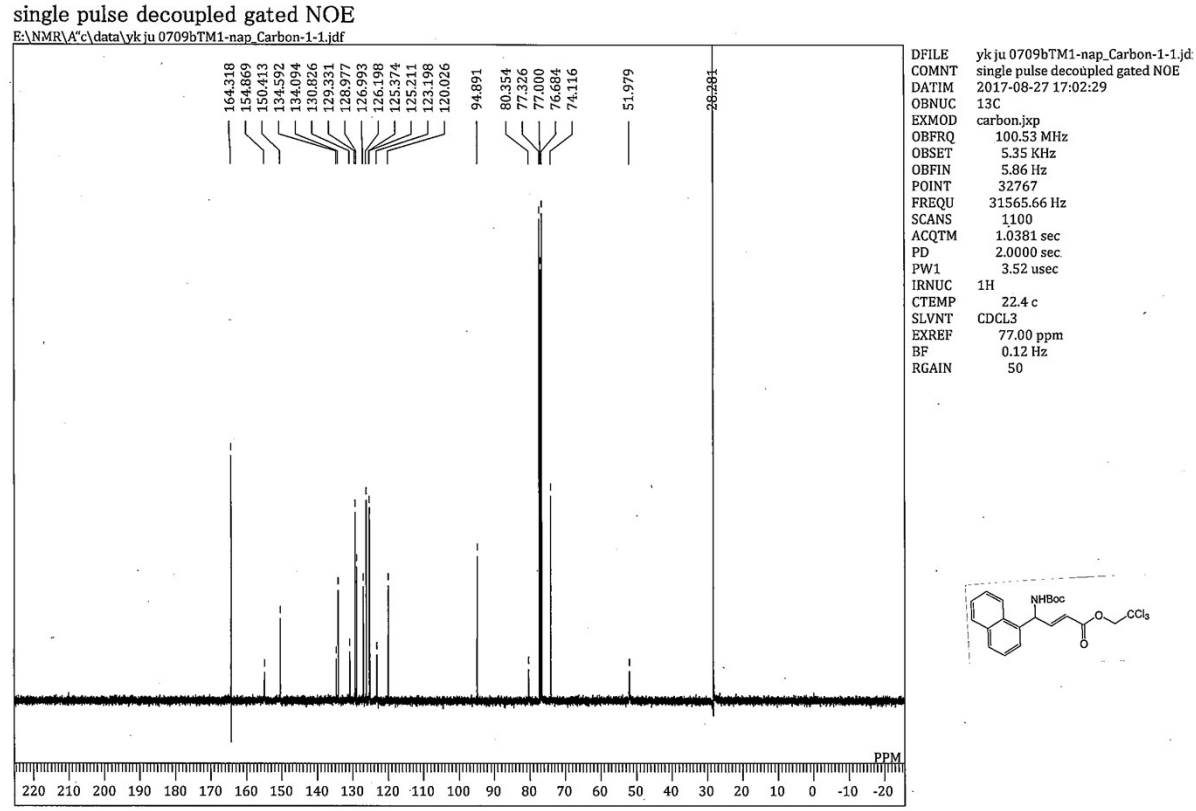
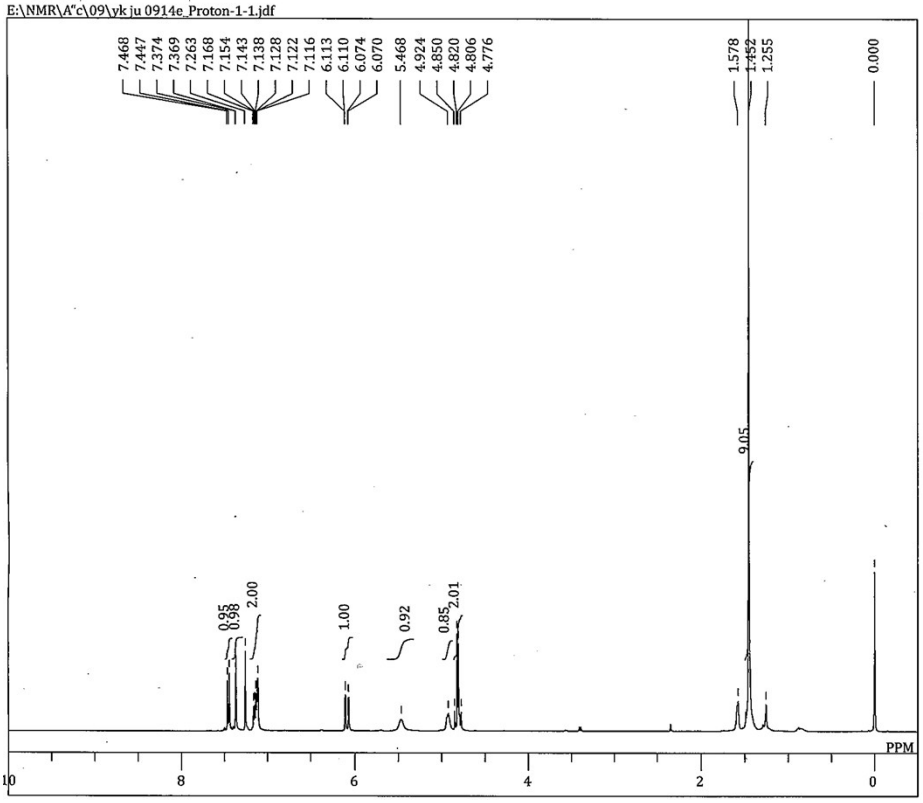
1.551 1.469
0.070 0.008 0.000
1.00 2.01 2.09 1.99 0.98 1.93 0.86 2.00 9.00
PPM
10 8 6 4 2 0
DFILE yk ju TM1-nap_Proton-1-1.jdf
COMNT single_pulse
DATIM 2017-08-28 11:19:15
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 7503.00 Hz
SCANS 4
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.00 usec
IRNUC 1H
CTEMP 23.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 50
NHBoc
O
CCl3


single pulse decoupled gated NOE
E:\NMR\A"c\data\yk ju 0709bTM1-nap_Carbon-1-1.jdf
164.318 154.869 150.413 134.592 134.094 130.826 129.331 128.977 126.993 126.198 125.374 125.211 123.198 120.026 94.891 80.354 77.326 77.000 76.684 74.116 51.979 28.281
PPM
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
DFILE yk ju 0709bTM1-nap_Carbon-1-1.jd
COMNT single pulse decoupled gated NOE
DATIM 2017-08-27 17:02:29
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 32767
FREQU 31565.66 Hz
SCANS 1100
ACQTM 1.0381 sec
PD 2.0000 sec
PW1 3.52 usec
IRNUC 1H
CTEMP 22.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50
NHBoc
O
CCl3

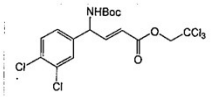
3bj

single_pulse

E:\NMR\A"c\09\yk ju 0914e_Proton-1-1.jdf

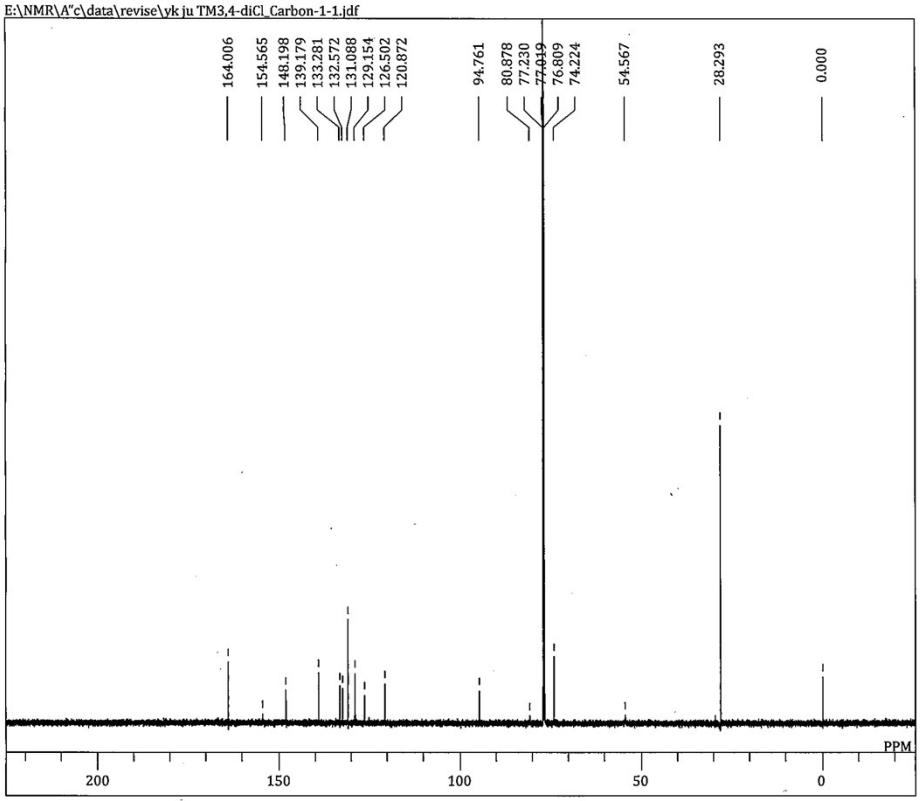


DFILE yk ju 0914e_Proton-1-1.jdf
COMNT single_pulse
DATIM 2018-05-16 04:22:32
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 7494.01 Hz
SCANS 8
ACQTM 2.1863 sec
PD 5.0000 sec
PW1 6.47 usec
IRNUC 1H
CTEMP 23.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 56

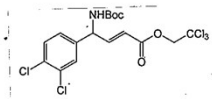


single pulse decoupled gated NOE

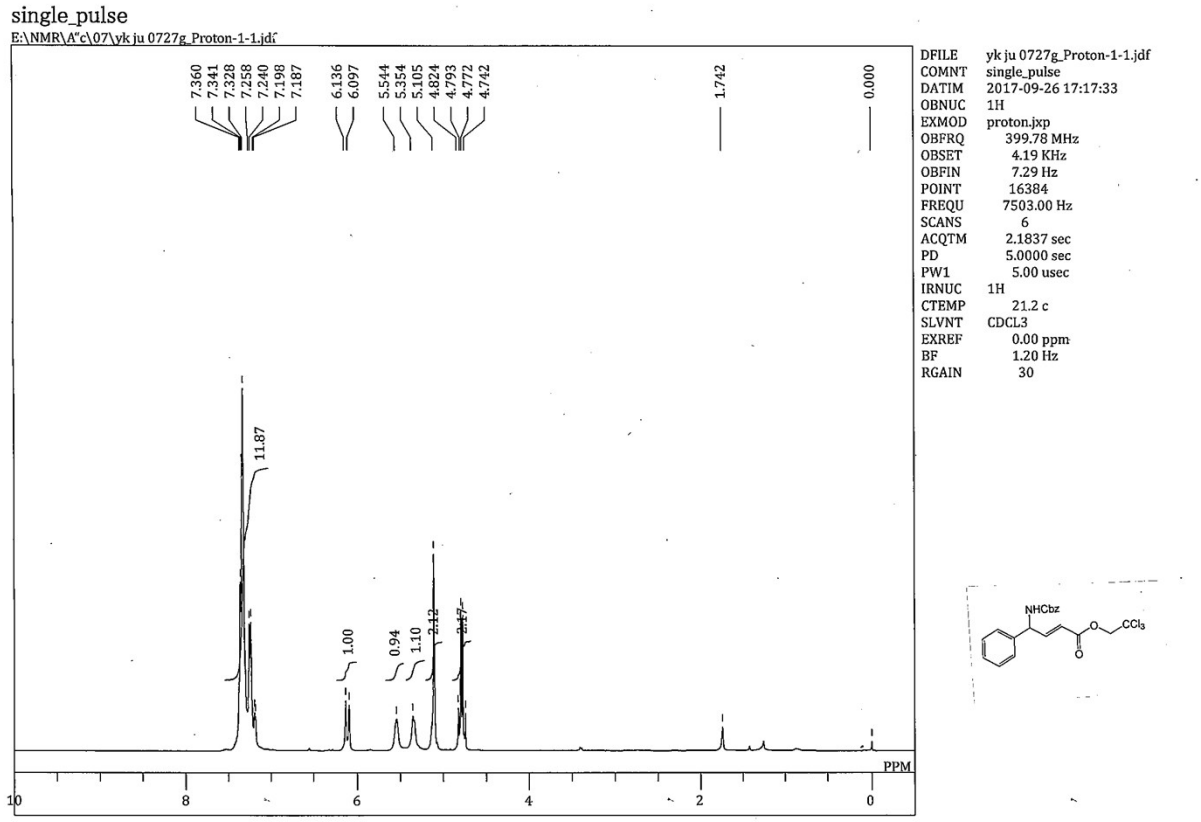
E:\NMR\A"c\data\revise\yk ju TM3,4-diCl_Carbon-1-1.jdf

