Supporting Information

Visible light-induced N-radicals 5-exo/6-endo cyclization of alkenyl amide: facile access to isoindolinones/isoquinolinones

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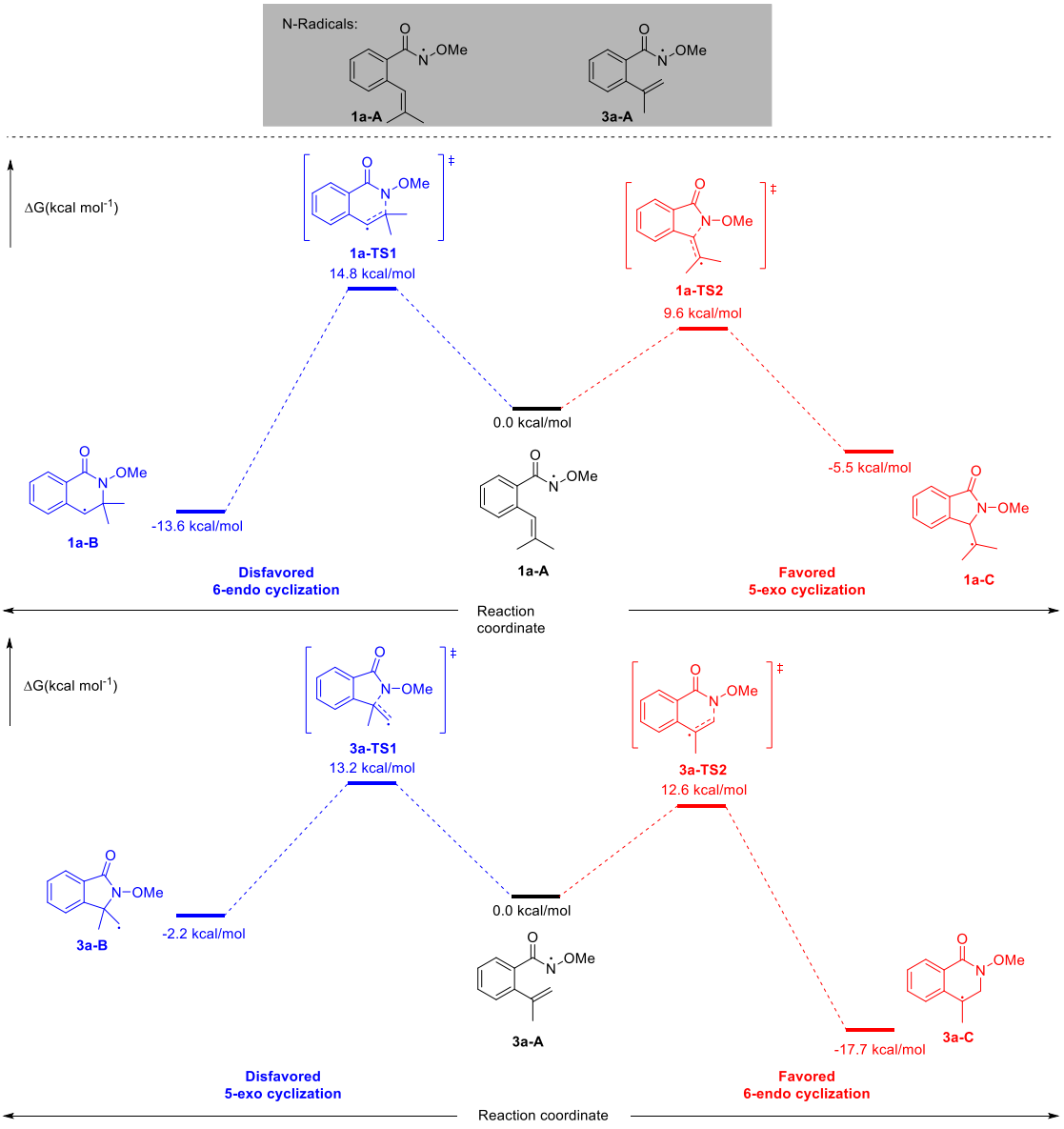
1. General Information

Unless otherwise noted, reagents obtained from commercial suppliers were used without further purification. All glasswares were washed with detergent, rinsed with acetone, and dried in an oven at 125 °C prior to use. Moisture-sensitive reactions were carried out in the argon atmosphere and sensitive reagents were added via syringe and cannula techniques. TLC (Thin Layer Chromatography) was performed on precoated silica gel HSGF254 plates which were visualized by use of UV light (254 nm), iodine, $KMnO_4$ solution or alcoholic solution of phosphomolybdic acid. CC (column chromatography) was performed on silica gel 100-200/, 200–300/, 300–400 mesh obtained from Qingdao Haiyang Chemical. NMR spectra were recorded on Bruker AVANCE-300 spectrometer at 300 MHz for ^{1}H NMR, 75 MHz for ^{13}C NMR in $CDCl_3$ with tetramethylsilane (TMS) as internal standard. The chemical shifts are expressed in ppm and coupling constants are given in Hz. Data for ^{1}H NMR are recorded as follows: chemical shift (ppm), multiplicity (s, singlet; d, doublet; t, triplet; q, quarter; p, pentet, m, multiplet; br, broad), coupling constant (Hz), integration. Data for ^{13}C NMR are reported in terms of chemical shift

(δ, ppm). High-resolution mass spectrometry (HRMS) spectra were obtained on an Ultimate 3000 UHPLC-Thermo QE Focus MS instrument. IR spectra were obtained on a Bruker Mobile-IR instrument and the photoreactor is Penn PhD Photoreactor M2 from Merck.

2. Density Functional Theory (DFT) calculation

Density functional theory (DFT) is exploited to investigate the cyclization step of N-centred radical intermediates **1a-A** and **3a-A** electronically diverse substituents on olefins. It shows that *5-exo-trig* radical cyclization of **1a-A** with an activation free energy of only 9.6 kcal mol^{-1} via **1a-TS2**, which is much more favored than the *6-endo-trig* variant **1a-TS1** (activation free energy of 14.8 kcal mol^{-1}). Moreover, in order to reach the transition states **3a-TS1** and **3a-TS2**, the energy barriers that N-radical intermediate **3a-A** has to cross are 13.2 kcal mol^{-1} and 12.6 kcal mol^{-1}. More energy is reduced from the transition state, so generation for **3a-C** is easier than **3a-B**.



Complete reference for Gaussian 16

Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

Computational details

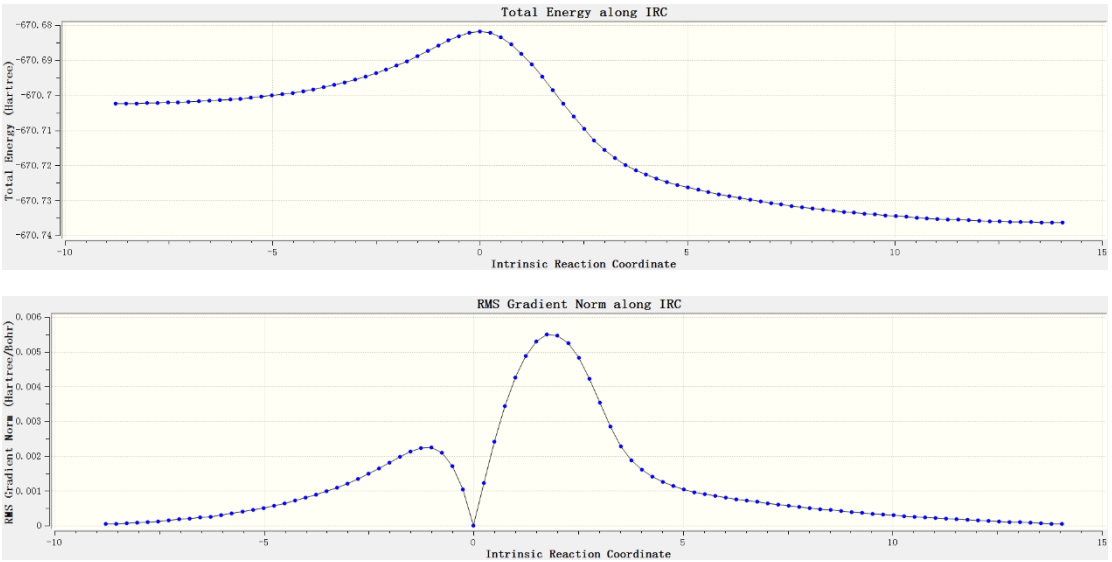
All calculations were carried out with the density functional theory (DFT) at the M06-2X level[1] of theory using Gaussian 16 series of programs. The 6-311G(d,p) basis set was used for all the atoms. The gas-phase geometries of all intermediates and transition states were fully optimized without any symmetry restriction, following harmonic frequency calculations to ensure that the local minima had zero imaginary frequencies and the transition state one and to derive the thermal corrections for Gibbs free energies. The transition states had been verified by intrinsic reaction coordinate (IRC) calculation and imaginary vibration modes, which linked reactants and products. Double hybrid functional (B2PLYP method)[2], which could give more accurate energetic information, was used to calculate single point energies with cc-pvqz basis set. Solvation free energies were differences between electronic energies in dichloroethane solvent with an SMD continuum solvation model[3] and electronic energies gas phase, which were calculated with M06-2X/6-31G(d) level of theory. Gibbs free energies of all stationary points in dichloroethane solvent were obtained by the thermal correction to Gibbs free energy in the gas phase, single-point energy in the gas phase and the solvation free energy.

Geometry	$E_{(gas\text{-}B2PLYP)}$[a]	$G_{(corr\text{-}M062X)}$ [b]	ΔG_{solv}[c]	IF[d]	ΔG[e] (kcal/mol)
1a-A	-670.573229	0.193922	-0.014129	-	0.0
1a-TS1	-670.551096	0.196323	-0.015013	-577.64	14.824996
1a-B	-670.600208	0.198993	-0.013905	-	-13.605879
1a-TS2	-670.557511	0.194427	-0.015074	-523.01	9.581941
1a-C	-670.582157	0.194848	-0.014832	-	-5.458968
3a-A	-631.275229	0.166799	-0.012982	-	0.0
3a-TS1	-631.254417	0.168022	-0.013946	-646.42	13.209669
3a-B	-631.280266	0.168708	-0.013406	-	-2.232887

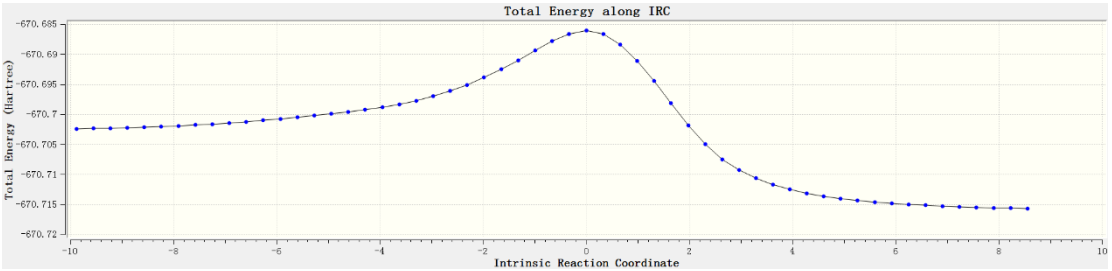
3a-TS2	-631.255171	0.168547	-0.014658	-604.45	12.624608
3a-C	-631.305326	0.170949	-0.015237	-	-17.686451

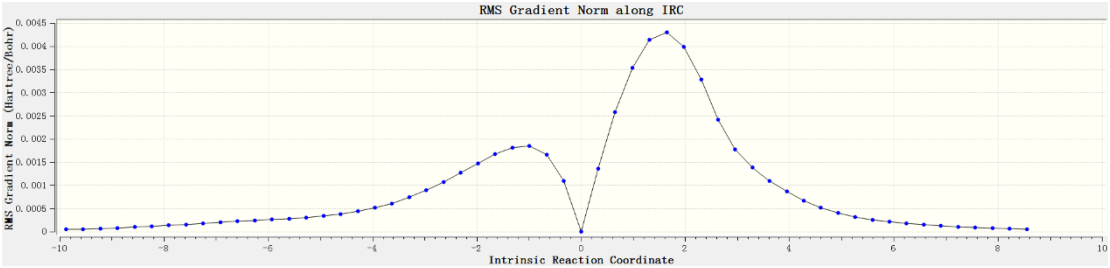
[a] The electronic energy calculated by B2PLYP in gas phase. [b] The thermal correction to Gibbs free energy calculated by M062X in gas phase. [c] ΔG_{solv} (solvation free energy) = G_{sol} (The electronic energy calculated by M062X in dichloroethane solvent with a SMD continuum solvation model) – G_{gas} (The electronic energy calculated by M062X in gas phase) + 1.89/627.15 [d] The M062X calculated imaginary frequencies for the transition states. [e] $\Delta G = [G_{(corr\text{-}M062X)} + E_{(gas\text{-}B2PLYP)} + \Delta G_{solv}]$ (Sum of electronic and thermal free energies in dichloroethane solvent for transition state) - $[G_{(corr\text{-}M062X)} + E_{(gas\text{-}B2PLYP)} + \Delta G_{solv}]$ (Sum of electronic and thermal free energies in dichloroethane solvent for reactant) or $\Delta G = [G_{(corr\text{-}M062X)} + E_{(gas\text{-}B2PLYP)} + \Delta G_{solv}]$ (Sum of electronic and thermal free energies in dichloroethane solvent for product) - $[G_{(corr\text{-}M062X)} + E_{(gas\text{-}B2PLYP)} + \Delta G_{solv}]$ (Sum of electronic and thermal free energies in dichloroethane solvent for reactant)

Plots of total energy and root-mean-squared (RMS) gradient norm along IRC for **1a-TS1**:

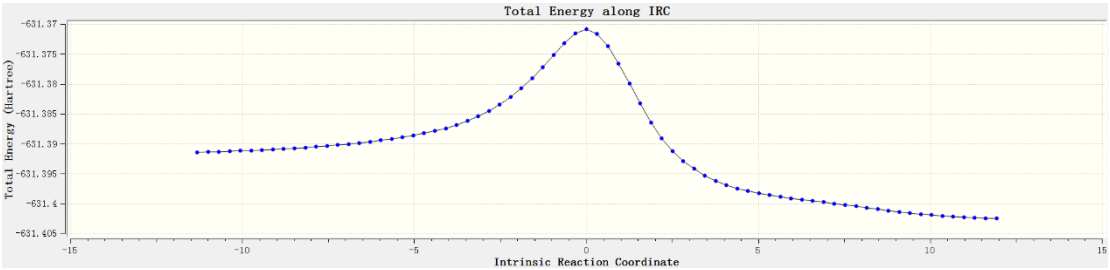


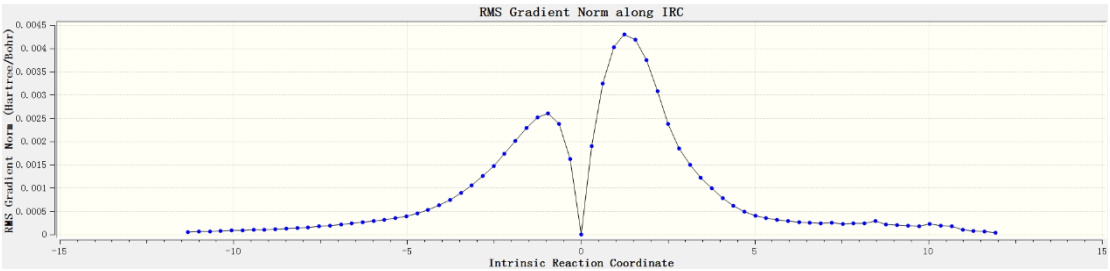
Plots of total energy and root-mean-squared (RMS) gradient norm along IRC for **1a-TS2**:



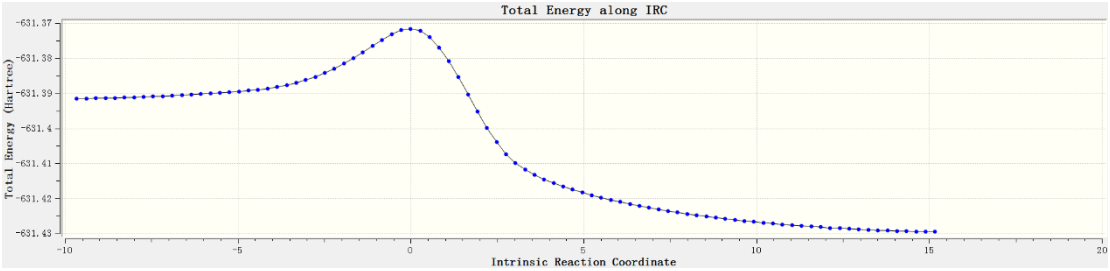


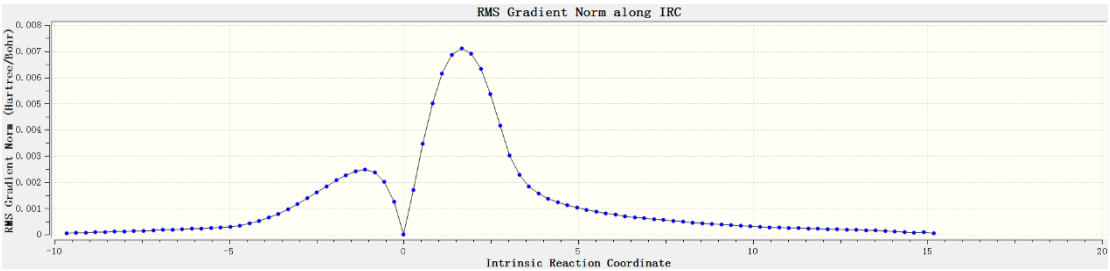
Plots of total energy and root-mean-squared (RMS) gradient norm along IRC for **3a-TS1**:





Plots of total energy and root-mean-squared (RMS) gradient norm along IRC for **3a-TS2**:





Optimized Geometries for All the Compounds and Transition State

1a-A

C	-2.41177600	1.25877200	-0.68782300
C	-3.57464600	0.52283800	-0.50898000
C	-3.51061100	-0.78104100	-0.02021600
C	-2.27494400	-1.34184700	0.26309400
C	-1.10039500	-0.61437100	0.05515900
C	-1.15433400	0.71806000	-0.38923000
H	-2.46833900	2.28175400	-1.04429500
H	-4.53452300	0.96918300	-0.74202800
H	-4.41670500	-1.35593200	0.12846700
H	-2.19955200	-2.35948800	0.62890400
C	0.18677600	-1.32248600	0.32292700
O	0.33999000	-2.10127100	1.23866900
N	1.16560400	-1.06554600	-0.65754800
O	2.34454000	-1.44881400	-0.20274800
C	3.35142000	-1.31002100	-1.21485000
H	3.40292600	-0.26806300	-1.53224300
H	4.28339600	-1.62022300	-0.74889300
H	3.10541700	-1.95519200	-2.05855100
C	1.00005700	1.78910600	0.37417500
C	0.03779000	1.58125000	-0.53579700
H	0.09256800	2.13300200	-1.47178700
C	1.03677000	1.17446800	1.74571300
H	1.31552300	1.93596300	2.47947600
H	0.08422400	0.73796600	2.04682200
H	1.80538600	0.39347300	1.79344800
C	2.16125400	2.69250300	0.06677600
H	2.18605700	3.53624700	0.76390500
H	3.10322200	2.14893900	0.19906700
H	2.12075800	3.07847400	-0.95250000

1a-TS1

C	-2.56389000	1.33423600	-0.50174400
C	-3.67618500	0.51248000	-0.40793100
C	-3.52756600	-0.83746500	-0.08516800
C	-2.25918800	-1.36194900	0.12353500
C	-1.13248200	-0.54841700	0.01990100
C	-1.27894300	0.82614200	-0.26083400
H	-2.67735400	2.38603900	-0.74050900
H	-4.66447700	0.92172900	-0.58252900
H	-4.39815600	-1.47794500	-0.01046300
H	-2.12228300	-2.41214300	0.35255200
C	0.21087000	-1.20081900	0.18660900
O	0.34563700	-2.23392300	0.81138700
N	1.23835400	-0.55999200	-0.50419900
O	2.44430600	-1.04249900	-0.09618500
C	3.36654300	-1.02789400	-1.18319700
H	3.41347700	-0.03714200	-1.63896600
H	4.33402700	-1.29336100	-0.75928000
H	3.06866500	-1.76494500	-1.93242100
C	1.05911500	1.38144300	0.36679700
C	-0.09474600	1.65748500	-0.35545600
H	-0.04896000	2.38366800	-1.16222100
C	1.04017000	0.92488700	1.80522700
H	1.80538900	0.16214300	1.97665100
H	1.29471200	1.78835100	2.42795200
H	0.07011000	0.54802700	2.12723300
C	2.34281000	2.04963900	-0.02889000
H	2.37828000	2.26651100	-1.09661000
H	2.44914600	2.98587100	0.52887600
H	3.19034900	1.41591200	0.24441200

1a-B

C	2.61827500	-1.33474200	-0.33024000
C	3.70939500	-0.49378600	-0.26614300
C	3.54176900	0.87821800	-0.02746100
C	2.26287300	1.39875400	0.13765500
C	1.15342700	0.56728900	0.07165800
C	1.30441300	-0.82663100	-0.15345500
H	2.74830100	-2.39648200	-0.50841700
H	4.70658900	-0.89745100	-0.39909200
H	4.40490800	1.53040300	0.02252700
H	2.10775600	2.45665700	0.31281400
C	-0.20003500	1.16707200	0.21517700
O	-0.37574600	2.35206200	0.43750500
N	-1.24201900	0.30330300	-0.01543200
O	2.49580000	0.81719500	0.26896200
C	-3.02173500	1.50738100	-0.86451700
H	-3.09375500	0.83793900	-1.72497600
H	-4.01609400	1.83880200	-0.56593700

H	-2.39996000	2.37131300	-1.10454100
C	-1.20520900	-1.16570500	0.11585900
C	0.17534400	-1.65595200	-0.18105700
H	0.28740900	-2.72351200	-0.33258300
C	-1.58673400	-1.55804500	1.55673800
H	-2.59215800	-1.19920300	1.78408300
H	-1.56694500	-2.64460800	1.66245500
H	-0.88104800	-1.12108500	2.26686800
C	-2.20238200	-1.77379600	-0.87621200
H	-1.94374700	-1.49335900	-1.89927400
H	-2.17564100	-2.86206300	-0.79252900
H	-3.21552500	-1.43487500	-0.65311200

1a-TS2

C	-2.11699000	1.39315300	-0.77258800
C	-3.39858700	0.90478800	-0.53248800
C	-3.59124200	-0.37451800	-0.00711800
C	-2.49780000	-1.18445500	0.27344000
C	-1.22179000	-0.69829200	0.01302400
C	-1.01802900	0.58841100	-0.48399700
H	-1.97293900	2.39515700	-1.16126200
H	-4.25760600	1.52955500	-0.74848100
H	-4.59603000	-0.73497600	0.17834300
H	-2.62229400	-2.18220600	0.67899000
C	0.03356600	-1.45515800	0.25461200
O	0.16662900	-2.39210400	1.01561900
N	1.01840500	-0.92767300	-0.57233100
O	2.26276400	-1.13540700	-0.06914100
C	3.21973900	-1.06961600	-1.12071200
H	3.17772200	-0.09475000	-1.61411500
H	4.19267400	-1.20782100	-0.65152600
H	3.03425200	-1.86189200	-1.84921900
C	1.13573700	1.55660200	0.40501500
C	0.40161700	1.02075900	-0.63759000
H	0.72294600	1.26365500	-1.64698300
C	0.75200200	1.35664600	1.83518300
H	1.07437100	2.20378100	2.44544400
H	-0.31906800	1.20575000	1.97329100
H	1.27276200	0.46833500	2.22226600
C	2.49527800	2.12011900	0.15395000
H	2.62067300	3.07767300	0.66922900
H	3.25463900	1.43998400	0.56370800
H	2.69292400	2.26091800	-0.90959300

1a-C

C	-1.94973300	1.43754700	-0.71460400
C	-3.27350600	1.07013000	-0.47863200
C	-3.59833800	-0.20035100	0.00626300
C	-2.60055800	-1.13361200	0.26846300
C	-1.28651100	-0.75831300	0.02832100
C	-0.95832800	0.50387200	-0.45280000
H	-1.70277400	2.42748600	-1.08230200
H	-4.06692000	1.78318800	-0.67065300
H	-4.63674000	-0.45543800	0.18118800
H	-2.83224400	-2.12167400	0.64981200
C	-0.03940100	-1.53899100	0.25390300
O	0.09855500	-2.63246200	0.75697500
N	0.95327400	-0.73886800	-0.25772100
O	2.25632800	-0.96513800	0.09987200
C	3.00355400	-1.44555100	-1.01936600
H	2.99988900	-0.71141000	-1.82968700
H	4.01994600	-1.58685000	-0.65396300
H	2.59555900	-2.39606700	-1.36901200
C	1.17711300	1.64809000	0.32192300
C	0.54199300	0.64297500	-0.59425500
H	0.81353300	0.85676300	-1.63290500
C	0.95977600	1.47774500	1.78852300
H	1.19097200	2.39829800	2.33002800
H	-0.06712500	1.18563500	2.02406700
H	1.62247200	0.69252100	2.18382400
C	2.40978200	2.34773400	-0.14225400
H	2.56575600	3.28220800	0.40390300
H	3.29796800	1.72067700	0.03370500
H	2.37267100	2.56989600	-1.21163700

3a-A

C	-2.40046300	0.99154400	-0.16442700
C	-3.37002200	0.02486300	-0.39961400
C	-3.03246100	-1.32655000	-0.38057300
C	-1.71845900	-1.69965900	-0.14010600
C	-0.73633200	-0.73018200	0.07247200
C	-1.07420500	0.63176400	0.09325900

H	-2.67805600	2.03974400	-0.14761800
H	-4.39434300	0.32588200	-0.58640600
H	-3.78852900	-2.08211600	-0.55686100
H	-1.43206700	-2.74508500	-0.13292400
C	0.66753100	-1.20999100	0.25372300
O	0.95615500	-2.21439100	0.86482700
N	1.59673700	-0.42281300	-0.45901800
O	2.81877100	-0.76955200	-0.10667100
C	3.79434500	-0.02296600	-0.84674900
H	3.67598500	1.03864600	-0.62599600
H	4.76195900	-0.38296600	-0.50623800
H	3.66182200	-0.21077700	-1.91237600
C	0.56217600	1.63653500	1.61627100
H	1.28637600	2.39788000	1.88737400
C	-0.07977300	1.68520800	0.44845000
H	0.37844900	0.84145300	2.33210100
C	0.14607800	2.76828400	-0.56794300
H	0.52216600	2.32908900	-1.49704400
H	-0.78753400	3.28406500	-0.80952900
H	0.86671400	3.50231700	-0.20519000

3a-TS1

C	-2.06846100	1.38424100	0.00448500
C	-3.28399600	0.71884500	-0.12238900
C	-3.33575900	-0.67559600	-0.18921200
C	-2.16417900	-1.41852200	-0.13811300
C	-0.95125200	-0.74689000	-0.02521300
C	-0.89193900	0.64114400	0.06890800
H	-2.03814200	2.46592100	0.07530000
H	-4.20384100	1.29083400	-0.16126600
H	-4.29230800	-1.17528800	-0.28434100
H	-2.17673300	-2.50109400	-0.19433300
C	0.37299800	-1.41094100	0.00916500
O	0.58453200	-2.58032900	0.24634400
N	1.33649900	-0.46428300	-0.34190400
O	2.55244400	-0.79758700	0.14838500
C	3.56945600	-0.04551800	-0.50275500
H	3.52683100	1.00116500	-0.19004500
H	4.51420200	-0.48440400	-0.18606200
H	3.45958500	-0.11852500	-1.58671300
C	0.94963300	1.35236200	1.55757300
H	1.83719700	1.93833100	1.76717300
C	0.46627300	1.24611300	0.26507800
H	0.50837800	0.78109700	2.36575400
C	0.90475800	2.22719300	-0.79336200
H	0.91532500	1.75179200	-1.77518900
H	0.19778600	3.06166100	-0.82634600
H	1.89523400	2.62723000	-0.57342400

3a-B

C	-2.09460900	1.28248700	-0.09699000
C	-3.28092600	0.55624300	-0.18942700
C	-3.27903600	-0.84169700	-0.17496900
C	-2.08401000	-1.54675300	-0.06971800
C	-0.90857700	-0.81518700	0.01747100
C	-0.90619100	0.57495200	0.00715400
H	-2.10389600	2.36706900	-0.09941200
H	-4.22373500	1.08462000	-0.27150700
H	-4.21798600	-1.37747600	-0.24657300
H	-2.06298000	-2.63064200	-0.05726200
C	0.49042200	-1.30471700	0.14661200
O	0.90130800	-2.43904600	0.26955600
N	1.24979900	-0.16714300	0.06446000
O	2.57140100	-0.18319100	0.42621000
C	3.39173800	-0.51690300	-0.69835000
H	3.25511000	0.20866600	-1.50330300
H	4.41665600	-0.48012500	-0.33110100
H	3.15829400	-1.52363700	-1.04951500
C	0.71311600	1.74741300	1.48001400
H	0.76507500	2.82455400	1.56459200
C	0.51333100	1.10774200	0.14354600
H	0.65209400	1.13832800	2.37307600
C	0.91155500	2.04167600	-0.99636700
H	0.75995200	1.55239800	-1.95988000
H	0.30766800	2.95079600	-0.95758600
H	1.96259600	2.32180800	-0.89274000

3a-TS2

C	-2.47880300	0.97754600	-0.00204300
C	-3.43972800	-0.00477800	-0.19052300
C	-3.06704300	-1.34682200	-0.25024200
C	-1.72883300	-1.69542500	-0.13363000

C	-0.75070100	-0.71814400	0.04995800
C	-1.12723300	0.63950400	0.14833400
H	-2.77583400	2.01822800	0.05851800
H	-4.48264100	0.27392400	-0.28692000
H	-3.81639600	-2.11528900	-0.39730700
H	-1.41890900	-2.73135500	-0.19921600
C	0.67557200	-1.20487800	0.09685900
O	0.94290000	-2.35698200	0.36438400
N	1.62805100	-0.25474100	-0.28501800
O	2.86586100	-0.67088500	0.08728900
C	3.84942500	0.05266700	-0.64267400
H	3.77066700	1.12295100	-0.43314700
H	4.81226300	-0.32251400	-0.30001200
H	3.73220800	-0.12470800	-1.71378300
C	1.03997500	1.27004800	1.02369300
H	1.90134600	1.92970900	1.05310600
C	-0.09420000	1.65646800	0.35247100
H	0.99243400	0.52197800	1.80780900
C	-0.19407400	2.96177800	-0.37314300
H	-0.36580500	2.80242800	-1.44247200
H	-1.03619300	3.55305800	0.00107800
H	0.71427300	3.54992700	-0.24027000

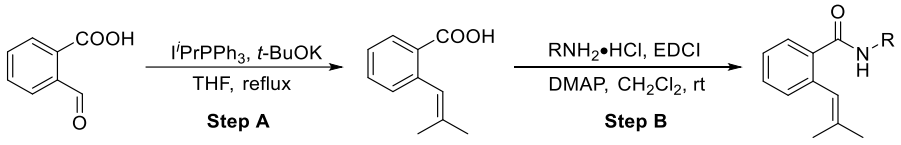
3a-C

C	2.56116800	0.69541200	0.15403800
C	3.38386900	-0.41249300	0.20155700
C	2.85277900	-1.70482100	0.10879000
C	1.47883800	-1.87029400	-0.02952500
C	0.63548200	-0.76934700	-0.07706400
C	1.15522700	0.55273500	0.00972600
H	2.99034200	1.68754800	0.22463300
H	4.45403400	-0.27760800	0.31088800
H	3.50549100	-2.56818100	0.14537400
H	1.03897000	-2.85787200	-0.10106300
C	-0.82607700	-1.01826100	-0.21723700
O	-1.30492100	-2.13554600	-0.31939700
N	-1.59790900	0.10206000	-0.16466600
O	-2.94424500	-0.05112100	-0.41545000
C	-3.63708000	-0.38417600	0.78948600
H	-3.47945600	0.38650400	1.54862500
H	-4.69141600	-0.42648500	0.51852200
H	-3.30747200	-1.35711600	1.15757500
C	-1.17250500	1.48564700	-0.24164900
H	-1.72020000	2.05614900	0.52018200
C	0.29416100	1.66709600	-0.05447600
H	-1.47733000	1.89540000	-1.21725200
C	0.78975500	3.07517100	0.00174000
H	1.31133300	3.27664800	0.94356500
H	1.49727400	3.28161200	-0.80833800
H	-0.03658100	3.78229200	-0.08357500

3. Synthesis and Characterization of Substrates

3.1 General Procedure for preparation of substrates

General synthesis of substrates **1a-1g** (Method A):

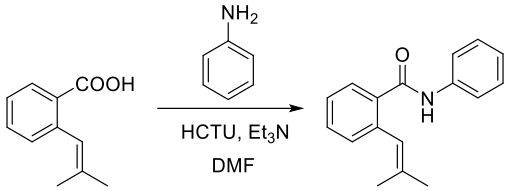


Step A. A solution of isopropyltriphenylphosphinium iodide (32 mmol, 2.0 equiv) and potassium tert-butoxide (48 mmol, 3.0 equiv) in THF(120 mL) was stirred at room temperature for 1.5 h. 2-formylbenzoic acid (16mmol, 1.0 equiv) was added and the solution was refluxed overnight. Until the reaction was completed, as monitored by TLC, the resulting mixture was quenched with water, basified with aqueous NaOH (3.0 M) and washed with diethyl ether. The resulting aqueous phase was acidified with aqueous HCl (3.0 M) until pH 1-2 and extracted twice with ethyl acetate. The combined organic layers were washed with water, brine, dried over with Na_2SO_4, filtered and concentrated in vacuo. The

resulting crude product was purified by flash column chromatography to afford the desired unsaturated benzoic acid derivatives.[4]

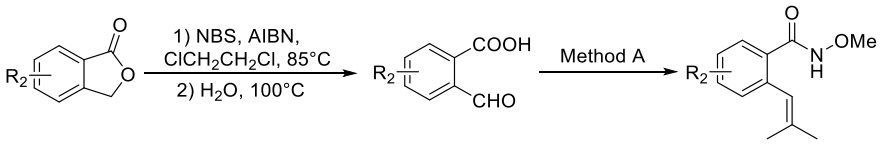
Step B. To a solution of 2-(2-methylprop-1-en-1-yl)benzoic acid (13 mmol, 1 equiv) in CH_2Cl_2 (90 mL) was added RNH_2·HCl (1.5 equiv), EDCI (2.0 equiv.) and DMAP (2 equiv) successively. The resulting mixture was stirred at room temperature overnight. The reaction was quenched by adding HCl (3 M). The organic layer was separated and the aqueous layer was extracted with CH_2Cl_2. The combined extracts were washed with brine, dried over Na_2SO_4, and filtrated. The filtrate was concentrated and purified by column chromatography on silica gel to yield the product.[5]

Synthesis of substrates **1h** (Method B)[6]:



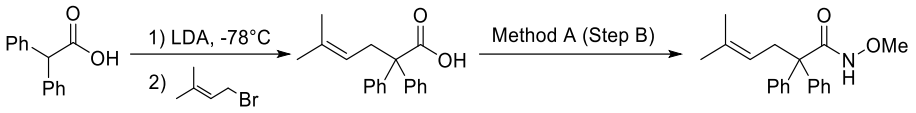
To a solution of 2-(2-methylprop-1-en-1-yl)benzoic acid (648 mg, 4.0mmol, 1 equiv), O-(6-Chloro-1-hydrocibenzotriazol-1-yl)-1,1,3,3-tetramethyluronium (HCTU, 1.82 g, 4.4 mmol, 1.1 equiv) in DMF (8 mL) was added Et_3N (609 μL, 4.4 mmol, 1.1 equiv). The reaction mixture was stirred at room temperature for 10 minutes. Then aniline (401 μL, 4.4 mmol, 1.1 equiv) was added. The reaction mixture was stirred at room temperature for 4 h and then was diluted with DCM (30 mL) and water (30 mL). The organic layer was separated and the aqueous layer was extracted with DCM (20 mL×3). The combined organic layers were dried over Na_2SO_4, filtered, and concentrated in vacuo. The residue was purified by column chromatography on silica gel using Petroleum/EtOAc as the eluent to yield the compound 1h (872 mg, 91.8%) as a white solid.

General synthesis of substrates **1i-1m** (Method C)[7]:



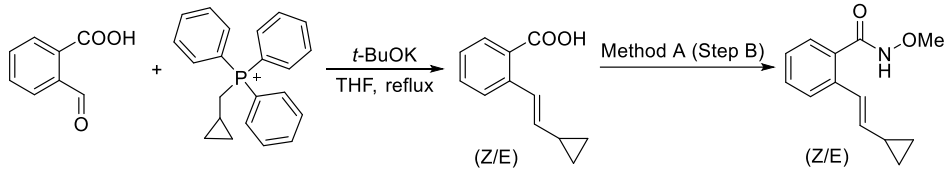
To a solution of phthalides (12 mmol，1 equiv) in 60 mL 1,2-dichloroethane was added NBS (13.2 mmol，1.1equiv) and AIBN (0.6 mmol, 0.05 equiv) was added at room temperature. Then the mixture was refluxed at 85 ºC overnight. It was cooled to room temperature and purified by flash chromatography (silica gel, petroleum ether and ethyl acetate as eluent). The product was then suspended in 100 mL of H_2O and heated to 100 ºC. After 1 h, the mixture was cooled to room temperature and then extracted with EtOAc (3×30 mL). The combined extracts were dried overNa_2SO_4, filtered and concentrated under reduced pressure to give a corresponding 2-formylbenzoic acid as a solid. From the benzoic acid derivative, the corresponding benzamide derivate was synthesized by the same method A.

Synthesis of substrates **1n** (Method D)[8]:



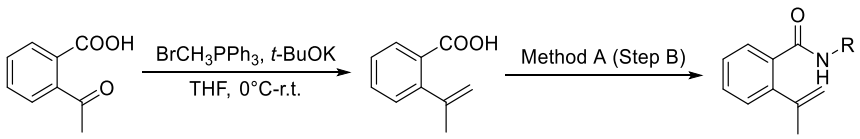
Under N_2 protection, the solution of LDA (5.25 mL, 2.1 equiv) was carefully injected into a 100 mL flask and cooled to -78℃. A solution of diphenylacetic acid (1.06 g, 1 equiv) in THF was added dropwise. The reaction turned cloudy and bright yellow. The reaction was allowed to stir for 1 hour at -78 ℃ before prenyl bromide (0.85 mL, 1.5 equiv) was added dropwise to the enolate solution. Upon completion of the addition, the reaction was warmed to ambient temperature and stirred for an additional 3 hours. The reaction was then quenched with saturated ammonium chloride (30 mL), and diluted with ether(20 mL). The organics were separated, and the aqueous was extracted with 3×40 mL portions of diethyl ether. The combined organics were washed with 1M HCl (30 mL), water (30 mL), and brine (30 mL), then dried over Na_2SO_4, filtered, and concentrated to give a viscous oil. The material was recrystallized from EtOAc/Hexanes to give 903 mg of fine white crystals (65 %). From the carboxylic acid derivative, the next product was synthesized by the same method A (step B).

Synthesis of substrates **1p** (Method E):



A solution of (Cyclopropylmethyl)triphenylphosphonium bromide (3 mmol, 2.0 equiv) and potassium tert-butoxide (4.5 mmol, 3.0 equiv) in THF(20 mL) was stirred at room temperature for 1.5 h. 2-formylbenzoic acid (1.5 mmol, 1.0 equiv) was added and the solution was refluxed overnight. Until the reaction was completed, as monitored by TLC, the resulting mixture was quenched with water, basified with aqueous NaOH (3.0 M) and washed with diethyl ether. The resulting aqueous phase was acidified with aqueous HCl (3.0 M) until pH 1-2 and extracted twice with ethyl acetate. The combined organic layers were washed with water, brine, dried over with Na_2SO_4, filtered and concentrated in vacuo. The resulting crude product was purified by flash column chromatography to afford the desired unsaturated benzoic acid derivatives. From benzoic acid derivative, the corresponding benzamide derivate was synthesized by the same method A (step B).

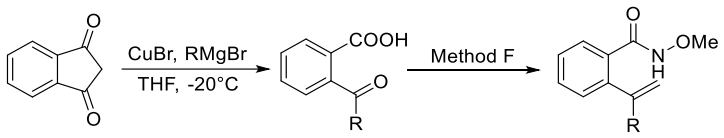
General synthesis of substrates **3a-3e** (Method F)[9]:



To a stirred suspension of methyltriphenylphosphonium bromide (18 mmol, 3.0 equiv) in THF, potassium tert-butoxide (18 mmol, 3.0 equiv) was added at 0 °C and stirred for 0.5 hour under Ar. A solution of 2-ketobenzoic acid (6 mmol, 1.0 equiv) in THF was added dropwise. Until the reaction was completed, as monitored by TLC, the resulting mixture was quenched with water, basified with aqueous

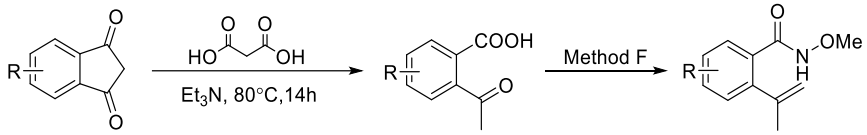
NaOH (3.0 M) and washed with diethyl ether. The resulting aqueous phase was acidified with aqueous HCl (3.0 M) until pH 1-2 and extracted twice with ethyl acetate. The combined organic layers were washed with water, brine, dried over with Na_2SO_4, filtered and concentrated in vacuo. The resulting crude product was purified by flash column chromatography to afford the desired unsaturated benzoic acid derivatives. From the benzoic acid derivative, the corresponding benzamide derivate was synthesized by the same method A (Step B).

General synthesis of substrates **3f-3n** (Method G)[10]:



Phthalicacidanhydrid (6.7 g, 45.0 mmol, 1.0 equiv), copper bromide (0.46 g, 3.2 mmol) and anhydrous THF (60 mL) were added to a flame-dried flask and cooled to - 20 °C under N_2 atmosphere. RMgBr (50 mmol, in 40 mL THF, prepared from alkylbromides and magnesium powder) was added dropwise to the mixture over 1 h. The reaction mixture was stirred overnight at -20 °C, then allowed to warm to room temperature, quenched with water, basified with aqueous NaOH (3.0 M) until pH 12- 14 and washed with diethyl ether. The resulting aqueous phase was acidified with aqueous HCl (2.0 M) until pH 1-2 and extracted twice with ethyl acetate. The combined organic layers were washed with water, brine, dried over Na_2SO_4, filtered and concentrated in vacuo. The crude product was dissolved in DCM and the solid was filtered off. The crude benzoic acid derivative was used for the next step without further purification. From the benzoic acid derivative, the corresponding benzamide derivate was synthesized by the same method F**.**

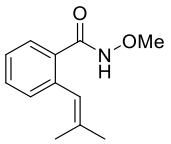
General synthesis of substrates **3o-3u** (Method H)[11]:



A stirred mixture of phthalicanhydrides and triethylamine (1.5 equiv) were heated to 80 °C. Ten equal portions of malonic acid (10 × 0.12 equiv; 1.2 equiv total) were charged for 4 h, and the reaction mixture was maintained at 80°C for a further 10 h. Hydrochloric acid was charged and the reaction stirred for a further 30 min at 80 °C before being cooled to 25 °C, and the resulting slurry was filtered. The damp cake was washed with water and then dried under vacuum at 50 °C to give the title compound light-brown crystals. From the benzoic acid derivative, the corresponding benzamide derivate was synthesized by the same method F.

3.2 Characterizations of substrates

N-methoxy-2-(2-methylprop-1-en-1-yl)benzamide, 1a



Colorless oil (2.59 g), yield: 96.9%

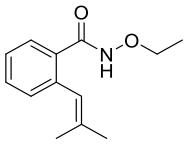
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.80 (s, 1H), 7.70 – 7.57 (m, 1H), 7.41 (td, *J* = 7.5, 1.5 Hz, 1H), 7.31 – 7.24 (m, 1H), 7.20 (d, *J* = 7.7 Hz, 1H), 6.40 (s, 1H), 3.84 (s, 3H), 1.93 (d, *J* = 1.4 Hz, 3H), 1.74 (d, *J* = 1.3 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 167.31 , 138.59 , 136.35 , 131.79 , 130.57 , 130.38 , 128.72 , 126.69 , 122.95 , 64.58 , 26.24 , 19.46 .