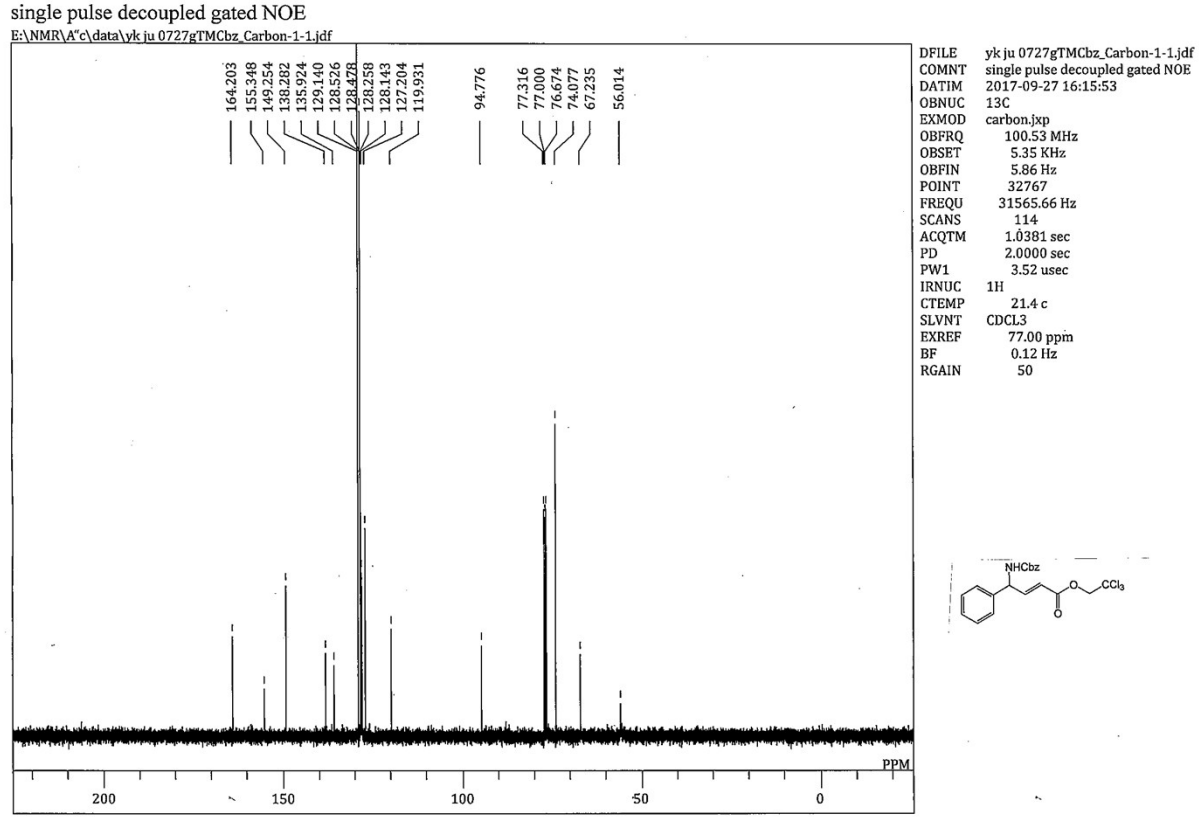


DFILE yk ju TM3,4-diCl_Carbon-1-1.jdf
COMNT single pulse decoupled gated NOE
DATIM 2018-05-16 09:26:19
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 32767
FREQU 47348.49 Hz
SCANS 1881
ACQTM 0.6921 sec
PD 2.0000 sec
PW1 4.28 usec
IRNUC 1H
CTEMP 22.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 56



3cc

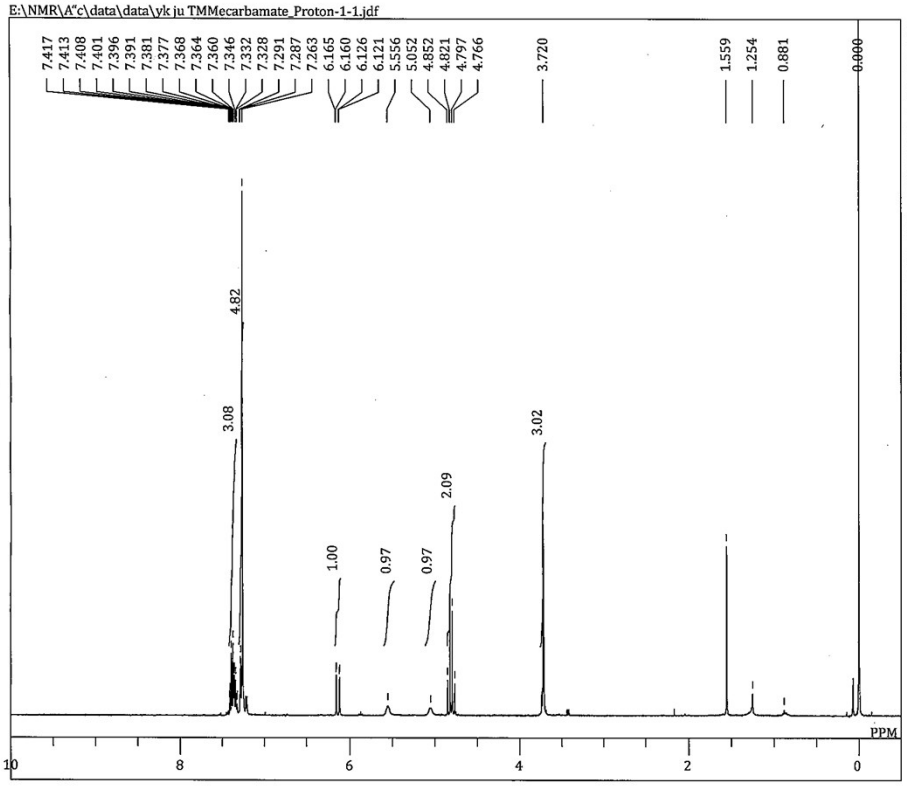

single_pulse
E:\NMR\A"c\07\yk ju 0727g_Proton-1-1.jdf
7.360
7.341
7.328
7.258
7.240
7.198
7.187
6.136
6.097
5.544
5.354
5.105
4.824
4.793
4.772
4.742
1.742
0.000
11.87
1.00
0.94
1.10
2.12
2.17
PPM
10
8
6
4
2
0
DFILE yk ju 0727g_Proton-1-1.jdf
COMNT single_pulse
DATIM 2017-09-26 17:17:33
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 7503.00 Hz
SCANS 6
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.00 usec
IRNUC 1H
CTEMP 21.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 30
NHCbz
O
CCl3
O


single pulse decoupled gated NOE
E:\NMR\A"c\data\yk ju 0727gTMCbz_Carbon-1-1.jdf
164.203
155.348
149.254
138.282
135.924
129.140
128.526
128.478
128.258
128.143
127.204
119.931
94.776
77.316
77.000
76.674
74.077
67.235
56.014
PPM
200
150
100
50
0
DFILE yk ju 0727gTMCbz_Carbon-1-1.jdf
COMNT single pulse decoupled gated NOE
DATIM 2017-09-27 16:15:53
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 32767
FREQU 31565.66 Hz
SCANS 114
ACQTM 1.0381 sec
PD 2.0000 sec
PW1 3.52 usec
IRNUC 1H
CTEMP 21.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50
NHCbz
O
CCl3
O

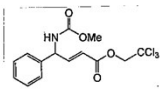
3dc

single_pulse

E:\NMR\A"c\data\data\yk ju TMMecarbamate_Proton-1-1.jdf

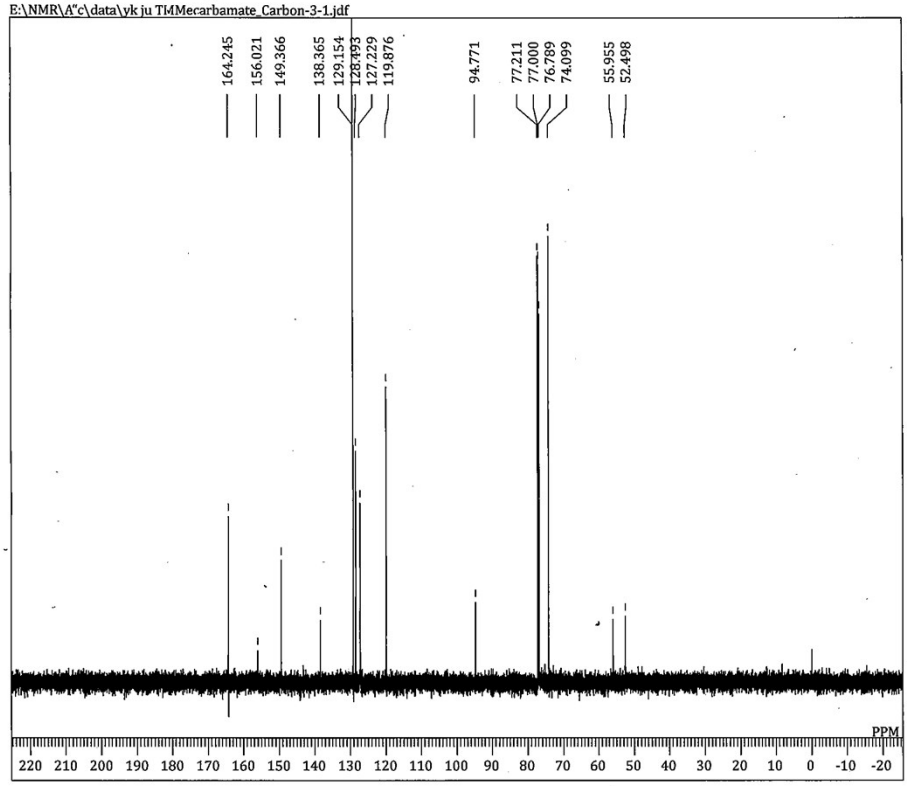


DFILE	yk ju TMMecarbamate_Proton-1-1.j
COMNT	single_pulse
DATIM	2018-01-09 22:00:24
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	16384
FREQU	7494.01 Hz
SCANS	4
ACQTM	2.1863 sec
PD	5.0000 sec
PW1	6.47 usec
IRNUC	1H
CTEMP	460.0 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	46

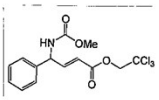


single pulse decoupled gated NOE

E:\NMR\A"c\data\yk ju TMMecarbamate_Carbon-3-1.jdf



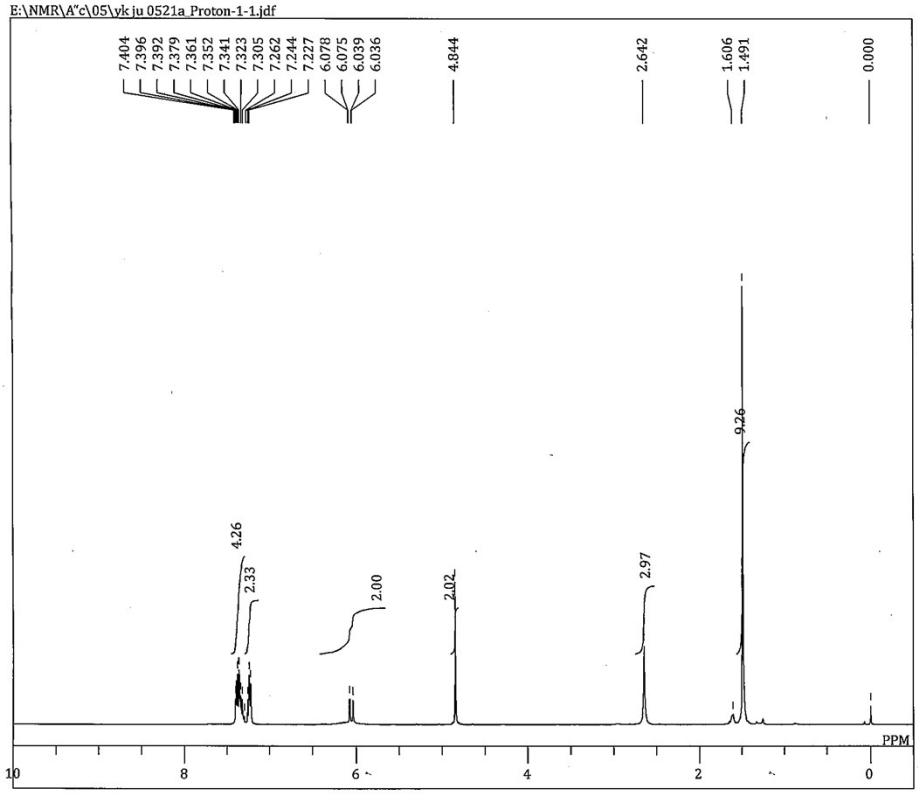
DFILE	yk ju TMMecarbamate_Carbon-3-1.j
COMNT	single pulse decoupled gated NOE
DATIM	2018-01-25 15:48:46
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	150.92 MHz
OBSET	8.52 KHz
OBFIN	1.74 Hz
POINT	32767
FREQU	47348.49 Hz
SCANS	200
ACQTM	0.6921 sec
PD	2.0000 sec
PW1	4.67 usec
IRNUC	1H
CTEMP	17.3 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	56