IR(neat)**:** ν_{max} 3179, 2970, 2933, 1653, 1596, 1440, 1303, 1159, 1034, 891, 747, 677 cm^{-1}

HRMS (ESI) m/z calcd for $C_{12}H_{16}NO_2$ $[M+H]^+$: 206.1181, found: 206.1171

N-ethoxy-2-(2-methylprop-1-en-1-yl)benzamide, 1b



Colorless oil (482 mg), yield: 73.3%

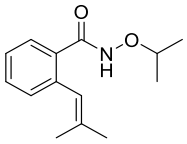
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.68 (s, 1H), 7.70 – 7.55 (m, 1H), 7.40 (td, *J* = 7.6, 1.5 Hz, 1H), 7.32 – 7.23 (m, 1H), 7.20 (d, *J* = 7.7 Hz, 1H), 6.41 (s, 1H), 4.06 (q, *J* = 7.1 Hz, 2H), 1.93 (d, *J* = 1.5 Hz, 3H), 1.75 (d, *J* = 1.3 Hz, 3H), 1.32 (t, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 167.29 , 138.35 , 136.35 , 132.06 , 130.43 , 130.34 , 128.67 , 126.63 , 123.04 , 72.33 , 26.23 , 19.43 , 13.49 .

IR(neat)**:** ν_{max} 3178, 2977, 2932, 2910, 1650, 1502, 1442, 1381, 1304, 1158, 1034, 904, 746, 668 cm^{-1}

HRMS (ESI) m/z calcd for $C_{13}H_{17}NO_2$ $[M+H]^+$: 220.1338 , found: 220.1327

N-isopropoxy-2-(2-methylprop-1-en-1-yl)benzamide, 1c



White solid (495 mg), yield: 84.8%

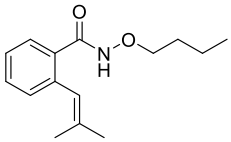
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.49 (s, 1H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.40 (td, *J* = 7.5, 1.5 Hz, 1H), 7.27 (td, *J* = 7.8, 7.4, 1.3 Hz, 1H), 7.20 (d, *J* = 7.6 Hz, 1H), 6.43 (s, 1H), 4.39 – 4.10 (m, 1H), 1.93 (d, *J* = 1.5 Hz, 3H), 1.75 (d, *J* = 1.3 Hz, 3H), 1.31 (d, *J* = 6.2 Hz, 6H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 167.38 , 138.21 , 136.35 , 132.27 , 130.37 , 128.67 , 126.65 , 123.22 , 26.25 , 20.52 , 19.43 .

IR(neat)**:** ν_{max} 3179, 2973, 2931, 1647, 1596, 1503, 1443, 1374, 1303, 1146, 1115, 1021, 915, 745, 679, 635 cm^{-1}

HRMS (ESI) m/z calcd for $C_{14}H_{20}NO_2$ $[M+H]^+$: 234.1494 , found: 234.1484

N-butoxy-2-(2-methylprop-1-en-1-yl)benzamide, 1d



Colorless oil (449 mg), yield: 90.7%

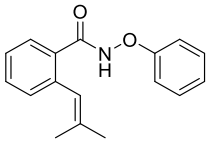
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.55 (s, 1H), 7.67 (d, *J* = 7.7 Hz, 1H), 7.39 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.34 – 7.23 (m, 1H), 7.20 (d, *J* = 7.6 Hz, 1H), 6.42 (s, 1H), 4.00 (d, *J* = 6.8 Hz, 2H), 1.93 (d, *J* = 1.4 Hz, 3H), 1.75 (d, *J* = 1.3 Hz, 3H), 1.70 (t, *J* = 7.5 Hz, 2H), 1.44 (d, *J* = 7.6 Hz, 2H), 0.94 (d, *J* = 7.4 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 167.14 , 138.27 , 136.35 , 132.08 , 130.40 , 130.33 , 128.67 , 126.61 , 123.10 , 30.02 , 26.22 , 19.43 , 19.04 , 13.89 .

IR(neat)**:** ν_{max} 3181, 2959, 2933, 2872, 1646, 1596, 1506, 1466, 1376, 1304, 1159, 1060, 1028, 899, 677, 634, 512 cm^{-1}

HRMS (ESI) m/z calcd for $C_{15}H_{22}NO_2$ $[M+H]^+$: 248.1651, found: 248.1639

2-(2-methylprop-1-en-1-yl)-N-phenoxybenzamide, 1e



Light yellow oil (235 mg), yield: 44%

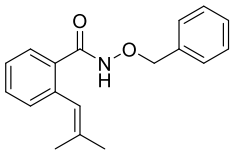
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.97 (s, 1H), 7.77 (d, *J* = 7.7 Hz, 1H), 7.46 (td, *J* = 7.6, 1.5 Hz, 1H), 7.32 (ddd, *J* = 8.9, 7.1, 2.1 Hz, 3H), 7.24 (d, *J* = 8.3 Hz, 1H), 7.18 – 7.01 (m, 3H), 6.52 (s, 1H), 1.97 (d, *J* = 1.4 Hz, 3H), 1.77 (d, *J* = 1.3 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 159.54 , 139.36 , 136.61 , 131.29 , 131.03 , 130.57 , 129.50 , 129.04 , 126.90 , 123.08 , 123.04 , 113.29 , 26.23 , 19.48 .

IR(neat)**:** ν_{max} 3141, 2967, 2930, 1654, 1590, 1487, 1444, 1376, 1299, 1198, 1026, 903, 746, 686 cm^{-1}

HRMS (ESI) m/z calcd for $C_{17}H_{18}NO_2$ $[M+H]^+$: 268.1338, found: 268.1324

N-(benzyloxy)-2-(2-methylprop-1-en-1-yl)benzamide, 1f



White solid (536 mg), yield: 95.2%

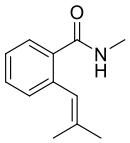
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.59 (s, 1H), 7.69 (d, *J* = 7.7 Hz, 1H), 7.50 – 7.31 (m, 6H), 7.30 – 7.22 (m, 1H), 7.14 (d, *J* = 7.6 Hz, 1H), 6.26 (s, 1H), 5.02 (s, 2H), 1.77 (d, *J* = 1.4 Hz, 3H), 1.63 (d, *J* = 1.3 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 166.79 , 138.72 , 136.42 , 135.50 , 130.63 , 130.49 , 129.22 , 128.88 , 128.80 , 128.70 , 126.71 , 123.11 , 78.14 , 26.02 , 19.34 .

IR(neat)**:** ν_{max} 3181, 2971, 2911, 1646, 1496, 1443, 1375, 1301, 1210, 1158, 1019, 906, 831,739, 696, 678, 614 cm^{-1}

HRMS (ESI) m/z calcd for $C_{18}H_{20}NO_2$ $[M+H]^+$: 282.1494, found: 282.1483

N-methyl-2-(2-methylprop-1-en-1-yl)benzamide, 1g



White solid (412 mg), yield: 83.7%

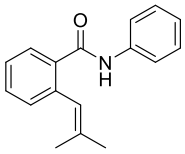
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.71 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.37 (td, *J* = 7.5, 1.5 Hz, 1H), 7.27 (td, *J* = 7.6, 1.4 Hz, 1H), 7.22 – 7.16 (m, 1H), 6.40 (s, 1H), 6.12 (s, 1H), 2.97 (d, *J* = 4.9 Hz, 3H), 1.93 (d, *J* = 1.4 Hz, 3H), 1.76 (d, *J* = 1.3 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 169.58 , 137.67 , 135.88 , 134.90 , 130.44 , 129.84 , 128.53 , 126.60 , 123.48 , 26.75 , 26.26 , 19.44 .

IR(neat)**:** ν_{max} 3232, 2980, 2935, 2853, 1630, 1571, 1547, 1442, 1316, 1151, 1040, 1004, 840, 740, 670, 635, 564, 517 cm^{-1}

HRMS (ESI) m/z calcd for $C_{12}H_{16}NO$ $[M+H]^+$: 190.1232, found: 190.1220

2-(2-methylprop-1-en-1-yl)-N-phenylbenzamide, 1h



White solid (403 mg), yield: 45.8%

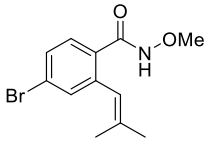
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.10 (s, 1H), 7.88 (d, *J* = 7.9 Hz, 1H), 7.58 (d, *J* = 7.1 Hz, 2H), 7.44 (t, *J* = 6.8 Hz, 1H), 7.34 (q, *J* = 6.9, 6.3 Hz, 3H), 7.23 (d, *J* = 7.6 Hz, 1H), 7.13 (t, *J* = 7.4 Hz, 1H), 6.51 (s, 1H), 1.98 (d, *J* = 1.4 Hz, 3H), 1.79 (d, *J* = 1.4 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 166.62 , 138.94 , 138.10 , 135.91 , 134.55 , 130.66 , 130.54 , 129.24 , 129.12 , 127.01 , 124.35 , 123.56 , 119.68 , 26.20 , 19.50 .

IR(neat)**:** ν_{max} 3282, 3059, 2909, 1650, 1619, 1597, 1568, 1527, 1498, 1436, 1318, 1251, 1053, 907, 830, 751, 690, 589, 509 cm^{-1}

HRMS (ESI) m/z calcd for $C_{17}H_{18}NO$ $[M+H]^+$: 252.1388, found: 252.1380

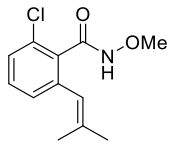
4-bromo-N-methoxy-2-(2-methylprop-1-en-1-yl)benzamide, 1i



Light green solid (630 mg), yield: 71.7%

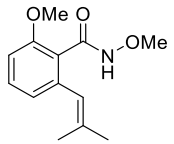
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.84 (s, 1H), 7.50 (d, *J* = 8.3 Hz, 1H), 7.40 (dd, *J* = 8.3, 2.0 Hz, 1H), 7.35 (d, *J* = 1.9 Hz, 1H), 6.32 (s, 1H), 3.83 (s, 3H), 1.93 (d, *J* = 1.4 Hz, 3H), 1.75 (d, *J* = 1.3 Hz, 3H).
^{13}C NMR (75 MHz, Chloroform-*d*) δ 166.27 , 139.95 , 138.32 , 133.12 , 130.64 , 130.30 , 129.74 , 124.97 , 121.81 , 64.56 , 26.22 , 19.50 .
IR(neat)**:** ν_{max} 3153, 2973, 2933, 1651, 1463, 1439, 1080, 1036, 900, 824, 730, 645 cm^{-1}
HRMS (ESI) m/z calcd for $C_{12}H_{15}BrNO_2$ $[M+H]^+$: 284.0286, found: 284.0276

2-chloro-N-methoxy-6-(2-methylprop-1-en-1-yl)benzamide, 1j



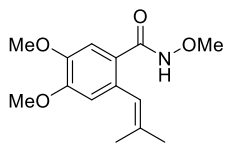
White solid (509 mg), yield: 26.5%
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.34 (s, 1H), 7.36 – 7.20 (m, 2H), 7.20 – 7.09 (m, 1H), 6.31 – 6.17 (m, 1H), 3.90 (s, 3H), 1.88 (d, *J* = 1.4 Hz, 3H), 1.76 (d, *J* = 1.4 Hz, 3H).
^{13}C NMR (75 MHz, Chloroform-*d*) δ 164.46 , 139.46 , 138.97 , 132.18 , 131.67 , 130.35 , 128.12 , 127.16 , 120.86 , 64.51 , 26.41 , 19.62 .
IR(neat)**:** ν_{max} 3154, 2975, 2935, 1652, 1447, 1295, 1196, 1132, 1033, 884, 781, 717, 671 cm^{-1}
HRMS (ESI) m/z calcd for $C_{12}H_{15}ClNO_2$ $[M+H]^+$: 240.0791, found: 240.0782

N,2-dimethoxy-6-(2-methylprop-1-en-1-yl)benzamide, 1k



White solid (543 mg), yield: 51.3%
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.37 (s, 1H), 7.30 (t, *J* = 8.0 Hz, 1H), 6.85 (d, *J* = 7.7 Hz, 1H), 6.77 (d, *J* = 8.3 Hz, 1H), 6.27 (s, 1H), 3.83 (d, *J* = 11.0 Hz, 6H), 1.86 (d, *J* = 1.4 Hz, 3H), 1.76 (d, *J* = 1.3 Hz, 3H).
^{13}C NMR (75 MHz, Chloroform-*d*) δ 165.80 , 156.69 , 138.79 , 137.87 , 130.36 , 122.23 , 122.05 , 121.68 , 108.75 , 64.37 , 55.82 , 26.41 , 19.63 .
IR(neat)**:** ν_{max} 3191, 2970, 2935, 1653, 1573, 1467, 1435, 1271, 1090, 1047, 883, 759, 729, 678, 613 cm^{-1}
HRMS (ESI) m/z calcd for $C_{13}H_{18}NO_3$ $[M+H]^+$: 236.1287 , found: 236.1277

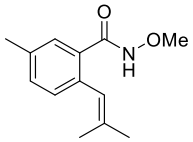
N,4,5-trimethoxy-2-(2-methylprop-1-en-1-yl)benzamide, 1l



Light green oil (545 mg), yield: 96%

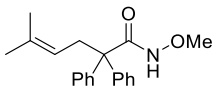
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.86 (s, 1H), 7.38 (s, 1H), 6.61 (s, 1H), 6.38 (p, *J* = 1.5 Hz, 1H), 3.92 (s, 3H), 3.89 (s, 3H), 3.85 (s, 3H), 1.95 (d, *J* = 1.5 Hz, 3H), 1.73 (d, *J* = 1.3 Hz, 3H).
^{13}C NMR (75 MHz, Chloroform-*d*) δ 166.92 , 150.60 , 147.73 , 138.95 , 129.59 , 123.65 , 123.44 , 112.78 , 111.89 , 64.60 , 56.05 , 55.98 , 25.93 , 19.47 .
IR(neat)**:** ν_{max} 3176, 2935, 1646, 1601, 1568, 1508, 1463, 1333, 1262, 1216, 1175, 1104, 1032, 992, 875, 804, 729, 607 cm^{-1}
HRMS (ESI) m/z calcd for $C_{14}H_{20}NO_4$ $[M+H]^+$: 266.1392, found: 266.1382

N-methoxy-5-methyl-2-(2-methylprop-1-en-1-yl)benzamide, 1m



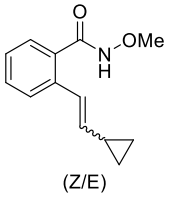
Colorless oil (533 mg), yield: 68.7%
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.75 (s, 1H), 7.49 (s, 1H), 7.22 (dd, *J* = 7.8, 1.9 Hz, 1H), 7.08 (d, *J* = 7.9 Hz, 1H), 6.36 (s, 1H), 3.84 (s, 3H), 2.35 (s, 3H), 1.92 (d, *J* = 1.5 Hz, 3H), 1.73 (d, *J* = 1.4 Hz, 3H).
^{13}C NMR (75 MHz, Chloroform-*d*) δ 167.47 , 138.21 , 136.55 , 133.35 , 131.54 , 131.36 , 130.31 , 129.27 , 122.88 , 64.54 , 26.17 , 20.93 , 19.40 .
IR(neat)**:** ν_{max} 3189, 2970, 2931, 1651, 1491, 1439, 1377, 1305, 1149, 1108, 1039, 946, 858, 677, 563 cm^{-1}
HRMS (ESI) m/z calcd for $C_{13}H_{18}NO_2$ $[M+H]^+$: 220.1338, found: 220.1327

N-methoxy-5-methyl-2,2-diphenylhex-4-enamide, 1n[12]



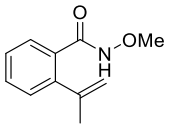
White solid (733 mg), yield: 79.1%
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.18 (s, 1H), 7.36 – 7.21 (m, 10H), 5.12 (tp, *J* = 7.0, 1.4 Hz, 1H), 3.71 (s, 3H), 3.13 (dt, *J* = 6.9, 1.2 Hz, 2H), 1.60 (d, *J* = 1.5 Hz, 3H), 1.40 (d, *J* = 1.4 Hz, 3H).
^{13}C NMR (75 MHz, Chloroform-*d*) δ 172.28 , 142.28 , 134.98 , 128.86 , 128.31 , 127.09 , 119.79 , 64.17 , 59.35 , 37.32 , 25.98 , 17.88 .
IR(neat)**:** ν_{max} 3258, 2970, 2930, 1656, 1493, 1442, 1071, 1034, 909, 729, 697 cm^{-1}
HRMS (ESI) m/z calcd for $C_{20}H_{24}NO_2$ $[M+H]^+$: 310.1807, found: 310.1792

2-(2-cyclopropylvinyl)-N-methoxybenzamide, 1p



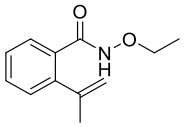
^{1}H NMR (300 MHz, Chloroform-*d*) δ 9.01 (d, *J* = 5.6 Hz, 1H), 7.63 – 7.11 (m, 4H), 6.61 (dd, *J* = 75.9, 13.5 Hz, 1H), 5.75 – 5.06 (m, 1H), 3.84 (d, *J* = 7.3 Hz, 3H), 1.74 – 1.47 (m, 1H), 0.81 (tt, *J* = 8.2, 3.1 Hz, 2H), 0.50 (dq, *J* = 6.6, 4.4 Hz, 2H).
^{13}C NMR (75 MHz, Chloroform-*d*) δ 139.44 , 138.53 , 136.43 , 135.74 , 131.79 , 130.56 , 130.08 , 128.72 , 127.89 , 126.94 , 126.37 , 125.79 , 124.62 , 123.87 , 64.52 , 14.93 , 11.06 , 8.03 , 7.56 .
IR(neat)**:** ν_{max} 3179, 3004, 1639, 1499, 1282, 1034, 907, 725, 645 cm^{-1}
HRMS (ESI) m/z calcd for $C_{13}H_{16}NO_2$ $[M+H]^+$: 218.1181, found: 218.1171

N-methoxy-2-(prop-1-en-2-yl)benzamide, 3a



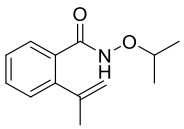
White solid (840 mg), yield: 88%
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.68 (s, 1H), 7.75 – 7.51 (m, 1H), 7.43 (td, *J* = 7.5, 1.6 Hz, 1H), 7.34 (td, *J* = 7.5, 1.5 Hz, 1H), 7.24 (dd, *J* = 7.5, 1.4 Hz, 1H), 5.27 (s, 1H), 5.11 (dd, *J* = 1.8, 1.0 Hz, 1H), 3.86 (s, 3H), 2.11 (d, *J* = 0.7 Hz, 3H).
^{13}C NMR (75 MHz, Chloroform-*d*) δ 167.45 , 145.56 , 142.00 , 130.89 , 128.83 , 128.67 , 127.56 , 116.61 , 64.27 , 24.23 .
IR(neat)**:** ν_{max} 3165, 2970, 2936, 1635, 1499, 1437, 1303, 1030, 884, 769, 657, 545 cm^{-1}
HRMS (ESI) m/z calcd for $C_{11}H_{14}NO_2$ $[M+H]^+$: 192.1025, found: 192.1012

N-ethoxy-2-(prop-1-en-2-yl)benzamide, 3b



White solid (520mg), yield: 72.4%
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.62 (s, 1H), 7.68 – 7.52 (m, 1H), 7.42 (td, *J* = 7.5, 1.6 Hz, 1H), 7.33 (td, *J* = 7.5, 1.5 Hz, 1H), 7.24 (dd, *J* = 7.5, 1.4 Hz, 1H), 5.30 – 5.22 (m, 1H), 5.13 – 5.06 (m, 1H), 4.07 (q, *J* = 7.0 Hz, 2H), 2.11 (t, *J* = 1.1 Hz, 3H), 1.32 (t, *J* = 7.1 Hz, 3H).
^{13}C NMR (75 MHz, Chloroform-*d*) δ 167.45 , 145.71 , 141.97 , 131.09 , 130.83 , 128.86 , 128.67 , 127.57 , 116.51 , 72.21 , 24.30 , 13.53 .
IR(neat)**:** ν_{max} 3182, 2978, 1650, 1500, 1480, 1382, 1303, 1033, 899, 769, 659, 549 cm^{-1}
HRMS (ESI) m/z calcd for $C_{12}H_{16}NO_2$ $[M+H]^+$: 206.1181, found: 206.1170

N-isopropoxy-2-(prop-1-en-2-yl)benzamide, 3c



White solid (642 mg), yield: 97.6%

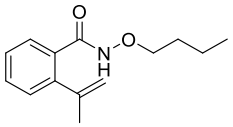
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.51 (s, 1H), 7.67 – 7.50 (m, 1H), 7.41 (td, *J* = 7.5, 1.6 Hz, 1H), 7.32 (td, *J* = 7.5, 1.5 Hz, 1H), 7.24 (dd, *J* = 7.5, 1.4 Hz, 1H), 5.30 – 5.19 (m, 1H), 5.09 (d, *J* = 1.7 Hz, 1H), 4.26 (p, *J* = 6.2 Hz, 1H), 2.11 (t, *J* = 1.2 Hz, 3H), 1.29 (d, *J* = 6.2 Hz, 6H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 167.69 , 145.71 , 141.96 , 131.37 , 130.71 , 128.81 , 128.65 , 127.53 , 116.36 , 78.22 , 24.37 , 20.62 .

IR(neat)**:** ν_{max} 3187, 2975, 1647, 1466, 1372, 1303, 1114, 1020, 974, 892, 768, 660, 554 cm^{-1}

HRMS (ESI) m/z calcd for $C_{13}H_{18}NO_2$ $[M+H]^+$: 220.1338, found: 220.1328

N-butoxy-2-(prop-1-en-2-yl)benzamide, 3d



Colorless oil (520 mg), yield: 89.1%

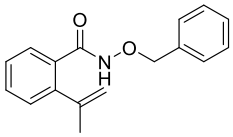
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.60 (s, 1H), 7.60 (d, *J* = 7.5 Hz, 1H), 7.41 (td, *J* = 7.5, 1.5 Hz, 1H), 7.33 (td, *J* = 7.5, 1.4 Hz, 1H), 7.24 (dd, *J* = 7.5, 1.4 Hz, 1H), 5.25 (t, *J* = 1.9 Hz, 1H), 5.09 (s, 1H), 4.01 (t, *J* = 6.8 Hz, 2H), 2.11 (d, *J* = 1.4 Hz, 3H), 1.67 (q, *J* = 7.3 Hz, 2H), 1.43 (q, *J* = 7.5 Hz, 2H), 0.95 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 167.30 , 145.74 , 141.97 , 131.12 , 130.80 , 128.86 , 128.67 , 127.56 , 116.48 , 76.51 , 30.07 , 24.32 , 19.03 , 13.90 .

IR(neat)**:** ν_{max} 3185, 2959, 1649, 1503, 1467, 1304, 1028, 895, 769, 659, 548 cm^{-1}

HRMS (ESI) m/z calcd for $C_{14}H_{20}NO_2$ $[M+H]^+$: 234.1494, found: 234.1484

N-(benzyloxy)-2-(prop-1-en-2-yl)benzamide, 3e



White solid (370 mg), yield: 55.4%

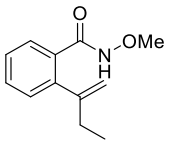
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.56 (s, 1H), 7.57 (d, *J* = 7.5 Hz, 1H), 7.48 – 7.25 (m, 7H), 7.20 (dd, *J* = 7.6, 1.4 Hz, 1H), 5.12 (t, *J* = 1.6 Hz, 1H), 5.10 – 4.68 (m, 3H), 2.02 (t, *J* = 1.1 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 167.22 , 145.56 , 142.08 , 135.40 , 130.95 , 130.83 , 129.04 , 128.81 , 128.76 , 128.66 , 127.49 , 116.49 , 78.13 , 24.30 .

IR(neat)**:** ν_{max} 3184, 2972, 1649, 1496, 1454, 1302, 1019, 897, 745, 697, 659, 545 cm^{-1}

HRMS (ESI) m/z calcd for $C_{17}H_{18}NO_2$ $[M+H]^+$: 268.1338, found: 268.1325

2-(but-1-en-2-yl)-N-methoxybenzamide, 3f



Colorless oil (688 mg), yield: 90.6%

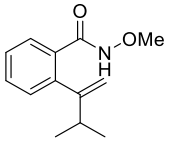
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.87 (s, 1H), 7.62 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.42 (td, *J* = 7.5, 1.6 Hz, 1H), 7.33 (td, *J* = 7.5, 1.4 Hz, 1H), 7.19 (dd, *J* = 7.5, 1.4 Hz, 1H), 5.25 (d, *J* = 1.6 Hz, 1H), 5.10 (d, *J* = 1.4 Hz, 1H), 3.82 (s, 3H), 2.46 – 2.30 (m, 2H), 1.05 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 167.29 , 151.91 , 141.58 , 130.94 , 130.79 , 129.22 , 128.92 , 127.54 , 114.34 , 64.25 , 30.62 , 12.47 .

IR(neat)**:** ν_{max} 3189,2966, 2935, 1654, 1498, 1463, 1439, 1299, 1032, 891, 770, 659 cm^{-1}

HRMS (ESI) m/z calcd for $C_{12}H_{16}NO_2$ $[M+H]^+$: 206.1181, found: 206.1172

N-methoxy-2-(3-methylbut-1-en-2-yl)benzamide, 3g



Colorless oil (1.31 g), yield: 85.3%

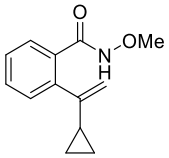
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.77 (s, 1H), 7.70 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.47 – 7.32 (m, 2H), 7.17 (dd, *J* = 7.5, 1.4 Hz, 1H), 5.27 (t, *J* = 1.4 Hz, 1H), 5.11 (t, *J* = 0.9 Hz, 1H), 3.84 (s, 3H), 2.55 (p, *J* = 6.7 Hz, 1H), 1.06 (d, *J* = 6.8 Hz, 6H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 167.27 , 157.22 , 141.68 , 130.82 , 130.77 , 129.80 , 129.23 , 127.62 , 112.96 , 64.37 , 34.88 , 21.47 .

IR(neat)**:** ν_{max} 3193, 2963, 1654, 1496, 1467, 1439, 1304, 1043, 886, 771, 760, 658, 586 cm^{-1}

HRMS (ESI) m/z calcd for $C_{13}H_{18}NO_2$ $[M+H]^+$: 220.1338, found: 220.1328

2-(1-cyclopropylvinyl)-N-methoxybenzamide, 3h



Colorless oil (1.37 g), yield: 85.2%

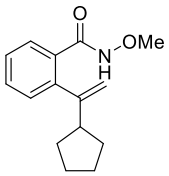
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.94 (s, 1H), 7.72 (dd, *J* = 7.5, 1.8 Hz, 1H), 7.46 – 7.32 (m, 2H), 7.19 (dd, *J* = 7.4, 1.6 Hz, 1H), 5.18 (s, 1H), 5.03 (d, *J* = 1.2 Hz, 1H), 3.86 (s, 3H), 1.64 (td, *J* = 8.3, 4.1 Hz, 1H), 0.84 – 0.75 (m, 2H), 0.55 – 0.45 (m, 2H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 167.12 , 151.86 , 139.79 , 131.30 , 130.76 , 129.55 , 129.17 , 127.78 , 112.54 , 64.37 , 17.46 , 7.49 .

IR(neat)**:** ν_{max} 3201, 3005, 2935, 1655, 1468, 1304, 1032, 886, 769, 726 cm^{-1}

HRMS (ESI) m/z calcd for $C_{13}H_{16}NO_2$ $[M+H]^+$: 218.1181, found: 218.1172

2-(1-cyclopentylvinyl)-N-methoxybenzamide, 3i



Colorless oil (1.38 g), yield: 86.9%

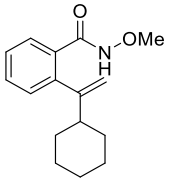
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.87 (s, 1H), 7.70 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.45 – 7.31 (m, 2H), 7.16 (dd, *J* = 7.3, 1.5 Hz, 1H), 5.30 (s, 1H), 5.11 (s, 1H), 3.84 (s, 3H), 2.70 (s, 1H), 1.82 – 1.33 (m, 8H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 167.24 , 154.59 , 141.90 , 130.80 , 130.74 , 129.46 , 129.16 , 127.52 , 113.35 , 64.38 , 47.16 , 31.69 , 24.51 .

IR(neat)**:** ν_{max} 3201, 2951, 2868, 1655, 1468, 1304, 1042, 886, 768, 657 cm^{-1}

HRMS (ESI) m/z calcd for $C_{15}H_{20}NO_2$ $[M+H]^+$: 246.1494, found: 246.1484

2-(1-cyclohexylvinyl)-N-methoxybenzamide, 3j



Colorless oil (908 mg), yield: 70%

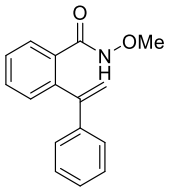
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.82 (s, 1H), 7.71 (dd, *J* = 7.4, 1.7 Hz, 1H), 7.45 – 7.32 (m, 2H), 7.15 (d, *J* = 6.9 Hz, 1H), 5.24 (s, 1H), 5.10 (d, *J* = 1.3 Hz, 1H), 3.84 (s, 3H), 2.14 (d, *J* = 10.9 Hz, 1H), 1.81 – 1.63 (m, 5H), 1.29 – 1.08 (m, 5H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 167.23 , 156.41 , 141.63 , 130.78 , 130.69 , 129.83 , 129.25 , 127.55 , 113.27 , 64.32 , 44.74 , 32.09 , 26.47 , 26.18 .

IR(neat)**:** ν_{max} 3201, 2924, 2851, 1655, 1496, 1468, 1448, 1304, 1045, 886, 764, 734, 664, 557 cm^{-1}

HRMS (ESI) m/z calcd for $C_{16}H_{22}NO_2$ $[M+H]^+$: 260.1651, found: 260.1640

N-methoxy-2-(1-phenylvinyl)benzamide, 3k



White solid (520 mg), yield: 93.3%

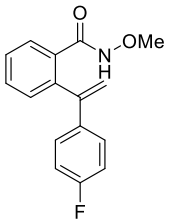
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.45 (s, 1H), 7.65 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.50 (td, *J* = 7.5, 1.6 Hz, 1H), 7.42 (td, *J* = 7.5, 1.5 Hz, 1H), 7.35 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.32 – 7.22 (m, 5H), 5.82 (s, 1H), 5.40 (d, *J* = 0.9 Hz, 1H), 3.41 (s, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 166.49 , 148.59 , 139.93 , 139.71 , 132.43 , 131.04 , 130.97 , 129.01 , 128.56 , 128.35 , 128.23 , 126.94 , 116.33 , 63.89 .

IR(neat)**:** ν_{max} 3170, 2975, 2935, 1652, 1493, 1439, 1304, 1029, 906, 888, 769, 727, 706, 660, 597 cm^{-1}

HRMS (ESI) m/z calcd for $C_{16}H_{16}NO_2$ $[M+H]^+$: 254.1181, found: 254.1171

2-(1-(4-fluorophenyl)vinyl)-N-methoxybenzamide, 3l



White solid (417 mg), yield: 90.4%

^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.47 (s, 1H), 7.62 (d, *J* = 7.4 Hz, 1H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.42 (t, *J* = 7.0 Hz, 1H), 7.35 (d, *J* = 7.5 Hz, 1H), 7.27 – 7.21 (m, 2H), 6.98 (t, *J* = 8.6 Hz, 2H), 5.73 (s, 1H), 5.37 (s, 1H), 3.48 (s, 3H).

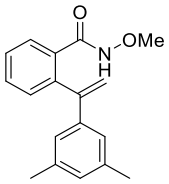
^{13}C NMR (75 MHz, Chloroform-*d*) δ 166.46 , 162.69 (d, *J* = 248.2 Hz), 147.69 , 139.89 , 136.08 , 132.40 , 131.07 , 130.87 , 128.87 , 128.80 , 128.70 , 128.31 , 116.03 (d, *J* = 1.6 Hz), 115.52 , 115.23 , 63.95 .

^{19}F NMR (282 MHz, Chloroform-*d*) δ -113.52 .

IR(neat)**:** ν_{max} 3171, 2977, 2936, 1654, 1600, 1506, 1468, 1439, 1222, 1159, 1035, 937, 907, 888, 841, 772, 728, 651, 556 cm^{-1}

HRMS (ESI) m/z calcd for $C_{16}H_{15}FNO_2$ $[M+H]^+$: 272.1087, found: 272.1076

2-(1-(3,5-dimethylphenyl)vinyl)-N-methoxybenzamide, 3m



White solid (721mg), yield: 80%

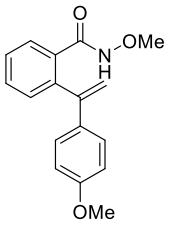
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.46 (s, 1H), 7.68 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.45 (ddd, *J* = 13.0, 7.4, 1.6 Hz, 2H), 7.32 (dd, *J* = 7.3, 1.5 Hz, 1H), 6.90 (d, *J* = 11.9 Hz, 3H), 5.80 (d, *J* = 1.0 Hz, 1H), 5.34 (d, *J* = 1.0 Hz, 1H), 3.46 (s, 3H), 2.26 (s, 6H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 166.52 , 148.67 , 140.05 , 139.62 , 138.04 , 132.37 , 130.89 , 130.06 , 129.11 , 128.10 , 124.82 , 116.13 , 63.78 , 21.34 .

IR(neat)**:** ν_{max} 3193, 2934, 1656, 1597, 1467, 1304, 1038, 908, 886, 852, 769, 727, 646 cm^{-1}

HRMS (ESI) m/z calcd for $C_{18}H_{20}NO_2$ $[M+H]^+$: 282.1494, found: 282.1483

N-methoxy-2-(1-(4-methoxyphenyl)vinyl)benzamide, 3n



White solid (416 mg), yield: 97.8%

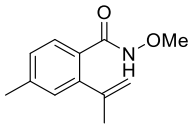
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.54 (s, 1H), 7.68 (dd, *J* = 7.4, 1.6 Hz, 1H), 7.53 – 7.39 (m, 2H), 7.37 – 7.29 (m, 1H), 7.20 (d, *J* = 8.9 Hz, 2H), 6.82 (d, *J* = 8.9 Hz, 2H), 5.74 (d, *J* = 1.0 Hz, 1H), 5.28 (d, *J* = 1.0 Hz, 1H), 3.78 (s, 3H), 3.47 (s, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 166.56 , 159.76 , 148.08 , 140.03 , 132.37 , 132.16 , 131.04 , 130.80 , 129.16 , 128.20 , 128.12 , 114.32 , 113.90 , 63.97 , 55.30 .

IR(neat)**:** ν_{max} 3195, 2935, 1655, 1607, 1509, 1464, 1292, 1246, 1179, 1030, 907, 888, 835, 772, 727, 566 cm^{-1}

HRMS (ESI) m/z calcd for $C_{17}H_{18}NO_3$ $[M+H]^+$: 284.1287, found: 284.1275

N-methoxy-4-methyl-2-(prop-1-en-2-yl)benzamide, 3o



White solid (500 mg), yield: 43.5%

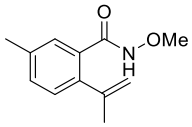
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.82 (s, 1H), 7.51 (d, *J* = 7.8 Hz, 1H), 7.13 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.04 (d, *J* = 1.7 Hz, 1H), 5.29 – 5.18 (m, 1H), 5.14 – 5.01 (m, 1H), 3.83 (s, 3H), 2.36 (s, 3H), 2.09 (t, *J* = 1.1 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 167.50 , 145.98 , 141.97 , 141.24 , 129.32 , 128.99 , 128.25 , 127.95 , 116.33 , 64.24 , 24.30 , 21.37 .

IR(neat)**:** ν_{max} 3188, 2974, 2934, 1655, 1463, 1305, 1046, 893, 824 cm^{-1}

HRMS (ESI) m/z calcd for $C_{12}H_{16}NO_2$ $[M+H]^+$: 206.1181, found: 206.1171

N-methoxy-5-methyl-2-(prop-1-en-2-yl)benzamide, 3p



White solid (188 mg), yield: 16.3%

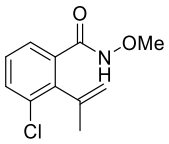
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.73 (s, 1H), 7.42 (d, *J* = 1.8 Hz, 1H), 7.22 (ddd, *J* = 7.8, 1.9, 0.8 Hz, 1H), 7.13 (d, *J* = 7.9 Hz, 1H), 5.23 (t, *J* = 1.6 Hz, 1H), 5.08 (dd, *J* = 1.9, 1.0 Hz, 1H), 3.84 (s, 3H), 2.35 (s, 3H), 2.08 (dd, *J* = 1.5, 0.9 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 167.61 , 145.51 , 139.05 , 137.53 , 131.61 , 130.61 , 129.38 , 128.62 , 116.37 , 64.26 , 24.30 , 20.91 .

IR(neat)**:** ν_{max} 3176, 2971, 2933, 1651, 1490, 1438, 1304, 1041, 897, 823, 547 cm^{-1}

HRMS (ESI) m/z calcd for $C_{12}H_{16}NO_2$ $[M+H]^+$: 206.1181, found: 206.1171

3-chloro-N-methoxy-2-(prop-1-en-2-yl)benzamide, **3q**



White solid (227 mg), yield: 72%

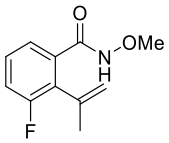
^{1}H NMR (300 MHz, Chloroform-*d*) δ 9.12 (s, 1H), 7.46 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.42 – 7.30 (m, 1H), 7.23 (t, *J* = 7.8 Hz, 1H), 5.41 – 5.27 (m, 1H), 4.93 (t, *J* = 1.3 Hz, 1H), 3.80 (s, 3H), 2.10 (t, *J* = 1.2 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 166.11 , 142.80 , 140.57 , 133.85 , 133.05 , 131.76 , 128.19 , 126.45 , 117.67 , 64.27 , 23.73 .

IR(neat)**:** ν_{max} 3192, 2975, 2938, 1657, 1436, 1288, 1148, 1114, 1064, 994, 907, 756, 727, 646, 561 cm^{-1}

HRMS (ESI) m/z calcd for $C_{11}H_{13}ClNO_2$ $[M+H]^+$: 226.0635, found: 226.0626

3-fluoro-N-methoxy-2-(prop-1-en-2-yl)benzamide, 3r



White solid (94 mg), yield: 54%

^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.83 (s, 1H), 7.39 – 7.27 (m, 1H), 7.13 – 6.77 (m, 2H), 5.25 – 5.13 (m, 1H), 5.06 (s, 1H), 3.82 (s, 3H), 2.08 (s, 3H).

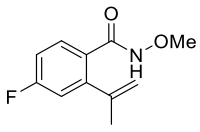
^{13}C NMR (75 MHz, Chloroform-*d*) δ 162.87 , 159.65 (d, *J* = 249.4 Hz), 144.65 , 142.79 (d, *J* = 2.1 Hz), 131.36 (d, *J* = 8.9 Hz), 123.92 , 119.90 (d, *J* = 17.2 Hz), 116.92 , 114.40 (d, *J* = 21.8 Hz), 64.29 , 23.83 .

^{19}F NMR (282 MHz, Chloroform-*d*) δ -115.18 (dd, *J* = 9.2, 5.8 Hz).

IR(neat)**:** ν_{max} 3159, 2974, 2939, 1655, 1439, 1240, 1148, 1036, 896, 803, 724, 577 cm^{-1}

HRMS (ESI) m/z calcd for $C_{11}H_{13}FNO_2$ $[M+H]^+$: 210.0930, found: 210.0921

4-fluoro-N-methoxy-2-(prop-1-en-2-yl)benzamide, 3s



White solid (840 mg), yield: 65.9%

^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.89 (s, 1H), 7.58 (dd, *J* = 8.5, 5.7 Hz, 1H), 7.07 – 6.86 (m, 2H), 5.32 – 5.23 (m, 1H), 5.11 (s, 1H), 3.83 (s, 3H), 2.09 (t, *J* = 1.1 Hz, 3H).

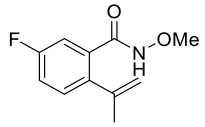
^{13}C NMR (75 MHz, Chloroform-*d*) δ 165.94 (d, *J* = 86.2 Hz), 162.03 , 144.71 (d, *J* = 8.2 Hz), 144.54 , 131.25 (d, *J* = 9.2 Hz), 127.10 , 117.28 , 115.68 (d, *J* = 22.2 Hz), 114.54 (d, *J* = 21.7 Hz), 64.26 , 23.90 .

^{19}F NMR (282 MHz, Chloroform-*d*) δ -108.77 (d, *J* = 7.8 Hz).

IR(neat)**:** ν_{max} 3179, 2977, 2938, 1655, 1608, 1578, 1478, 1301, 1259, 1201, 1036, 900, 606 cm^{-1}

HRMS (ESI) m/z calcd for $C_{11}H_{13}FNO_2$ $[M+H]^+$: 210.0930, found: 210.0921

5-fluoro-N-methoxy-2-(prop-1-en-2-yl)benzamide, 3t



White solid (290 mg), yield: 22.8%

^{1}H NMR (300 MHz, Chloroform-*d*) δ 9.00 (s, 1H), 7.33 – 7.18 (m, 2H), 7.10 (td, *J* = 8.3, 2.7 Hz, 1H), 5.32 – 5.19 (m, 1H), 5.07 (s, 1H), 3.84 (s, 3H), 2.08 (s, 3H).

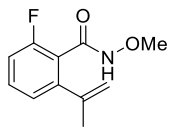
^{13}C NMR (75 MHz, Chloroform-*d*) δ 164.59 (d, *J* = 203.6 Hz), 159.95 , 144.65 , 138.01 (d, *J* = 3.6 Hz), 132.61 , 130.64 (d, *J* = 7.6 Hz), 117.85 (d, *J* = 20.9 Hz), 117.10 , 115.79 (d, *J* = 23.2 Hz), 64.26 , 24.30 .

^{19}F NMR (282 MHz, Chloroform-*d*) δ -113.84 (d, *J* = 6.7 Hz).

IR(neat)**:** ν_{max} 3191, 2977, 2939, 1656, 1558, 1490, 1303, 1266, 1212, 1039, 827, 673, 545 cm^{-1}

HRMS (ESI) m/z calcd for $C_{11}H_{13}FNO_2$ $[M+H]^+$: 210.0930, found: 210.0921

2-fluoro-N-methoxy-6-(prop-1-en-2-yl)benzamide, 3u



White solid (849 mg), yield: 84%

^{1}H NMR (300 MHz, Chloroform-*d*) δ 9.02 (s, 1H), 7.36 – 7.23 (m, 2H), 7.20 – 7.10 (m, 1H), 5.37 (s, 1H), 5.04 (s, 1H), 3.82 (s, 3H), 2.11 (s, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 165.93 , 159.17 (d, *J* = 246.9 Hz), 138.91 , 133.73 , 129.74 (d, *J* = 18.4 Hz), 128.75 (d, *J* = 8.5 Hz), 124.00 , 118.46 , 118.03 (d, *J* = 22.9 Hz), 64.28 , 24.00 .

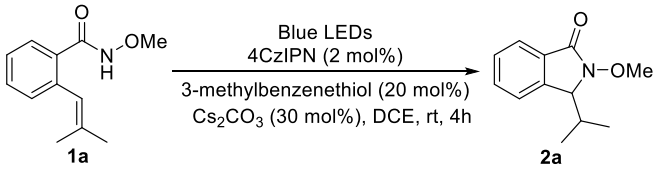
^{19}F NMR (282 MHz, Chloroform-*d*) δ -114.29 (dd, *J* = 9.4, 4.4 Hz).

IR(neat)**:** ν_{max} 3189, 2975, 2939, 1660, 1455, 1241, 1053, 830, 803, 755 cm^{-1}

HRMS (ESI) m/z calcd for $C_{11}H_{13}FNO_2$ $[M+H]^+$: 210.0930, found: 210.0921

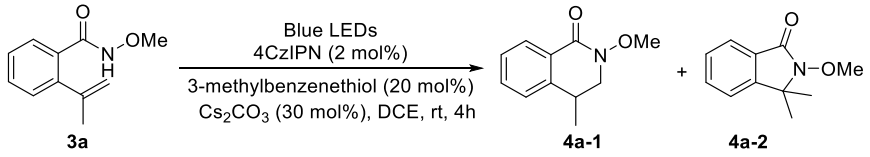
4. Synthesis and Characterization of Products

4.1 General Procedure for preparation of products



1a 2a

To a Schlenk tube were added 1a (51.32 mg, 0.25 mmol), 4CzIPN (3.94 mg, 0.005 mmol, 2 mol%), Cs_2CO_3 (24.4mg, 0.075mmol, 30 mol%). The tube was degassed and refilled with N_2 three times, anhydrous DCE (2.5 mL) was added before m-toluenethiol (5.94 µL, 0.05 mmol, 20 mol%) via a syringe. The mixture was then placed around the Blue LEDs (450 nm, 100% light intensity) and stirred until the substrate was consumed (monitored by TLC), the solvent was removed by rotary evaporation and the resulting residue was purified directly by flash column chromatography (33% EtOAc in hexanes) to give the desired product 2a (43 mg, 83 % yield).

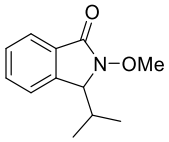


3a 4a-1 4a-2

To a Schlenk tube were added 3a (47.8 mg, 0.25 mmol), 4CzIPN (3.94 mg, 0.005 mmol, 2 mol%), Cs_2CO_3 (24.4mg, 0.075mmol, 30 mol%). The tube was degassed and refilled with N_2 three times, anhydrous DCE (2.5 mL) was added before m-toluenethiol (5.94 µL, 0.05 mmol, 20 mol%) via a syringe. The mixture was then placed around the Blue LEDs (450 nm, 100% light intensity) and stirred until the substrate was consumed (monitored by TLC), the solvent was removed by rotary evaporation and the resulting residue was purified directly by flash column chromatography (33% EtOAc in hexanes) to give the desired product 4a-1 (34 mg, 71 % yield) and 4a-2 (5 mg, 10 % yield)

4.2 Characterizations of products

3-isopropyl-2-methoxyisoindolin-1-one, 2a



White solid (43 mg), yield: 83%

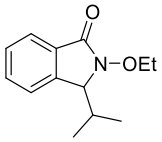
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.93 – 7.75 (m, 1H), 7.55 (td, *J* = 7.5, 1.4 Hz, 1H), 7.51 – 7.43 (m, 1H), 7.41 (dq, *J* = 7.6, 0.9 Hz, 1H), 4.68 (d, *J* = 2.9 Hz, 1H), 3.96 (s, 3H), 2.61 – 2.38 (m, 1H), 1.08 (d, *J* = 7.1 Hz, 3H), 0.78 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 165.05 , 140.69 , 131.72 , 130.71 , 128.34 , 123.72 , 122.93 , 64.38 , 63.20 , 29.52 , 17.67 , 16.63 .

IR(neat)**:** ν_{max} 2965, 2934, 1703, 1617, 1468, 1372, 1319, 1164, 1095, 1004, 910, 792, 731, 691, 521 cm^{-1}

HRMS (ESI) m/z calcd for $C_{12}H_{16}NO_2$ $[M+H]^+$: 206.1181, found: 206.1171

2-ethoxy-3-isopropylisoindolin-1-one, 2b



Colorless oil (44.3 mg), yield: 81%

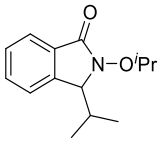
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.86 (d, *J* = 7.7 Hz, 1H), 7.54 (td, *J* = 7.5, 1.4 Hz, 1H), 7.51 – 7.37 (m, 2H), 4.66 (d, *J* = 2.9 Hz, 1H), 4.19 (q, *J* = 7.1 Hz, 2H), 2.53 (qd, *J* = 7.0, 3.0 Hz, 1H), 1.38 (t, *J* = 7.1 Hz, 3H), 1.08 (d, *J* = 7.1 Hz, 3H), 0.75 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 165.13 , 140.71 , 131.57 , 130.86 , 128.29 , 123.71 , 122.89 , 71.26 , 64.98 , 29.54 , 17.75 , 16.53 , 13.83 .

IR(neat)**:** ν_{max} 2965, 2932, 2876, 1705, 1470, 1389, 1095, 1026, 973, 945, 734, 565, 531 cm^{-1}

HRMS (ESI) m/z calcd for $C_{13}H_{18}NO_2$ $[M+H]^+$: 220.1338, found: 220.1327

2-isopropoxy-3-isopropylisoindolin-1-one, 2c



White solid (51.7 mg), yield: 87%

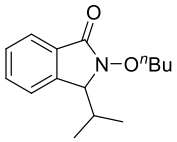
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.86 (d, *J* = 7.5 Hz, 1H), 7.54 (td, *J* = 7.5, 1.4 Hz, 1H), 7.46 (t, *J* = 7.0 Hz, 1H), 7.43 – 7.37 (m, 1H), 4.65 (d, *J* = 3.1 Hz, 1H), 4.43 (p, *J* = 6.2 Hz, 1H), 2.54 (ddt, *J* = 10.1, 7.0, 3.1 Hz, 1H), 1.35 (dd, *J* = 6.2, 2.8 Hz, 6H), 1.10 (d, *J* = 7.1 Hz, 3H), 0.66 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 165.47 , 140.67 , 131.41 , 130.97 , 128.25 , 123.67 , 122.98 , 77.79 , 65.81 , 29.47 , 21.12 , 21.10 , 17.98 , 16.13 .

IR(neat)**:** ν_{max} 2967, 1703, 1468, 1373, 1319, 1110, 973, 949, 792, 741, 692, 530 cm^{-1}

HRMS (ESI) m/z calcd for $C_{14}H_{20}NO_2$ $[M+H]^+$: 234.1494, found: 234.1483

2-butoxy-3-isopropylisoindolin-1-one, 2d



Colorless oil (48.9 mg), yield: 79%

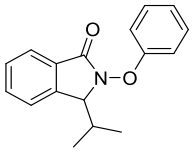
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.85 (dt, *J* = 7.4, 1.0 Hz, 1H), 7.54 (td, *J* = 7.5, 1.4 Hz, 1H), 7.50 – 7.37 (m, 2H), 4.65 (d, *J* = 3.0 Hz, 1H), 4.19 – 4.06 (m, 2H), 2.53 (td, *J* = 7.0, 3.0 Hz, 1H), 1.75 (dq, *J* = 13.5, 6.8 Hz, 2H), 1.49 (q, *J* = 7.5 Hz, 2H), 1.09 (d, *J* = 7.1 Hz, 3H), 0.97 (t, *J* = 7.3 Hz, 3H), 0.74 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 164.92 , 140.65 , 131.52 , 130.93 , 128.27 , 123.65 , 122.89 , 75.50 , 64.84 , 30.32 , 29.53 , 19.15 , 17.82 , 16.52 , 13.92 .

IR(neat)**:** ν_{max} 2960, 2874, 1705, 1467, 1371, 1165, 977, 786, 732, 691, 529 cm^{-1}

HRMS (ESI) m/z calcd for $C_{15}H_{22}NO_2$ $[M+H]^+$: 248.1606, found: 248.1639

3-isopropyl-2-phenoxyisoindolin-1-one, 2e



White solid (58 mg), yield: 84%

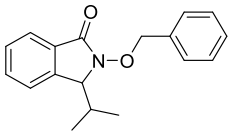
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.94 (d, *J* = 7.5 Hz, 1H), 7.62 (td, *J* = 7.5, 1.3 Hz, 1H), 7.57 – 7.48 (m, 1H), 7.44 (d, *J* = 7.5 Hz, 1H), 7.37 – 7.28 (m, 2H), 7.15 – 7.04 (m, 3H), 4.78 (d, *J* = 2.9 Hz, 1H), 2.52 (ddq, *J* = 9.9, 7.0, 3.5, 3.0 Hz, 1H), 1.04 (d, *J* = 7.1 Hz, 3H), 0.79 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 166.58 , 158.80 , 141.37 , 132.43 , 129.80 , 129.64 , 128.63 , 124.25 , 123.37 , 123.23 , 113.91 , 65.90 , 29.62 , 17.60 , 16.98 .

IR(neat)**:** ν_{max} 2965, 1716, 1590, 1487, 1469, 1370, 1194, 1155, 1075, 1022, 861, 729, 687 cm^{-1}

HRMS (ESI) m/z calcd for $C_{17}H_{18}NO_2$ $[M+H]^+$: 268.1338, found: 268.1325

2-(benzyloxy)-3-isopropylisoindolin-1-one, 2f



White solid (65.1 mg), yield: 92%

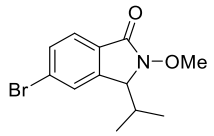
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.91 – 7.80 (m, 1H), 7.55 – 7.42 (m, 4H), 7.41 – 7.34 (m, 3H), 7.30 (d, *J* = 7.4 Hz, 1H), 5.16 (s, 2H), 4.20 (d, *J* = 3.0 Hz, 1H), 2.47 (td, *J* = 7.0, 3.0 Hz, 1H), 0.99 (d, *J* = 7.1 Hz, 3H), 0.67 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 140.82 , 135.30 , 131.58 , 130.68 , 129.64 , 128.93 , 128.60 , 128.24 , 123.67 , 122.86 , 77.83 , 65.76 , 29.35 , 17.85 , 16.44 .

IR(neat)**:** ν_{max} 2963, 1703, 1467, 1371, 1205, 1164, 1094, 976, 730, 691, 530 cm^{-1}

HRMS (ESI) m/z calcd for $C_{18}H_{20}NO_2$ $[M+H]^+$: 282.1494, found: 282.1482

5-bromo-3-isopropyl-2-methoxyisoindolin-1-one, 2i



Colorless oil (65.6 mg), yield: 92%

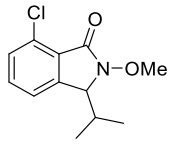
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.72 (d, *J* = 8.1 Hz, 1H), 7.62 (dd, *J* = 8.1, 1.6 Hz, 1H), 7.57 (q, *J* = 0.8 Hz, 1H), 4.66 (d, *J* = 2.9 Hz, 1H), 3.96 (s, 3H), 2.52 (pd, *J* = 7.0, 3.0 Hz, 1H), 1.08 (d, *J* = 7.1 Hz, 3H), 0.79 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 164.20 , 142.44 , 131.84 , 129.63 , 126.48 , 126.27 , 125.20 , 64.12 , 63.31 , 29.54 , 17.62 , 16.64 .

IR(neat)**:** ν_{max} 2964, 2932, 1704, 1608, 1461, 1370, 1204, 1057, 1001, 908, 834, 730, 685, 649, 582 cm^{-1}

HRMS (ESI) m/z calcd for $C_{12}H_{15}BrNO_2$ $[M+H]^+$: 284.0286, found: 284.0275

7-chloro-3-isopropyl-2-methoxyisoindolin-1-one, 2j



White solid (56.6 mg), yield: 93%

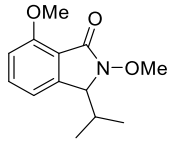
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.47 (dd, *J* = 8.0, 7.4 Hz, 1H), 7.39 (dd, *J* = 8.1, 1.1 Hz, 1H), 7.31 (dt, *J* = 7.4, 0.9 Hz, 1H), 4.63 (d, *J* = 2.8 Hz, 1H), 3.96 (s, 3H), 2.52 (td, *J* = 7.0, 2.9 Hz, 1H), 1.04 (d, *J* = 7.1 Hz, 3H), 0.82 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 163.37 , 143.33 , 132.46 , 131.56 , 130.04 , 126.82 , 121.42 , 63.67 , 63.19 , 29.70 , 17.43 , 16.92 .

IR(neat)**:** ν_{max} 2965, 2935, 1706, 1604, 1460, 1371, 1200, 1004, 914, 893, 782, 680, 575 cm^{-1}

HRMS (ESI) m/z calcd for $C_{12}H_{15}ClNO_2$ $[M+H]^+$: 240.0791, found: 240.0781

3-isopropyl-2,7-dimethoxyisoindolin-1-one, 2k



White solid (45 mg), yield: 75%

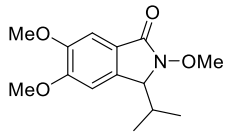
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.49 (t, *J* = 8.0 Hz, 1H), 6.93 (dd, *J* = 14.9, 8.0 Hz, 2H), 4.59 (d, *J* = 2.8 Hz, 1H), 3.96 (s, 3H), 3.93 (s, 3H), 2.48 (pd, *J* = 7.0, 2.8 Hz, 1H), 1.02 (d, *J* = 7.1 Hz, 3H), 0.83 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 164.96 , 157.34 , 143.56 , 133.42 , 117.69 , 115.00 , 110.42 , 64.09 , 63.05 , 55.82 , 29.78 , 17.35 , 17.00 .

IR(neat)**:** ν_{max} 2964, 2935, 1702, 1594, 1485, 1263, 1060, 1007, 902, 822, 803, 754, 691, 537 cm^{-1}

HRMS (ESI) m/z calcd for $C_{13}H_{18}NO_3$ $[M+H]^+$: 236.1287, found: 236.1277

3-isopropyl-2,5,6-trimethoxyisoindolin-1-one, 2l



Colorless oil (46.7 mg), yield: 70%

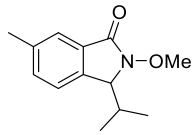
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.32 (s, 1H), 6.84 (s, 1H), 4.59 (d, *J* = 2.8 Hz, 1H), 3.98 – 3.91 (m, 9H), 2.49 (pd, *J* = 7.0, 2.9 Hz, 1H), 1.05 (d, *J* = 7.1 Hz, 3H), 0.82 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 166.28 , 152.69 , 149.75 , 134.51 , 122.77 , 105.43 , 105.28 , 64.40 , 63.29 , 56.26 , 56.20 , 29.67 , 17.48 , 16.86 .

IR(neat)**:** ν_{max} 2963, 2935, 1699, 1498, 1463, 1292, 1224, 1102, 1014, 863, 769, 727, 690 cm^{-1}

HRMS (ESI) m/z calcd for $C_{14}H_{20}NO_4$ $[M+H]^+$: 266.1392, found: 266.1380

3-isopropyl-2-methoxy-6-methylisoindolin-1-one, 2m



Colorless oil (50.2 mg), yield: 90%

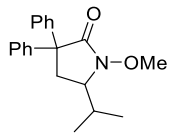
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.66 (dt, *J* = 1.7, 0.8 Hz, 1H), 7.39 – 7.32 (m, 1H), 7.29 (d, *J* = 7.8 Hz, 1H), 4.64 (d, *J* = 2.9 Hz, 1H), 3.95 (s, 3H), 2.50 (td, *J* = 7.0, 3.0 Hz, 1H), 2.43 (s, 3H), 1.07 (d, *J* = 7.1 Hz, 3H), 0.75 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 165.29 , 138.38 , 137.78 , 132.67 , 130.68 , 123.96 , 122.73 , 64.27 , 63.19 , 29.44 , 21.38 , 17.74 , 16.50 .

IR(neat)**:** ν_{max} 2963, 2933, 1704, 1490, 1370, 1106, 1013, 832, 738, 696, 560, 517 cm^{-1}

HRMS (ESI) m/z calcd for $C_{13}H_{18}NO_2$ $[M+H]^+$: 220.1338, found: 220.1328

5-isopropyl-1-methoxy-3,3-diphenylpyrrolidin-2-one, 2n



White solid (77mg), yield: 96%

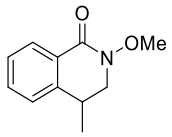
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.42 – 7.20 (m, 10H), 3.77 (s, 3H), 3.71 (ddd, *J* = 10.0, 6.0, 4.2 Hz, 1H), 2.74 (dd, *J* = 13.0, 6.1 Hz, 1H), 2.33 – 2.12 (m, 2H), 0.97 (dd, *J* = 14.8, 6.9 Hz, 6H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 144.39 , 141.22 , 128.58 , 128.39 , 127.90 , 127.74 , 127.27 , 126.78 , 61.45 , 58.97 , 54.24 , 33.93 , 28.16 , 18.31 , 16.01 .

IR(neat)**:** ν_{max} 2962, 2874, 1703, 1494, 1445, 1233, 1043, 978, 877, 759, 696, 642, 594 cm^{-1}

HRMS (ESI) m/z calcd for $C_{20}H_{24}NO_2$ $[M+H]^+$: 310.1807, found: 310.1793

2-methoxy-4-methyl-3,4-dihydroisoquinolin-1(2H)-one, 4a-1



Colorless oil (34 mg), yield: 71%

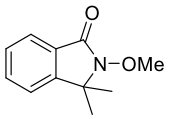
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.14 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.48 (td, *J* = 7.5, 1.5 Hz, 1H), 7.36 (td, *J* = 7.6, 1.3 Hz, 1H), 7.26 – 7.19 (m, 1H), 3.95 (dd, *J* = 11.3, 5.0 Hz, 1H), 3.89 (s, 3H), 3.55 (dd, *J* = 11.3, 6.0 Hz, 1H), 3.28 (q, *J* = 6.2 Hz, 1H), 1.42 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 162.99 , 142.33 , 132.43 , 128.40 , 127.80 , 127.14 , 126.00 , 61.60 , 54.10 , 33.56 , 19.20 .

IR(neat)**:** ν_{max} 3255, 2968, 2931, 1666, 1604, 1460, 1288, 1015, 902, 757, 695, 558 cm^{-1}

HRMS (ESI) m/z calcd for $C_{11}H_{14}NO_2$ $[M+H]^+$: 192.1025, found: 192.1014

2-methoxy-3,3-dimethylisoindolin-1-one，4a-2



White solid (4.8 mg), yield: 10%

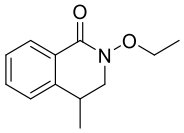
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.80 (dt, *J* = 7.5, 1.0 Hz, 1H), 7.54 (td, *J* = 7.5, 1.2 Hz, 1H), 7.41 (td, *J* = 7.5, 1.1 Hz, 1H), 7.33 (dt, *J* = 7.6, 0.9 Hz, 1H), 4.04 (s, 3H), 1.54 (s, 6H).

^{13}C NMR (75 MHz, Deuterium Oxide) δ 146.23 , 129.69 , 125.90 , 125.63 , 121.23 , 118.14 , 74.97 , 74.55 , 74.13 , 62.71 , 60.90 , 22.49 .

IR(neat)**:** ν_{max} 2977, 2936, 1707, 1465, 1342, 1176, 1080, 992, 763, 566 cm^{-1}

HRMS (ESI) m/z calcd for $C_{11}H_{14}NO_2$ $[M+H]^+$: 192.1025, found: 192.1014

2-ethoxy-4-methyl-3,4-dihydroisoquinolin-1(2H)-one, 4b-1



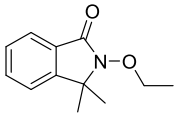
White solid (34 mg), yield: 65%

^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.14 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.47 (td, *J* = 7.5, 1.5 Hz, 1H), 7.36 (td, *J* = 7.6, 1.3 Hz, 1H), 7.26 – 7.17 (m, 1H), 4.14 (qd, *J* = 7.0, 2.0 Hz, 2H), 3.94 (dd, *J* = 11.3, 5.0 Hz, 1H), 3.56 (dd, *J* = 11.3, 6.0 Hz, 1H), 3.28 (q, *J* = 6.2 Hz, 1H), 1.45 – 1.30 (m, 6H).

IR(neat)**:** ν_{max} 2974, 2931, 2873, 1668, 1474, 1401, 1285, 1229, 1027, 951, 756, 695, 562 cm^{-1}

HRMS (ESI) m/z calcd for $C_{12}H_{16}NO_2$ $[M+H]^+$: 206.1181, found: 206.1171

2-ethoxy-3,3-dimethylisoindolin-1-one, 4b-2



White solid (7.5 mg), yield: 15%

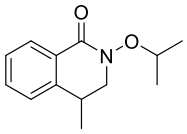
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.83 (dt, *J* = 7.6, 1.0 Hz, 1H), 7.57 (td, *J* = 7.5, 1.2 Hz, 1H), 7.44 (td, *J* = 7.5, 1.1 Hz, 1H), 7.36 (dt, *J* = 7.6, 0.9 Hz, 1H), 4.30 (q, *J* = 7.1 Hz, 2H), 1.56 (s, 6H), 1.41 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 164.25 , 148.84 , 132.13 , 128.58 , 128.15 , 123.81 , 120.69 , 73.16 , 63.39 , 25.15 , 14.03 .

IR(neat)**:** ν_{max} 2978, 1703, 1472, 1339, 1260, 1077, 1022, 987, 761, 691, 566 cm^{-1}

HRMS (ESI) m/z calcd for $C_{12}H_{16}NO_2$ $[M+H]^+$: 206.1181, found: 206.1170

2-isopropoxy-4-methyl-3,4-dihydroisoquinolin-1(2H)-one, 4c



Colorless oil (37.5 mg), yield: 67%

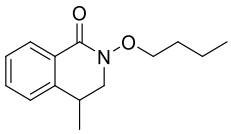
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.14 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.47 (td, *J* = 7.5, 1.5 Hz, 1H), 7.35 (td, *J* = 7.6, 1.3 Hz, 1H), 7.23 (dd, *J* = 7.7, 1.2 Hz, 1H), 4.43 (p, *J* = 6.2 Hz, 1H), 3.88 (dd, *J* = 11.3, 4.9 Hz, 1H), 3.54 (dd, *J* = 11.3, 6.3 Hz, 1H), 3.29 (td, *J* = 6.9, 5.2 Hz, 1H), 1.43 (d, *J* = 7.0 Hz, 3H), 1.34 (d, *J* = 6.2 Hz, 6H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 164.52 , 142.42 , 132.35 , 128.45 , 128.01 , 127.11 , 125.91 , 76.59 , 56.32 , 33.68 , 21.10 , 21.02 , 19.19 .

IR(neat)**:** ν_{max} 2973, 2930, 2871, 1672, 1604, 1463, 1371, 1284, 1230, 1113, 1013, 955, 756, 696, 521 cm^{-1}

HRMS (ESI) m/z calcd for $C_{13}H_{18}NO_2$ $[M+H]^+$: 220.1338, found: 220.1327

2-butoxy-4-methyl-3,4-dihydroisoquinolin-1(2H)-one, 4d



White solid (52.4 mg), yield: 86%

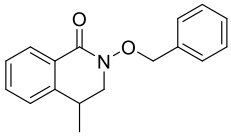
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.13 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.47 (td, *J* = 7.5, 1.5 Hz, 1H), 7.35 (td, *J* = 7.6, 1.3 Hz, 1H), 7.27 – 7.15 (m, 1H), 4.07 (td, *J* = 6.7, 4.5 Hz, 2H), 3.93 (dd, *J* = 11.3, 5.0 Hz, 1H), 3.55 (dd, *J* = 11.3, 6.0 Hz, 1H), 3.27 (q, *J* = 6.2 Hz, 1H), 1.77 – 1.67 (m, 2H), 1.54 – 1.44 (m, 2H), 1.41 (d, *J* = 7.0 Hz, 3H), 0.97 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 163.21 , 142.31 , 132.32 , 128.36 , 127.99 , 127.12 , 125.93 , 74.04 , 54.83 , 33.61 , 30.28 , 19.21 , 13.92 .

IR(neat)**:** ν_{max} 2959, 2872, 1671, 1462, 1285, 1014, 958, 756, 695, 563 cm^{-1}

HRMS (ESI) m/z calcd for $C_{14}H_{20}NO_2$ $[M+H]^+$: 234.1494, found: 234.1484

2-(benzyloxy)-4-methyl-3,4-dihydroisoquinolin-1(2H)-one, 4e



White solid (54.8 mg), yield: 80%

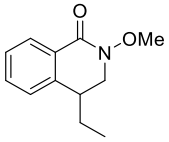
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.15 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.55 – 7.42 (m, 3H), 7.36 (tt, *J* = 7.4, 2.9 Hz, 4H), 7.17 (d, *J* = 7.5 Hz, 1H), 5.12 (d, *J* = 1.6 Hz, 2H), 3.74 (dd, *J* = 11.3, 5.0 Hz, 1H), 3.39 (dd, *J* = 11.3, 6.0 Hz, 1H), 3.10 (d, *J* = 6.4 Hz, 1H), 1.19 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 163.75 , 142.47 , 135.62 , 132.42 , 129.72 , 128.74 , 128.50 , 128.34 , 127.87 , 127.12 , 125.98 , 76.73 , 55.77 , 33.53 , 19.06 .

IR(neat)**:** ν_{max} 2967, 2928, 2872, 1668, 1455, 1285, 982, 753, 696, 556 cm^{-1}

HRMS (ESI) m/z calcd for $C_{17}H_{18}NO_2$ $[M+H]^+$: 268.1338, found: 268.1325

4-ethyl-2-methoxy-3,4-dihydroisoquinolin-1(2H)-one, 4f



Colorless oil (35.4 mg), yield: 69%

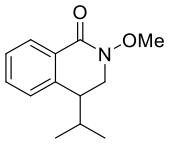
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.05 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.38 (td, *J* = 7.5, 1.5 Hz, 1H), 7.28 (td, *J* = 7.6, 1.3 Hz, 1H), 7.17 – 7.05 (m, 1H), 3.94 (dd, *J* = 11.6, 4.6 Hz, 1H), 3.81 (s, 3H), 3.60 (dd, *J* = 11.6, 3.4 Hz, 1H), 2.84 (dt, *J* = 7.4, 3.6 Hz, 1H), 1.70 (p, *J* = 7.4 Hz, 2H), 0.94 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 162.69 , 141.35 , 132.07 , 128.39 , 127.88 , 127.18 , 127.09 , 61.58 , 51.49 , 40.53 , 26.89 , 11.86 .

IR(neat)**:** ν_{max} 2964, 2929, 2874, 1670, 1458, 1310, 989, 902, 755, 696, 564 cm^{-1}

HRMS (ESI) m/z calcd for $C_{12}H_{16}NO_2$ $[M+H]^+$: 206.1181, found: 206.1171

4-isopropyl-2-methoxy-3,4-dihydroisoquinolin-1(2H)-one, 4g



Colorless oil (50.4 mg), yield: 87%

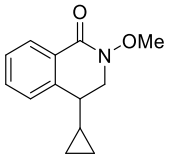
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.12 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.45 (td, *J* = 7.4, 1.6 Hz, 1H), 7.36 (td, *J* = 7.5, 1.4 Hz, 1H), 7.22 – 7.14 (m, 1H), 3.98 (dd, *J* = 12.0, 4.7 Hz, 1H), 3.90 (s, 3H), 3.82 (dd, *J* = 12.0, 2.8 Hz, 1H), 2.70 (ddd, *J* = 7.5, 4.7, 2.8 Hz, 1H), 2.12 – 2.02 (m, 1H), 1.05 (d, *J* = 6.7 Hz, 3H), 0.91 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 162.61 , 140.17 , 131.59 , 128.44 , 128.15 , 127.19 , 61.70 , 49.80 , 45.41 , 30.76 , 20.97 , 20.09 .

IR(neat)**:** ν_{max} 2961, 1669, 1458, 1288, 1025, 944, 895, 762, 713, 584 cm^{-1}

HRMS (ESI) m/z calcd for $C_{13}H_{18}NO_2$ $[M+H]^+$: 220.1338, found: 220.1327

4-cyclopropyl-2-methoxy-3,4-dihydroisoquinolin-1(2H)-one, 4h



Colorless oil (45.5 mg), yield: 81%

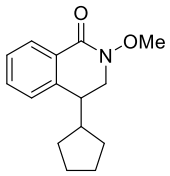
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.15 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.57 – 7.32 (m, 3H), 3.97 (dd, *J* = 11.2, 5.0 Hz, 1H), 3.91 (s, 3H), 3.78 (dd, *J* = 11.2, 6.8 Hz, 1H), 2.42 – 2.26 (m, 1H), 1.16 – 1.01 (m, 1H), 0.78 – 0.58 (m, 2H), 0.46 (dq, *J* = 9.0, 4.9 Hz, 1H), 0.33 (dt, *J* = 9.6, 4.9 Hz, 1H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 162.92 , 140.72 , 132.26 , 128.35 , 127.99 , 127.40 , 126.41 , 61.70 , 53.17 , 44.03 , 14.67 , 5.19 , 3.32 .

IR(neat)**:** ν_{max} 3000, 2931, 1668, 1457, 1290, 1009, 900, 750, 695, 585 cm^{-1}

HRMS (ESI) m/z calcd for $C_{13}H_{16}NO_2$ $[M+H]^+$: 218.1181, found: 218.1171

4-cyclopentyl-2-methoxy-3,4-dihydroisoquinolin-1(2H)-one, 4i



Colorless oil (58 mg), yield: 94%

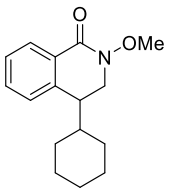
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.12 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.39 (dtd, *J* = 21.9, 7.5, 1.5 Hz, 2H), 7.18 (dd, *J* = 7.4, 1.4 Hz, 1H), 4.04 (dd, *J* = 11.7, 4.2 Hz, 1H), 3.90 (s, 3H), 3.77 (dd, *J* = 11.8, 2.0 Hz, 1H), 2.71 (d, *J* = 11.3 Hz, 1H), 2.25 – 2.10 (m, 1H), 2.03 – 1.92 (m, 1H), 1.72 – 1.25 (m, 7H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 162.57 , 141.10 , 131.62 , 128.28 , 128.07 , 127.81 , 127.20 , 61.76 , 51.85 , 44.79 , 43.02 , 31.53 , 31.24 , 25.09 , 24.73 .

IR(neat)**:** ν_{max} 2949, 2867, 1669, 1474, 1456, 1286, 1022, 1000, 897, 762, 698, 580 cm^{-1}

HRMS (ESI) m/z calcd for $C_{15}H_{20}NO_2$ $[M+H]^+$: 246.1494, found: 246.1484

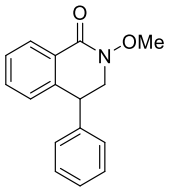
4-cyclohexyl-2-methoxy-3,4-dihydroisoquinolin-1(2H)-one, 4j



Colorless oil (52.5 mg), yield: 81%

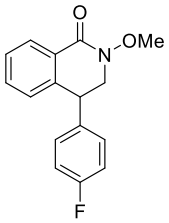
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.11 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.40 (dtd, *J* = 23.3, 7.4, 1.5 Hz, 2H), 7.17 – 7.11 (m, 1H), 3.98 (dd, *J* = 12.0, 4.6 Hz, 1H), 3.90 (s, 3H), 3.85 (dd, *J* = 12.0, 2.5 Hz, 1H), 2.70 (ddd, *J* = 7.3, 4.5, 2.5 Hz, 1H), 1.93 – 1.64 (m, 5H), 1.48 (d, *J* = 11.1 Hz, 1H), 1.21 – 0.95 (m, 5H).
^{13}C NMR (75 MHz, Chloroform-*d*) δ 162.49 , 140.03 , 131.46 , 128.54 , 128.27 , 128.15 , 127.15 , 61.67 , 49.67 , 44.77 , 40.28 , 31.36 , 30.58 , 26.46 , 26.37 , 26.23 .
IR(neat)**:** ν_{max} 2923, 2851, 1670, 1449, 1275, 1020, 997, 892, 838, 697, 572 cm^{-1}
HRMS (ESI) m/z calcd for $C_{16}H_{22}NO_2$ $[M+H]^+$: 260.1651, found: 260.1639

2-methoxy-4-phenyl-3,4-dihydroisoquinolin-1(2H)-one, 4k



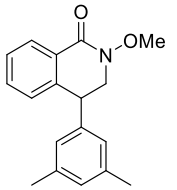
White solid (59.3 mg), yield: 92%
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.24 (q, *J* = 3.8 Hz, 1H), 7.52 – 7.25 (m, 5H), 7.17 (d, *J* = 7.2 Hz, 2H), 6.97 (d, *J* = 5.0 Hz, 1H), 4.47 (q, *J* = 5.4 Hz, 1H), 4.22 – 4.00 (m, 1H), 3.91 (t, *J* = 9.6 Hz, 1H), 3.71 (d, *J* = 3.2 Hz, 3H).
^{13}C NMR (75 MHz, Chloroform-*d*) δ 163.15 , 140.46 , 139.87 , 132.51 , 128.85 , 128.46 , 128.41 , 127.79 , 127.61 , 61.68 , 54.87 , 45.36 .
IR(neat)**:** ν_{max} 2932, 1669, 1453, 1325, 1288, 1010, 902, 729, 695, 645, 590, 514 cm^{-1}
HRMS (ESI) m/z calcd for $C_{16}H_{16}NO_2$ $[M+H]^+$: 254.1181, found: 254.1170

4-(4-fluorophenyl)-2-methoxy-3,4-dihydroisoquinolin-1(2H)-one, 4l



White solid (62.2 mg), yield: 91%
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.23 (dd, *J* = 7.0, 2.3 Hz, 1H), 7.42 (td, *J* = 7.8, 6.8, 3.9 Hz, 2H), 7.15 (dd, *J* = 8.6, 5.4 Hz, 2H), 7.09 – 6.91 (m, 3H), 4.55 – 4.36 (m, 1H), 4.11 (dd, *J* = 11.4, 5.3 Hz, 1H), 3.86 (dd, *J* = 11.5, 7.2 Hz, 1H), 3.72 (s, 3H).
^{13}C NMR (75 MHz, Chloroform-d) δ 163.13 , 162.08 (d, J = 246.6 Hz), 139.62 , 136.26 (d, J = 3.3 Hz), 132.63 , 129.98 (d, J = 8.0 Hz), 128.73 , 128.53 , 127.74 (d, J = 7.4 Hz), 115.89 , 115.61 , 61.72 , 54.93 , 44.60 .
^{19}F NMR (282 MHz, Chloroform-*d*) δ -114.68 .
IR(neat)**:** ν_{max} 2932, 1669, 1601, 1507, 1222, 1159, 1010, 903, 837, 778, 742, 694, 587 cm^{-1}
HRMS (ESI) m/z calcd for $C_{16}H_{15}FNO_2$ $[M+H]^+$: 272.1087, found: 272.1074

4-(3,5-dimethylphenyl)-2-methoxy-3,4-dihydroisoquinolin-1(2H)-one, 4m



White solid (68.1 mg), yield: 96%

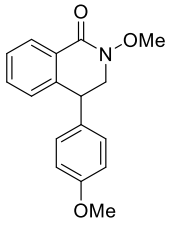
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.40 – 8.08 (m, 1H), 7.50 – 7.32 (m, 2H), 6.95 (d, *J* = 8.7 Hz, 2H), 6.80 (s, 2H), 4.39 (dd, *J* = 8.1, 5.5 Hz, 1H), 4.06 (dd, *J* = 11.4, 5.5 Hz, 1H), 3.91 (dd, *J* = 11.4, 8.1 Hz, 1H), 3.75 (s, 3H), 2.29 (s, 6H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 163.25 , 140.29 , 140.25 , 138.41 , 132.43 , 129.25 , 128.70 , 128.35 , 127.79 , 127.47 , 126.29 , 61.69 , 54.79 , 45.36 , 21.35 .

IR(neat)**:** ν_{max} 2928, 1672, 1603, 1455, 1286, 1001, 770, 696 cm^{-1}

HRMS (ESI) m/z calcd for $C_{18}H_{20}NO_2$ $[M+H]^+$: 282.1494, found: 282.1482

2-methoxy-4-(4-methoxyphenyl)-3,4-dihydroisoquinolin-1(2H)-one, 4n



Colorless oil (61.3 mg), yield: 86%

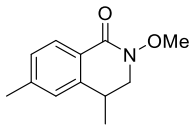
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.39 – 8.07 (m, 1H), 7.48 – 7.34 (m, 2H), 7.14 – 7.03 (m, 2H), 7.02 – 6.92 (m, 1H), 6.92 – 6.83 (m, 2H), 4.42 (dd, *J* = 7.7, 5.4 Hz, 1H), 4.07 (dd, *J* = 11.4, 5.3 Hz, 1H), 3.87 (dd, *J* = 11.4, 7.7 Hz, 1H), 3.80 (s, 3H), 3.73 (s, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 163.18 , 158.93 , 140.29 , 132.47 , 132.42 , 129.49 , 128.73 , 128.39 , 127.72 , 127.53 , 114.18 , 61.70 , 55.30 , 54.97 , 44.61 .

IR(neat)**:** ν_{max} 2931, 1669, 1509, 1456, 1246, 1178, 1031, 1008, 903, 833, 774, 740, 695, 559 cm^{-1}

HRMS (ESI) m/z calcd for $C_{17}H_{18}NO_3$ $[M+H]^+$: 284.1287, found: 284.1273

2-methoxy-4,6-dimethyl-3,4-dihydroisoquinolin-1(2H)-one, 4o-1



Colorless oil (31.3 mg), yield: 57%

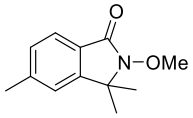
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.02 (d, *J* = 7.9 Hz, 1H), 7.16 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.02 (s, 1H), 3.97 – 3.83 (m, 4H), 3.52 (dd, *J* = 11.2, 5.9 Hz, 1H), 3.22 (q, *J* = 6.2 Hz, 1H), 2.39 (s, 3H), 1.40 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 163.34 , 143.02 , 142.36 , 128.47 , 127.99 , 126.64 , 125.10 , 61.59 , 54.19 , 33.52 , 21.67 , 19.22 .

IR(neat)**:** ν_{max} 2966, 2928, 1668, 1611, 1459, 1284, 1019, 898, 774, 695, 608 cm^{-1}

HRMS (ESI) m/z calcd for $C_{12}H_{16}NO_2$ $[M+H]^+$: 206.1181, found: 206.1170

2-methoxy-3,3,5-trimethylisoindolin-1-one, 4o-2



White solid (6.7 mg), yield: 12%

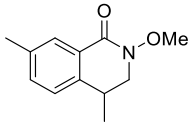
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.72 (d, *J* = 7.7 Hz, 1H), 7.25 (d, *J* = 7.7 Hz, 1H), 7.15 (s, 1H), 4.06 (s, 3H), 2.46 (s, 3H), 1.55 (s, 6H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 164.33 , 149.12 , 142.98 , 129.14 , 125.70 , 123.70 , 121.19 , 65.30 , 63.35 , 25.09 , 22.12 .

IR(neat)**:** ν_{max} 2978, 2927, 1698, 1344, 986, 697, 547 cm^{-1}

HRMS (ESI) m/z calcd for $C_{12}H_{16}NO_2$ $[M+H]^+$: 206.1181, found: 206.1170

2-methoxy-4,7-dimethyl-3,4-dihydroisoquinolin-1(2H)-one, 4p-1



Colorless oil (27.1 mg), yield: 51%

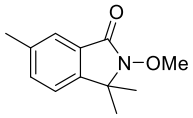
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.00 – 7.87 (m, 1H), 7.32 – 7.25 (m, 1H), 7.11 (d, *J* = 7.8 Hz, 1H), 4.00 – 3.81 (m, 4H), 3.53 (dd, *J* = 11.3, 6.1 Hz, 1H), 3.24 (q, *J* = 6.3 Hz, 1H), 2.37 (s, 3H), 1.39 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 163.21 , 139.40 , 136.94 , 133.22 , 128.67 , 127.52 , 125.91 , 61.55 , 54.22 , 33.16 , 20.97 , 19.17 .

IR(neat)**:** ν_{max} 2966, 2928, 1670, 1425, 1287, 1032, 1008, 837, 825, 781, 562 cm^{-1}

HRMS (ESI) m/z calcd for $C_{12}H_{16}NO_2$ $[M+H]^+$: 206.1181, found: 206.1171

2-methoxy-3,3,6-trimethylisoindolin-1-one, 4p-2



Colorless oil (5.9 mg), yield: 11%

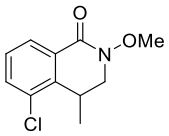
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.64 (dt, *J* = 1.6, 0.8 Hz, 1H), 7.41 – 7.33 (m, 1H), 7.24 (d, *J* = 7.8 Hz, 1H), 4.06 (s, 3H), 2.43 (s, 3H), 1.54 (s, 6H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 164.19 , 146.07 , 138.24 , 133.11 , 128.44 , 124.03 , 120.45 , 77.24 , 65.27 , 63.37 , 25.13 , 21.38 .

IR(neat)**:** ν_{max} 2977, 2935, 1710, 1493, 1436, 1331, 1077, 992, 833, 704, 572 cm^{-1}

HRMS (ESI) m/z calcd for $C_{12}H_{16}NO_2$ $[M+H]^+$: 206.1181, found: 206.1171

5-chloro-2-methoxy-4-methyl-3,4-dihydroisoquinolin-1(2H)-one, 4q-1



Colorless oil (29.5 mg), yield: 52%

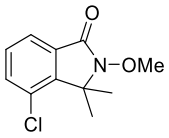
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.08 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.51 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.31 (t, *J* = 7.9 Hz, 1H), 4.12 – 4.04 (m, 1H), 3.89 (s, 3H), 3.60 – 3.51 (m, 2H), 1.41 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 161.41 , 139.95 , 133.15 , 132.14 , 129.53 , 128.18 , 127.27 , 61.39 , 53.42 , 31.31 , 18.27 .

IR(neat)**:** ν_{max} 2970, 2931, 1672, 1440, 1284, 1322, 1120, 1019, 909, 826, 753, 569 cm^{-1}

HRMS (ESI) m/z calcd for $C_{11}H_{13}ClNO_2$ $[M+H]^+$: 226.0635, found: 226.0625

4-chloro-2-methoxy-3,3-dimethylisoindolin-1-one, 4q-2



Colorless oil (14 mg), yield: 25%

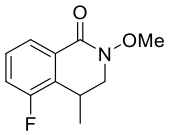
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.77 (dd, *J* = 7.4, 1.1 Hz, 1H), 7.51 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.40 (dd, *J* = 8.1, 7.4 Hz, 1H), 4.10 (s, 3H), 1.71 (s, 6H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 161.90 , 143.95 , 133.30 , 131.42 , 129.65 , 128.55 , 122.33 , 65.37 , 64.51 , 22.12 .

IR(neat)**:** ν_{max} 2994, 2940, 1710, 1456, 1349, 1095, 994, 756, 705, 561 cm^{-1}

HRMS (ESI) m/z calcd for $C_{11}H_{13}ClNO_2$ $[M+H]^+$: 226.0635, found: 226.0625

5-fluoro-2-methoxy-4-methyl-3,4-dihydroisoquinolin-1(2H)-one, 4r-1



Colorless oil (17.1 mg), yield: 32%

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.48 – 7.37 (m, 1H), 7.10 – 6.96 (m, 2H), 3.97 (dd, *J* = 11.8, 4.7 Hz, 1H), 3.89 (s, 3H), 3.55 (dd, *J* = 11.8, 5.3 Hz, 1H), 3.25 (dt, *J* = 7.1, 5.1 Hz, 1H), 1.41 (d, *J* = 7.0 Hz, 3H).

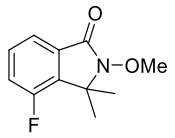
^{13}C NMR (75 MHz, Chloroform-d) δ 164.19 , 160.70 , 159.51 (d, J = 3.9 Hz), 145.29 , 133.64 (d, J = 10.0 Hz), 121.89 (d, J = 3.9 Hz), 115.96 (d, J = 22.3 Hz), 61.70 , 53.62 , 34.02 (d, J = 2.2 Hz), 19.34 .

^{19}F NMR (282 MHz, Chloroform-*d*) δ -110.90 (d, *J* = 5.0 Hz).

IR(neat)**:** ν_{max} 2969, 2932, 1671, 1612, 1468, 1251, 1004, 900, 805, 691, 563 cm^{-1}

HRMS (ESI) m/z calcd for $C_{11}H_{13}FNO_2$ $[M+H]^+$: 210.0930, found: 210.0919

4-fluoro-2-methoxy-3,3-dimethylisoindolin-1-one, 4r-2



Colorless oil (24.6 mg), yield: 46%

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.55 (ddd, *J* = 8.4, 7.6, 4.8 Hz, 1H), 7.20 – 7.02 (m, 2H), 4.06 (s, 3H), 1.57 (s, 6H).