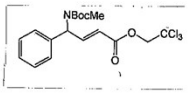
3ec

single_pulse

E:\NMR\A"c\05\yk ju 0521a_Proton-1-1.jdf

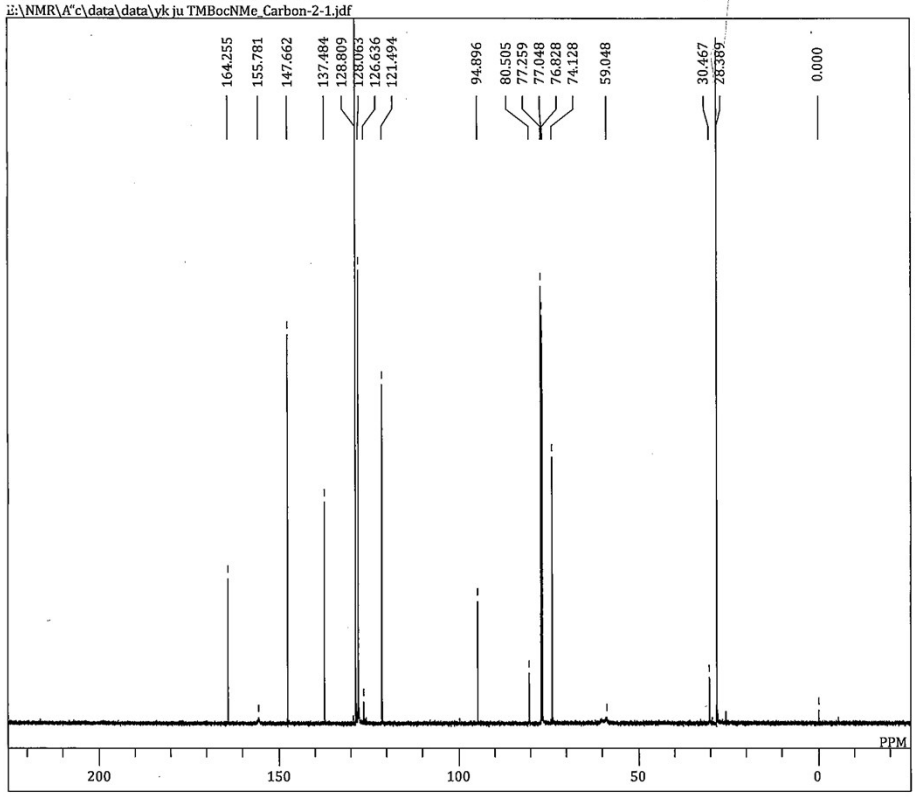


DFILE	yk ju 0521a_Proton-1-1.jdf
COMNT	single_pulse
DATIM	2017-02-23 12:26:10
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	16384
FREQU	7503.00 Hz
SCANS	4
ACQTM	2.1837 sec
PD	5.0000 sec
PW1	5.00 usec
IRNUC	1H
CTEMP	26.1 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	1.20 Hz
RGAIN	38

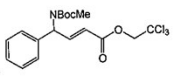


single pulse decoupled gated NOE

E:\NMR\A"c\data\data\yk ju TMBocNMe_Carbon-2-1.jdf



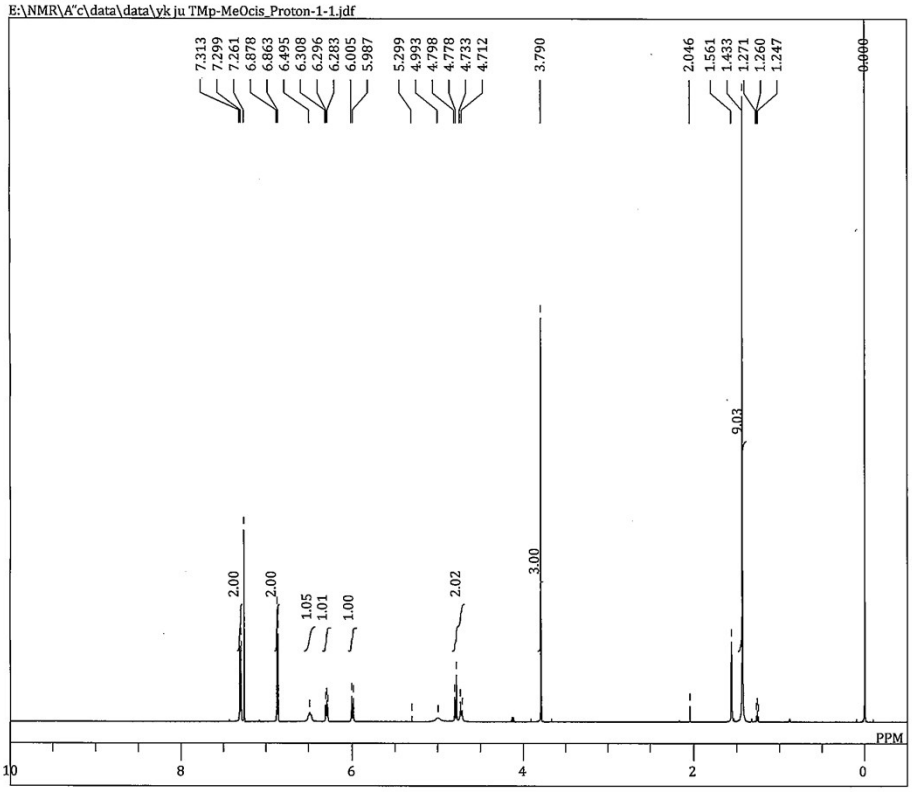
DFILE	yk ju TMBocNMe_Carbon-2-1.jdf
COMNT	single pulse decoupled gated NOE
DATIM	2018-02-06 15:14:47
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	150.92 MHz
OBSET	8.52 KHz
OBFIN	1.74 Hz
POINT	32767
FREQU	47348.49 Hz
SCANS	3863
ACQTM	0.6921 sec
PD	2.0000 sec
PW1	3.40 usec
IRNUC	1H
CTEMP	20.4 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	56



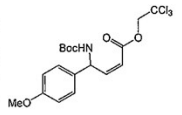
(*Z*)-3bg

single_pulse

E:\NMR\A"c\data\data\yk ju TMp-MeOcis_Proton-1-1.jdf

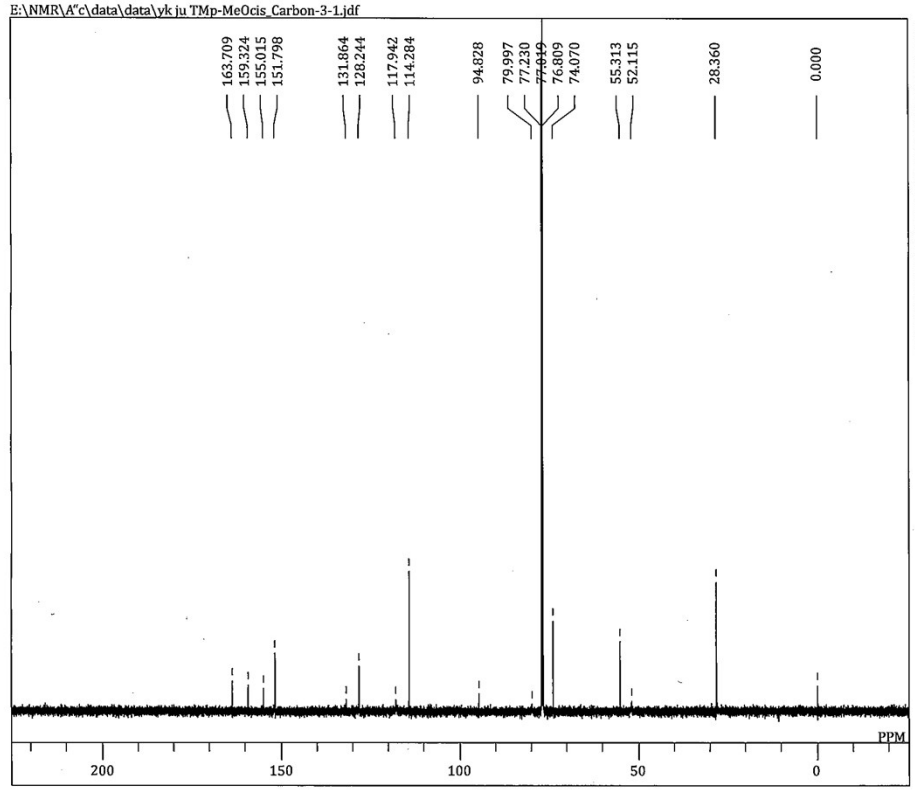


DFILE	yk ju TMp-MeOcis_Proton-1-1.jdf
COMNT	single_pulse
DATIM	2018-04-01 19:26:51
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	600.17 MHz
OBSET	5.30 KHz
OBFIN	5.47 Hz
POINT	16384
FREQU	11281.59 Hz
SCANS	8
ACQTM	1.4523 sec
PD	5.0000 sec
PW1	6.35 usec
IRNUC	1H
CTEMP	23.4 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	56

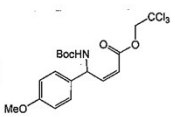


single pulse decoupled gated NOE

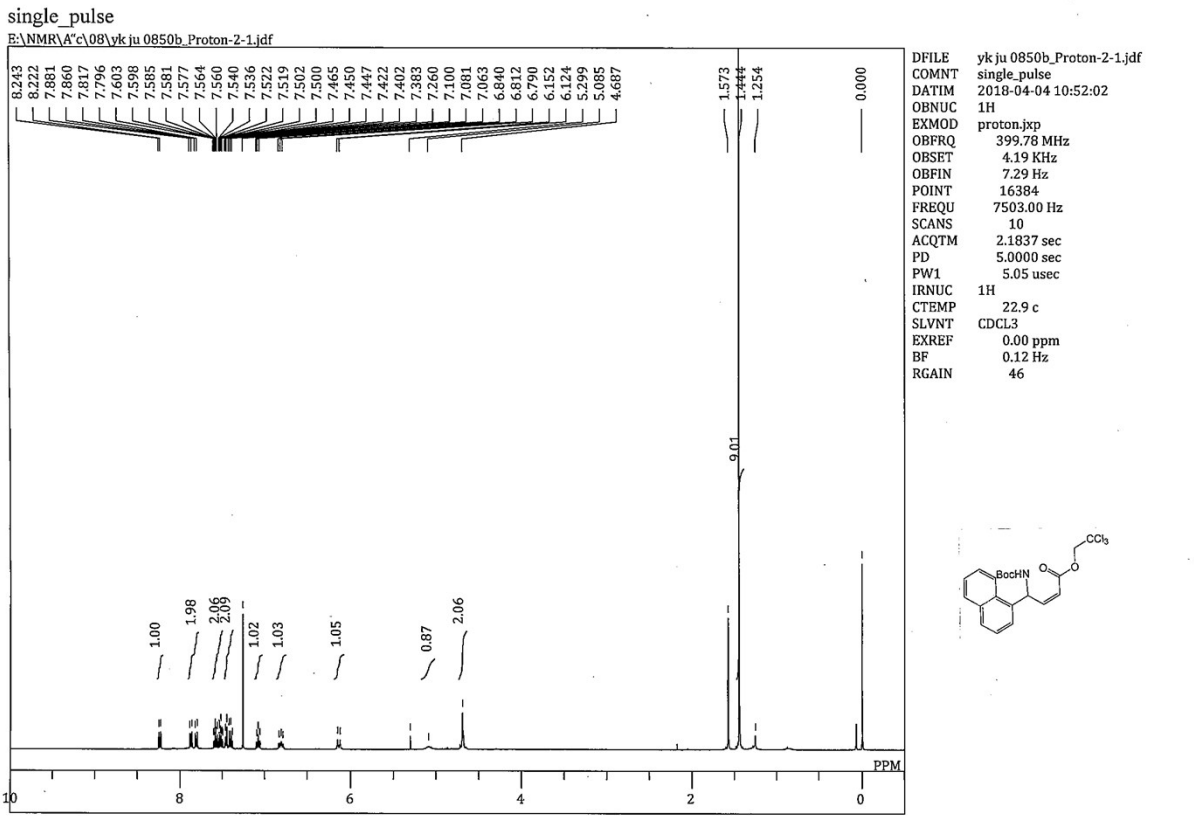
E:\NMR\A"c\data\data\yk ju TMp-MeOcis_Carbon-3-1.jdf

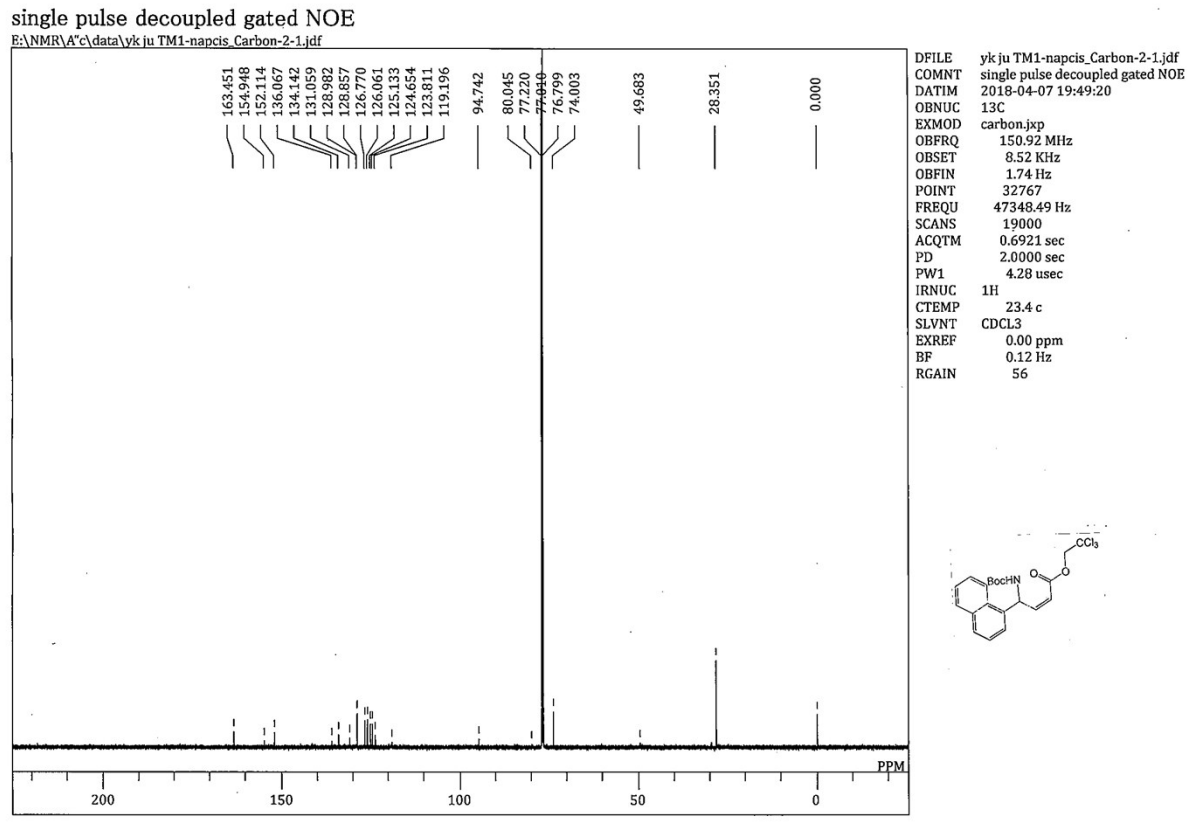


DFILE	yk ju TMp-MeOcis_Carbon-3-1.jdf
COMNT	single pulse decoupled gated NOE
DATIM	2018-04-08 13:43:42
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	150.92 MHz
OBSET	8.52 KHz
OBFIN	1.74 Hz
POINT	32767
FREQU	47348.49 Hz
SCANS	6325
ACQTM	0.6921 sec
PD	2.0000 sec
PW1	4.28 usec
IRNUC	1H
CTEMP	24.0 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	56