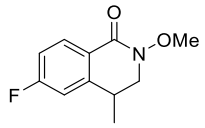
^{13}C NMR (75 MHz, Chloroform-d) δ 161.30 (d, J = 2.2 Hz), 160.48 , 157.02 , 151.32 (d, J = 2.6 Hz), 134.21 (d, J = 7.7 Hz), 116.75 (d, J = 4.1 Hz), 115.78 (d, J = 13.3 Hz), 115.54 (d, J = 19.3 Hz), 65.31 , 63.27 (d, J = 1.4 Hz), 25.09 .

^{19}F NMR (282 MHz, Chloroform-*d*) δ -116.85 (dd, *J* = 9.2, 5.0 Hz).

IR(neat)**:** ν_{max} 2981, 2942, 1702, 1479, 1343, 1249, 1108, 976, 857, 804, 776, 690, 554 cm^{-1}

HRMS (ESI) m/z calcd for $C_{11}H_{13}FNO_2$ $[M+H]^+$: 210.0930, found: 210.0919

6-fluoro-2-methoxy-4-methyl-3,4-dihydroisoquinolin-1(2H)-one, 4s-1



Colorless oil (36.8 mg), yield: 68%

^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.15 (dd, *J* = 8.7, 5.9 Hz, 1H), 7.12 – 6.78 (m, 2H), 3.98 – 3.83 (m, 4H), 3.56 (dd, *J* = 11.3, 6.5 Hz, 1H), 3.28 (q, *J* = 6.4 Hz, 1H), 1.42 (d, *J* = 7.0 Hz, 3H).

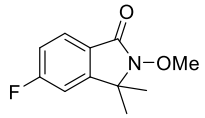
^{13}C NMR (75 MHz, Chloroform-*d*) δ 165.28 (d, *J* = 253.2 Hz), 162.42 , 145.27 (d, *J* = 8.4 Hz), 131.24 (d, *J* = 9.5 Hz), 124.11 (d, *J* = 2.8 Hz), 114.45 (d, *J* = 21.9 Hz), 112.89 (d, *J* = 22.4 Hz), 61.73 , 53.97 , 33.52 (d, *J* = 1.6 Hz), 18.76 .

^{19}F NMR (282 MHz, Chloroform-*d*) δ -106.51 (d, *J* = 5.9 Hz)

IR(neat)**:** ν_{max} 2970, 2933, 1671, 1611, 1478, 1401, 1254, 1018, 944, 772, 689, 609 cm^{-1}

HRMS (ESI) m/z calcd for $C_{11}H_{13}FNO_2$ $[M+H]^+$: 210.0930, found: 210.0919

5-fluoro-2-methoxy-3,3-dimethylisoindolin-1-one, 4s-2



Colorless oil (7 mg), yield: 13%

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.83 (dd, *J* = 8.4, 5.1 Hz, 1H), 7.14 (ddd, *J* = 9.2, 8.4, 2.3 Hz, 1H), 7.05 (dd, *J* = 8.1, 2.3 Hz, 1H), 4.06 (s, 3H), 1.56 (s, 6H).

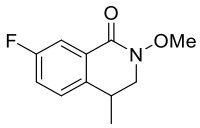
^{13}C NMR (75 MHz, Chloroform-*d*) δ 165.53 (d, *J* = 252.5 Hz), 163.26 , 151.25 (d, *J* = 9.1 Hz), 126.21 (d, *J* = 9.6 Hz), 124.41 (d, *J* = 2.4 Hz), 115.96 (d, *J* = 23.3 Hz), 108.39 (d, *J* = 23.9 Hz), 65.40 , 63.35 (d, *J* = 2.5 Hz), 24.98 .

^{19}F NMR (282 MHz, Chloroform-*d*) δ -105.47 (d, *J* = 5.1 Hz).

IR(neat)**:** ν_{max} 3054, 2974, 2942, 1701, 1480, 1346, 1213, 1064, 989, 893, 835, 777, 682, 551 cm^{-1}

HRMS (ESI) m/z calcd for $C_{11}H_{13}FNO_2$ $[M+H]^+$: 210.0930, found: 210.0920

7-fluoro-2-methoxy-4-methyl-3,4-dihydroisoquinolin-1(2H)-one, 4t-1



Colorless oil (39.8 mg), yield: 73%

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.81 (dd, *J* = 9.2, 2.6 Hz, 1H), 7.27 – 7.01 (m, 2H), 3.94 (dd, *J* = 11.4, 5.0 Hz, 1H), 3.89 (s, 3H), 3.55 (dd, *J* = 11.4, 6.1 Hz, 1H), 3.34 – 3.20 (m, 1H), 1.41 (d, *J* = 7.0 Hz, 3H).

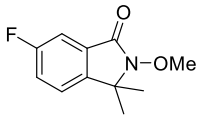
^{13}C NMR (75 MHz, Chloroform-*d*) δ 162.67 (d, *J* = 123.3 Hz), 160.23 , 138.05 (d, *J* = 3.2 Hz), 129.87 (d, *J* = 7.5 Hz), 127.87 (d, *J* = 7.7 Hz), 119.47 (d, *J* = 21.9 Hz), 114.92 (d, *J* = 23.4 Hz), 61.67 , 54.09 , 32.95 , 19.23 .

^{19}F NMR (282 MHz, Chloroform-*d*) δ -114.54 (d, *J* = 5.3 Hz).

IR(neat)**:** ν_{max} 2969, 2933, 1672, 1588, 1493, 1434, 1290, 1243, 1023, 848, 767, 570 cm^{-1}

HRMS (ESI) m/z calcd for $C_{11}H_{13}FNO_2$ $[M+H]^+$: 210.0930, found: 210.0921

6-fluoro-2-methoxy-3,3-dimethylisoindolin-1-one, 4t-2



White solid (7 mg), yield: 13%

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.51 (dd, *J* = 7.6, 2.4 Hz, 1H), 7.38 – 7.21 (m, 2H), 4.07 (d, *J* = 0.9 Hz, 3H), 1.56 (d, *J* = 0.8 Hz, 6H).

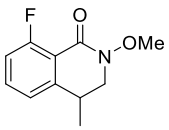
^{13}C NMR (75 MHz, Chloroform-*d*) δ 164.27 , 162.79 (d, *J* = 3.3 Hz), 160.99 , 144.22 (d, *J* = 2.8 Hz), 130.57 (d, *J* = 8.5 Hz), 122.49 (d, *J* = 8.3 Hz), 119.60 (d, *J* = 23.6 Hz), 110.69 (d, *J* = 23.6 Hz), 65.31 , 63.42 , 25.07 .

^{19}F NMR (282 MHz, Chloroform-*d*) δ -111.32 – -113.36 (m).

IR(neat)**:** ν_{max} 2985, 2943, 1698, 1488, 1351, 1236, 1179, 990, 832, 724, 578 cm^{-1}

HRMS (ESI) m/z calcd for $C_{11}H_{13}FNO_2$ $[M+H]^+$: 210.0930, found: 210.0920

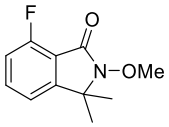
8-fluoro-2-methoxy-4-methyl-3,4-dihydroisoquinolin-1(2H)-one, 4u-1



Colorless oil (34.3 mg), yield: 64%

^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.01 – 7.85 (m, 1H), 7.33 (td, *J* = 7.8, 5.1 Hz, 1H), 7.26 – 7.15 (m, 1H), 4.07 (dd, *J* = 11.6, 4.6 Hz, 1H), 3.89 (s, 3H), 3.62 – 3.44 (m, 2H), 1.41 (d, *J* = 7.0 Hz, 3H).
^{13}C NMR (75 MHz, Chloroform-*d*) δ 161.67 (d, *J* = 3.3 Hz), 160.43 , 157.16 , 129.52 (d, *J* = 18.0 Hz), 128.36 (d, *J* = 8.1 Hz), 124.06 (d, *J* = 3.4 Hz), 119.07 (d, *J* = 21.6 Hz), 61.39 , 53.70 , 27.46 (d, *J* = 2.3 Hz), 19.30 .
^{19}F NMR (282 MHz, Chloroform-*d*) δ -121.28 (dd, *J* = 9.3, 5.4 Hz).
IR(neat)**:** ν_{max} 2971, 2932, 1673, 1581, 1476, 1452, 1287, 1244, 1023, 945, 860, 814, 751, 511 cm^{-1}
HRMS (ESI) m/z calcd for $C_{11}H_{13}FNO_2$ $[M+H]^+$: 210.0930, found: 210.0918

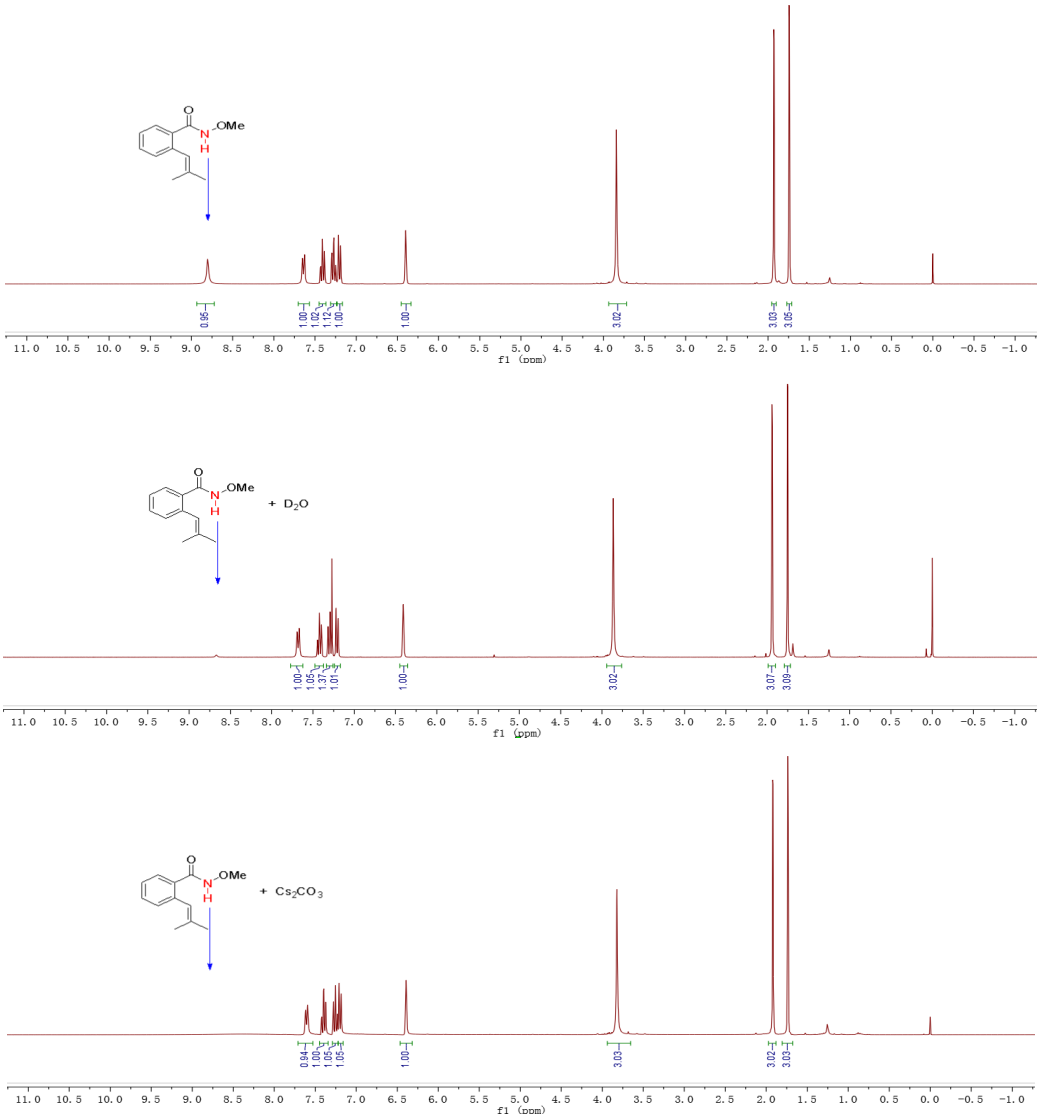
7-fluoro-2-methoxy-3,3-dimethylisoindolin-1-one, 4u-2



White solid (8 mg), yield: 15%
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.65 (d, *J* = 7.5 Hz, 1H), 7.44 (ddd, *J* = 8.3, 7.5, 4.6 Hz, 1H), 7.30 – 7.17 (m, 1H), 4.08 (s, 3H), 1.66 (s, 6H).
^{13}C NMR (75 MHz, Chloroform-*d*) δ 162.47 (d, *J* = 2.4 Hz), 158.75 , 155.42 , 133.95 (d, *J* = 15.7 Hz), 131.57 (d, *J* = 4.5 Hz), 130.20 (d, *J* = 6.8 Hz), 119.75 (d, *J* = 3.8 Hz), 119.29 (d, *J* = 20.1 Hz), 65.38 , 62.66 (d, *J* = 2.7 Hz), 23.60 .
^{19}F NMR (282 MHz, Chloroform-*d*) δ -121.53 (dd, *J* = 9.5, 4.6 Hz).
IR(neat)**:** ν_{max} 2983, 2940, 1713, 1595, 1485, 1464, 1346, 1246, 1056, 1015, 968, 850, 813, 754, 579 cm^{-1}
HRMS (ESI) m/z calcd for $C_{11}H_{13}FNO_2$ $[M+H]^+$: 210.0930, found: 210.0919

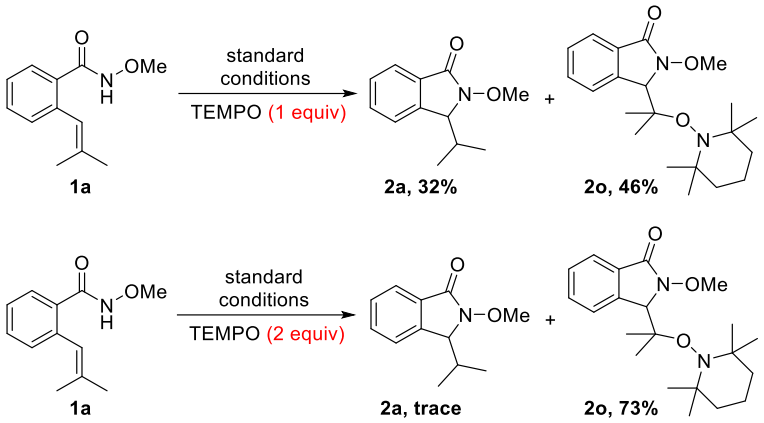
5. Mechanistic investigations

5.1 ^{1}H NMR Study on the effect of base with 1a



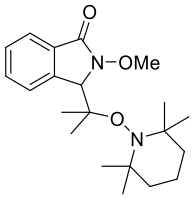
Under the basic condition (Cs_2CO_3 in $CDCl_3$), the signal of N-H disappeared in proton nuclear magnetic resonance (^{1}H NMR) spectra after stirring at room temperature for 30 min. These results suggested that the Cs_2CO_3 is able to abstract the proton of the N-H bond of N-methoxy-2-(2-methylprop-1-en-1-yl) benzamide to generate the corresponding nitrogen anion intermediate.

5.2 Radical Trapping Experiments



To a Schlenk tube were added 2a (51.32 mg, 0.25 mmol), 4CzIPN (3.94 mg, 0.005 mmol, 2 mol%), Cs_2CO_3 (24.4mg, 0.075mmol, 30 mol%) and TEMPO (39 mg, 0.25 mmol, 1 equiv.). The tube was degassed and refilled with N_2 three times, anhydrous DCE (2.5 mL) was added before m-toluenethiol (5.94 μL, 0.05 mmol, 20 mol%) via a syringe. The mixture was then placed around the Blue LEDs (450 nm, 100% light intensity) and stirred until the substrate was consumed (monitored by TLC), the solvent was removed by rotary evaporation and the resulting residue was purified directly by flash column chromatography (33% EtOAc in hexanes) to give the desired product 2p as a white solid (42 mg, 46% yield). When the amount of TEMPO is increased to 2.0 equivalents, the yield of 2o increased from 46% to 73%, which indicates that the reaction is likely to involve a free radical process.

2-methoxy-3-(2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)propan-2-yl)isoindolin-1-one, 2o



White solid (41.6 mg / 64 mg), yield: 46% / 73%

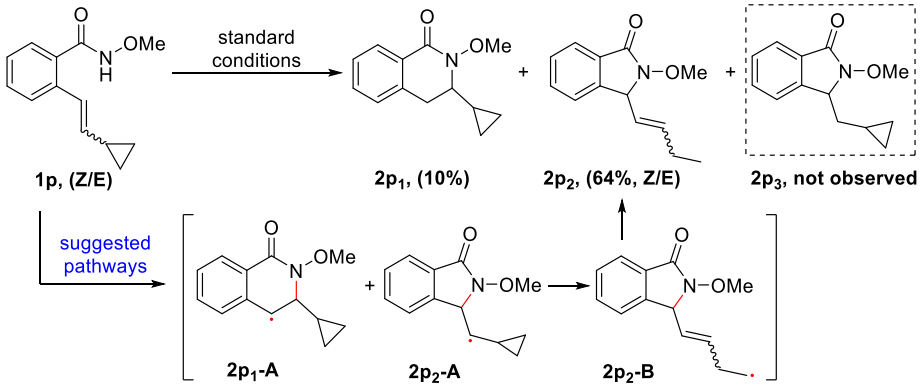
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.92 (d, *J* = 7.7 Hz, 1H), 7.87 – 7.78 (m, 1H), 7.57 (td, *J* = 7.6, 1.4 Hz, 1H), 7.52 – 7.43 (m, 1H), 4.98 (s, 1H), 3.94 (s, 3H), 1.57 (s, 9H), 1.28 (s, 6H), 1.22 (s, 3H), 1.17 (s, 3H), 0.98 (s, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 141.93 , 132.06 , 128.32 , 125.41 , 123.43 , 81.99 , 66.31 , 62.17 , 59.80 , 59.53 , 41.04 , 40.94 , 35.41 , 34.75 , 24.04 , 23.47 , 22.17 , 21.37 , 17.18 .

IR(neat)**:** ν_{max} 2931, 1717, 1467, 1376, 1362, 1131, 1011, 913, 734, 682, 562 cm^{-1}

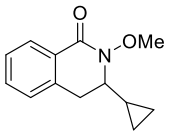
HRMS (ESI) m/z calcd for $C_{21}H_{33}N_2O_3$ $[M+H]^+$: 361.2491, found: 361.2475

5.3 Radical Clock Experiments



Following the standard procedure on 0.25 mmol scale. Purification by column chromatography (33% EtOAc in hexanes) gave $2p_2$ (36 mg, 64% yield) as a colorless oil and $2p_1$ (5.4 mg, 10% yield) as a colorless oil.

3-cyclopropyl-2-methoxy-3,4-dihydroisoquinolin-1(2H)-one, $2p_1$



Colorless oil (5.4 mg), yield: 10%

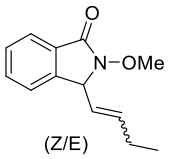
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.13 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.48 – 7.41 (m, 1H), 7.35 (t, *J* = 7.5 Hz, 1H), 7.21 (d, *J* = 7.5 Hz, 1H), 3.93 (s, 3H), 3.39 (dd, *J* = 15.4, 5.3 Hz, 1H), 3.22 – 3.06 (m, 2H), 1.03 (ddt, *J* = 12.4, 8.3, 3.6 Hz, 1H), 0.71 – 0.58 (m, 2H), 0.52 – 0.41 (m, 1H), 0.16 (ddd, *J* = 9.1, 4.6, 1.4 Hz, 1H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 161.21 , 134.44 , 130.44 , 126.69 , 126.35 , 125.84 , 125.30 , 75.49 , 62.76 , 61.25 , 33.34 , 11.87 , 3.23 .

IR(neat)**:** ν_{max} 2929, 1666, 1459, 1385, 1294, 1254, 1091, 1004, 907, 794, 745, 725, 690, 619 cm^{-1}

HRMS (ESI) m/z calcd for $C_{13}H_{16}NO_2$ $[M+H]^+$: 218.1181, found: 218.1171

3-(but-1-en-1-yl)-2-methoxyisoindolin-1-one, $2p_2$



Colorless oil (36 mg), yield: 64%

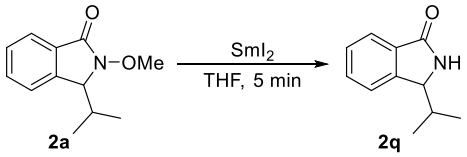
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.84 (d, *J* = 7.0 Hz, 1H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 1H), 7.30 (t, *J* = 9.1 Hz, 1H), 6.23 – 5.87 (m, 1H), 5.54 – 4.99 (m, 2H), 3.97 (d, *J* = 3.8 Hz, 3H), 2.43 – 2.15 (m, 2H), 1.12 (dt, *J* = 27.1, 7.5 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 142.01 , 140.13 , 139.09 , 132.38 , 132.29 , 129.49 , 128.65 , 128.62 , 124.25 , 124.15 , 123.73 , 123.63 , 123.10 , 122.91 , 64.58 , 64.53 , 63.90 , 58.15 , 25.38 , 21.09 , 14.53 , 13.25 .

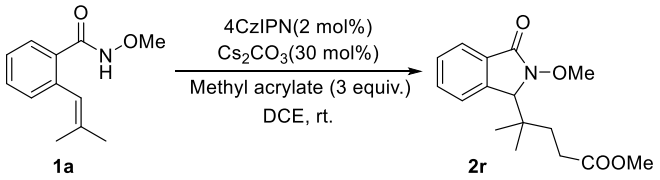
IR(neat)**:** ν_{max} 2964, 2934, 1708, 1467, 1346, 1200, 1162, 1089, 1000, 967, 921, 790, 747, 687, 559, 541 cm^{-1}

HRMS (ESI) m/z calcd for $C_{13}H_{16}NO_2$ $[M+H]^+$: 218.1181, found: 218.1171

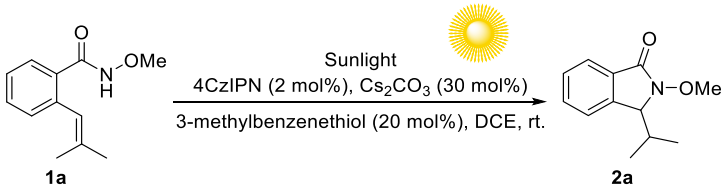
6. Further transformations



A round-bottom flask was charged with 2a (103 mg, 0.5 mmol). The flask was degassed and refilled with N_2 three times. Then SmI_2 (0.1 M in THF, 10 mL, 1 mmol) was added dropwise under N_2. The resulting mixture was stirred at room temperature for 5 min and then the reaction was quenched by the addition of a saturated aqueous solution of $Na_2S_2O_3$. The organic layer was separated and the aqueous layer was extracted with EtOAc. The combined organic solvent was dried over Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure. Purification by column chromatography (34% EtOAc in hexanes) gave 3-isopropylisoindolin-1-one 2q as a white solid (54.34 mg, 62 % yield);

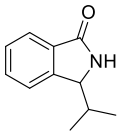


To a Schlenk tube were added 1a (51.32 mg, 0.25 mmol), 4CzIPN (3.94 mg, 0.005 mmol, 2 mol%), Cs_2CO_3(24.4mg, 0.075mmol, 30 mol%). The tube was degassed and refilled with N_2 three times. Anhydrous DCE (2.5 mL) was added before methyl acrylate (68 μL, 0.75 mmol, 3 equiv) via a syringe. The mixture was then placed around the Blue LEDs (450 nm, 100% light intensity) and stirred until the substrate was consumed (monitored by TLC), filtered, the solvent was removed by rotary evaporation and the resulting residue was purified directly by flash column chromatography (50% EtOAc in hexanes) to give the desired product 2r (57 mg, 78% yield).



To a Schlenk tube were added 1a (51.32 mg, 0.25 mmol), 4CzIPN (3.94 mg, 0.005 mmol, 2 mol%), Cs_2CO_3 (24.4mg, 0.075mmol, 30 mol%). The tube was degassed and refilled with N_2 three times, anhydrous DCE (2.5 mL) was added before m-toluenethiol (5.94 μL, 0.05 mmol, 20 mol%) via a syringe. The mixture was placed in the sunlight and stirred until the substrate was consumed (monitored by TLC), the solvent was removed by rotary evaporation and the resulting residue was purified directly by flash column chromatography (33% EtOAc in hexanes) to give the desired product 2a (43.2 mg, 82.44 % yield).

3-isopropylisoindolin-1-one, 2q



White solid (54.34 mg), yield: 62%

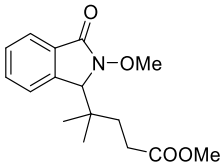
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.17 (s, 1H), 7.86 (d, *J* = 7.4 Hz, 1H), 7.63 – 7.31 (m, 3H), 4.58 (d, *J* = 3.5 Hz, 1H), 2.28 (ddp, *J* = 10.6, 7.0, 3.4 Hz, 1H), 1.12 (d, *J* = 6.9 Hz, 3H), 0.73 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 171.87 , 146.67 , 132.66 , 131.63 , 127.99 , 123.66 , 122.68 , 62.42 , 31.77 , 19.64 , 15.91 .

IR(neat)**:** ν_{max} 3206, 2962, 1685, 1467, 1370, 1315, 1139, 735, 584 cm^{-1}

HRMS (ESI) m/z calcd for $C_{11}H_{14}NO$ $[M+H]^+$: 176.1075, found: 176.1063

methyl 4-(2-methoxy-3-oxoisoindolin-1-yl)-4-methylpentanoate, 2r



Colorless oil (56.7 mg), yield: 78%

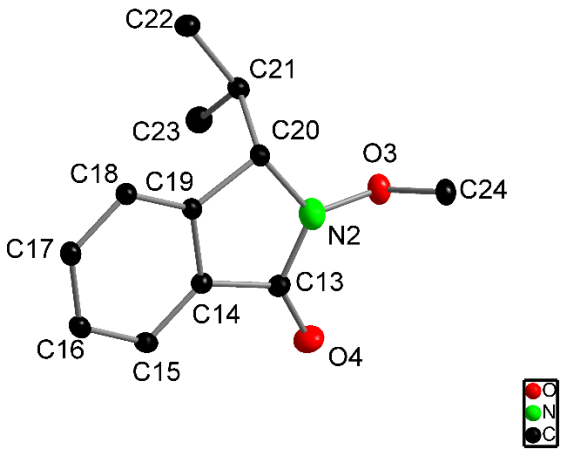
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.86 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.60 – 7.39 (m, 3H), 4.56 (s, 1H), 3.90 (s, 3H), 3.67 (s, 3H), 2.38 (ddd, *J* = 9.9, 6.3, 3.4 Hz, 2H), 1.97 – 1.85 (m, 1H), 1.70 (ddd, *J* = 13.9, 10.3, 6.6 Hz, 1H), 1.10 (s, 3H), 1.02 (s, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 174.09 , 164.88 , 140.48 , 131.47 , 130.90 , 128.51 , 124.42 , 123.83 , 65.88 , 62.21 , 51.79 , 37.97 , 33.84 , 29.19 , 24.40 , 23.98 .

7. X-Ray Date

The remaining non-hydrogen atoms were located from successive difference Fourier map calculations. The refinements were carried out by using full-matrix least-squares techniques on F^2 by using the program SHELXL. In each case, the locations of the largest peaks in the final difference Fourier map calculations, as well as the magnitude of the residual electron densities, were of no chemical significance. Positional parameters, hydrogen atom parameters, thermal parameters, bond distances and angles have been deposited as supporting information.

Crystal Structure Report for cu_20211228_Yang1_0m. (2a).



A colorless block-like specimen of $C_{12}H_{15}NO_2$, approximate dimensions 0.13 mm x 0.12 mm x 0.1 mm, was used for the single-crystal X-ray crystallographic analysis. The X-ray intensity data were measured. All structures were solved by using the program SHELXS/T and Olex2. Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as a supplementary publication no. CCDC 2131719. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+(44)1223-336-033; email: deposit@ccdc.cam.ac.uk)

Crystal data and structure refinement for cu_20211228_Yang1_0m.

Identification code	cu_20211228_Yang1_0m
Empirical formula	$C_{12}H_{15}NO_2$
Formula weight	205.25
Temperature / K	193.00
Crystal system	triclinic
Space group	P-1
a / Å	8.9132(5)
b / Å	11.7925(6)
c / Å	12.0168(6)
α /°	71.738(3)

β /°	69.902(3)
γ /°	72.397(3)
Volume / Å^3	1099.23(10)
Z	4
ρ $_{calc}$ / mg mm^{-3}	1.240
μ / mm^{-1}	0.680
F(000)	440.0
Crystal size / mm^3	0.13 × 0.12 × 0.1
2Θ range for data collection	8.058 to 137.114°
Index ranges	-10 ≤ h ≤ 10, -14 ≤ k ≤ 14, -14 ≤ l ≤ 14
Reflections collected	19166
Independent reflections	4022 [Rint = 0.0417, Rsigma = 0.0362]
Data/restraints/parameters	4022/0/277
Goodness-of-fit on F^2	1.068
Final R indexes [I>2(I) ， F$_o$>4 (F$_o$)]	R_1 = 0.0390, wR_2 = 0.1046
Final R indexes [all data]	R_1 = 0.0447, wR_2 = 0.1093
Largest diff. peak/hole / e Å^{-3}	0.36/-0.18

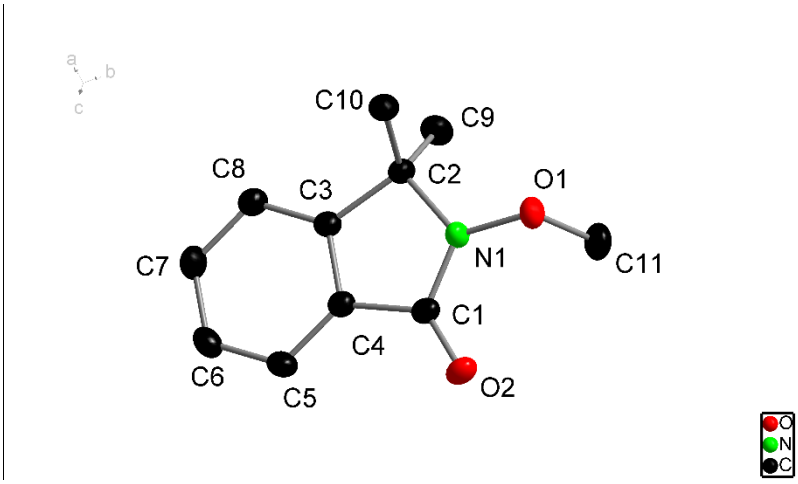
Bond Lengths for cu_20211228_Yang1_0m.

Bond	Length/Å	Bond	Length/Å
O1-N1	1.389(1)	O3-N2	1.391(1)
O1-C12	1.432(2)	O3-C24	1.432(2)
O2-C1	1.221(2)	O4-C13	1.223(2)
N1-C1	1.355(2)	N2-C13	1.358(2)
N1-C8	1.462(2)	N2-C20	1.464(2)
C1-C2	1.479(2)	C13-C14	1.485(2)
C2-C3	1.389(2)	C14-C15	1.383(2)
C2-C7	1.386(2)	C14-C19	1.389(2)
C3-C4	1.380(2)	C15-C16	1.384(2)
C4-C5	1.387(3)	C16-C17	1.389(2)
C5-C6	1.386(2)	C17-C18	1.386(2)
C6-C7	1.387(2)	C18-C19	1.387(2)
C7-C8	1.510(2)	C19-C20	1.511(2)
C8-C9	1.540(2)	C20-C21	1.541(2)
C9-C10	1.518(2)	C21-C22	1.518(2)
C9-C11	1.521(2)	C21-C23	1.525(2)

Bond Angles for cu_20211228_Yang1_0m.

Bond	Angle/°	Bond	Angle/°
N1-O1-C12	110.16(1)	N2-O3-C24	108.96(1)
O1-N1-C8	120.10(1)	C3-N2-C20	119.82(1)
C1-N1-O1	120.97(1)	C13-N2-O3	120.30(1)
C1-N1-C8	116.31(1)	C13-N2-C20	115.93(1)
O2-C1-N1	126.15(1)	O4-C13-N2	126.43(1)
O2-C1-C2	129.88(1)	O4-C13- C14	129.50(1)
N1-C1-C2	103.95(1)	N2-C13-C14	104.05(1)
C3-C2-C1	128.76(1)	C15-C14-C13	128.92(1)
C7-C2-C1	109.50(1)	C15-C14-C19	121.99(1)
C7-C2-C3	121.73(4)	C19-C14-C13	109.06(1)
C4-C3-C2	118.17(2)	C14-C15-C16	118.17(1)
C3-C4-C5	120.55(1)	C15-C16-C17	120.20(1)
C6-C5-C4	121.08(2)	C18-C17-C16	121.47(1)
C5-C6-C7	118.77(2)	C17-C18-C19	118.48(1)
C2-C7-C6	119.69(1)	C14-C19-C20	110.00(1)
C2-C7-C8	109.84(1)	C18-C19-C14	119.63(1)
C6-C7-C8	130.47(1)	C18-C19-C20	130.37(1)
N1-C8-C7	99.59(1)	N2-C20-C19	99.42(1)
N1-C8-C9	111.46(1)	N2-C20-C21	111.56(1)
C7-C8-C9	116.02(1)	C19-C20-C21	115.11(1)
C10-C9-C8	110.58(1)	C22-C21-C20	111.50(1)
C10-C9-C11	110.93(1)	C22-C21-C23	110.80(1)
C11-C9-C8	112.96(1)	C23-C21-C20	112.05(1)

Crystal Structure Report for exp_7641 (4a-2).



A colorless block-like specimen of $C_{11}H_{13}NO_2$, approximate dimensions 0.31 mm x 0.27 mm x 0.13 mm, was used for the single-crystal X-ray crystallographic analysis. The X-ray intensity data were measured. All structures were solved by using the program SHELXS/T and Olex2. Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as a supplementary publication no. CCDC 2125971. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+(44)1223-336-033; email: deposit@ccdc.cam.ac.uk)

Crystal data and structure refinement for exp_7641.

Identification code	exp_7641
Empirical formula	$C_{11}H_{13}NO_2$
Formula weight	191.22
Temperature / K	119(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a / Å	7.332(1)
b / Å	11.641(2)
c / Å	12.03(3)
α /°	90.00
β /°	96.75(1)
γ /°	90.00
Volume / Å^3	1019.80(3)
Z	4
ρ_{calc} / mg mm^{-3}	1.245
μ / mm^{-1}	0.086
F(000)	408

Crystal size / mm^3	0.31 × 0.27 × 0.13
2Θ range for data collection	6.2 to 51.98°
Index ranges	-9 ≤ h ≤ 8, -13 ≤ k ≤ 14, -9 ≤ l ≤ 14
Reflections collected	4091
Independent reflections	1958[R(int) = 0.0335]
Data/restraints/parameters	1958/0/130
Goodness-of-fit on F^2	1.062
Final R indexes [I>2(I) ， F$_o$>4 (F$_o$)]	R_1 = 0.0451, wR_2 = 0.0931
Final R indexes [all data]	R_1 = 0.0625, wR_2 = 0.1048
Largest diff. peak/hole / e Å^{-3}	0.193/-0.232

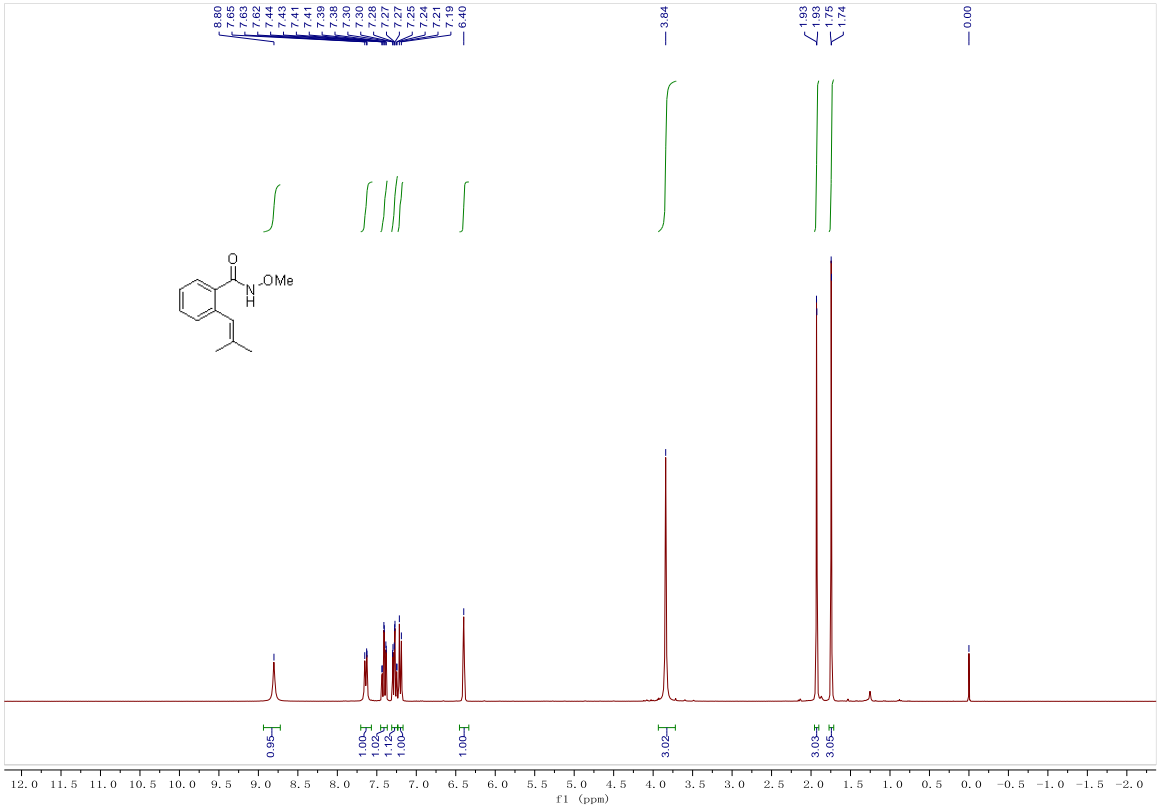
Bond Lengths for exp_7641.

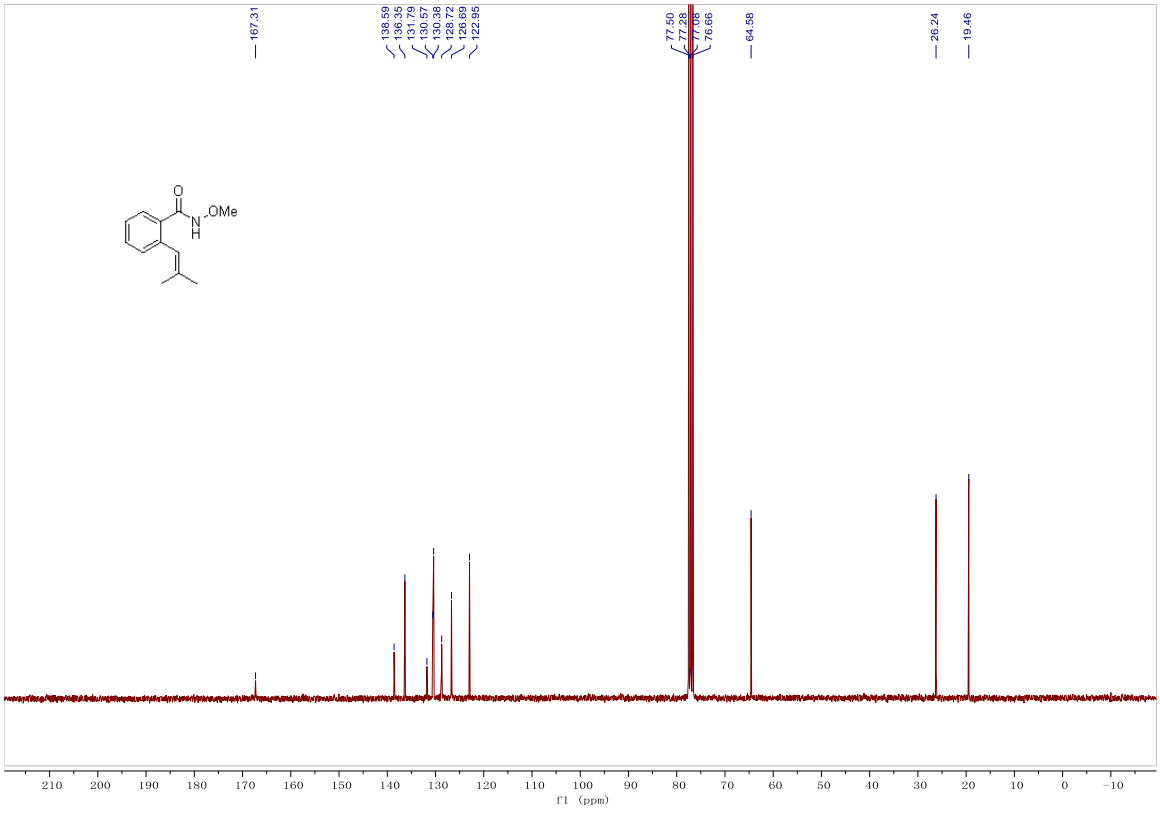
Bond	**Length/Å**	**Bond**	**Length/Å**
O1-N1	1.387 (2)	C4-C5	1.387(2)
O1-C11	1.444(2)	C3-C2	1.515(2)
O2-C1	1.231(2)	C3-C8	1.387(2)
N1-C1	1.355(2)	C2-C10	1.530(2)
N1-C2	1.473(2)	C5-C6	1.385(2)
C1-C4	1.480(2)	C7-C6	1.390(2)
C9-C2	1.526(2)	C7-C8	1.395(2)
C4-C3	1.389(2)		

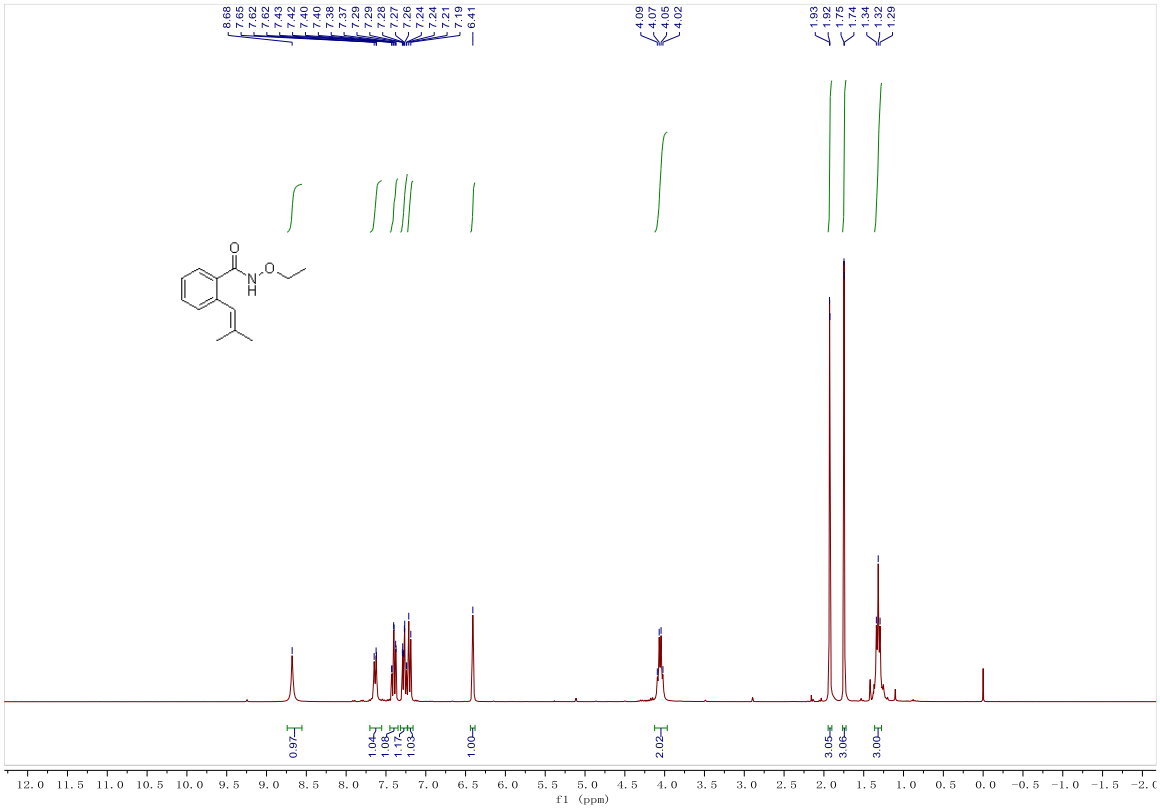
Bond Angles for exp_7641.

Bond	**Angle/°**	**Bond**	**Angle/°**
N1-O1-C11	110.3(1)	C8-C3-C2	128.8(1)
O1-N1-C2	119.6 (1)	N1-C2-C9	110.9(1)
C1-N1-O1	122.1(1)	N1-C2-C3	98.7(1)
C1-N1-C2	116.9(1)	N1-C2-C10	110.9(1)
O2-C1-N1	126.4(2)	C9-C2-C10	110.6(1)
O2-C1-C4	129.4 (2)	C3-C2-C9	113.8(1)
N1-C1-C4	104.2(1)	C3-C2-C10	111.5(1)
C3-C4-C1	109.1(1)	C6-C5-C4	117.8(2)
C5-C4-C1	129.0(2)	C6-C7-C8	121.5(2)
C5-C4-C3	121.9(2)	C5-C6-C7	120.6(2)
C4-C3-C2	110.8(1)	C3-C8-C7	117.9(2)
C8-C3-C4	120.3(2)		

8. NMR spectra



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4.07
4.05
4.02
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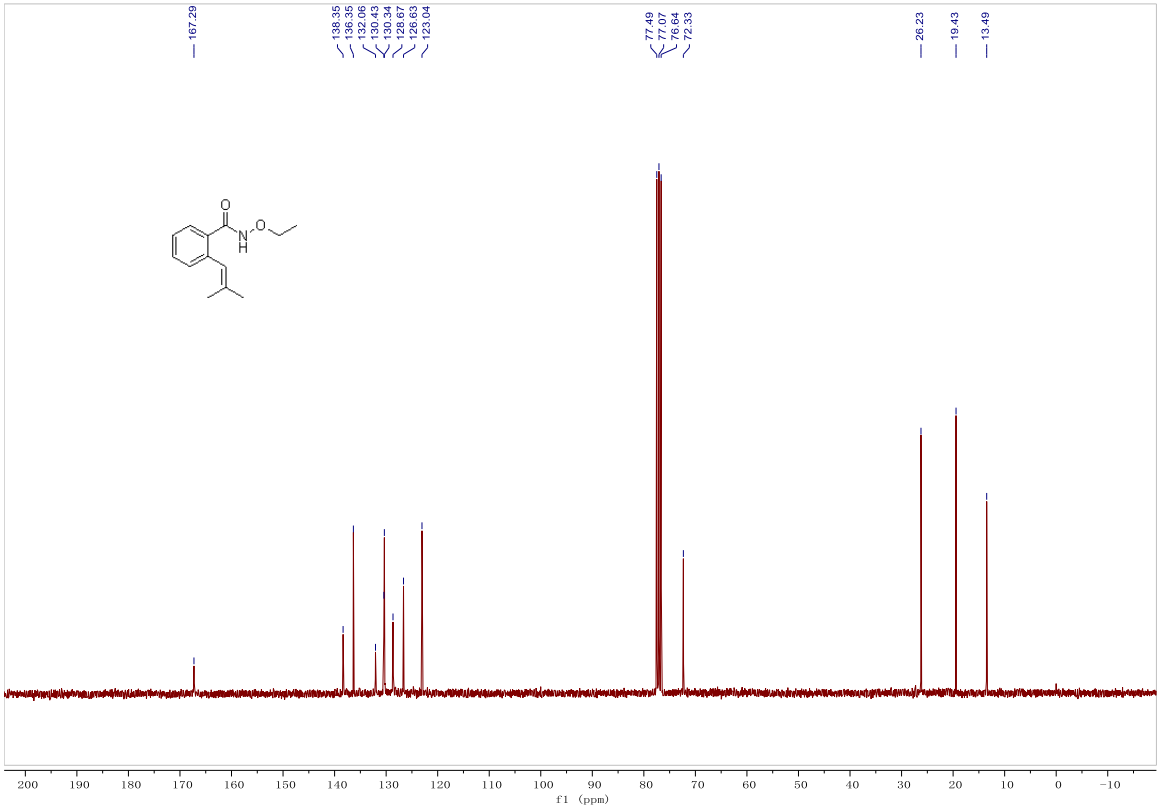
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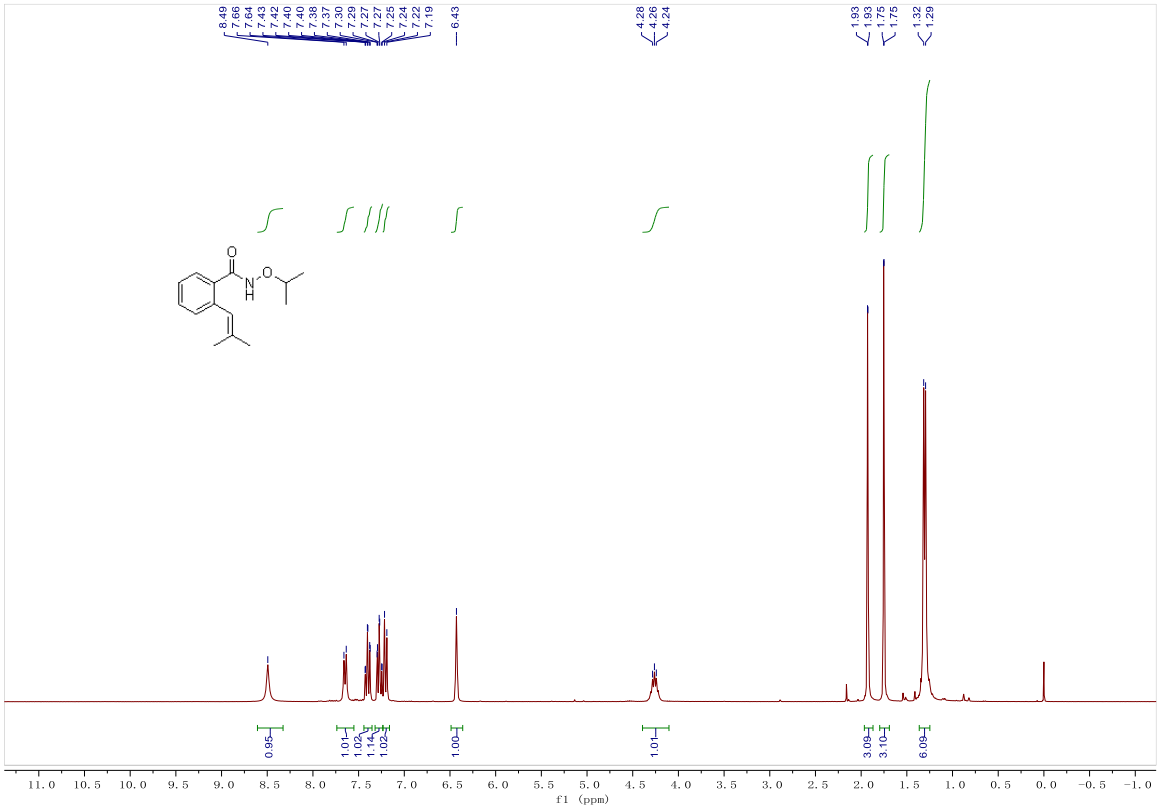
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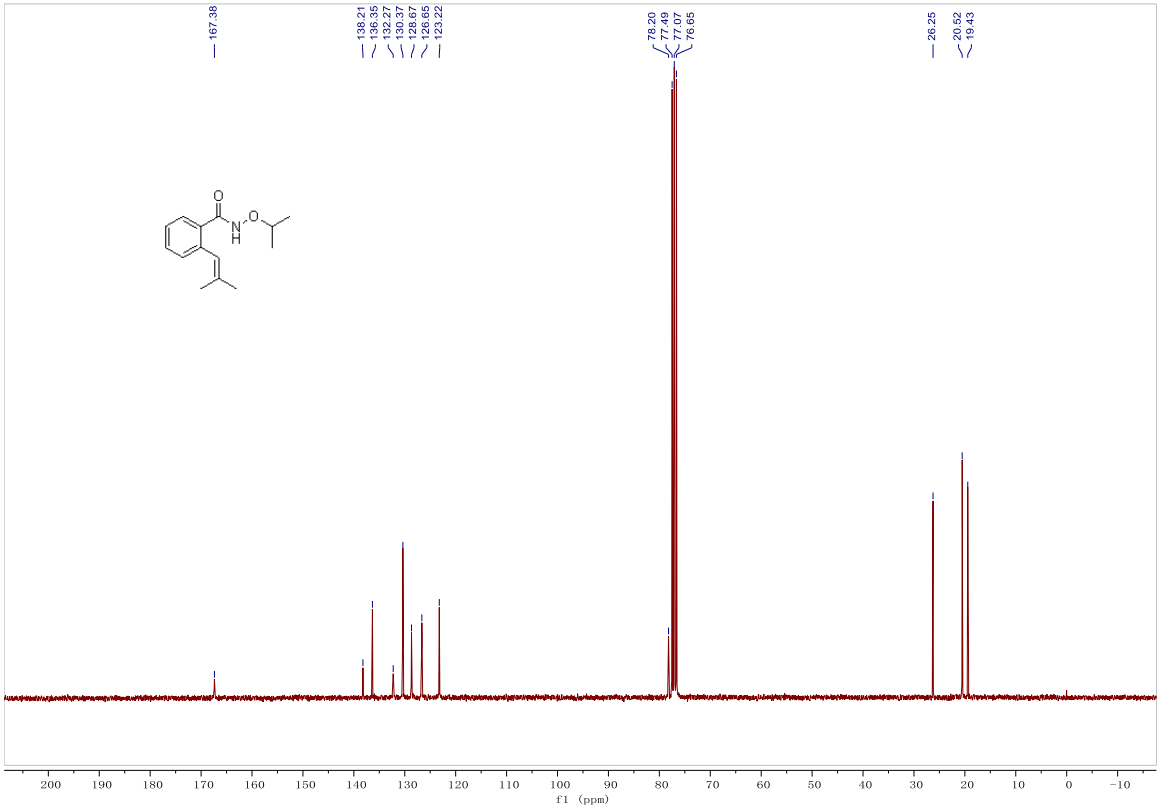
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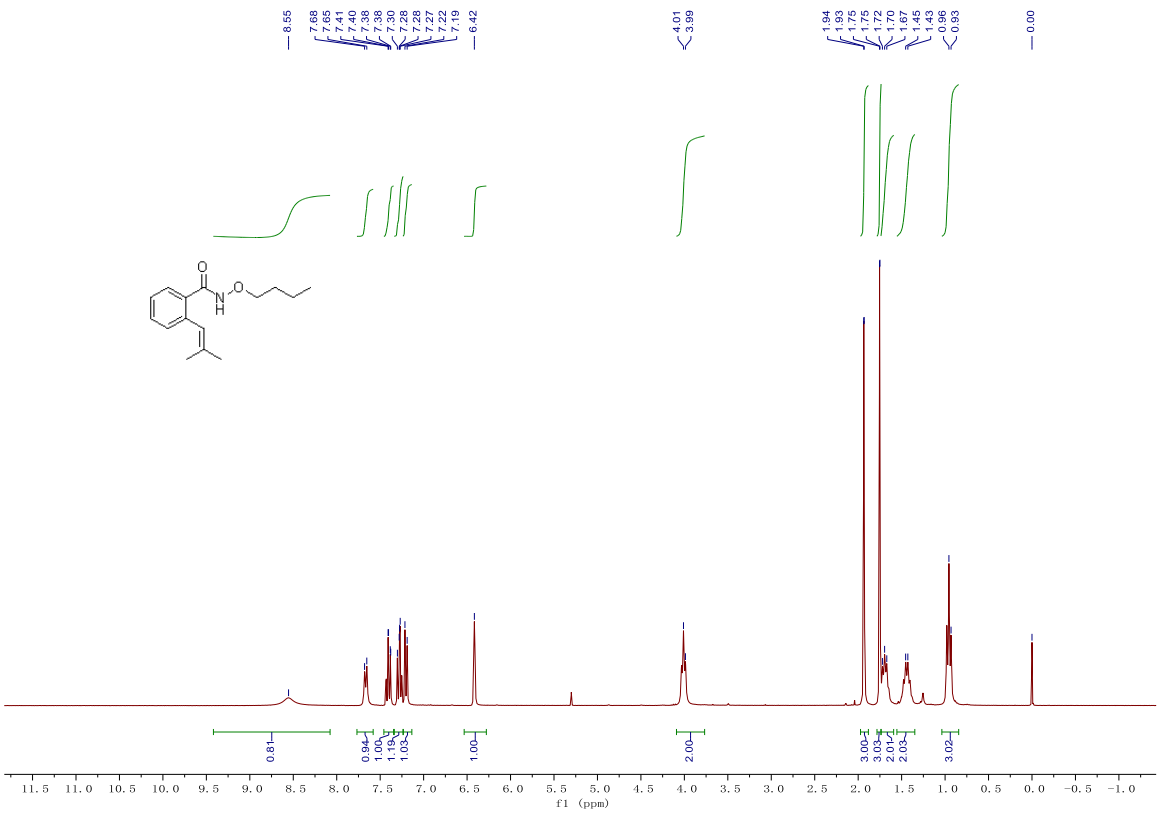
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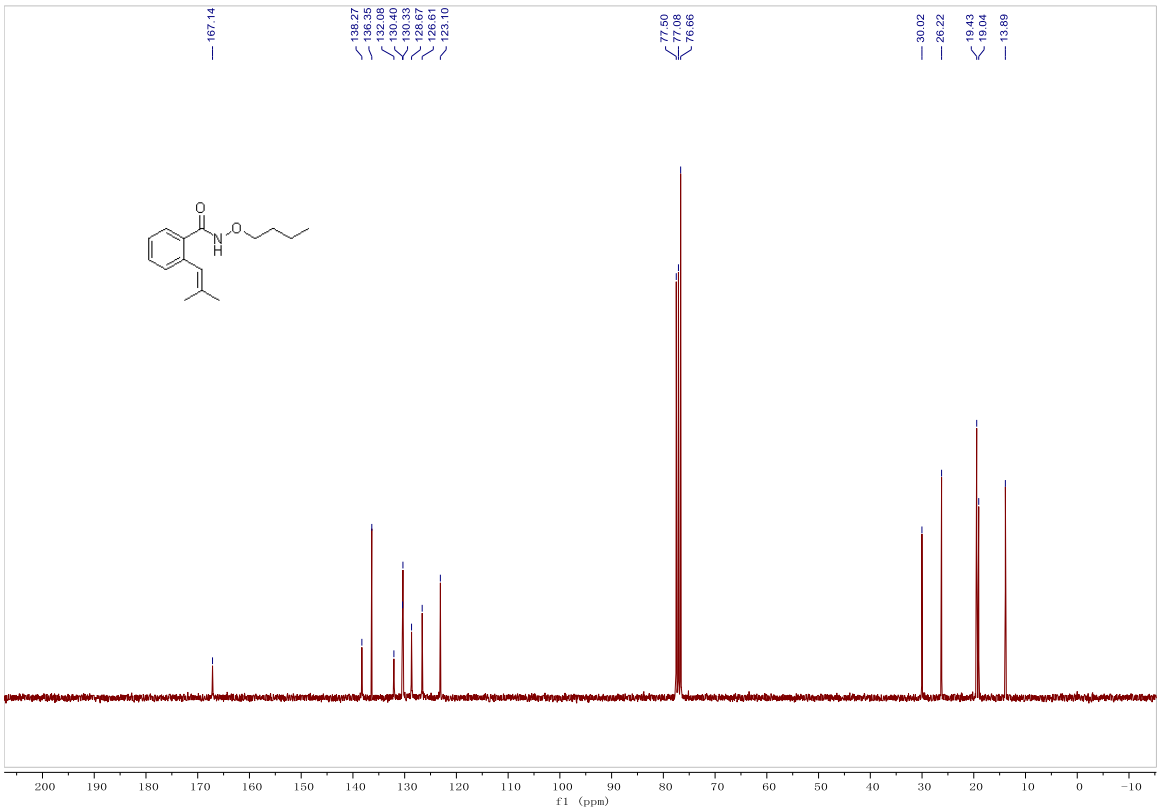
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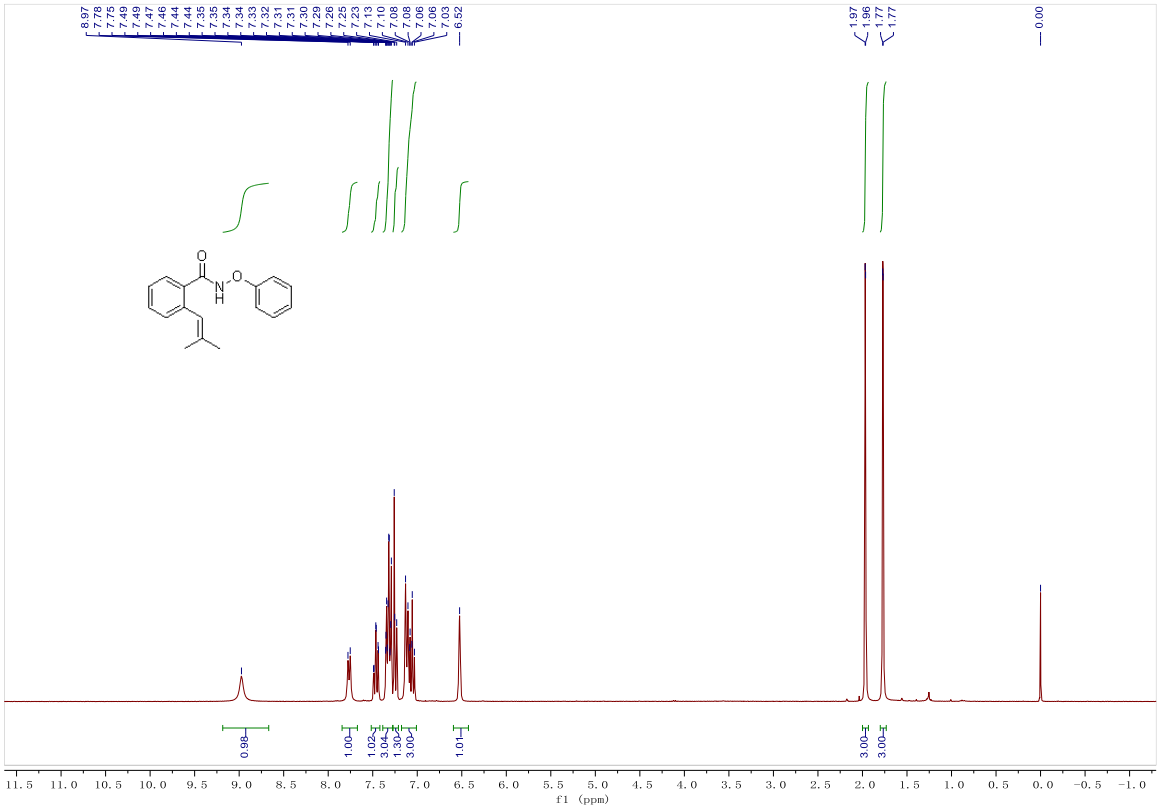
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7.03
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1.96
1.77
1.77
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1.30
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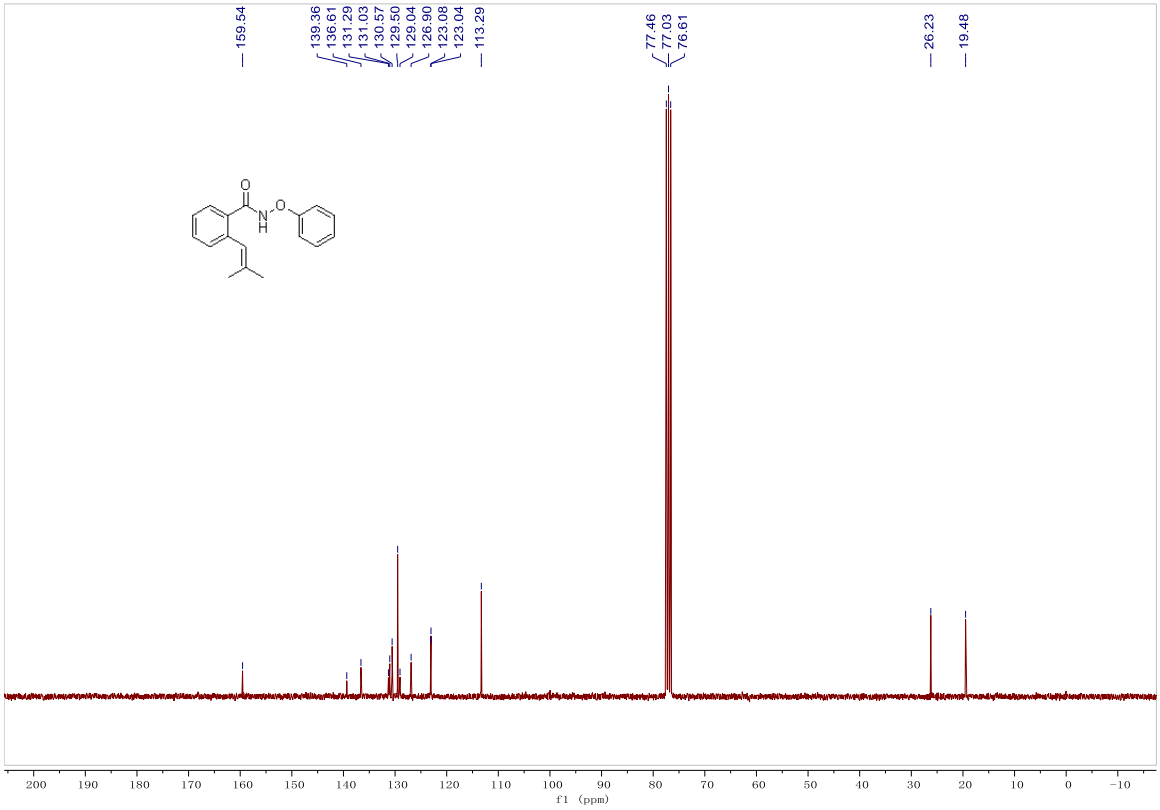
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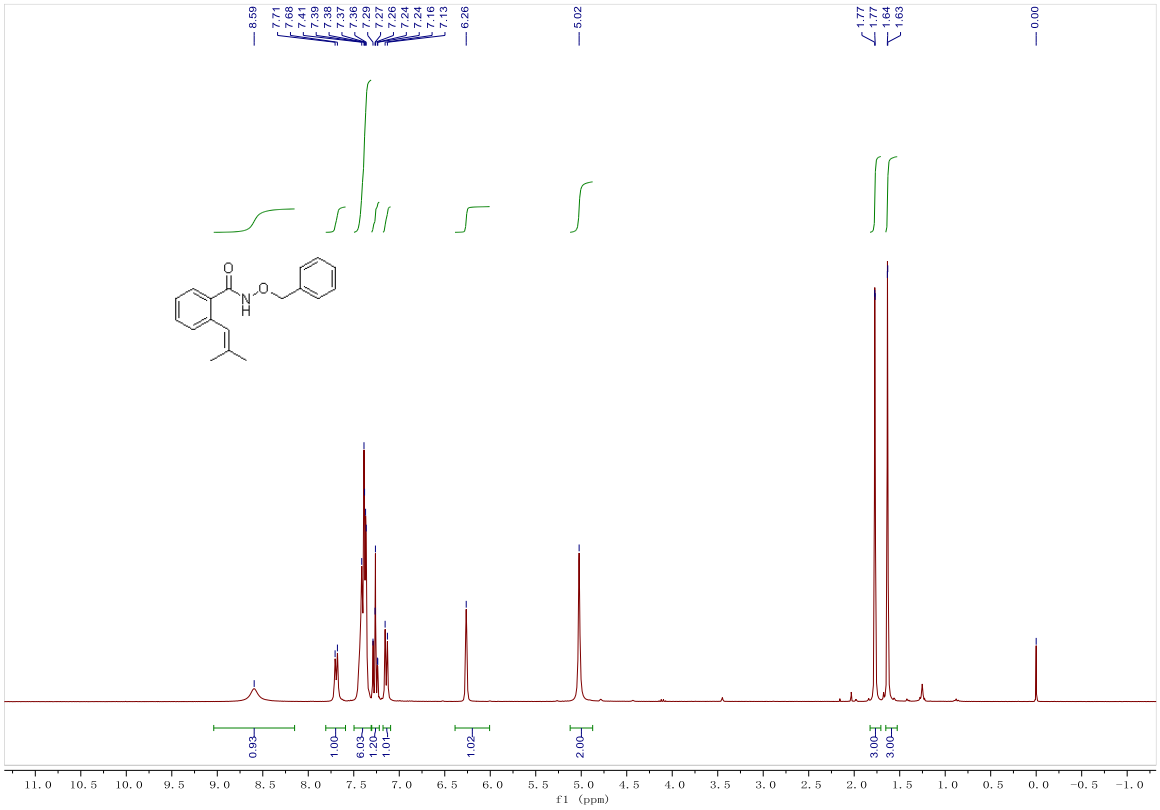
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6.26
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1.01
1.02
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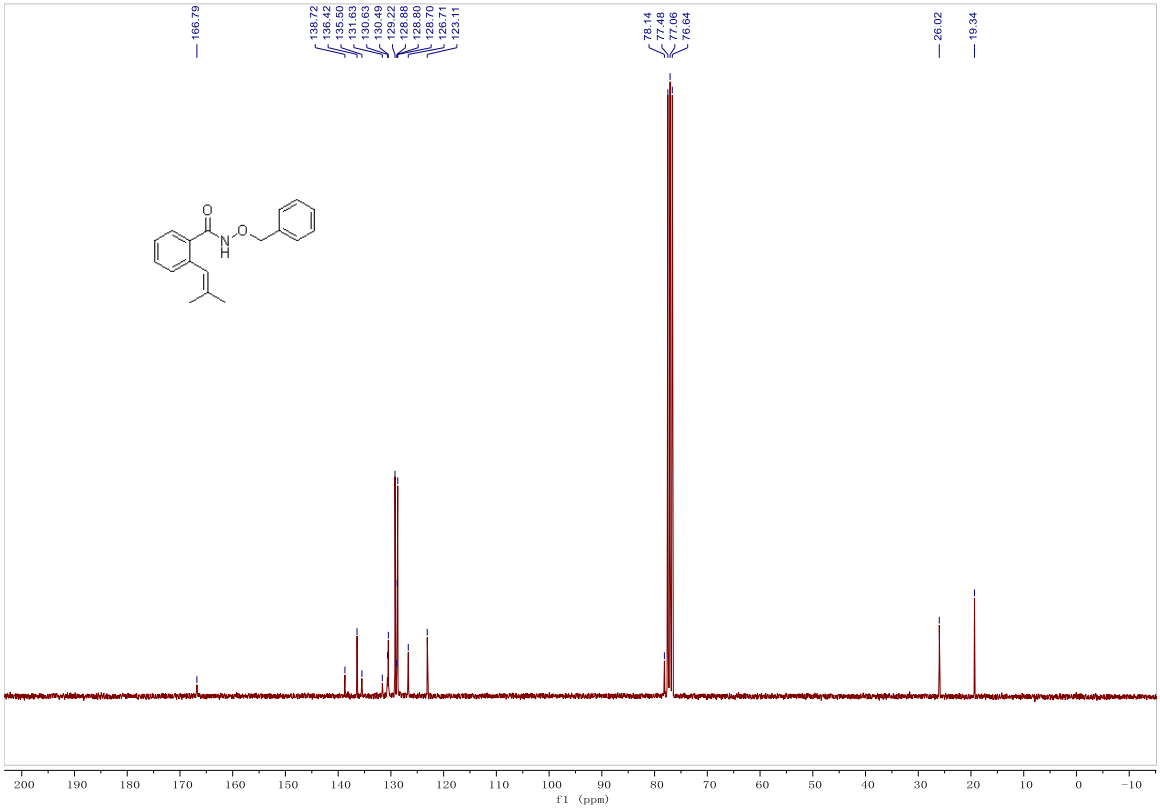
3.00
f1 (ppm)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130.49
129.22
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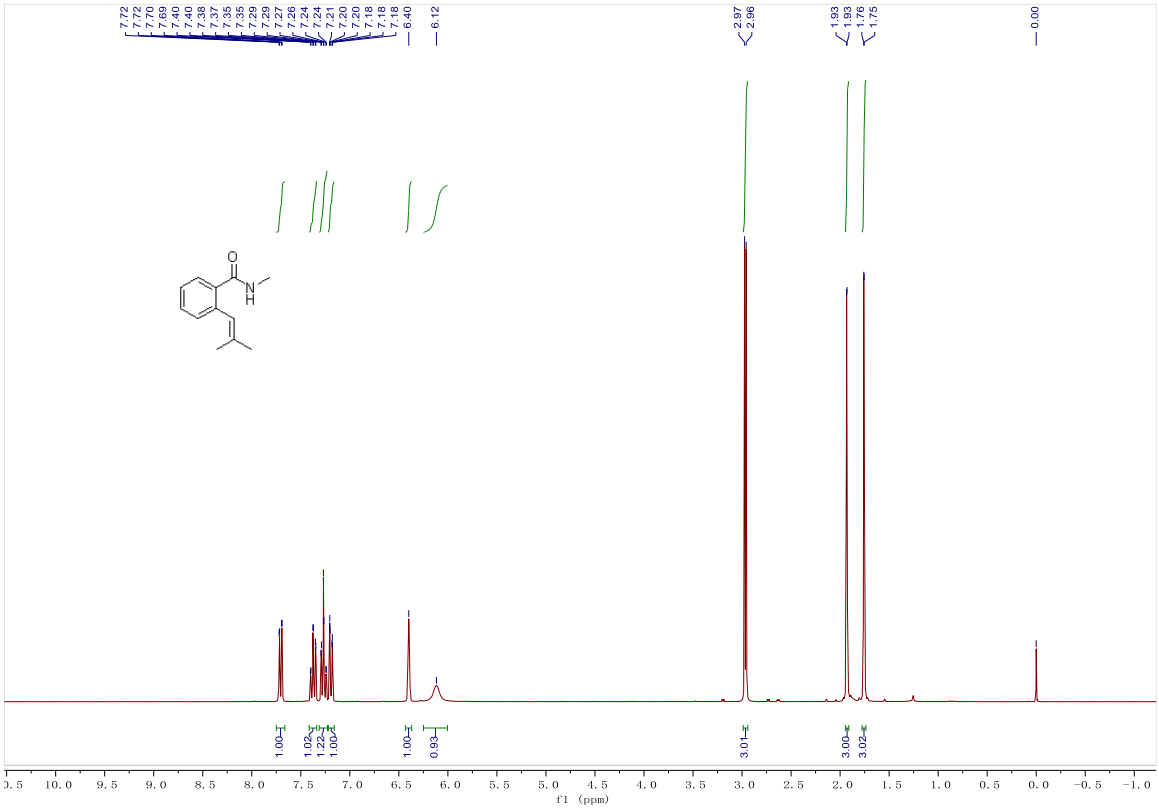
126.71
123.11
78.14
77.48
77.06
76.64
26.02
19.34
f1 (ppm)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7.72
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7.40
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7.37
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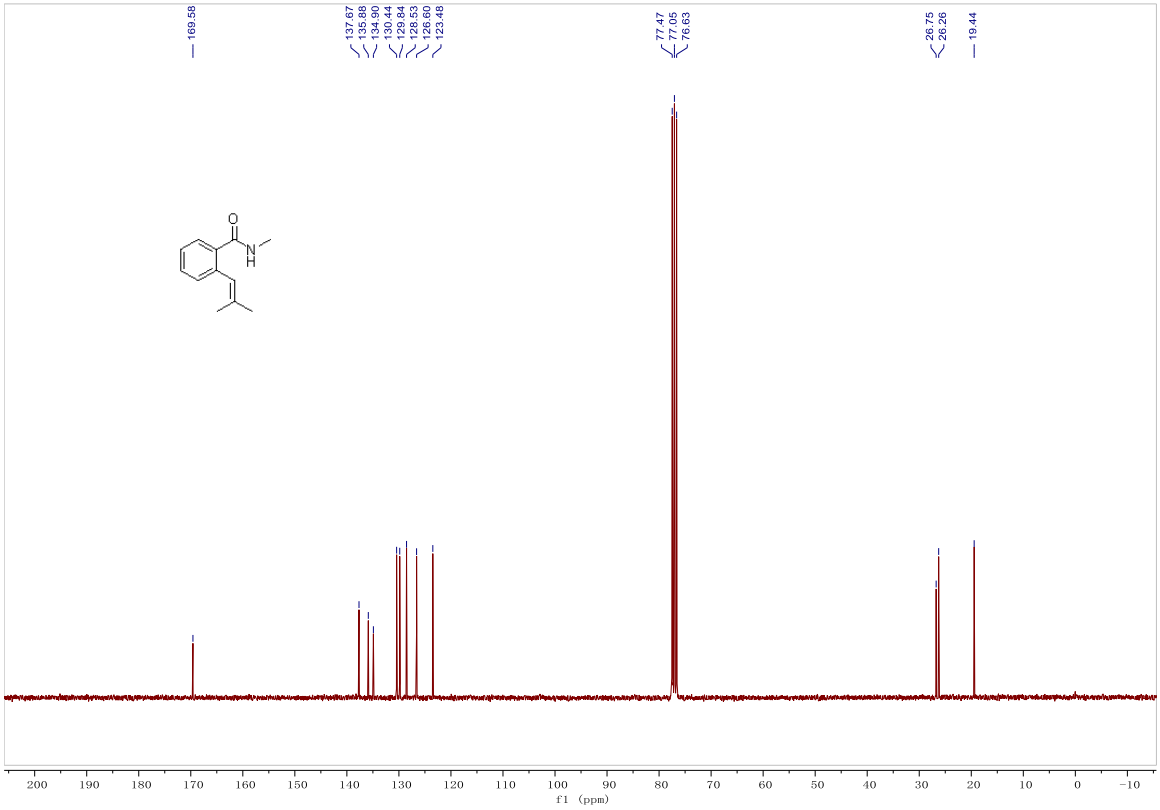
7.35
7.29
7.29
7.27
7.26
7.24
7.24
7.21
7.20
7.20
7.18
7.18
7.18
6.40
6.12
2.97
2.96
1.93
1.93
1.76
1.75
0.00
1.00
1.02
1.22
1.00
1.00
0.93
3.01
3.00
3.02
f1 (ppm)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126.60
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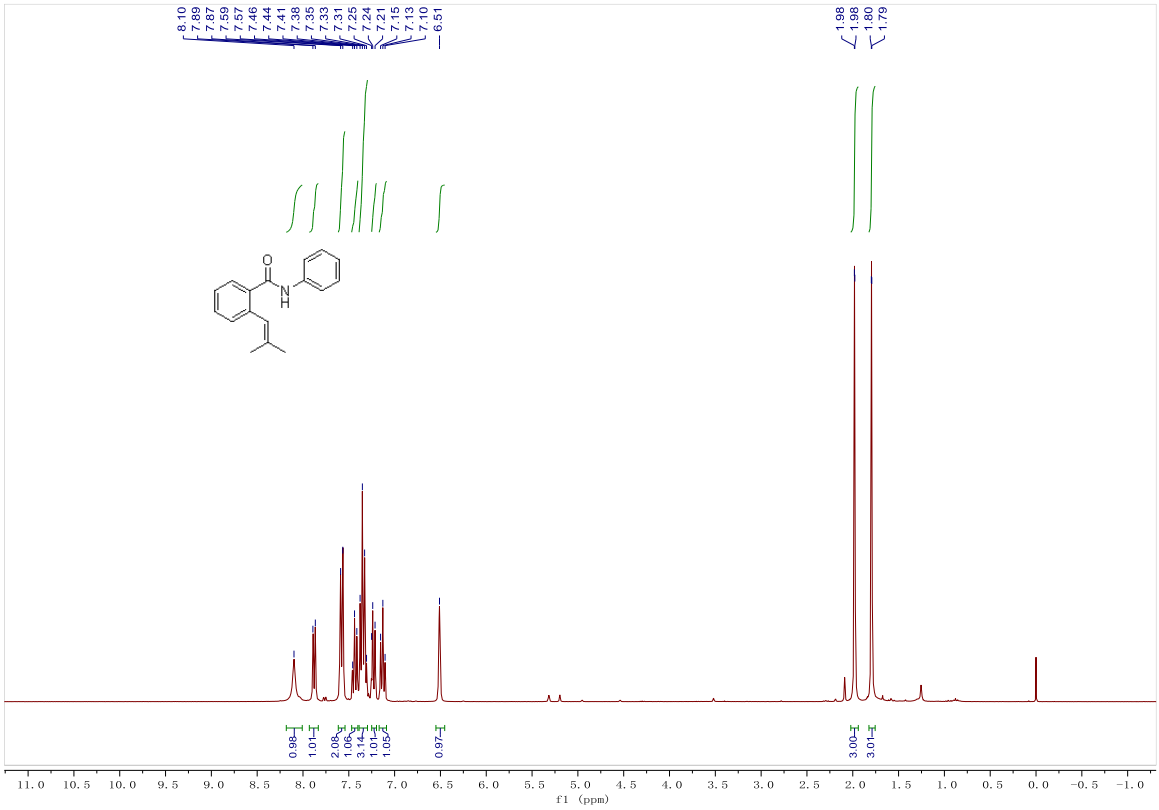
77.47
77.05
76.63
26.75
26.26
19.44
f1 (ppm)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7.44
7.41
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7.35
7.33
7.31
7.25
7.24
7.21
7.15
7.13
7.10
6.51
1.98
1.98
1.80
1.79
0.98