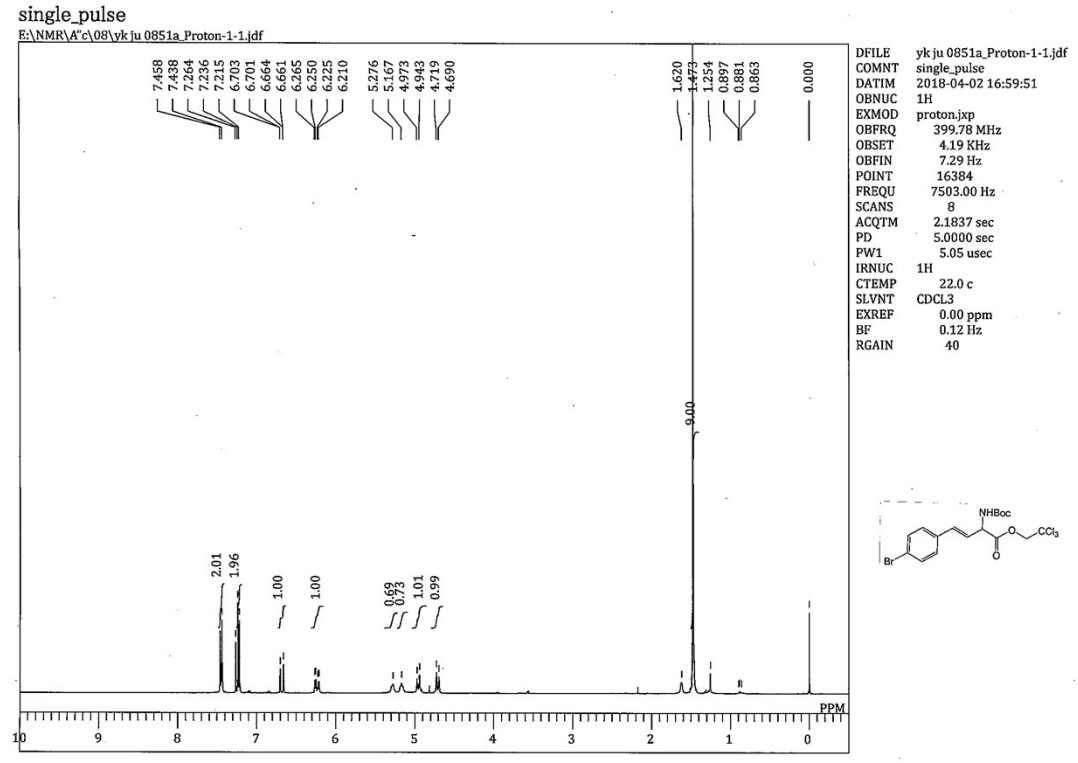


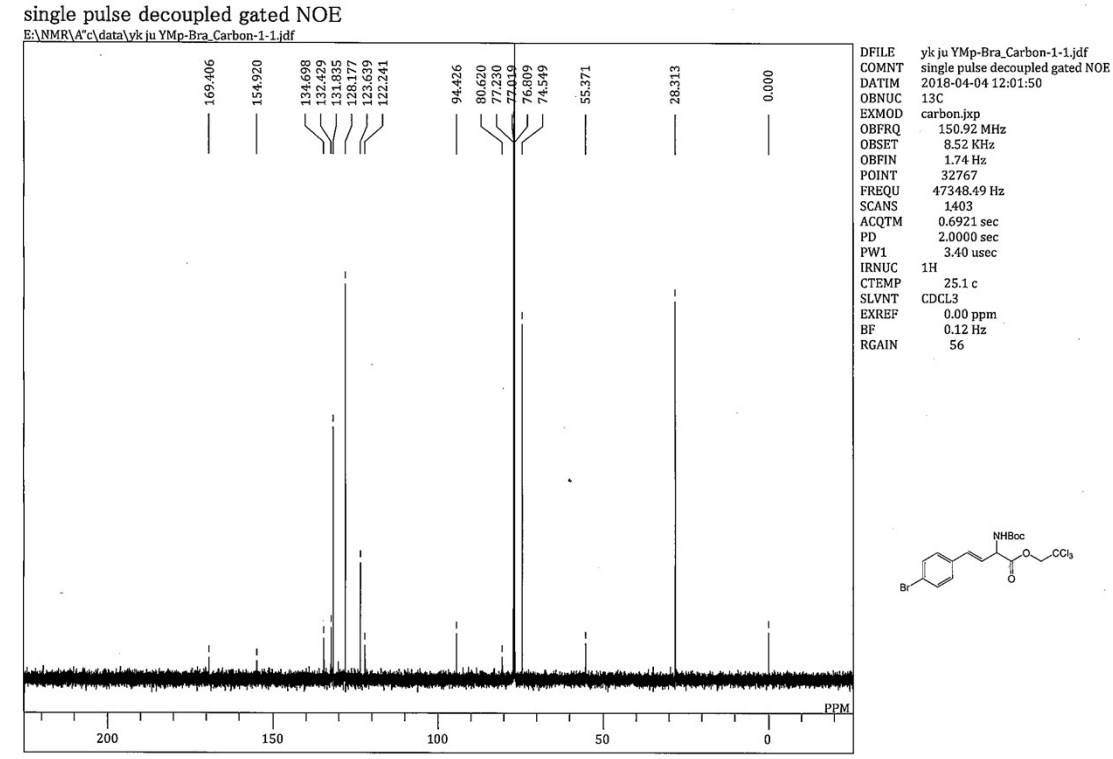
(*Z*)-3bi


single_pulse
E:\NMR\A"c\08\yk ju 0850b_Proton-2-1.jdf
8.243 8.222 7.881 7.860 7.817 7.796 7.603 7.598 7.585 7.581 7.577 7.564 7.560 7.540 7.536 7.522 7.519 7.502 7.500 7.465 7.450 7.447 7.422 7.402 7.383 7.260 7.100 7.081 7.063 6.840 6.812 6.790 6.152 6.124 5.299 5.085 4.687
1.573 1.444 1.254
0.000
9.01
1.00 1.98 2.06 2.09 1.02 1.03 1.05 0.87 2.06
PPM
10 8 6 4 2 0
DFILE yk ju 0850b_Proton-2-1.jdf
COMNT single_pulse
DATIM 2018-04-04 10:52:02
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 7503.00 Hz
SCANS 10
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.05 usec
IRNUC 1H
CTEMP 22.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 46
CCl3
BocHN
O
O


single pulse decoupled gated NOE
E:\NMR\A"c\data\yk ju TM1-napcis_Carbon-2-1.jdf
163.451 154.948 152.114 136.067 134.142 131.059 128.982 128.857 126.770 126.061 125.133 124.654 123.811 119.196
94.742 80.045 77.220 77.010 76.799 74.003
49.683
28.351
0.000
PPM
200 150 100 50 0
DFILE yk ju TM1-napcis_Carbon-2-1.jdf
COMNT single pulse decoupled gated NOE
DATIM 2018-04-07 19:49:20
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 32767
FREQU 47348.49 Hz
SCANS 19000
ACQTM 0.6921 sec
PD 2.0000 sec
PW1 4.28 usec
IRNUC 1H
CTEMP 23.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 56
CCl3
BocHN
O
O

4bh

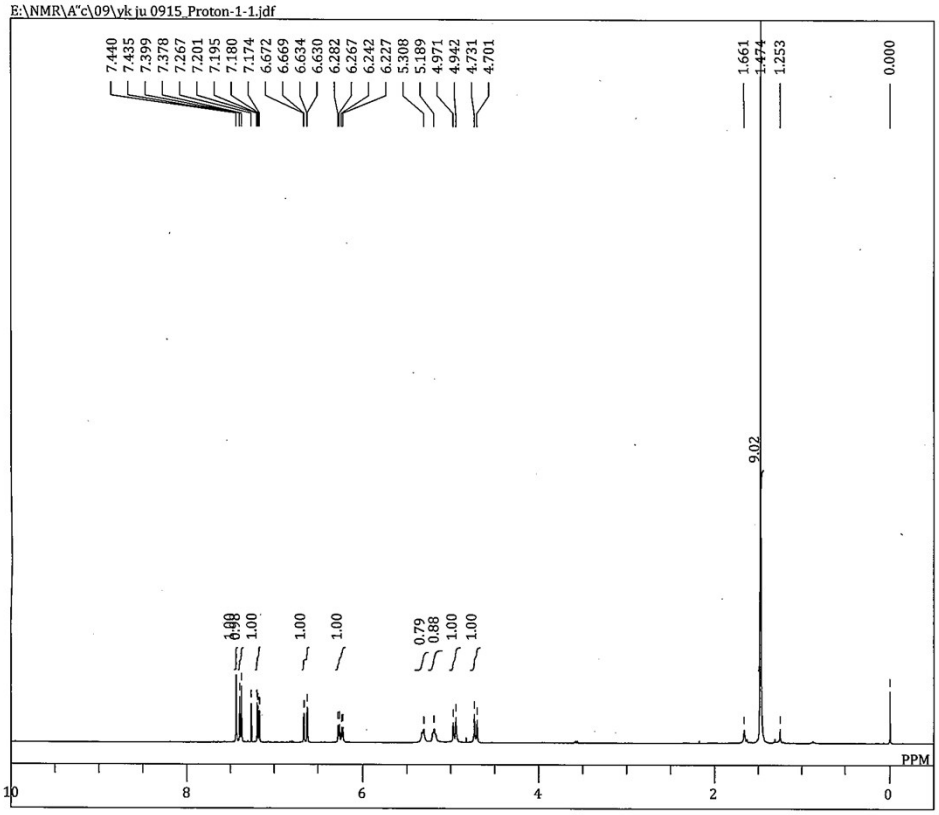

single_pulse
E:\NMR\A"c\08\yk ju 0851a_Proton-1-1.jdf
7.458
7.438
7.264
7.236
7.215
6.703
6.701
6.664
6.661
6.265
6.250
6.225
6.210
5.276
5.167
4.973
4.943
4.719
4.690
1.620
1.473
1.254
0.897
0.881
0.863
0.000
2.01
1.96
1.00
1.00
0.63
0.73
1.01
0.99
9.00
PPM
10
9
8
7
6
5
4
3
2
1
0
DFILE yk ju 0851a_Proton-1-1.jdf
COMNT single_pulse
DATIM 2018-04-02 16:59:51
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 7503.00 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.05 usec
IRNUC 1H
CTEMP 22.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 40
NHBoc
CCl3
Br
O
O


single pulse decoupled gated NOE
E:\NMR\A"c\data\yk ju YMp-Bra_Carbon-1-1.jdf
169.406
154.920
134.698
132.429
131.835
128.177
123.639
122.241
94.426
80.620
77.230
77.019
76.809
74.549
55.371
28.313
0.000
PPM
200
150
100
50
0
DFILE yk ju YMp-Bra_Carbon-1-1.jdf
COMNT single pulse decoupled gated NOE
DATIM 2018-04-04 12:01:50
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 32767
FREQU 47348.49 Hz
SCANS 1403
ACQTM 0.6921 sec
PD 2.0000 sec
PW1 3.40 usec
IRNUC 1H
CTEMP 25.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 56
NHBoc
CCl3
Br
O
O