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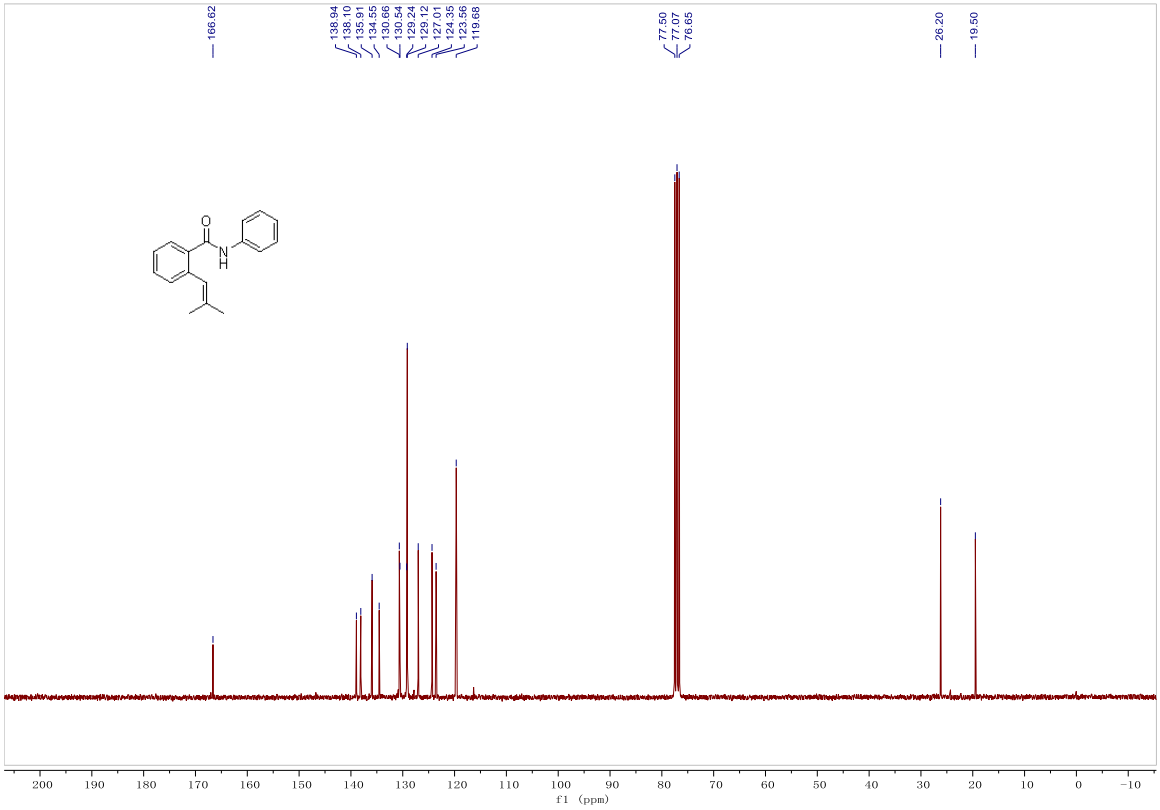
2.08
1.06
3.14
1.01
1.05
0.97
3.00
3.01
f1 (ppm)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130.54
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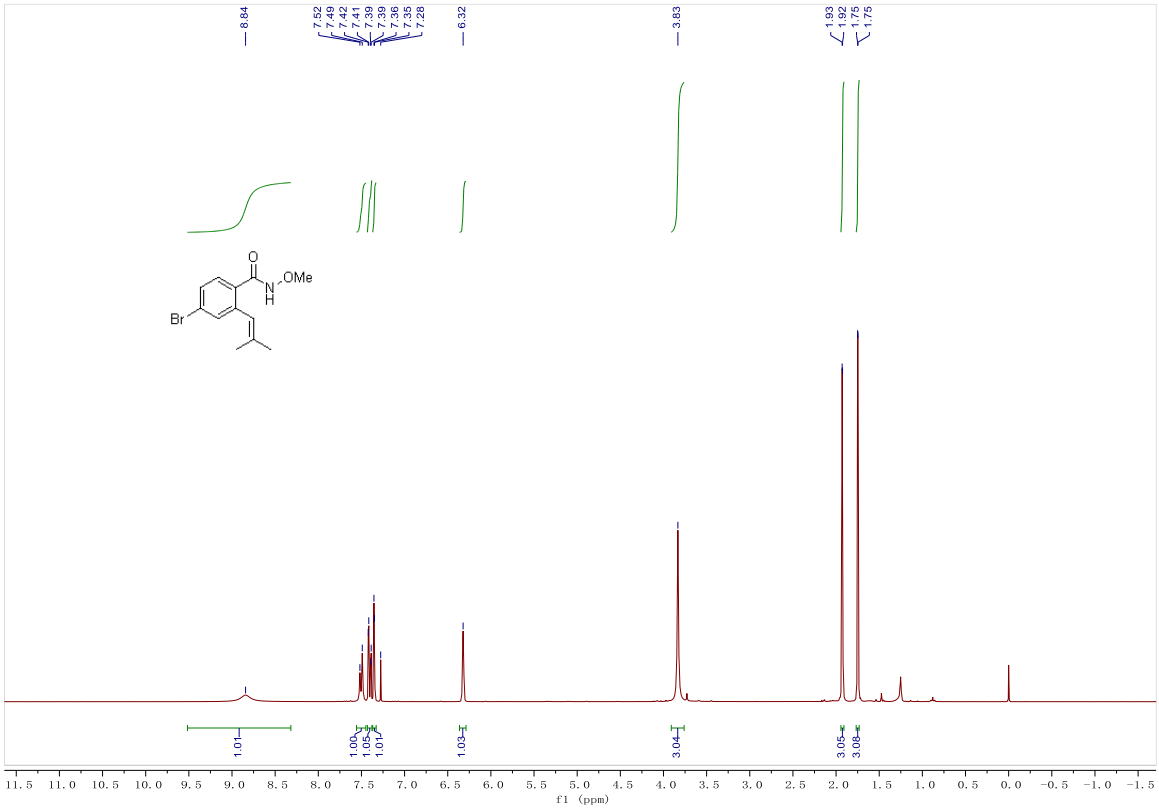
124.55
123.56
119.68
77.50
77.07
76.65
26.20
19.50
f1 (ppm)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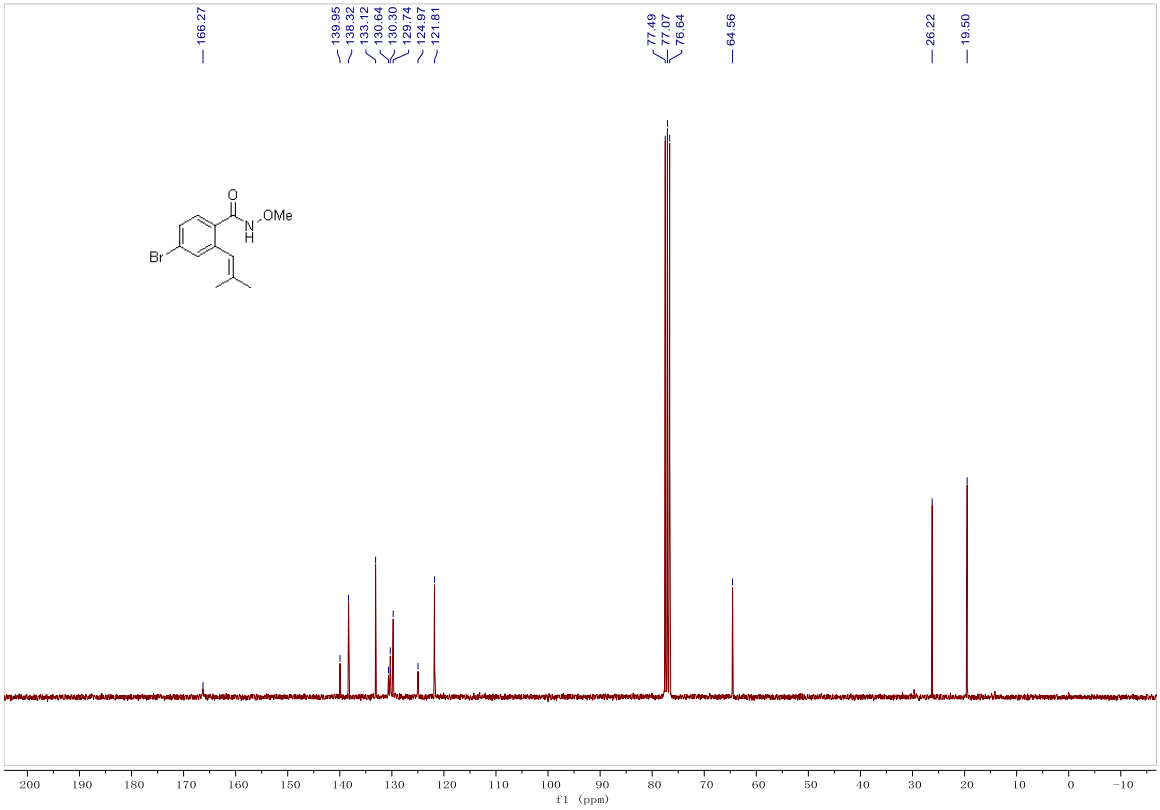
7.49
7.42
7.41
7.39
7.39
7.36
7.35
7.28
6.32
3.83
1.93
1.92
1.75
1.75
O
N
H
OMe
Br
1.01
1.00
1.05
1.01
1.03
3.04
3.05
3.08
f1 (ppm)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130.30
129.74
124.97
121.81
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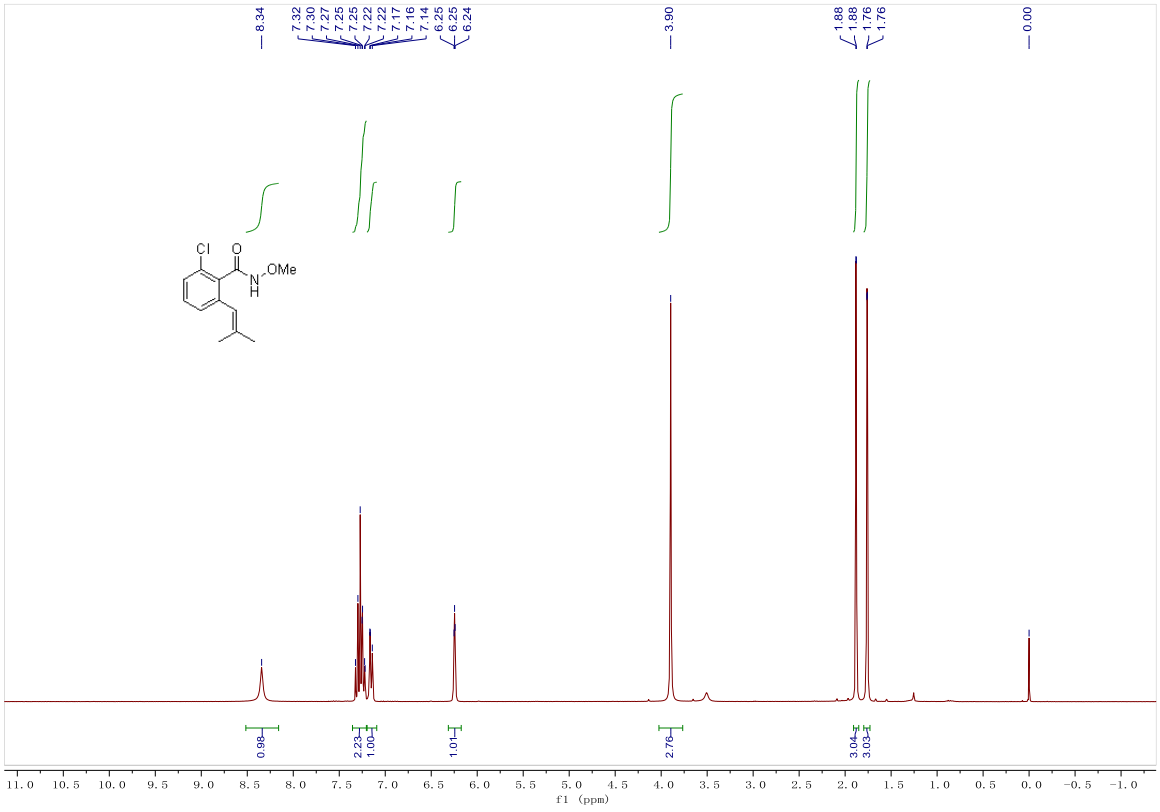
77.07
76.64
64.56
26.22
19.50
O
N
H
OMe
Br
f1 (ppm)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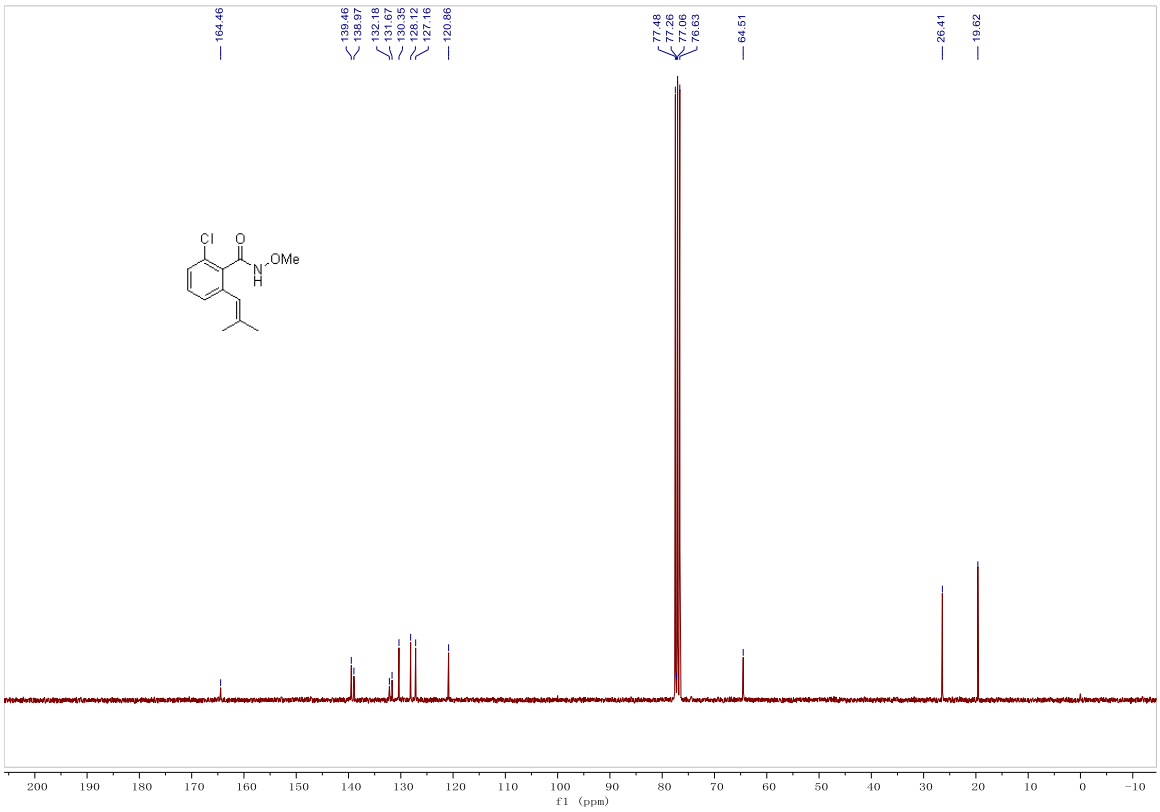
7.22
7.22
7.17
7.16
7.14
6.25
6.25
6.24
3.90
1.88
1.88
1.76
1.76
0.00
Cl
O
N
H
OMe
0.98
2.23
1.00
1.01
2.76
3.04
3.03
f1 (ppm)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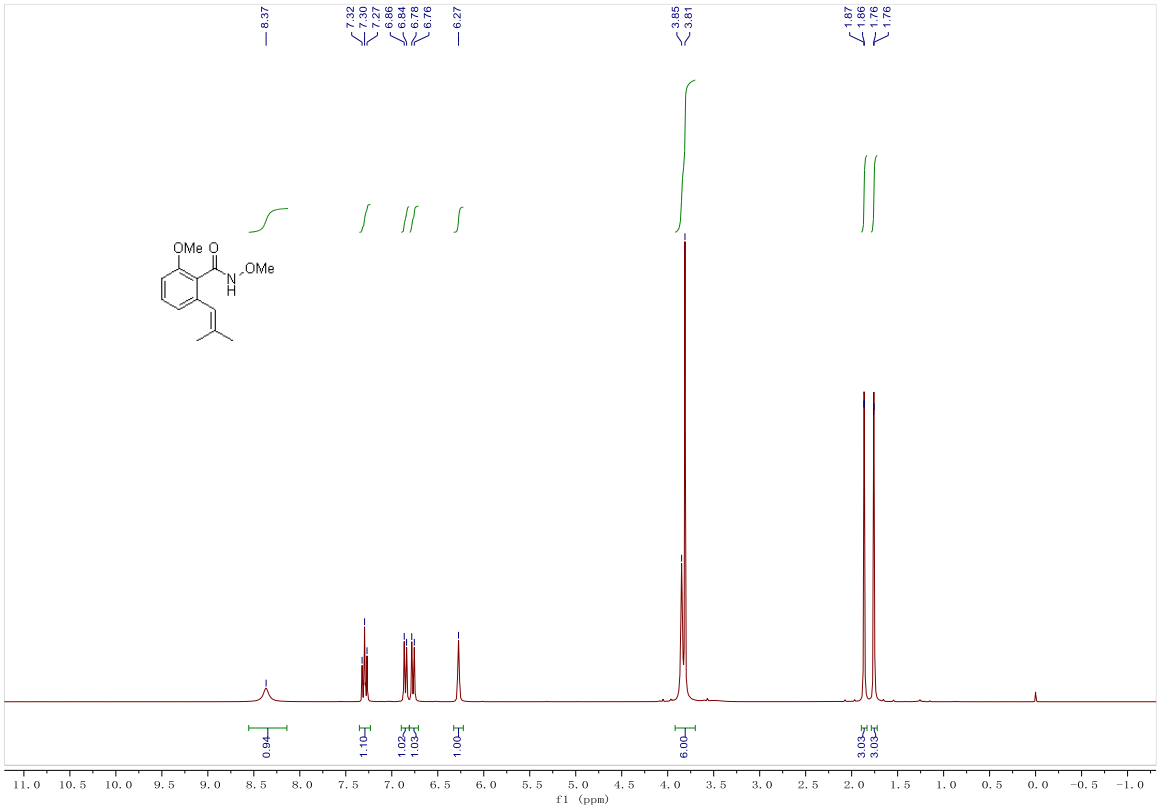
131.67
130.35
128.12
127.16
120.86
77.48
77.26
77.06
76.63
64.51
26.41
19.62
Cl
O
N
H
OMe
f1 (ppm)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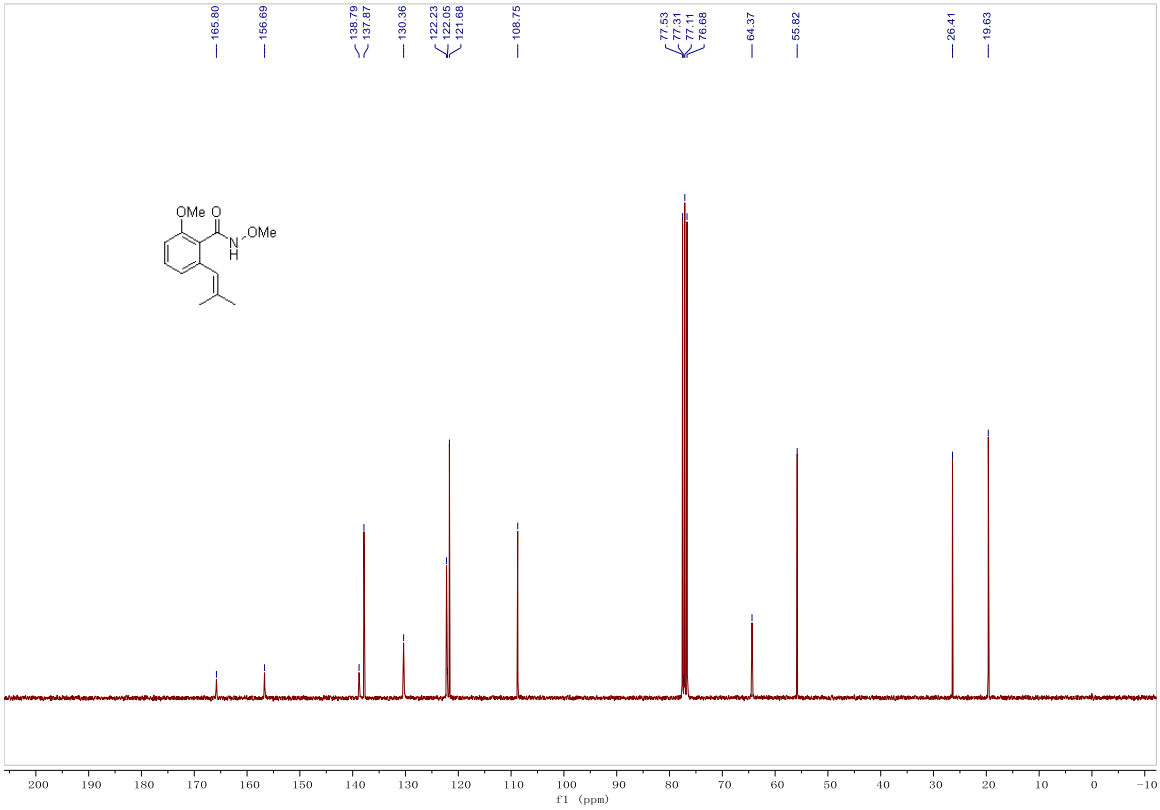
6.84
6.78
6.76
6.27
3.85
3.81
1.87
1.86
1.76
1.76
OMe
O
N
H
OMe
0.94
1.10
1.02
1.03
1.00
6.00
3.03
3.03
f1 (ppm)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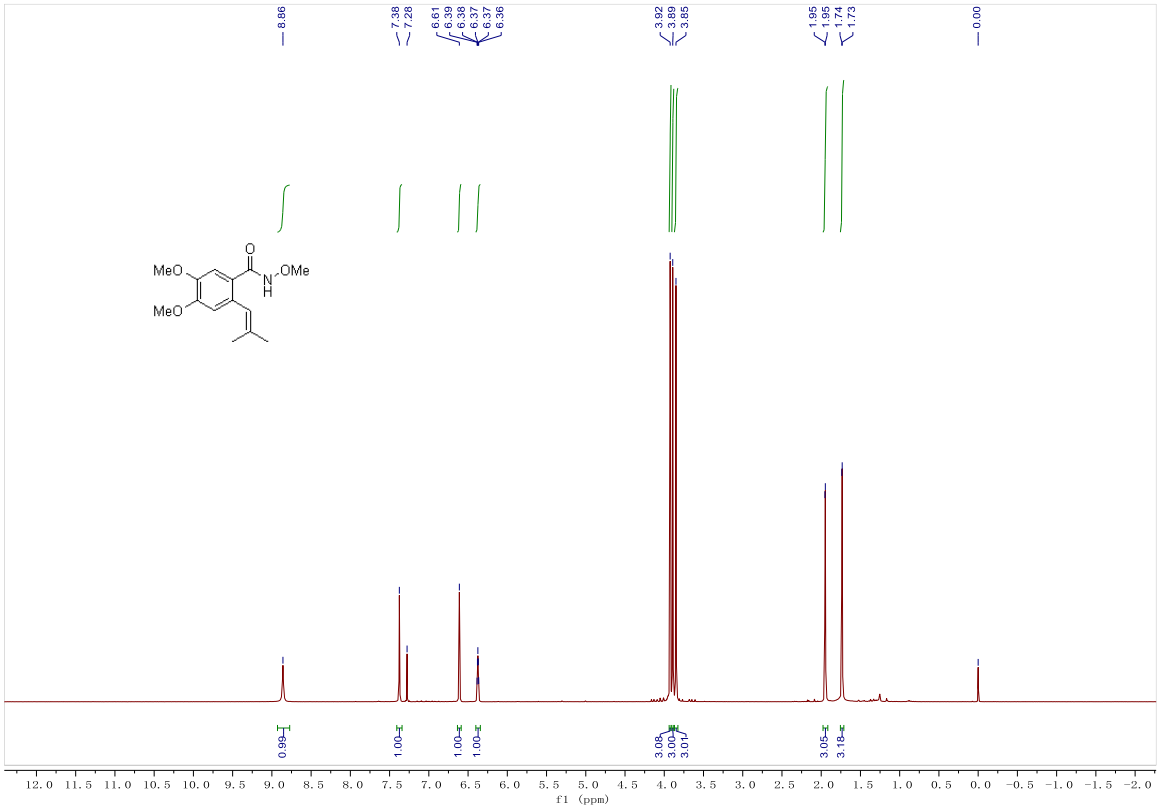
122.23
122.05
121.68
108.75
77.53
77.31
77.11
76.68
64.37
55.82
26.41
19.63
OMe
O
N
H
OMe
f1 (ppm)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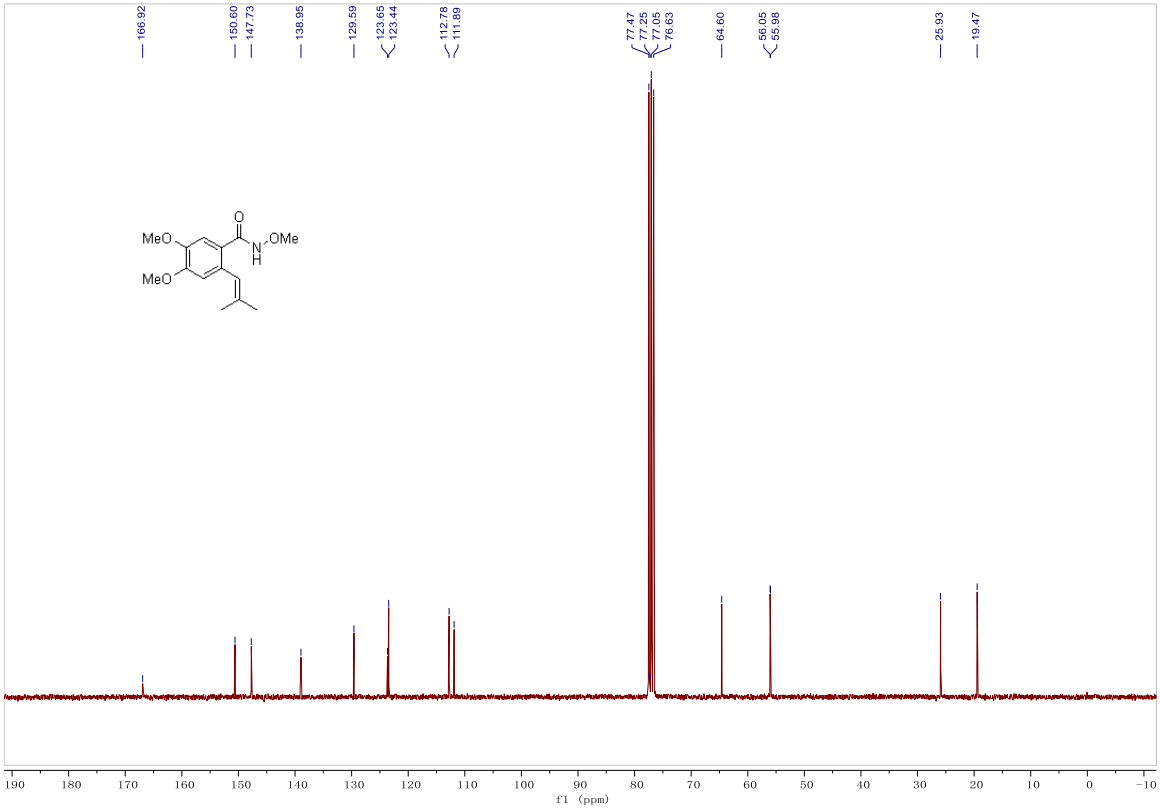
7.28
6.61
6.39
6.38
6.37
6.37
6.36
3.92
3.89
3.85
1.95
1.95
1.74
1.73
0.00
MeO
MeO
O
N
H
OMe
0.99
1.00
1.00
1.00
3.08
3.00
3.01
3.05
3.18
f1 (ppm)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129.59
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111.89
77.47
77.25
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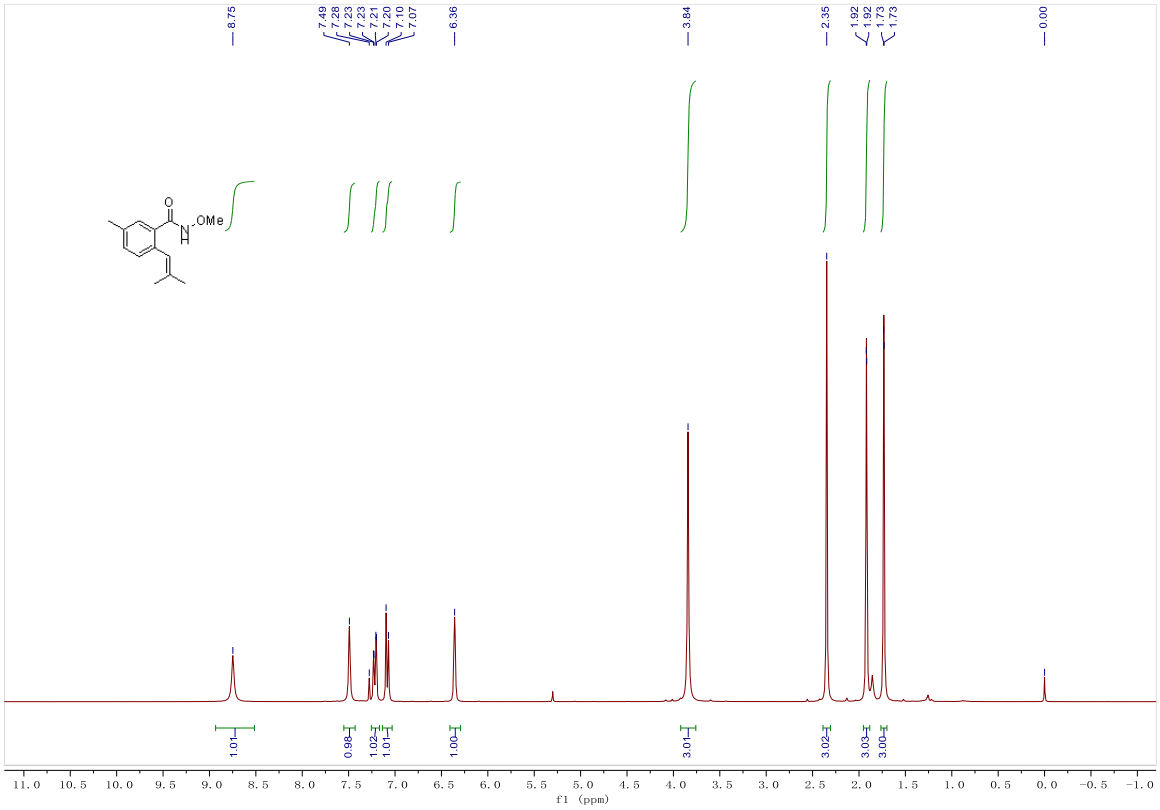
76.63
64.60
56.05
55.98
25.93
19.47
MeO
MeO
O
N
H
OMe
f1 (ppm)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7.26
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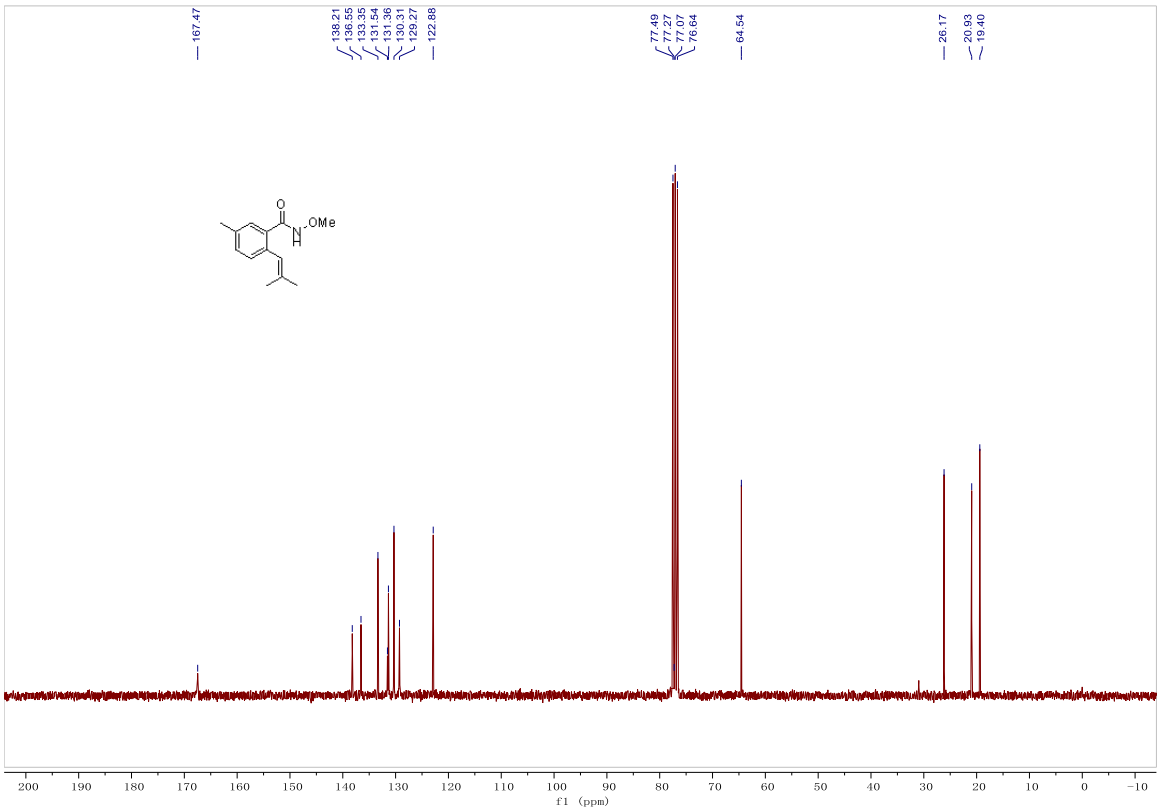
7.23
7.21
7.20
7.10
7.07
6.36
3.84
2.35
1.92
1.92
1.73
1.73
0.00
OMe
1.01
0.98
1.02
1.01
1.00
3.01
3.02
3.03
3.00
f1 (ppm)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138.21
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133.35
131.54
131.36
130.31
129.27
122.88
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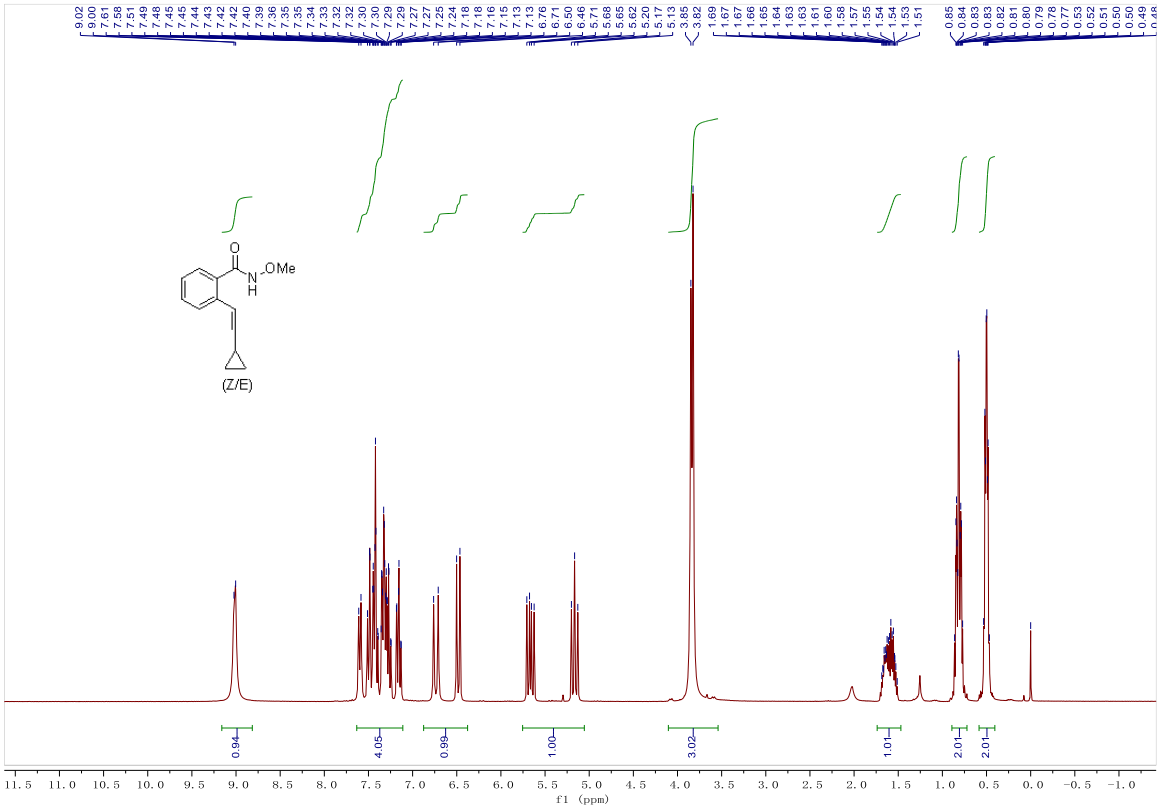
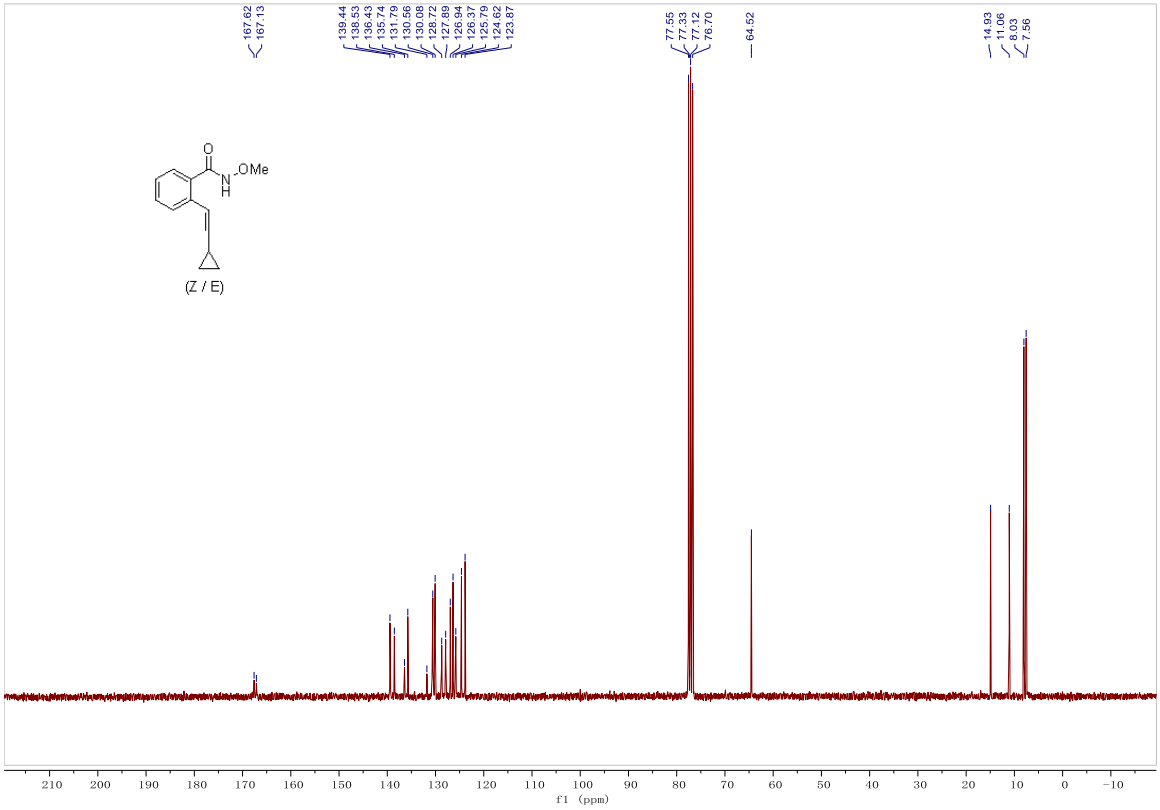
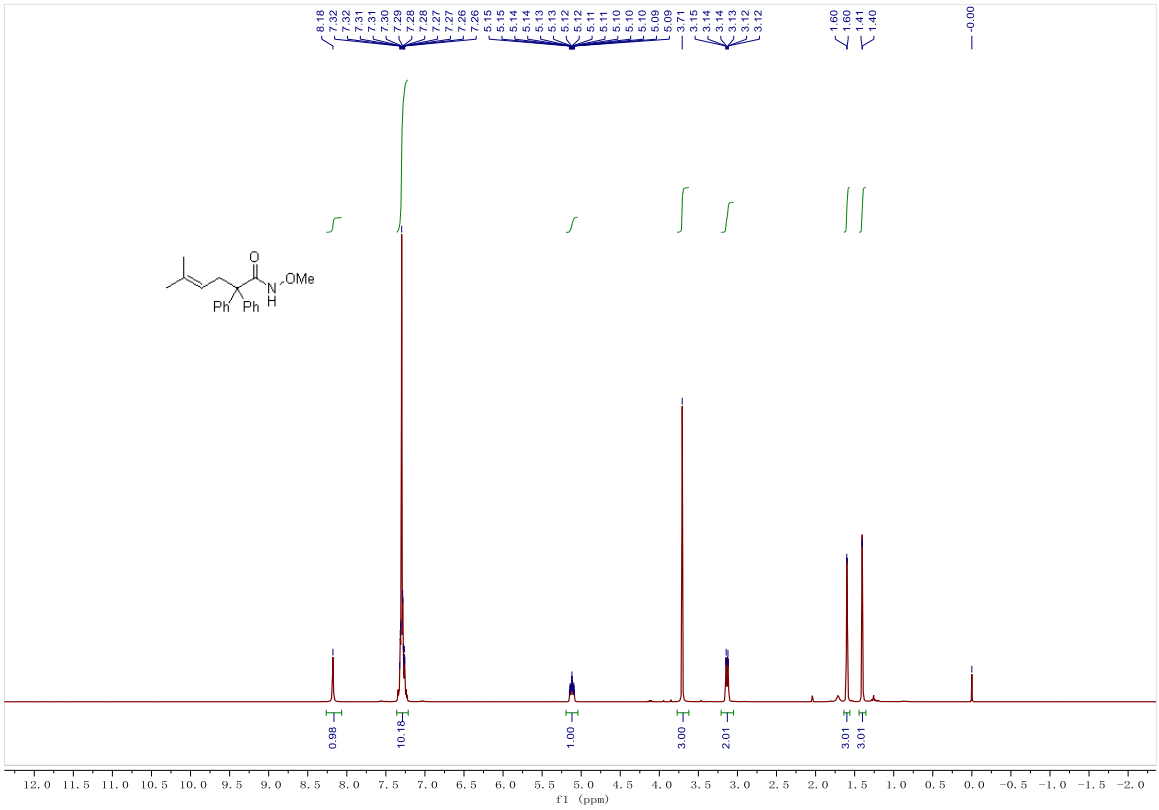
77.27
77.07
76.64
64.54
26.17
20.93
19.40
OMe
f1 (ppm)