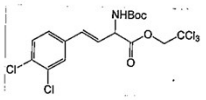
4bj

single_pulse

E:\NMR\A"c\09\yk ju 0915_Proton-1-1.jdf

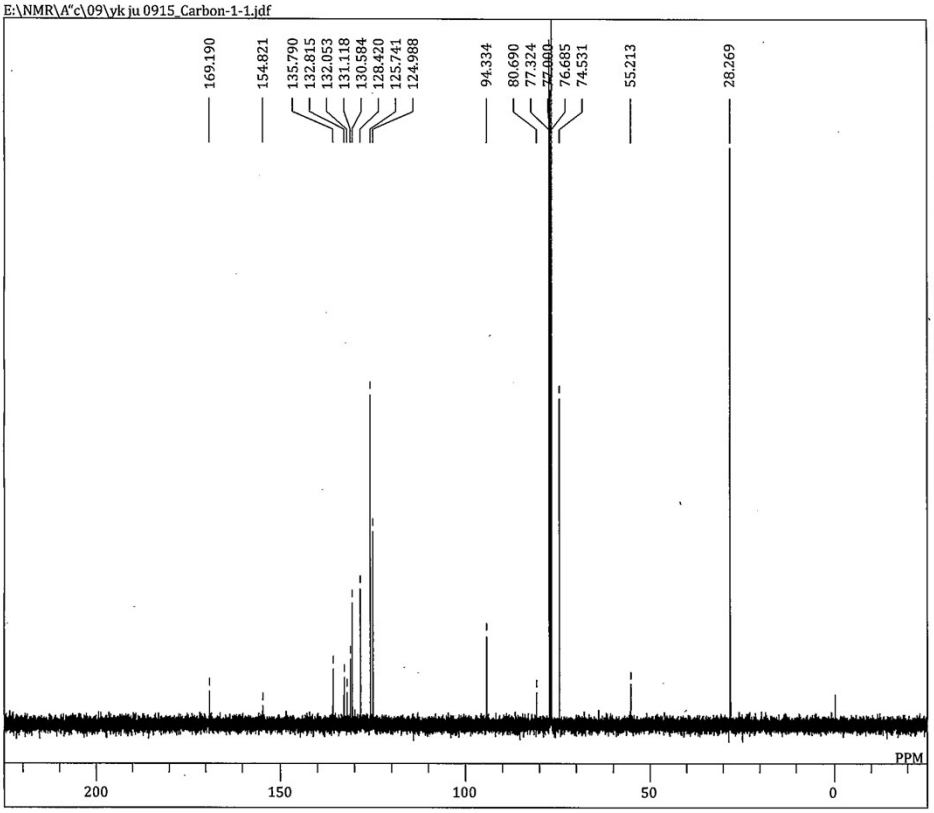


DFILE	yk ju 0915_Proton-1-1.jdf
COMNT	single_pulse
DATIM	2018-05-16 13:47:39
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	16384
FREQU	7503.00 Hz
SCANS	6
ACQTM	2.1837 sec
PD	5.0000 sec
PW1	5.05 usec
IRNUC	1H
CTEMP	20.4 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	36

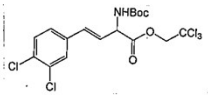


single pulse decoupled gated NOE

E:\NMR\A"c\09\yk ju 0915_Carbon-1-1.jdf



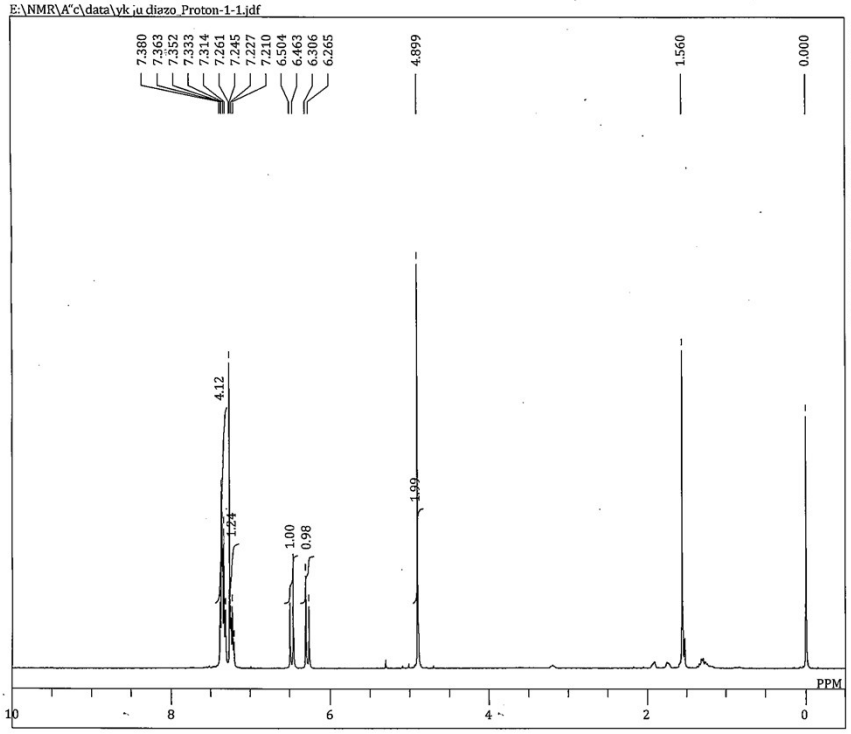
DFILE	yk ju 0915_Carbon-1-1.jdf
COMNT	single pulse decoupled gated N
DATIM	2018-05-16 13:48:39
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	32767
FREQU	31407.04 Hz
SCANS	233
ACQTM	1.0433 sec
PD	2.0000 sec
PW1	2.93 usec
IRNUC	1H
CTEMP	20.5 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	50



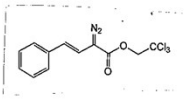
2c

single_pulse

E:\NMR\A"c\data\yk ju diazo_Proton-1-1.jdf

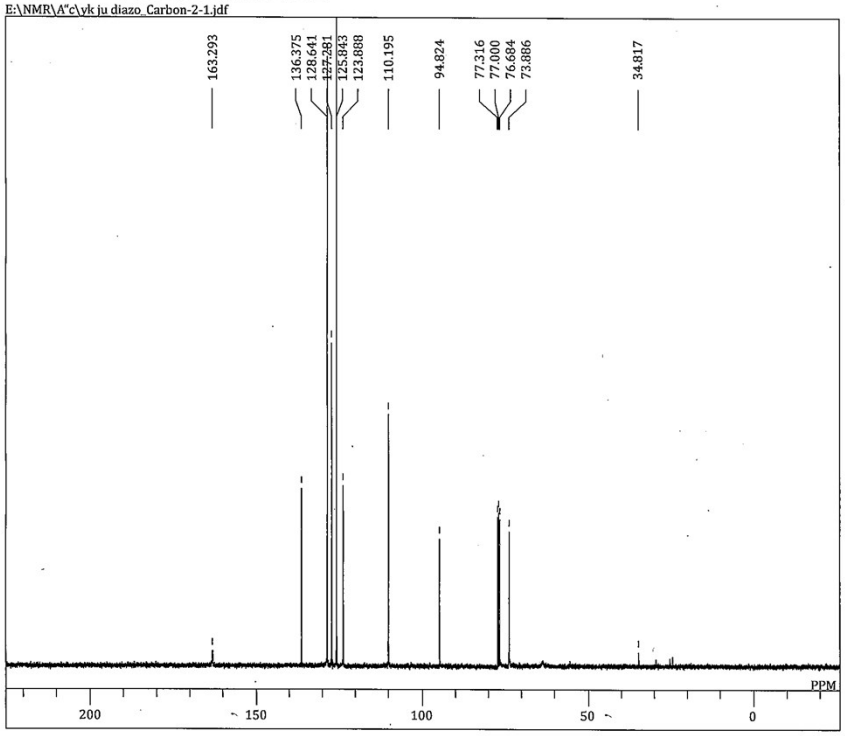


DFILE	yk ju diazo_Proton-1-1.jdf
COMNT	single_pulse
DATIM	2017-09-06 16:17:20
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	16384
FREQU	7503.00 Hz
SCANS	6
ACQTM	2.1837 sec
PD	5.0000 sec
PW1	5.00 usec
IRNUC	1H
CTEMP	21.1 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	1.20 Hz
RGAIN	50

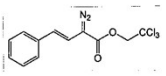


single pulse decoupled gated NOE

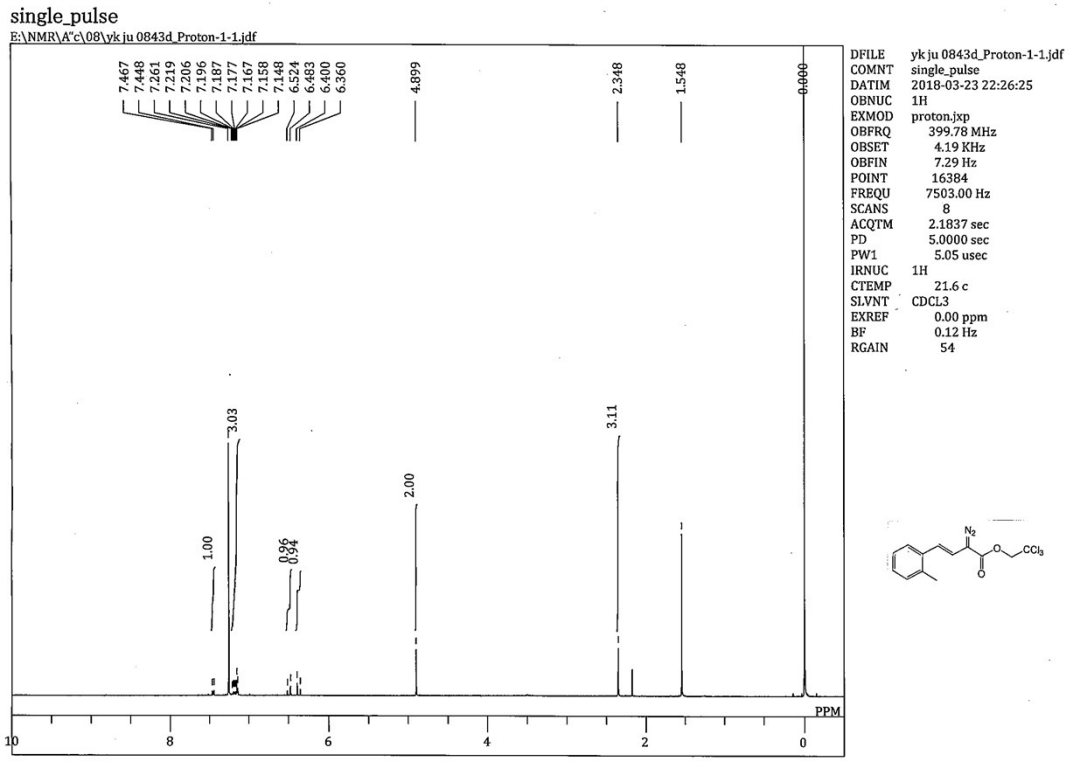
E:\NMR\A"c\yk ju diazo_Carbon-2-1.jdf

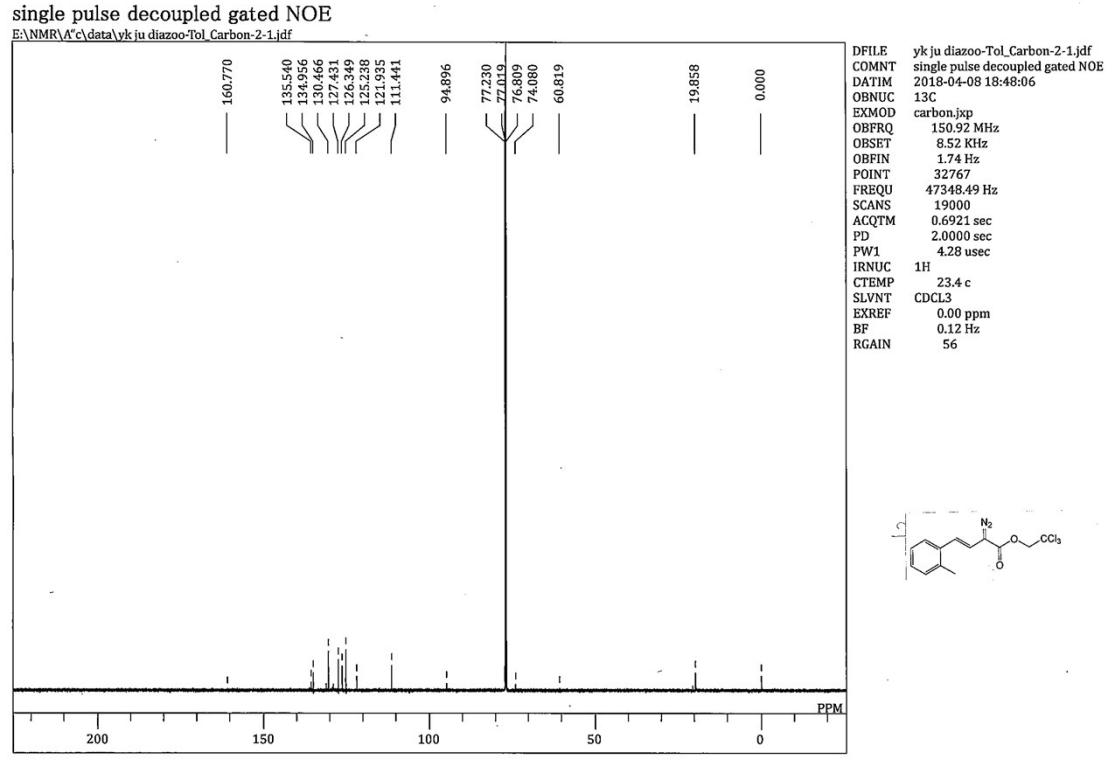


DFILE	yk ju diazo_Carbon-2-1.jdf
COMNT	single pulse decoupled gated NOE
DATIM	2017-09-20 19:10:29
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	32767
FREQU	31565.66 Hz
SCANS	193
ACQTM	1.0381 sec
PD	2.0000 sec
PW1	3.52 usec
IRNUC	1H
CTEMP	22.1 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.20 Hz
RGAIN	50



2d

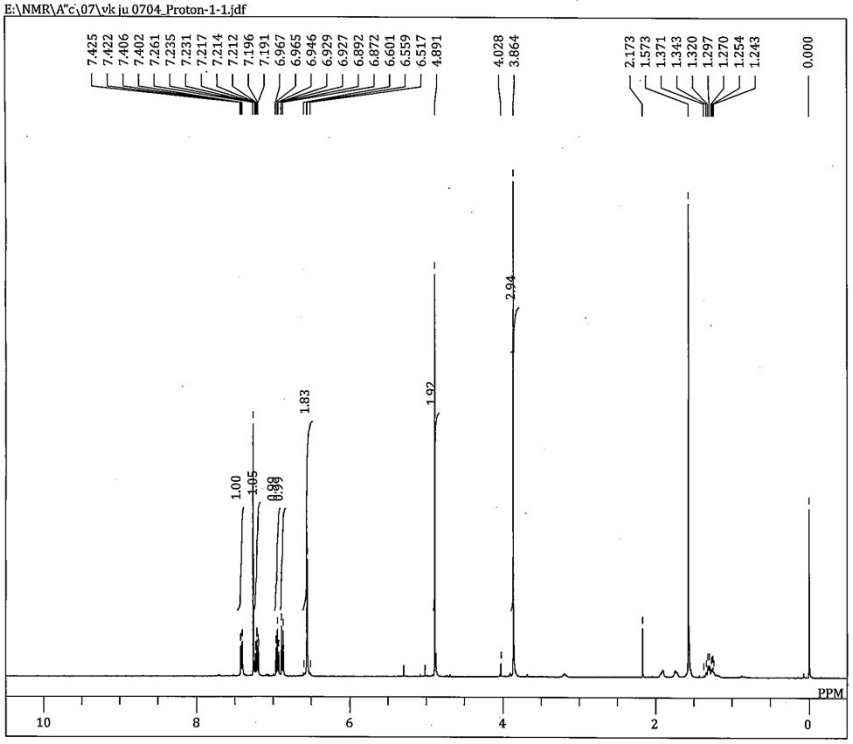

single_pulse
E:\NMR\A"c\08\yk ju 0843d_Proton-1-1.jdf
7.467
7.448
7.261
7.219
7.206
7.196
7.187
7.177
7.167
7.158
7.148
6.524
6.483
6.400
6.360
4.899
2.348
1.548
0.000
1.00
3.03
0.96
0.94
2.00
3.11
PPM
10
8
6
4
2
0
DFILE yk ju 0843d_Proton-1-1.jdf
COMNT single_pulse
DATIM 2018-03-23 22:26:25
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 7503.00 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.05 usec
IRNUC 1H
CTEMP 21.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 54
N2
O
CCl3
O


single pulse decoupled gated NOE
E:\NMR\A"c\data\yk ju diazoo-Tol_Carbon-2-1.jdf
160.770
135.540
134.956
130.466
127.431
126.349
125.238
121.935
111.441
94.896
77.230
77.019
76.809
74.080
60.819
19.858
0.000
PPM
200
150
100
50
0
DFILE yk ju diazoo-Tol_Carbon-2-1.jdf
COMNT single pulse decoupled gated NOE
DATIM 2018-04-08 18:48:06
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 32767
FREQU 47348.49 Hz
SCANS 19000
ACQTM 0.6921 sec
PD 2.0000 sec
PW1 4.28 usec
IRNUC 1H
CTEMP 23.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 56
N2
O
CCl3
O

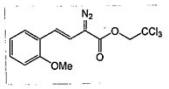
2e

single_pulse

E:\NMR\A"c\07\yk ju 0704_Proton-1-1.jdf

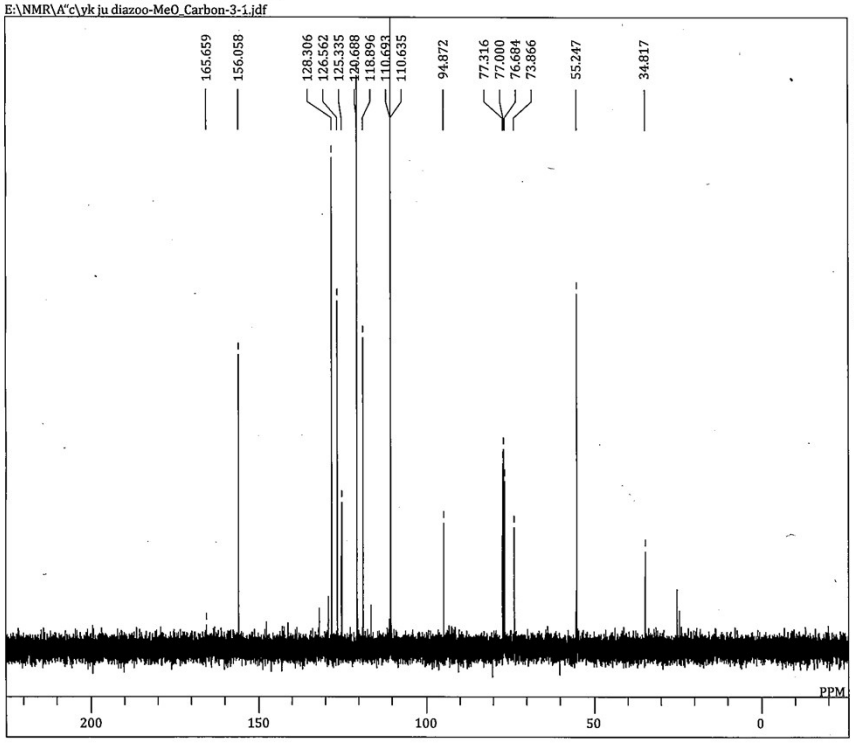


DFILE yk ju 0704_Proton-1-1.jdf
COMNT single_pulse
DATIM 2017-08-14 16:07:31
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 7503.00 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.00 usec
IRNUC 1H
CTEMP 22.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 50

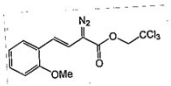


single pulse decoupled gated NOE

E:\NMR\A"c\yk ju diazoo-MeO_Carbon-3-1.jdf



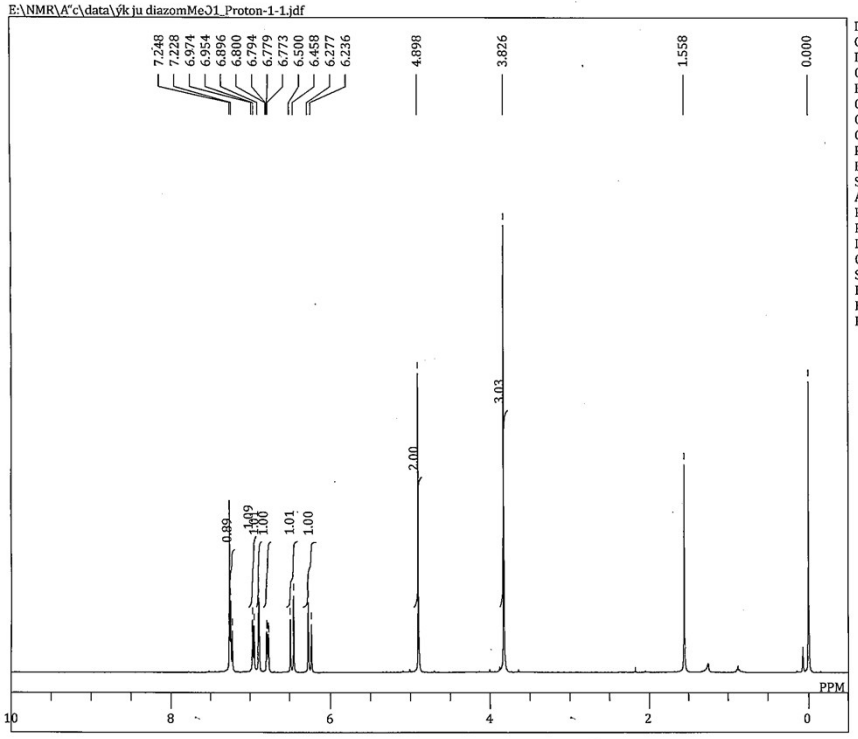
DFILE yk ju diazoo-MeO_Carbon-3-1.jdf
COMNT single pulse decoupled gated NOE
DATIM 2018-01-24 14:55:46
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 32767
FREQU 31565.66 Hz
SCANS 13
ACQTM 1.0381 sec
PD 2.0000 sec
PW1 4.08 usec
IRNUC 1H
CTEMP 18.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 56



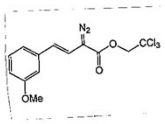
2f

single_pulse

E:\NMR\A"c\data\ýk ju diazomMeO1_Proton-1-1.jdf

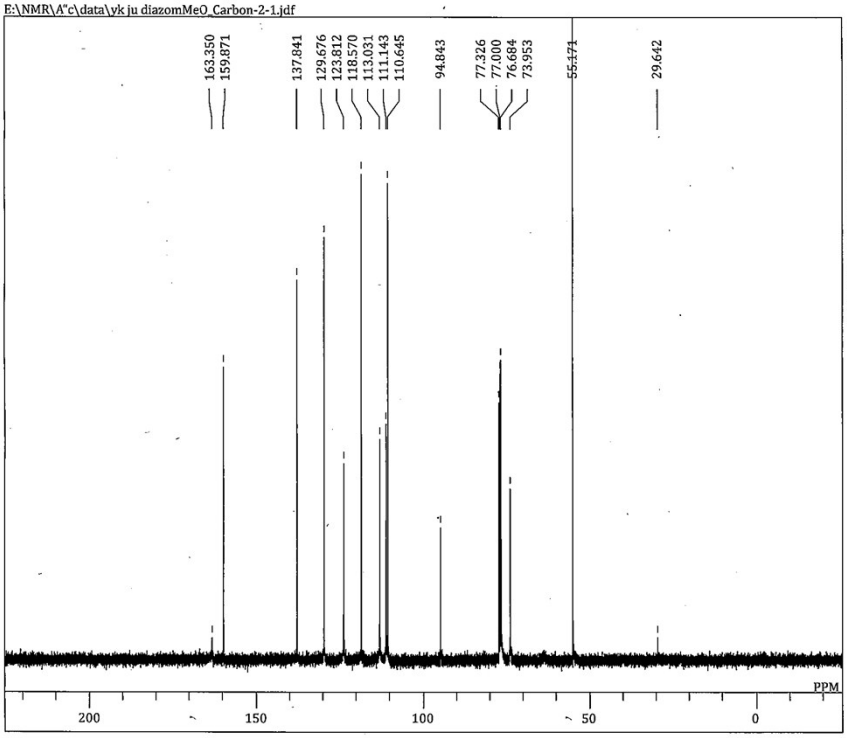


DFILE	yk ju diazomMeO1_Proton-1-1.jdf
COMNT	single_pulse
DATIM	2017-09-19 14:51:16
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	16384
FREQU	7503.00 Hz
SCANS	8
ACQTM	2.1837 sec
PD	5.0000 sec
PW1	5.00 usec
IRNUC	1H
CTEMP	21.4 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	1.20 Hz
RGAIN	50

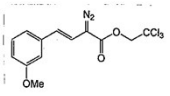


single pulse decoupled gated NOE

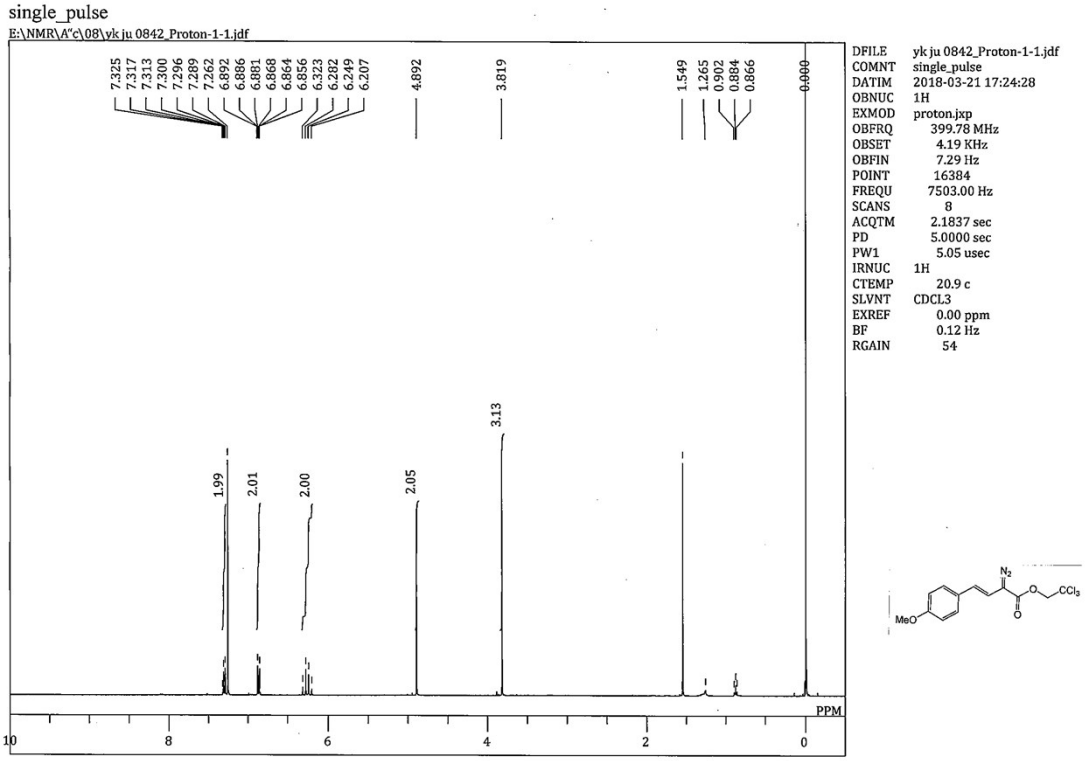
E:\NMR\A"c\data\yk ju diazomMeO_Carbon-2-1.jdf