(Z/E)
f1 (ppm)


(Z / E)
f1 (ppm)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7.30
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7.28
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7.27
7.27
7.26
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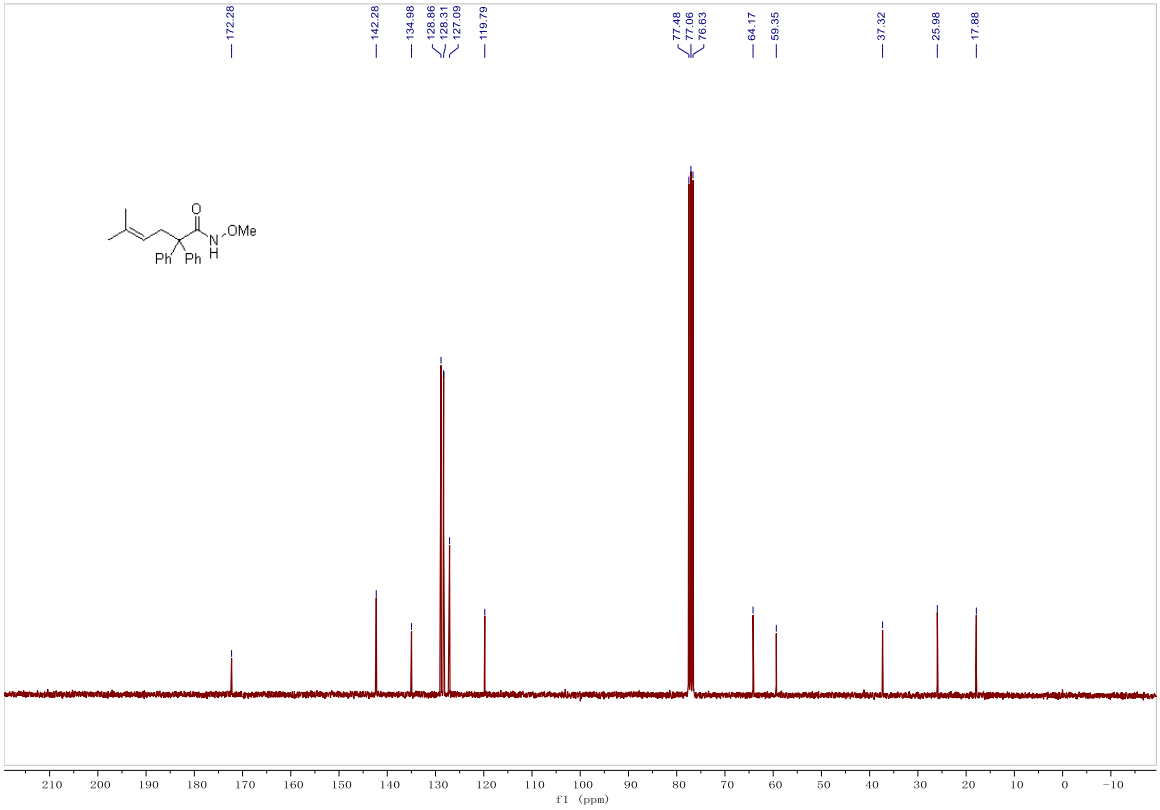
5.15
5.14
5.14
5.13
5.13
5.12
5.12
5.11
5.11
5.10
5.10
5.10
5.09
5.09
3.71
3.15
3.14
3.14
3.13
3.12
3.12
1.60
1.60
1.41
1.40
-0.00
O
N
H
OMe
Ph
Ph
0.98
10.18
1.00
3.00
2.01
3.01
3.01
f1 (ppm)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142.28
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128.86
128.31
127.09
119.79
77.48
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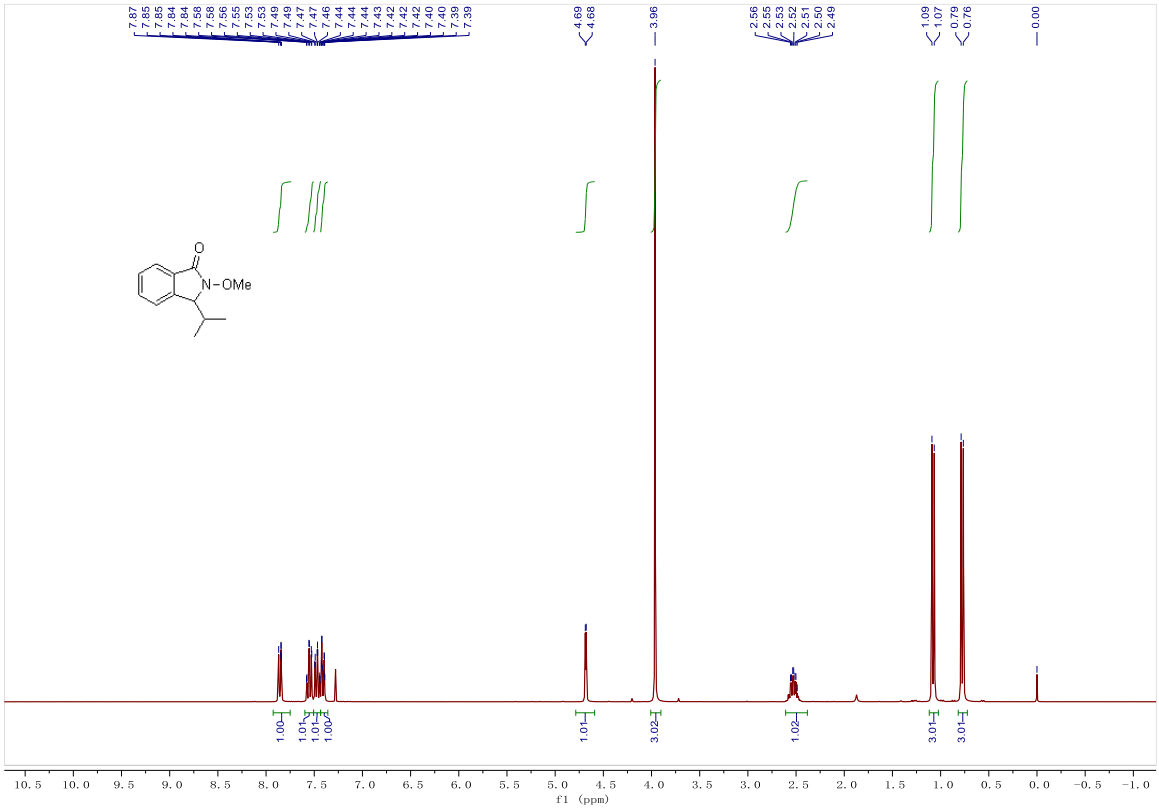
64.17
59.35
37.32
25.98
17.88
O
N
H
OMe
Ph
Ph
f1 (ppm)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7.85
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7.84
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7.58
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7.53
7.49
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7.47
7.47
7.46
7.44
7.44
7.43
7.42
7.42
7.40
7.40
7.39
7.39
4.69
4.68
3.96
2.56
2.55
2.53
2.52
2.51
2.50
2.49
1.09
1.07
0.79
0.76
0.00
N-OMe
1.00
1.01
1.01
1.00
1.01
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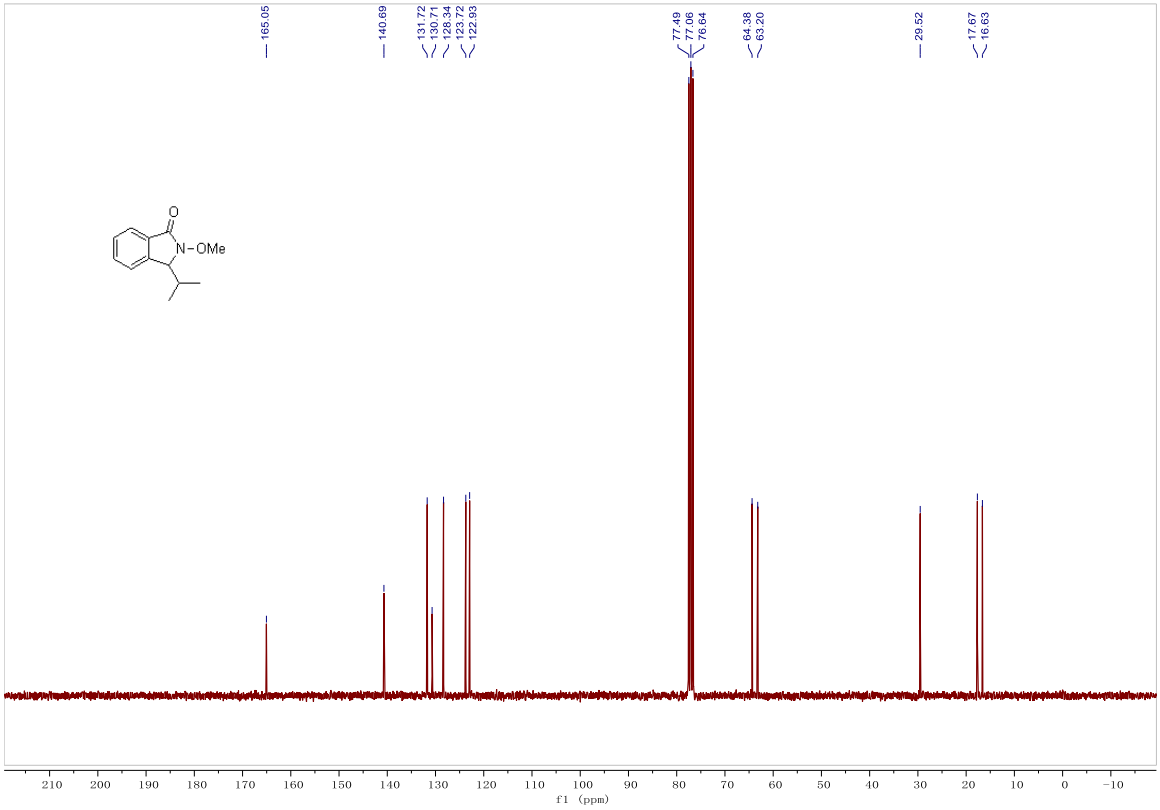
1.02
3.01
3.01
f1 (ppm)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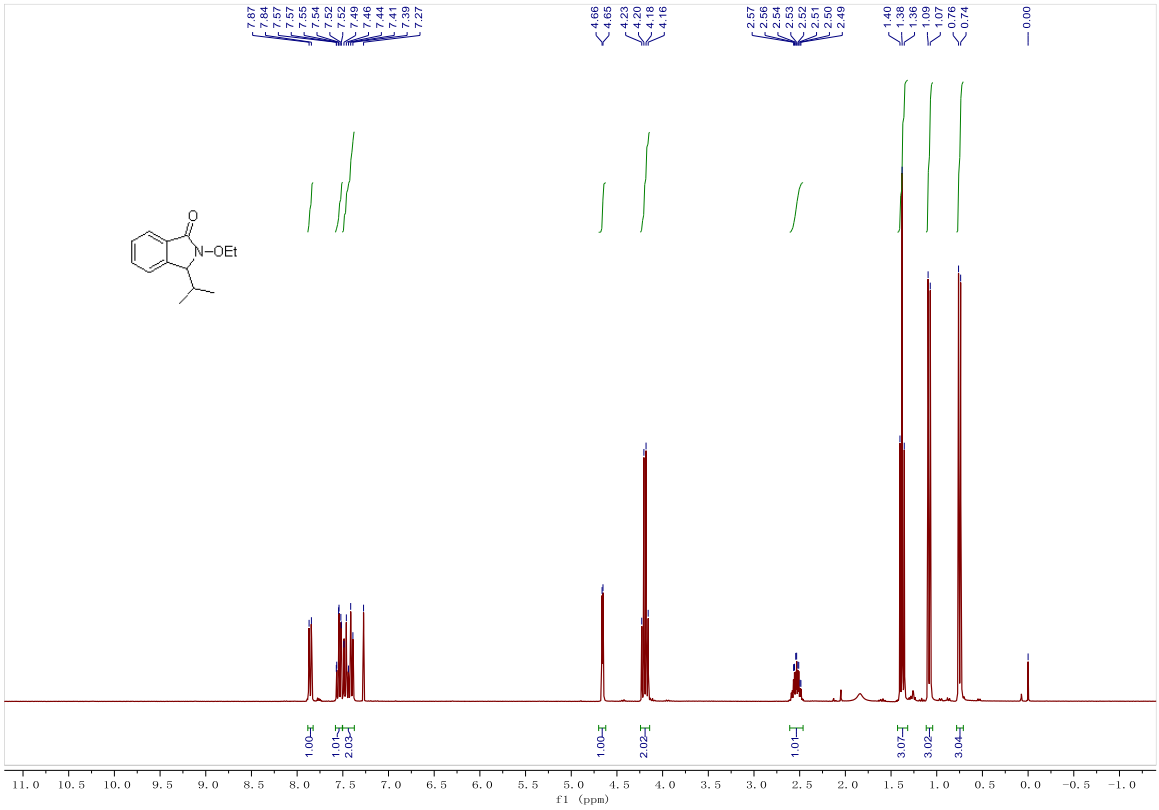
77.06
76.64
64.38
63.20
29.52
17.67
16.63
N-OMe
f1 (ppm)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7.54
7.52
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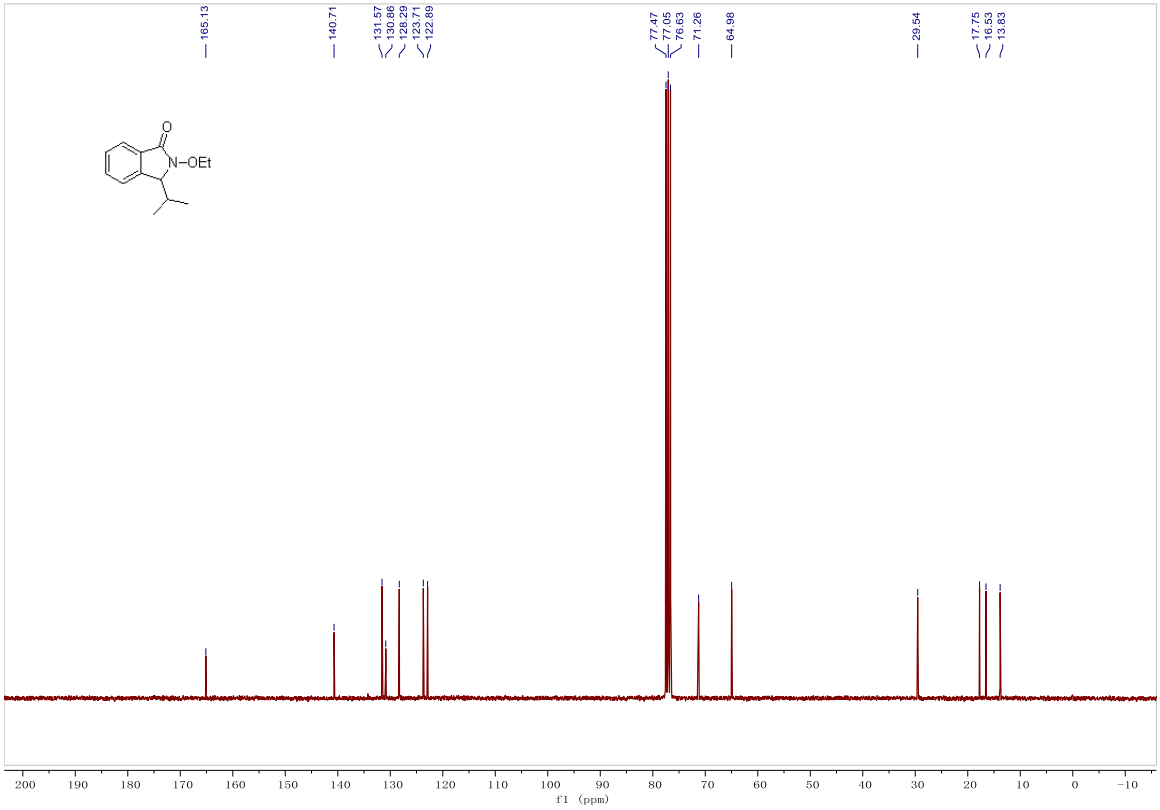
7.49
7.46
7.44
7.41
7.39
7.27
4.66
4.65
4.23
4.20
4.18
4.16
2.57
2.56
2.54
2.53
2.52
2.51
2.50
2.49
1.40
1.38
1.36
1.09
1.07
0.76
0.74
0.00
O
N–OEt
1.00
1.01
2.03
1.00
2.02
1.01
3.07
3.02
3.04
f1 (ppm)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123.71
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71.26
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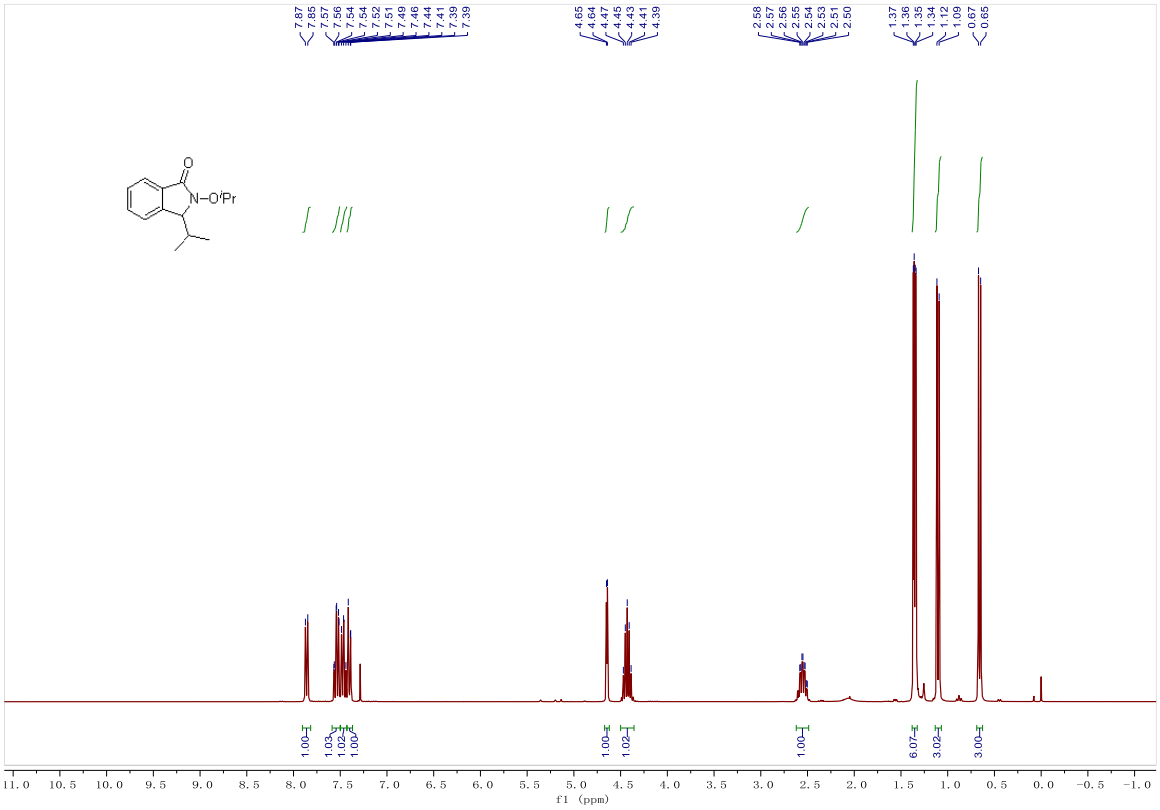
29.54
17.75
16.53
13.83
O
N–OEt
f1 (ppm)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7.44
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7.39
4.65
4.64
4.47
4.45
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4.41
4.39
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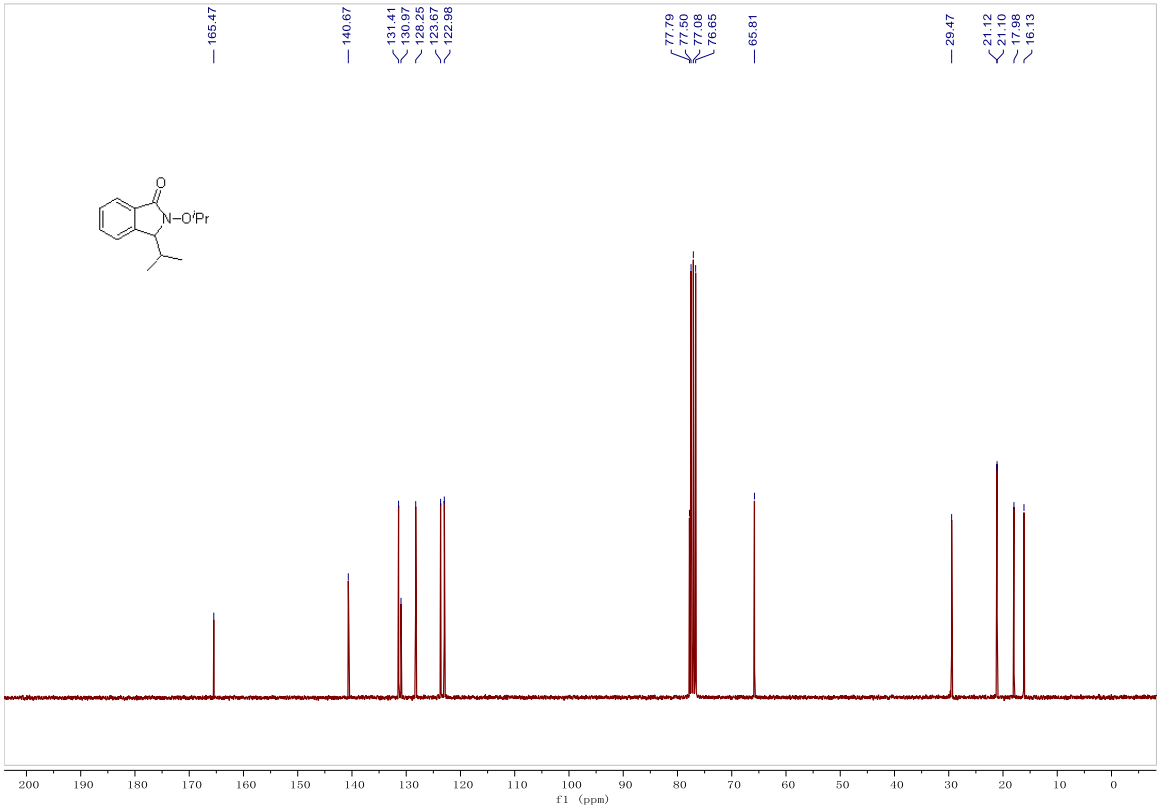
2.55
2.54
2.53
2.51
2.50
1.37
1.36
1.35
1.34
1.12
1.09
0.67
0.65
O
N–O'Pr
1.00
1.03
1.02
1.00
1.00
1.02
1.00
6.07
3.02
3.00
f1 (ppm)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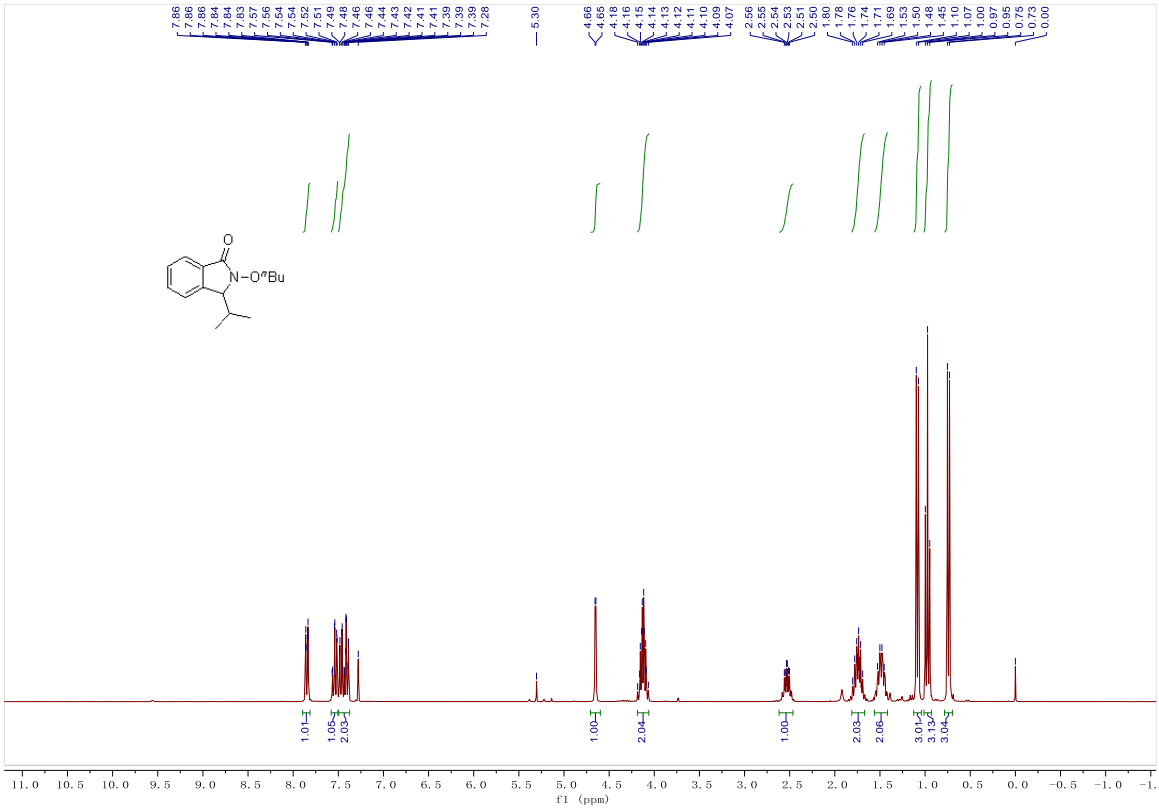
65.81
29.47
21.12
21.10
17.98
16.13
O
N–O'Pr
f1 (ppm)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7.52
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7.46
7.46
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7.41
7.39
7.39
7.39
7.28
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4.65
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4.16
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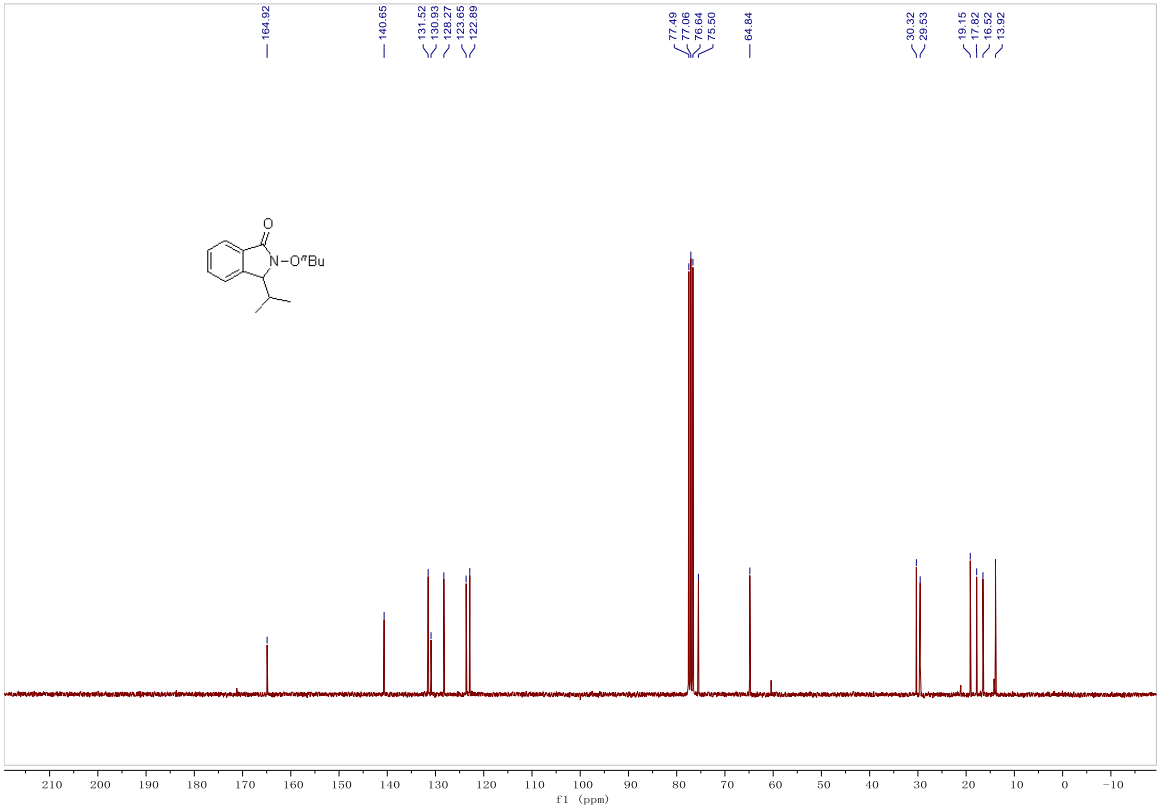
4.14
4.13
4.12
4.11
4.10
4.09
4.07
2.56
2.55
2.54
2.53
2.51
2.50
2.80
1.78
1.76
1.74
1.71
1.69
1.53
1.50
1.48
1.45
1.10
1.07
1.00
0.97
0.95
0.75
0.73
0.00
O
N–O^{n}Bu
1.01
1.05
2.03
1.00
2.04
1.00
2.03
2.06
3.01
3.13
3.04
f1 (ppm)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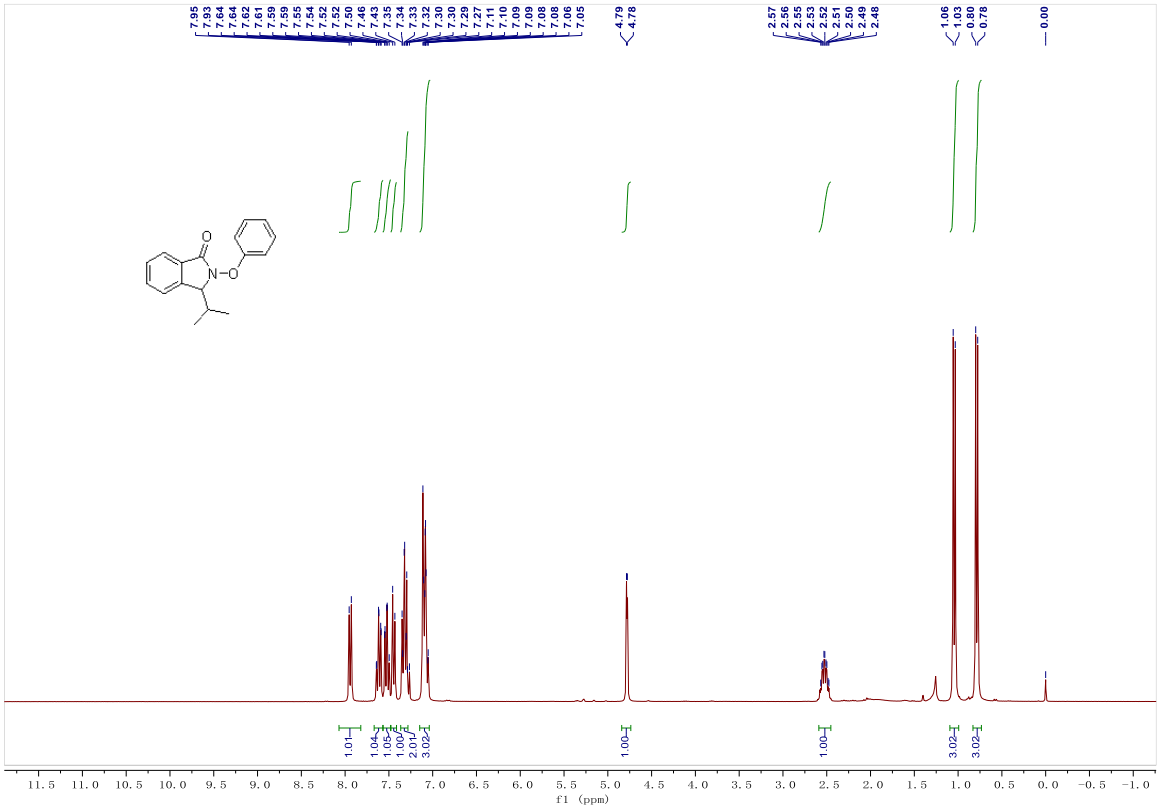
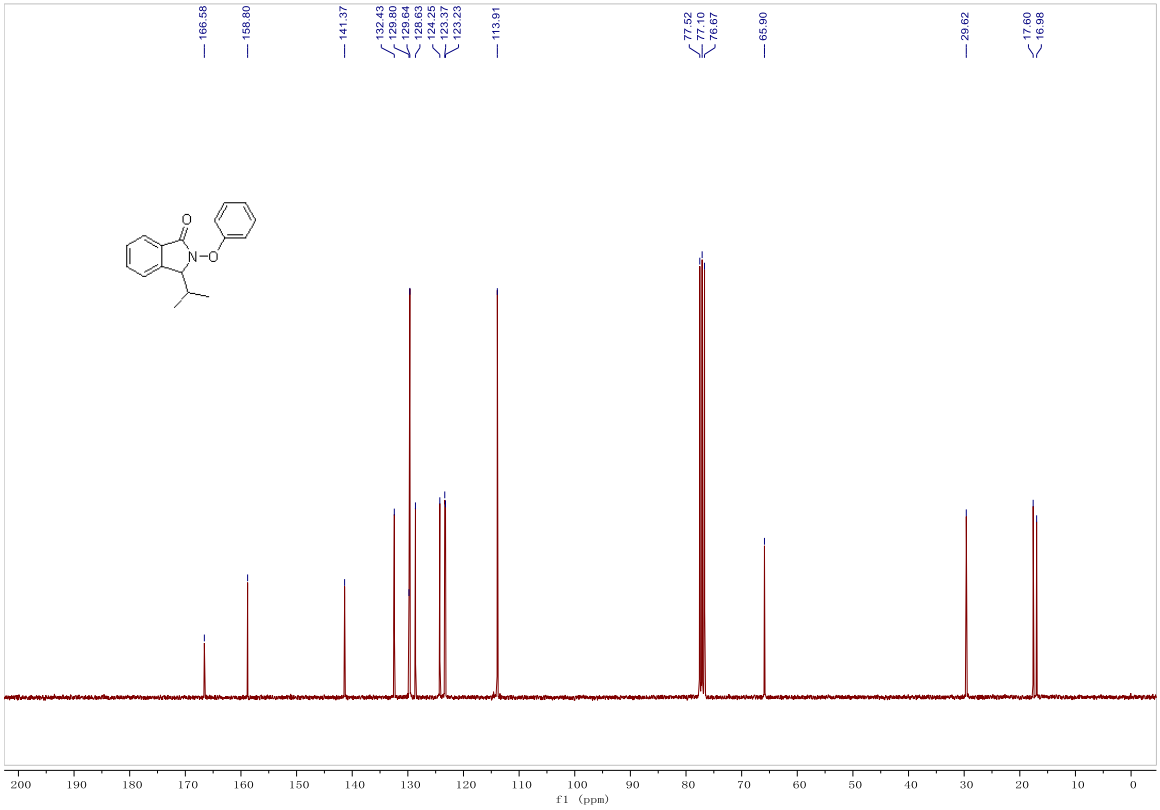
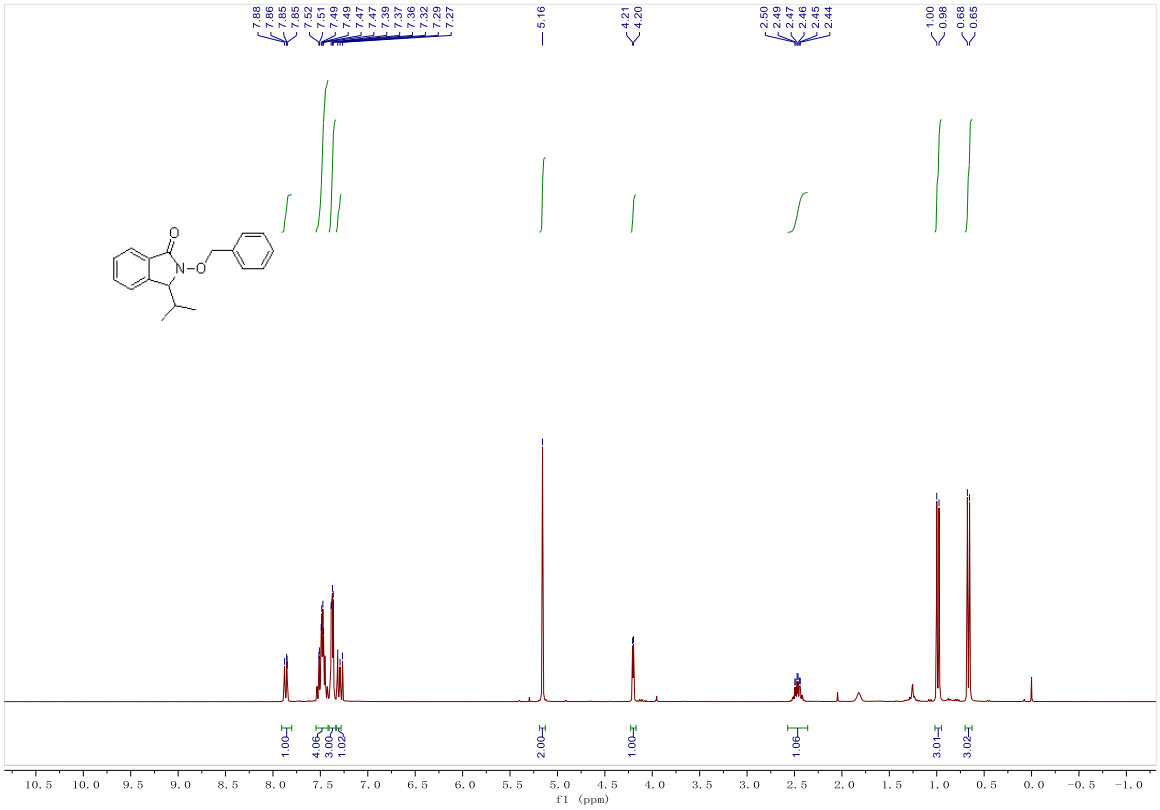
77.49
77.06
76.64
75.50
64.84
30.32
29.53
19.15
17.82
16.52
13.92
O
N–O^{n}Bu
f1 (ppm)


7.95 7.93 7.64 7.64 7.62 7.61 7.59 7.59 7.55 7.54 7.52 7.52 7.50 7.46 7.43 7.35 7.34 7.33 7.32 7.30 7.30 7.29 7.27 7.11 7.10 7.09 7.09 7.08 7.08 7.06 7.05
4.79 4.78
2.57 2.56 2.55 2.53 2.52 2.51 2.50 2.49 2.48
1.06 1.03 0.80 0.78
0.00
1.01 1.04 1.05 1.00 2.01 3.02 1.00 1.00 3.02 3.02
f1 (ppm)