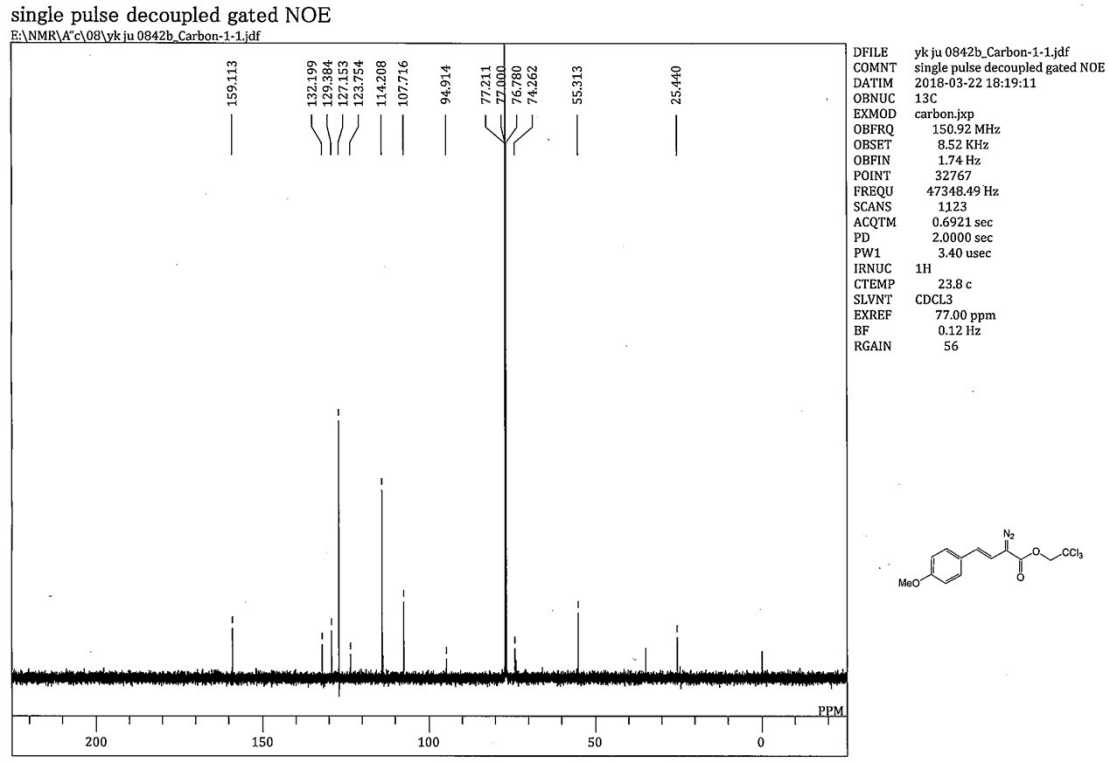


DFILE	yk ju diazomMeO_Carbon-2-1.jdf
COMNT	single pulse decoupled gated NOE
DATIM	2017-09-21 19:00:58
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	32767
FREQU	31565.66 Hz
SCANS	840
ACQTM	1.0381 sec
PD	2.0000 sec
PW1	3.52 usec
IRNUC	1H
CTEMP	22.1 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	50



2g

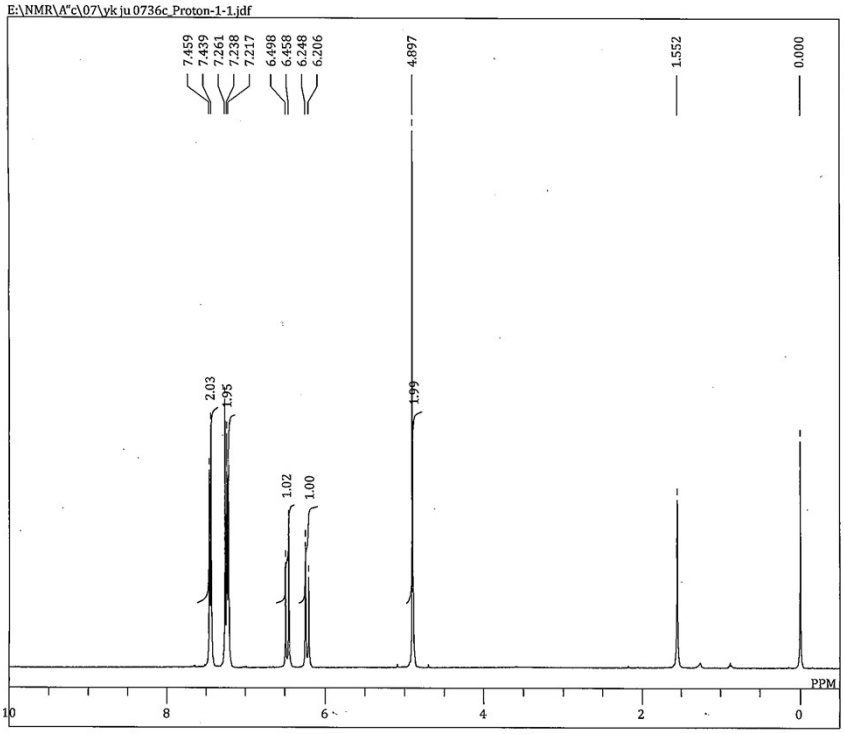

single_pulse
E:\NMR\A"c\08\yk ju 0842_Proton-1-1.jdf
7.325
7.317
7.313
7.300
7.296
7.289
7.262
6.892
6.886
6.881
6.868
6.864
6.856
6.323
6.282
6.249
6.207
4.892
3.819
1.549
1.265
0.902
0.884
0.866
0.000
1.99
2.01
2.00
2.05
3.13
PPM
10
8
6
4
2
0
DFILE yk ju 0842_Proton-1-1.jdf
COMNT single_pulse
DATIM 2018-03-21 17:24:28
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 7503.00 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.05 usec
IRNUC 1H
CTEMP 20.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 54
N2
O
CCl3
MeO


single pulse decoupled gated NOE
E:\NMR\A"c\08\yk ju 0842b_Carbon-1-1.jdf
159.113
132.199
129.384
127.153
123.754
114.208
107.716
94.914
77.211
77.000
76.780
74.262
55.313
25.440
PPM
200
150
100
50
0
DFILE yk ju 0842b_Carbon-1-1.jdf
COMNT single pulse decoupled gated NOE
DATIM 2018-03-22 18:19:11
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 32767
FREQU 47348.49 Hz
SCANS 1123
ACQTM 0.6921 sec
PD 2.0000 sec
PW1 3.40 usec
IRNUC 1H
CTEMP 23.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 56
N2
O
CCl3
MeO

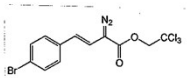
2h

single_pulse

E:\NMR\A"c\07\yk ju 0736c_Proton-1-1.jdf

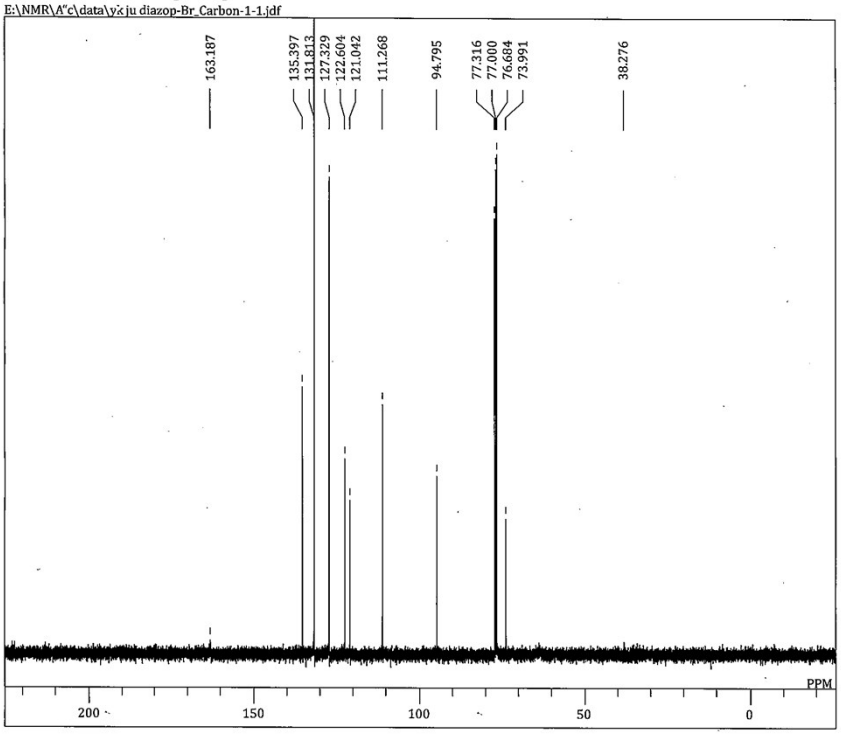


DFILE yk ju 0736c_Proton-1-1.jdf
COMNT single_pulse
DATIM 2017-10-02 11:00:15
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 7503.00 Hz
SCANS 6
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.00 usec
IRNUC 1H
CTEMP 22.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 52

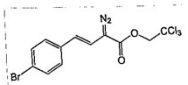


single pulse decoupled gated NOE

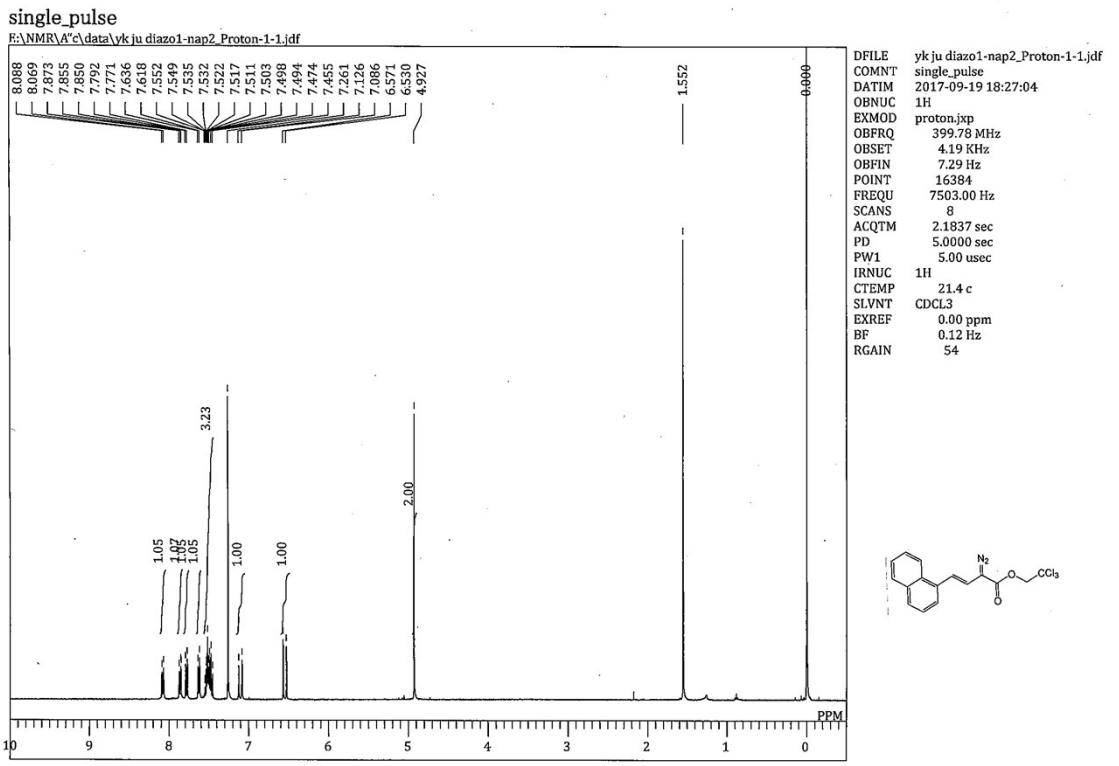
E:\NMR\A"c\data\yk ju diazop-Br_Carbon-1-1.jdf

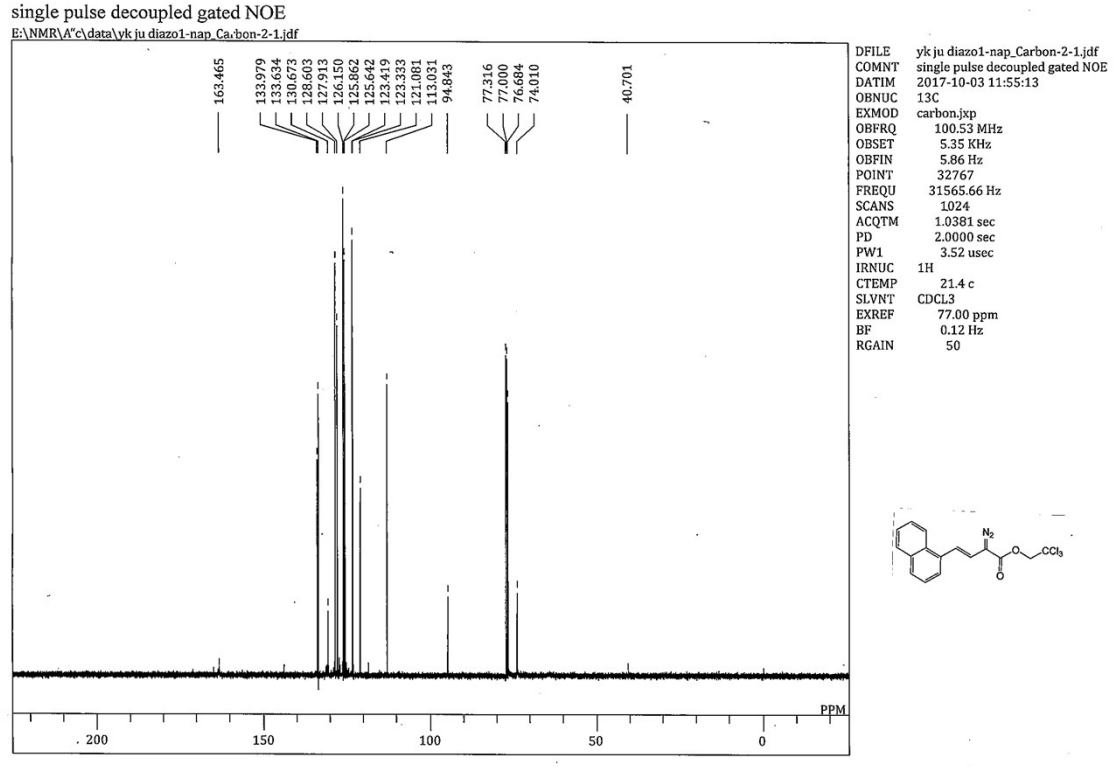


DFILE yk ju diazop-Br_Carbon-1-1.jdf
COMNT single pulse decoupled gated NOE
DATIM 2017-10-02 20:33:32
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 32767
FREQU 31565.66 Hz
SCANS 1024
ACQTM 1.0381 sec
PD 2.0000 sec
PW1 3.52 usec
IRNUC 1H
CTEMP 21.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50



2i

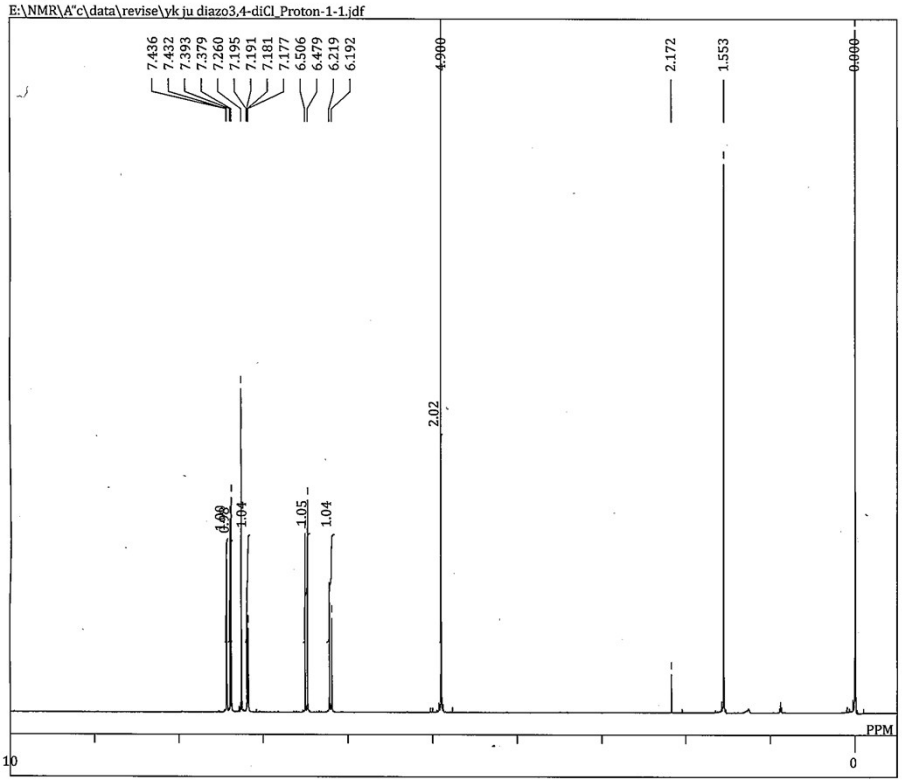

single_pulse
F:\NMR\A"c\data\yk ju diazo1-nap2_Proton-1-1.jdf
8.088
8.069
7.873
7.855
7.850
7.792
7.771
7.636
7.618
7.552
7.549
7.535
7.532
7.522
7.517
7.511
7.503
7.498
7.494
7.474
7.455
7.261
7.126
7.086
6.571
6.530
4.927
1.552
0.000
3.23
2.00
1.05
1.07
1.05
1.05
1.00
1.00
PPM
10
9
8
7
6
5
4
3
2
1
0
DFILE yk ju diazo1-nap2_Proton-1-1.jdf
COMNT single_pulse
DATIM 2017-09-19 18:27:04
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 7503.00 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.00 usec
IRNUC 1H
CTEMP 21.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 54
N2
O
O
CCl3


single pulse decoupled gated NOE
E:\NMR\A"c\data\yk ju diazo1-nap_Carbon-2-1.jdf
163.465
133.979
133.634
130.673
128.603
127.913
126.150
125.862
125.642
123.419
123.333
121.081
113.031
94.843
77.316
77.000
76.684
74.010
40.701
PPM
200
150
100
50
0
DFILE yk ju diazo1-nap_Carbon-2-1.jdf
COMNT single pulse decoupled gated NOE
DATIM 2017-10-03 11:55:13
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 32767
FREQU 31565.66 Hz
SCANS 1024
ACQTM 1.0381 sec
PD 2.0000 sec
PW1 3.52 usec
IRNUC 1H
CTEMP 21.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50
N2
O
O
CCl3

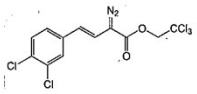
2j

single_pulse

E:\NMR\A"c\data\revise\yk ju diazo3,4-diCl_Proton-1-1.jdf

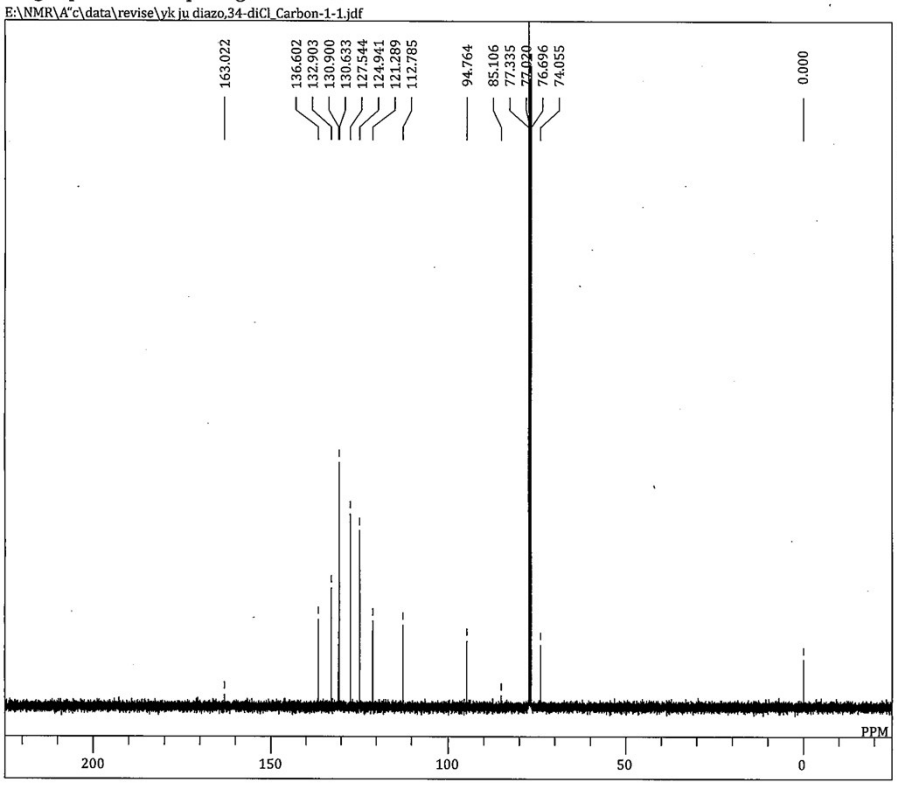


DFILE	yk ju diazo3,4-diCl_Proton-1-1.jdf
COMNT	single_pulse
DATIM	2018-05-15 17:32:53
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	600.17 MHz
OBSET	5.30 KHz
OBFIN	5.47 Hz
POINT	16384
FREQU	11281.59 Hz
SCANS	8
ACQTM	1.4523 sec
PD	5.0000 sec
PW1	4.03 usec
IRNUC	1H
CTEMP	22.7 c
SLVNT	CDCl3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	66

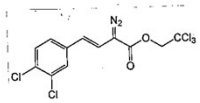


single pulse decoupled gated NOE

E:\NMR\A"c\data\revise\yk ju diazo,34-diCl_Carbon-1-1.jdf



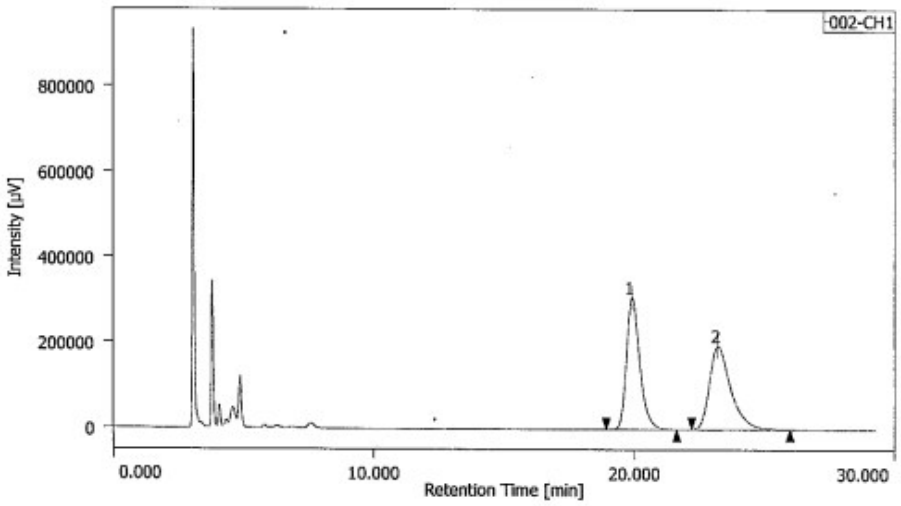
DFILE	yk ju diazo,34-diCl_Carbon-1-1.jdf
COMNT	single pulse decoupled gated NOE
DATIM	2018-05-16 14:03:44
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	32767
FREQU	31407.04 Hz
SCANS	606
ACQTM	1.0433 sec
PD	2.0000 sec
PW1	2.93 usec
IRNUC	1H
CTEMP	20.5 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	50



3. Racemic and Chiral HPLC Traces

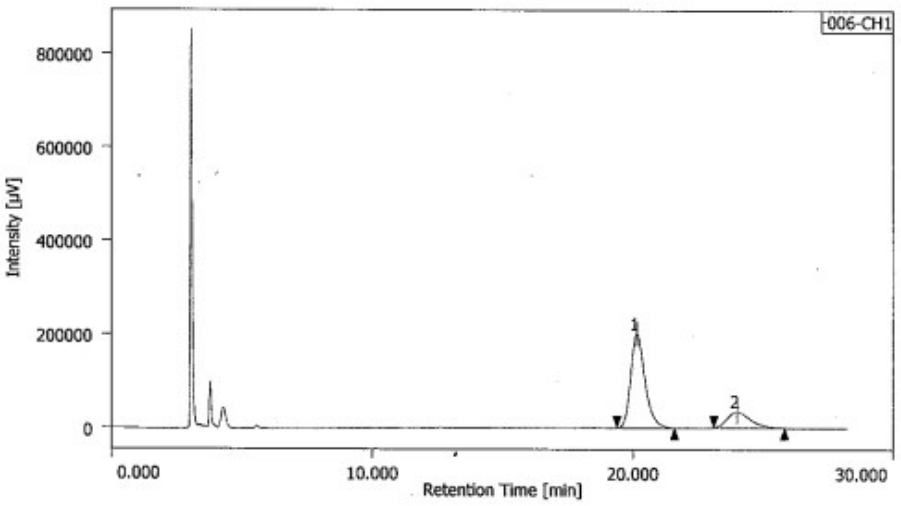
(±)-**3bc** and (–)-**3bc** (Scheme 2)

ju-0415_0415 002 2018/04/16 12:37:59



#	tR [min]	Area [μV*sec]	Height [μV]	Area%	Height%
1	19.900	10939848	309002	49.585	61.251
2	23.200	11122947	195484	50.415	38.749

ju-0415_0415 006 2018/04/16 12:36:20



#	tR [min]	Area [μV*sec]	Height [μV]	Area%	Height%
1	20.142	7662400	201062	77.785	85.357
2	23.992	2188379	34491	22.215	14.643

4. References

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