166.58 158.80 141.37 132.43 129.80 129.64 128.63 124.25 123.37 123.23 113.91
77.52 77.10 76.67 65.90 29.62 17.60 16.98
f1 (ppm)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7.49
7.49
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7.47
7.39
7.37
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7.32
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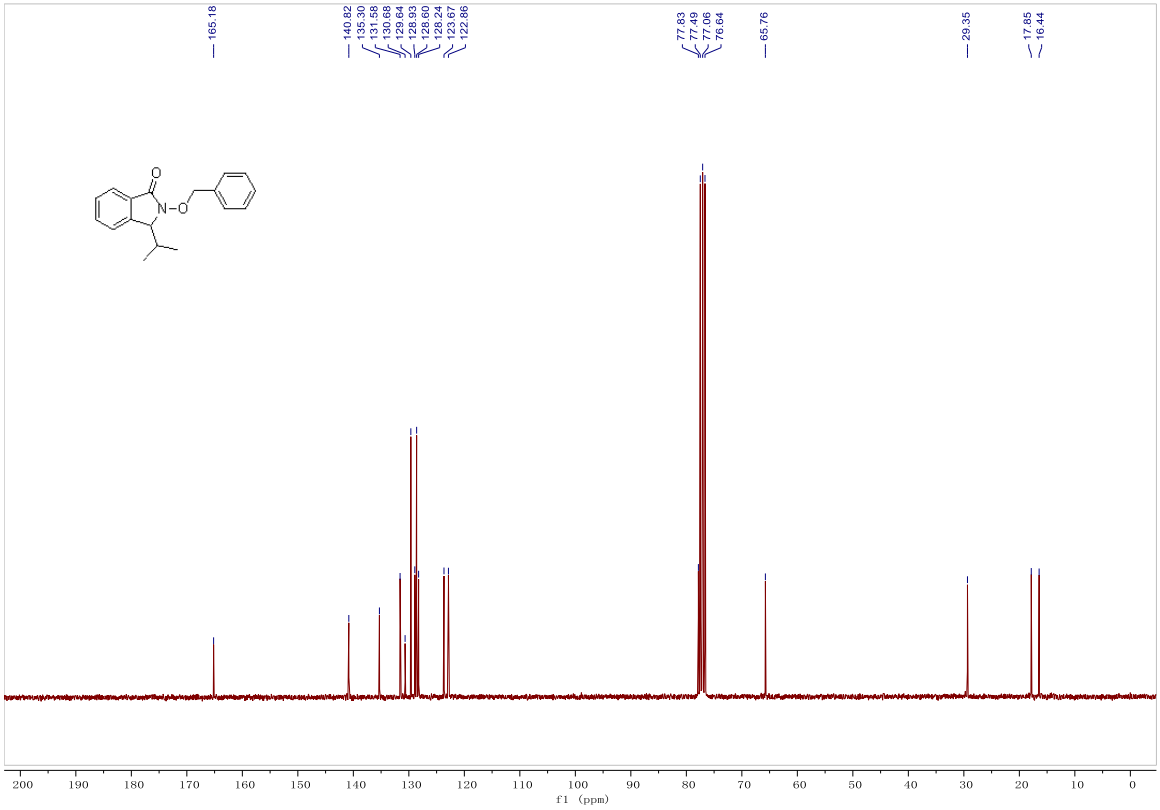
7.27
5.16
4.21
4.20
2.50
2.49
2.47
2.46
2.45
2.44
1.00
0.98
0.68
0.65
1.00
4.06
3.00
1.02
2.00
1.00
1.06
3.01
3.02
f1 (ppm)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135.30
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129.64
128.93
128.60
128.24
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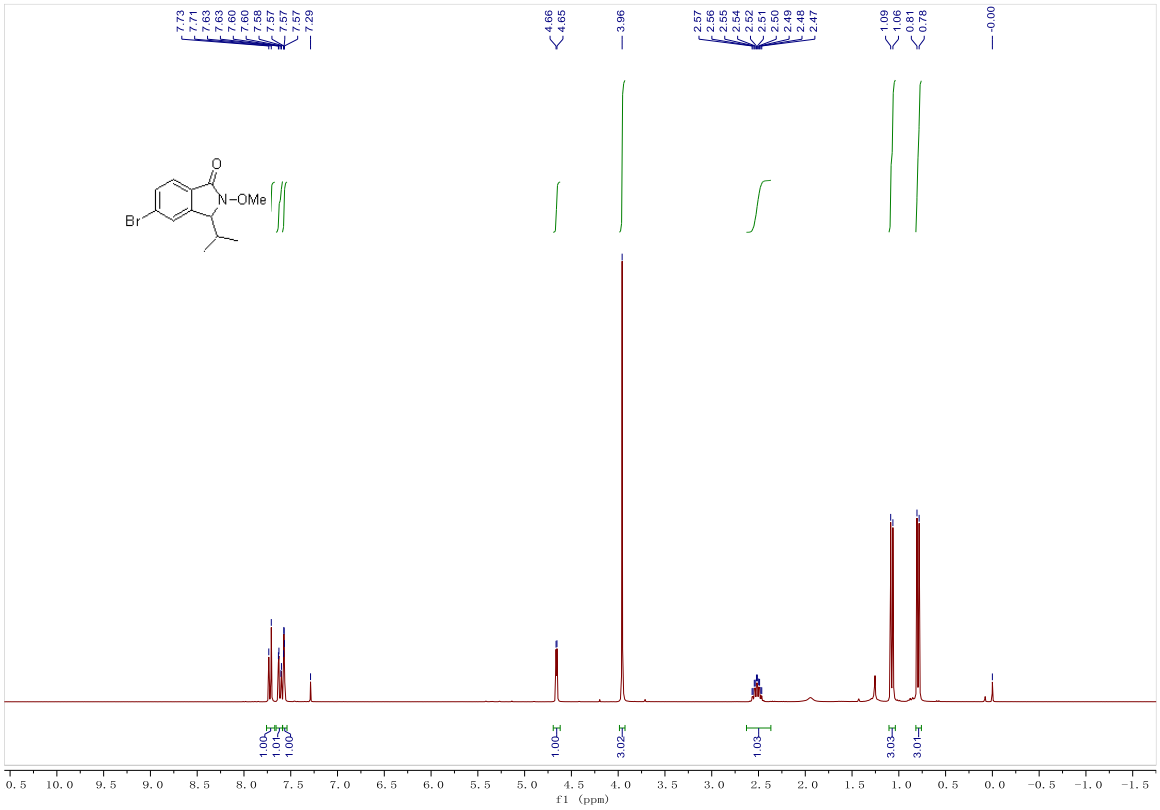
77.49
77.06
76.64
65.76
29.35
17.85
16.44
f1 (ppm)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7.29
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4.65
3.96
2.57
2.56
2.55
2.54
2.52
2.51
2.50
2.49
2.48
2.47
1.09
1.06
0.81
0.78
-0.00
O
N-OMe
Br
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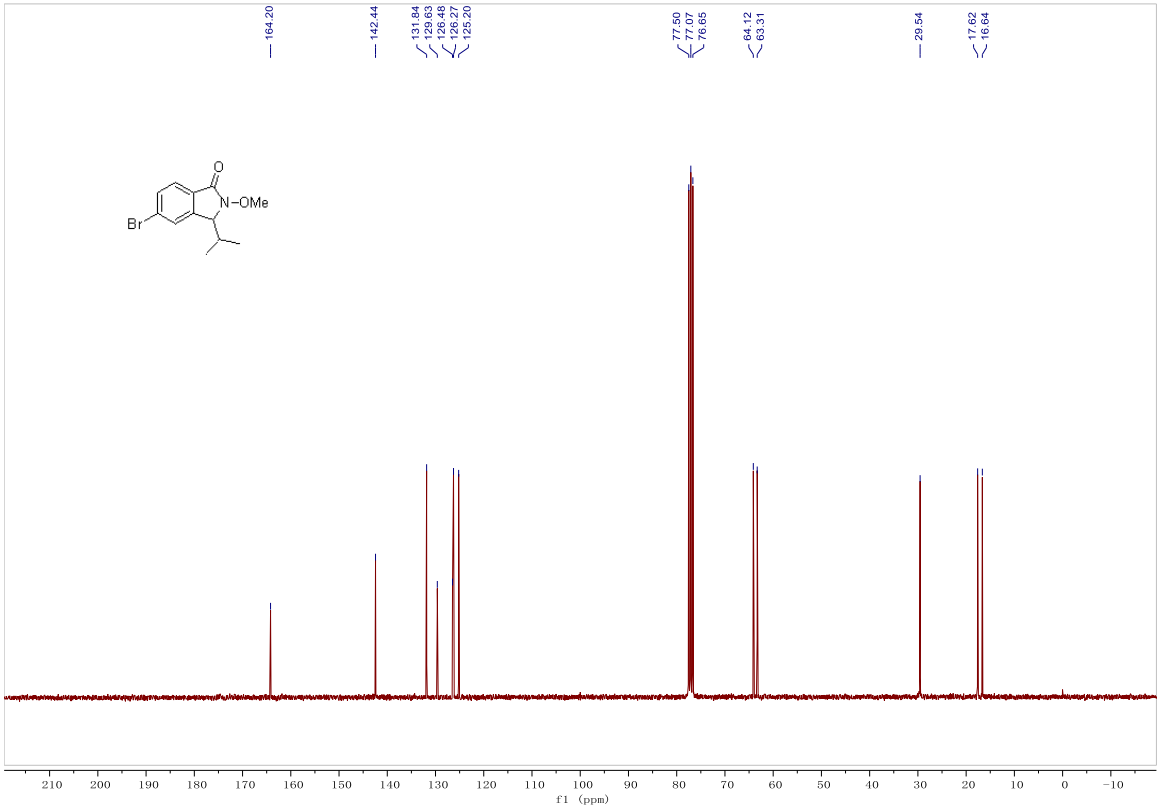
1.01
1.00
1.00
3.02
1.03
3.03
3.01
f1 (ppm)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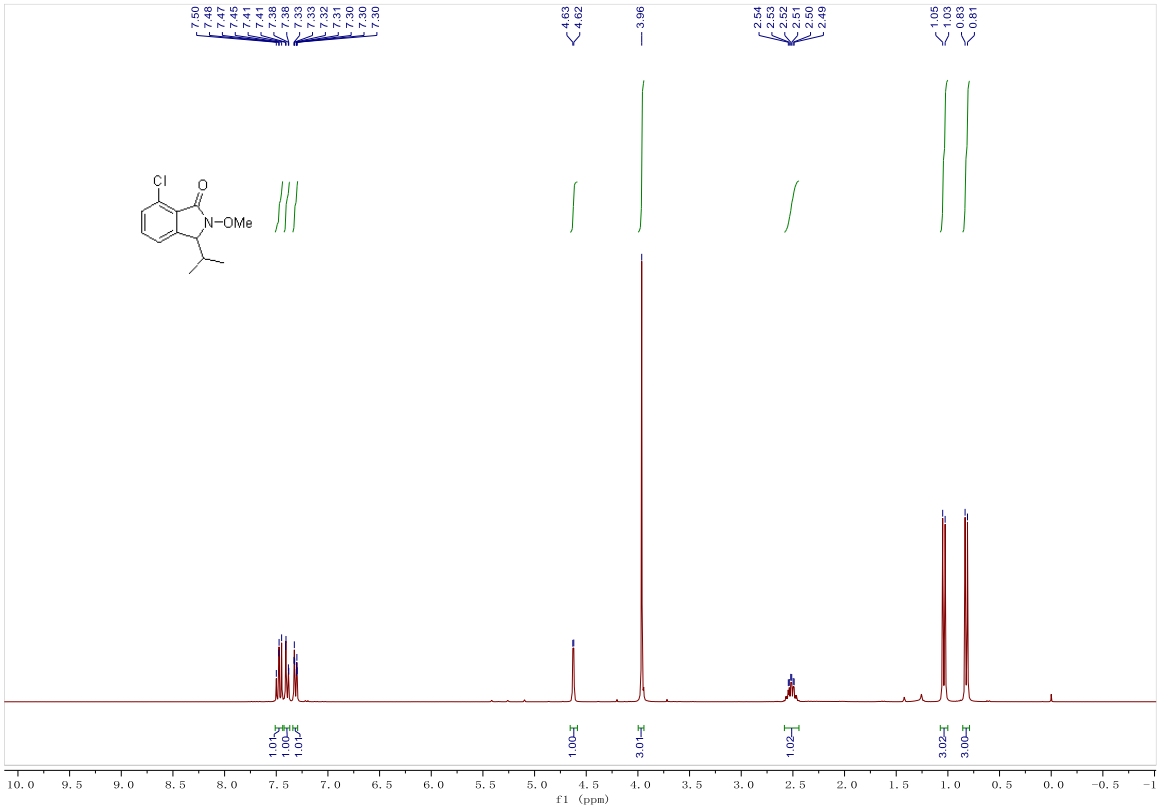
76.65
64.12
63.31
29.54
17.62
16.64
O
N-OMe
Br
f1 (ppm)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7.32
7.31
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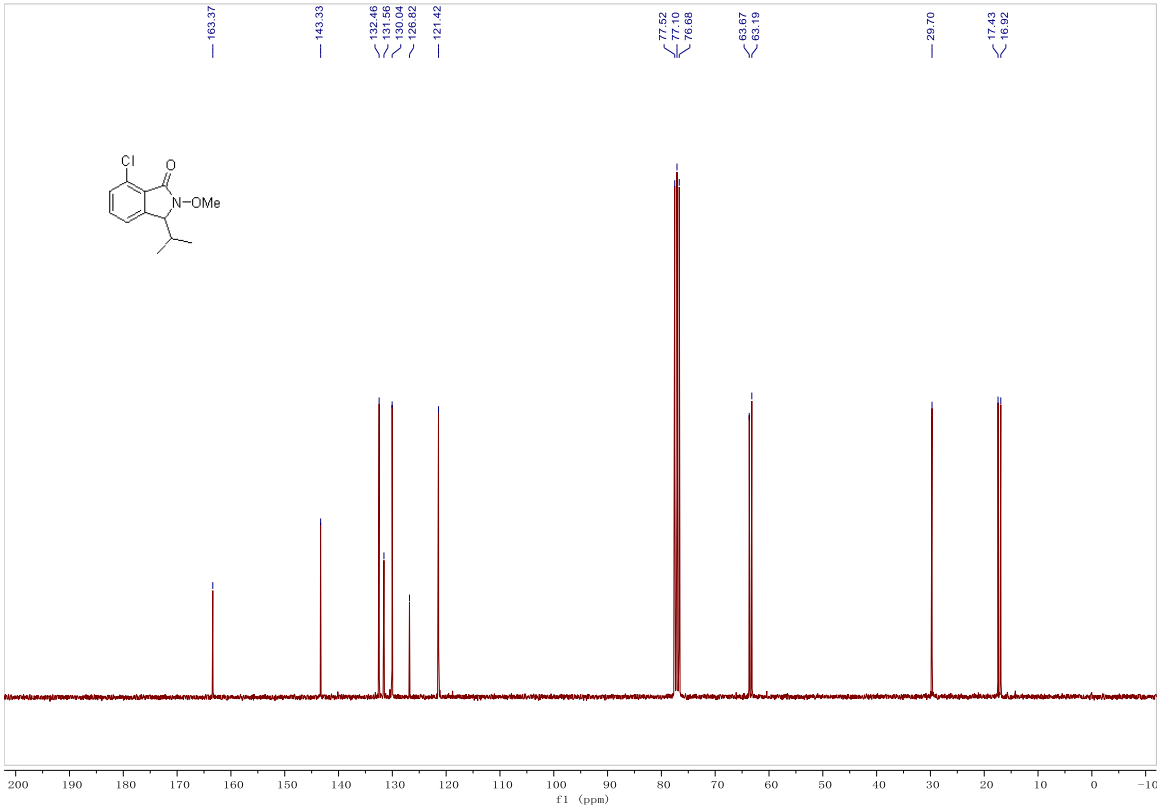
7.30
7.30
7.30
4.63
4.62
3.96
2.54
2.53
2.52
2.51
2.50
2.49
1.05
1.03
0.83
0.81
Cl
O
N–OMe
1.01
1.00
1.01
1.00
3.01
1.02
3.02
3.00
f1 (ppm)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126.82
121.42
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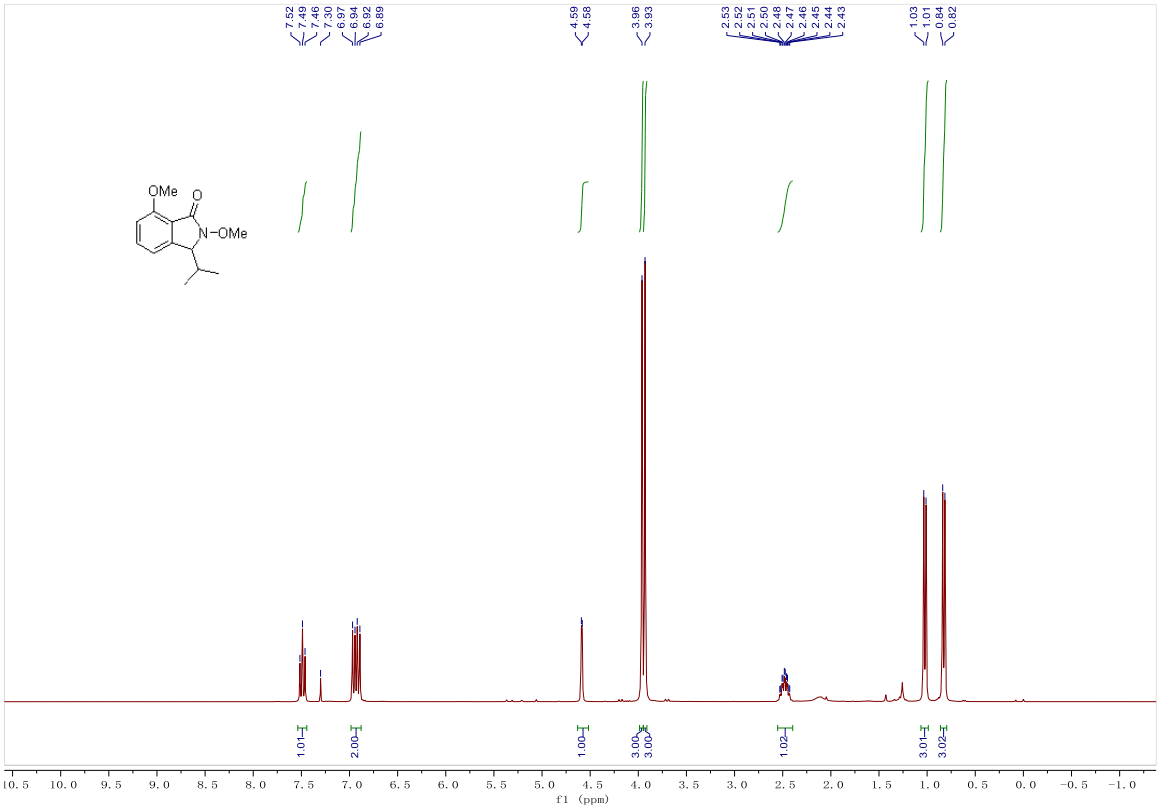
76.68
63.67
63.19
29.70
17.43
16.92
Cl
O
N–OMe
f1 (ppm)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7.49
7.46
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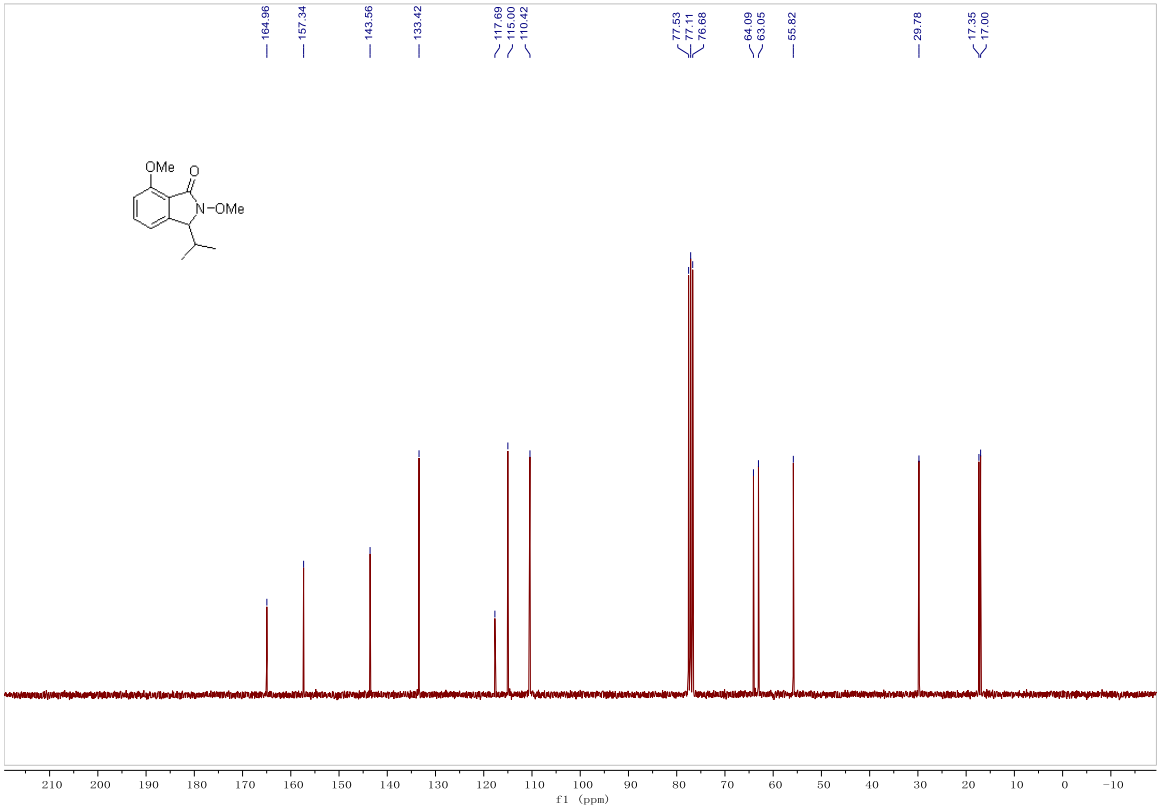
6.97
6.94
6.92
6.89
4.59
4.58
3.96
3.93
2.53
2.52
2.51
2.50
2.48
2.47
2.46
2.45
2.44
2.43
1.03
1.01
0.84
0.82
OMe
O
N–OMe
1.01
2.00
1.00
3.00
3.00
1.02
3.01
3.02
f1 (ppm)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115.00
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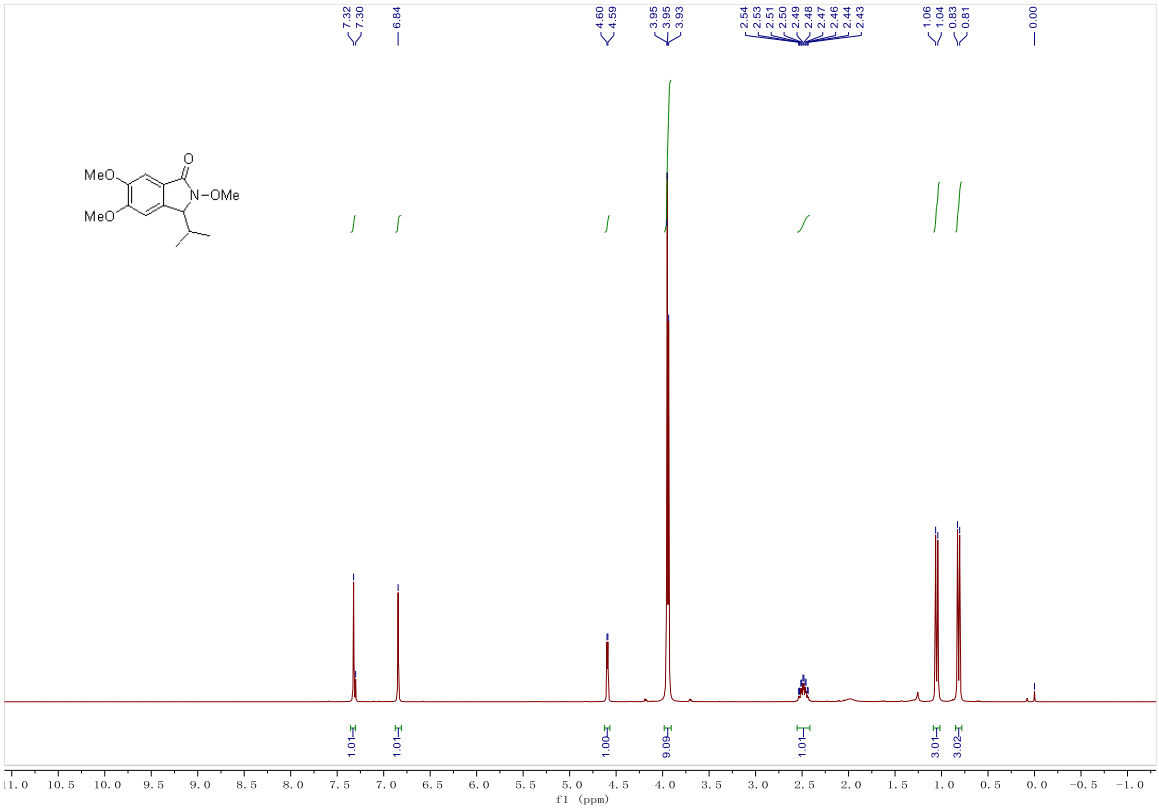
64.09
63.05
55.82
29.78
17.35
17.00
OMe
O
N–OMe
f1 (ppm)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3.95
3.95
3.93
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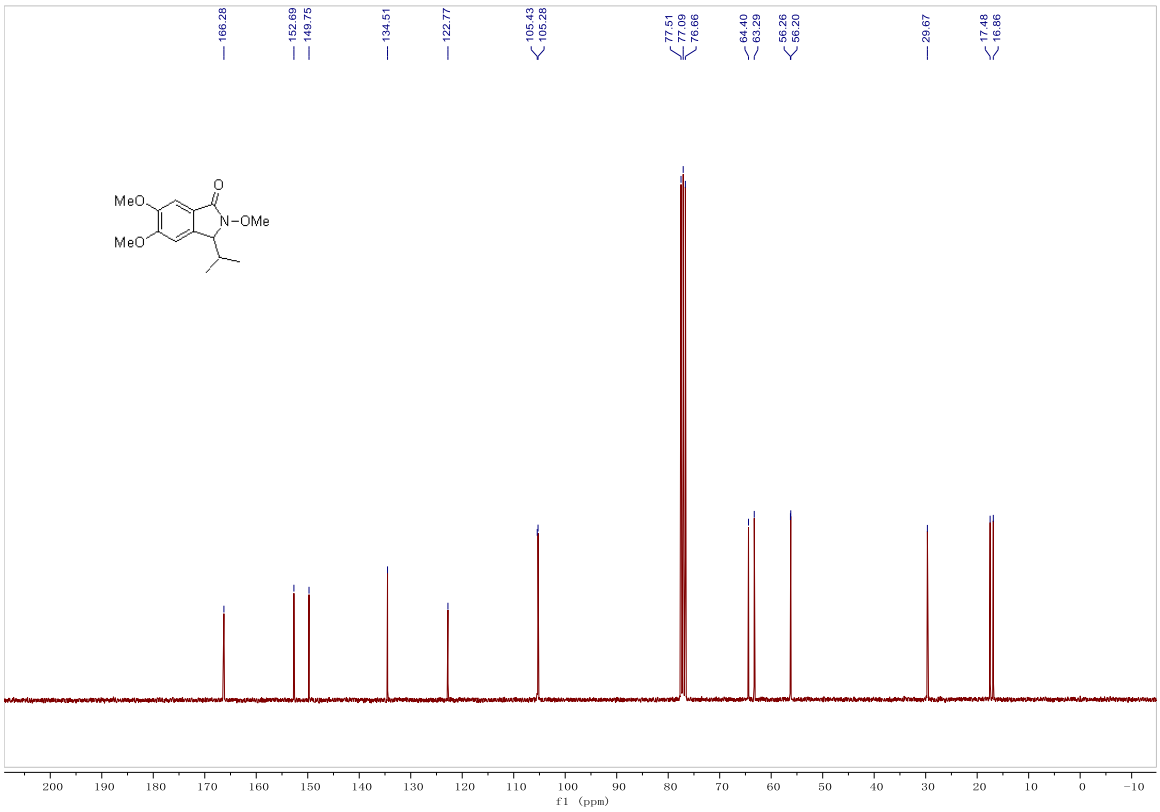
2.53
2.51
2.50
2.49
2.48
2.47
2.46
2.44
2.43
1.06
1.04
0.83
0.81
0.00
MeO
MeO
O
N–OMe
1.01
1.01
1.00
9.09
1.01
3.01
3.02
f1 (ppm)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149.75
134.51
122.77
105.43
105.28
77.51
77.09
76.66
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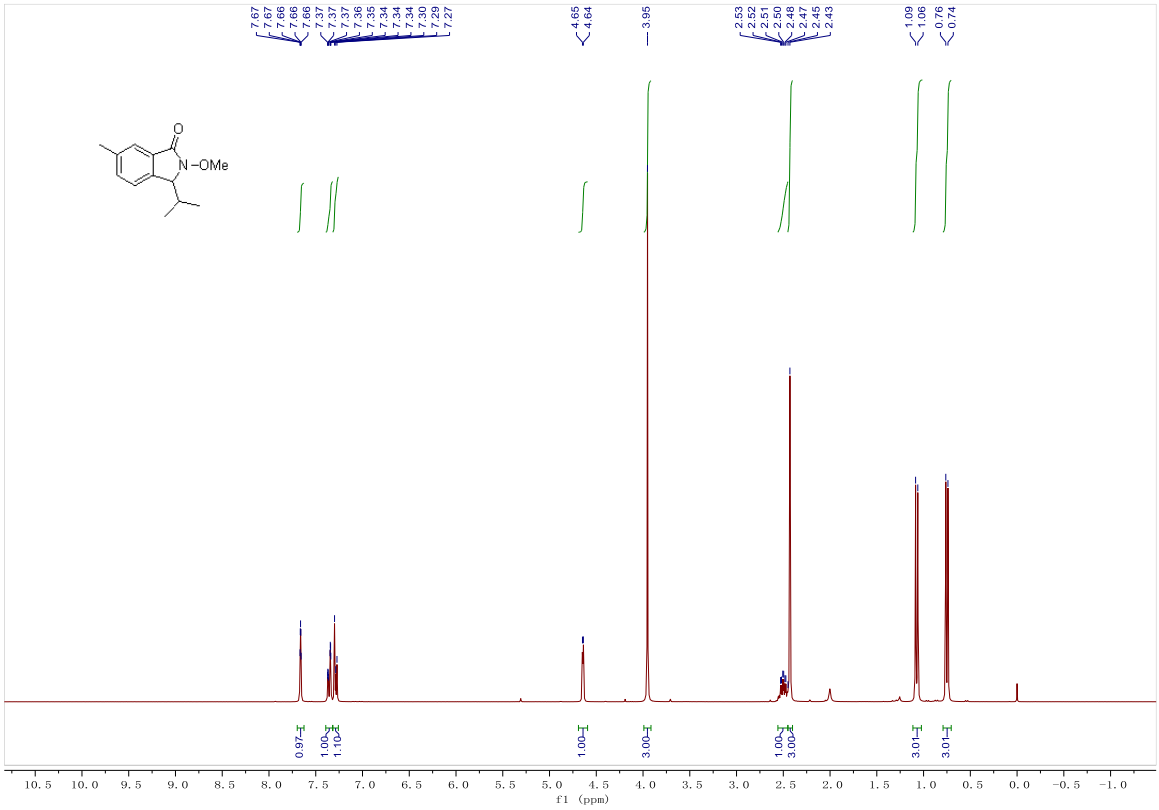
63.29
56.26
56.20
29.67
17.48
16.86
MeO
MeO
O
N–OMe
f1 (ppm)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7.66
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7.35
7.34
7.34
7.34
7.30
7.29
7.27
4.65
4.64
3.95
2.53
2.52
2.51
2.50
2.48
2.47
2.45
2.43
1.09
1.06
0.76
0.74
O
N–OMe
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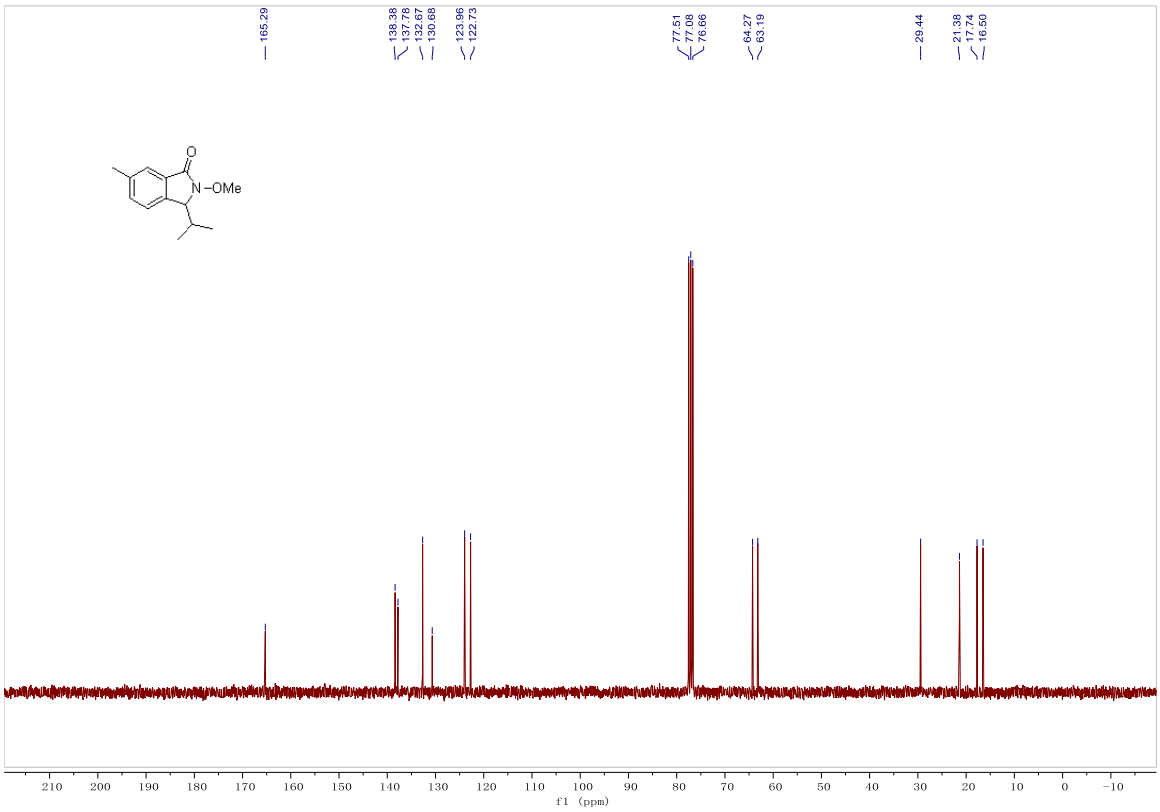
1.00
1.10
1.00
3.00
1.00
3.00
3.01
3.01
f1 (ppm)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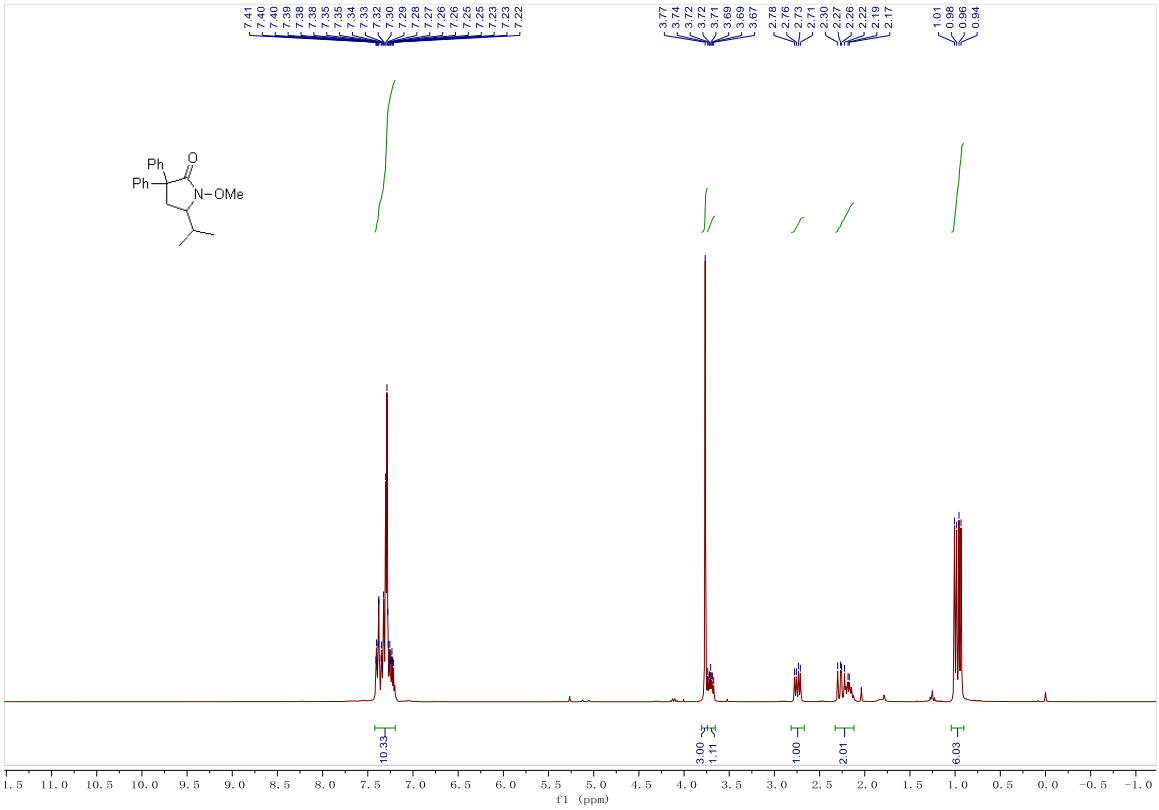
64.27
63.19
29.44
21.38
17.74
16.50
O
N–OMe
f1 (ppm)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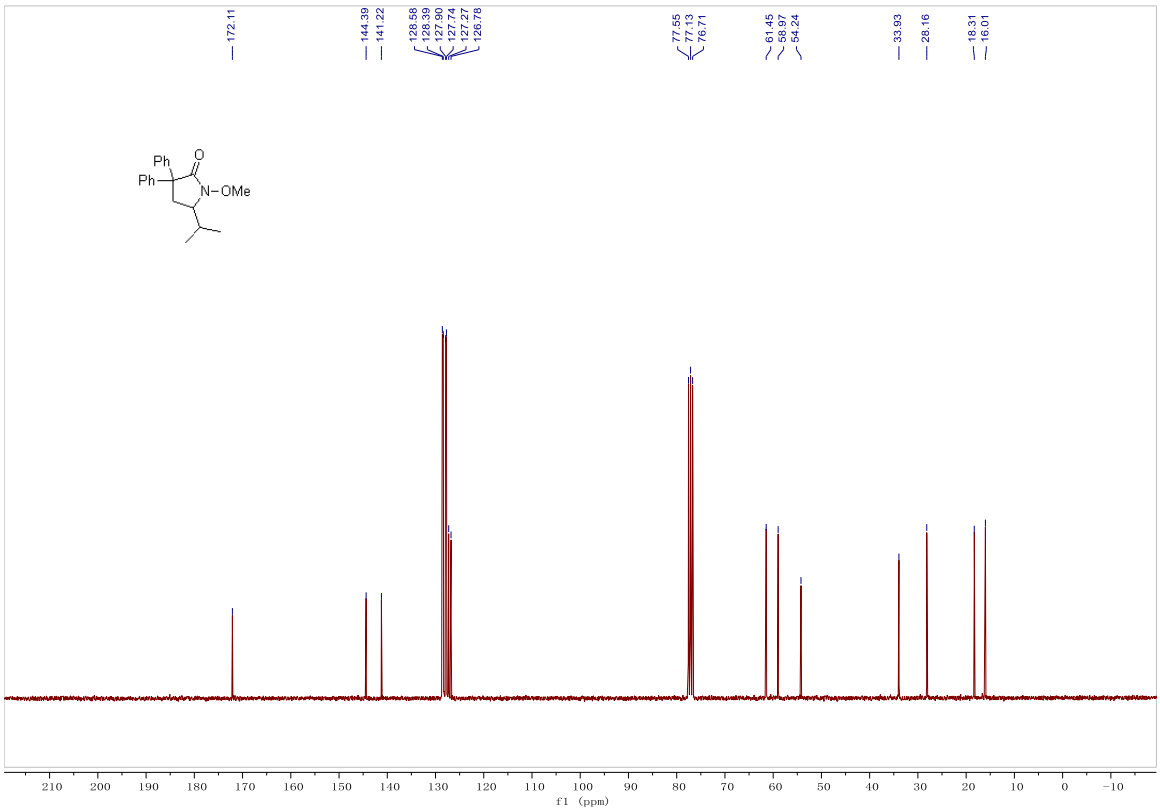
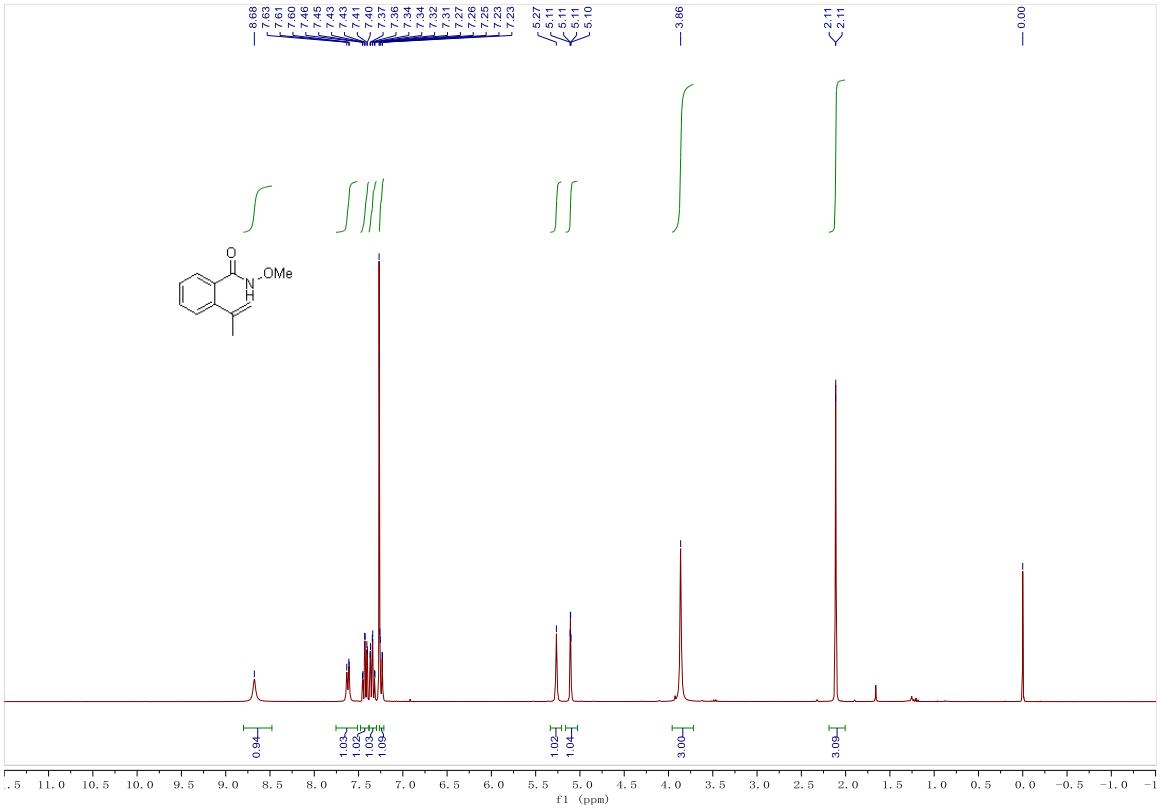
3.77 3.74 3.72 3.72 3.71 3.69 3.69 3.67
2.78 2.76 2.73 2.71 2.30 2.27 2.26 2.22 2.19 2.17
1.01 0.98 0.96 0.94
Ph
Ph
O
N–OMe
10.33
3.00
1.11
1.00
2.01
6.03
f1 (ppm)


172.11
144.39 141.22 128.58 128.39 127.90 127.74 127.27 126.78
77.55 77.13 76.71
61.45 58.97 54.24
33.93 28.16 18.31 16.01
Ph
Ph
O
N–OMe
f1 (ppm)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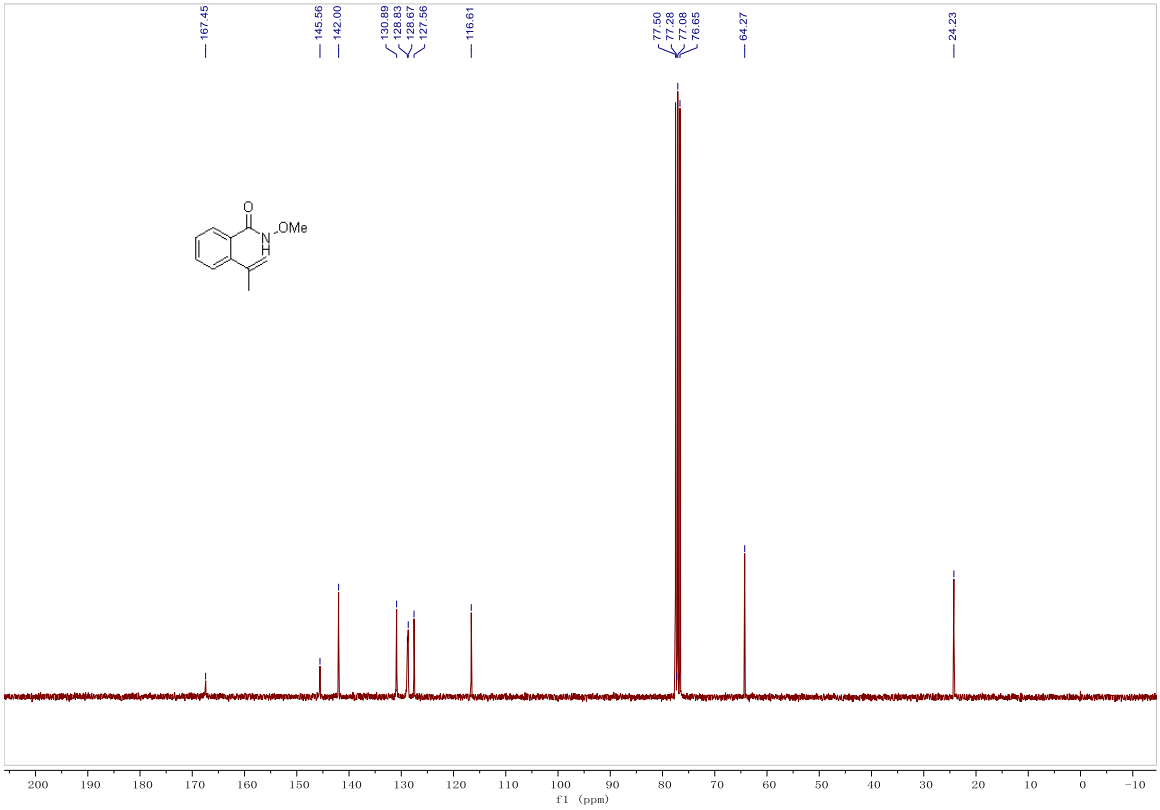
7.32
7.31
7.27
7.26
7.25
7.23
7.23
5.27
5.11
5.11
5.11
5.10
3.86
2.11
2.11
0.00
O
N
H
OMe
0.94
1.03
1.02
1.03
1.09
1.02
1.04
3.00
3.09
f1 (ppm)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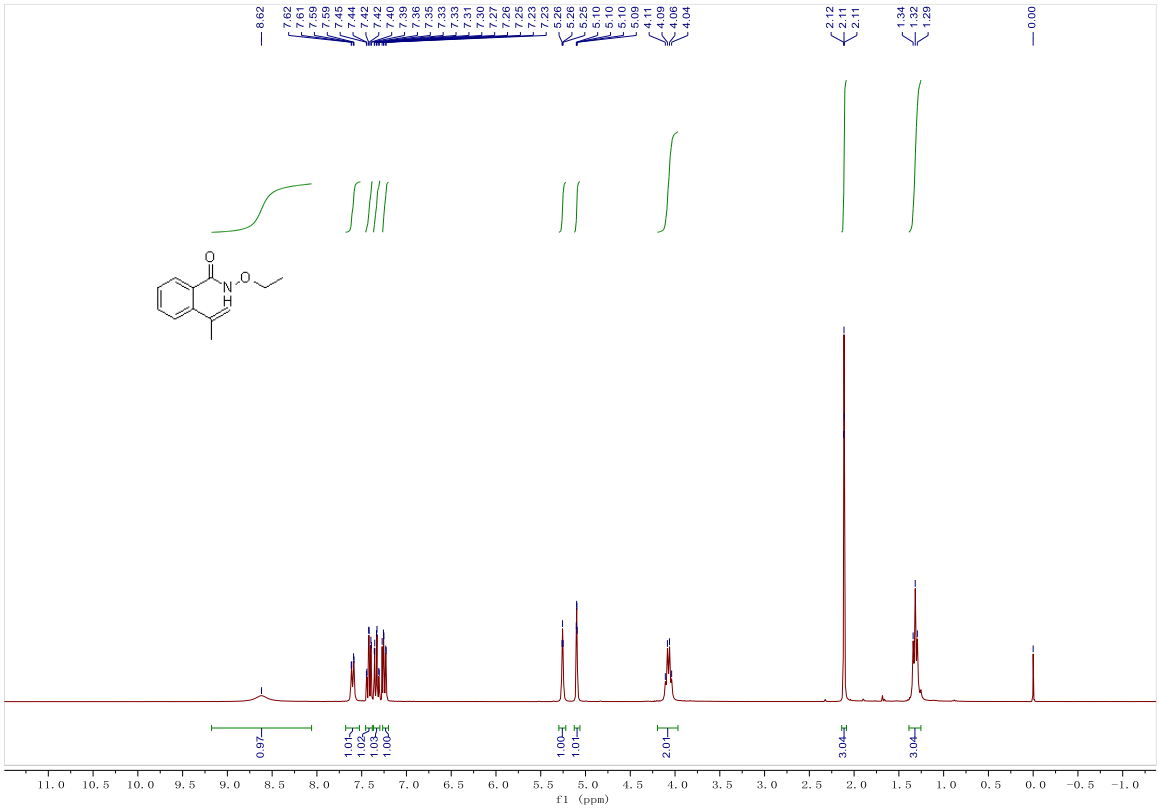
76.65
64.27
24.23
O
N
H
OMe
f1 (ppm)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7.36
7.35
7.33
7.33
7.31
7.30
7.27
7.26
7.25
7.23
7.23
5.26
5.26
5.25
5.10
5.10
5.09
4.11
4.09
4.06
4.04
2.12
2.11
2.11
1.34
1.32
1.29
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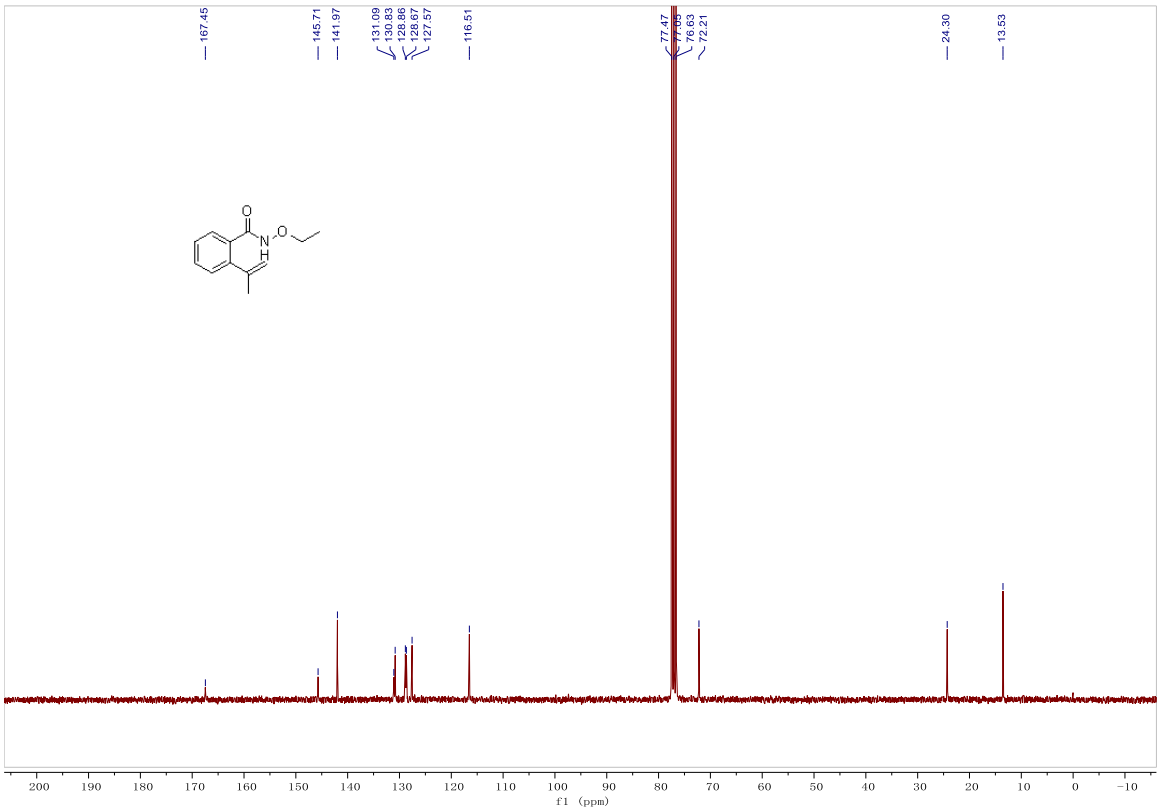
1.02
1.03
1.00
1.00
1.01
2.01
3.04
3.04
f1 (ppm)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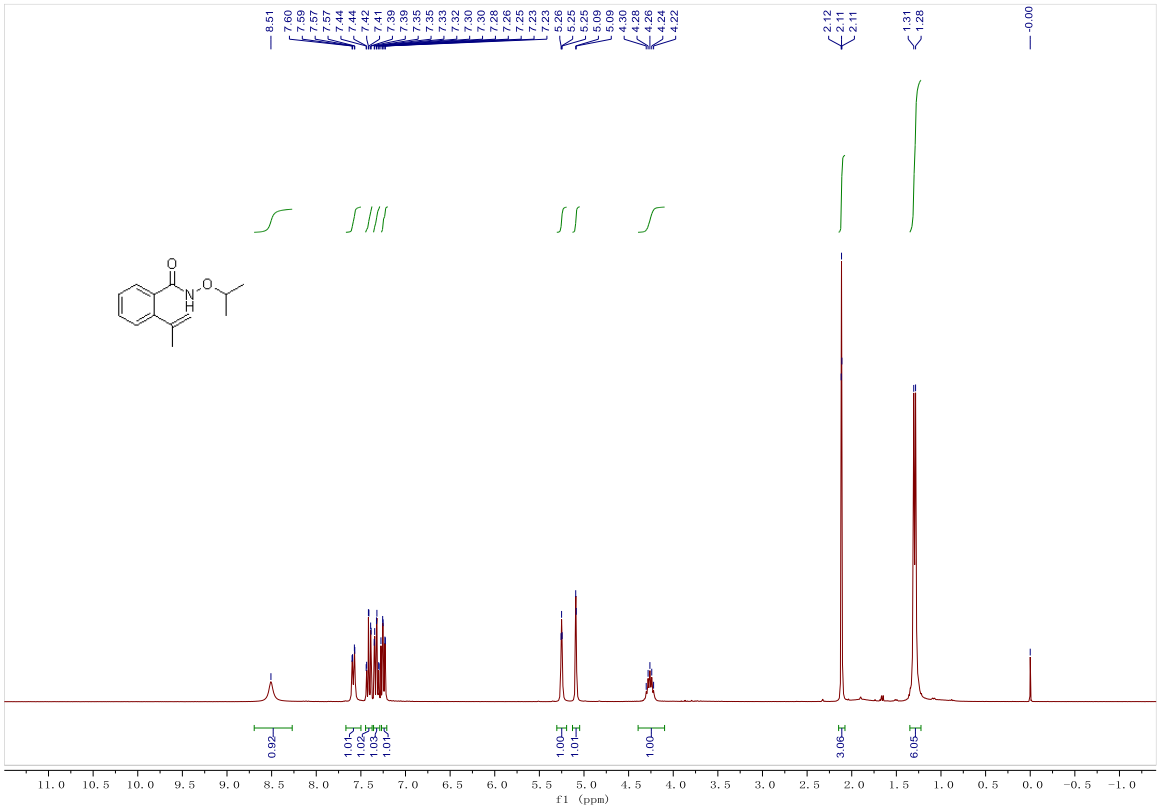
13.53
f1 (ppm)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7.39
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7.33
7.32
7.30
7.30
7.28
7.26
7.25
7.23
7.23
5.26
5.25
5.25
5.09
5.09
4.30
4.28
4.26
4.24
4.22
2.12
2.11
2.11
1.31
1.28
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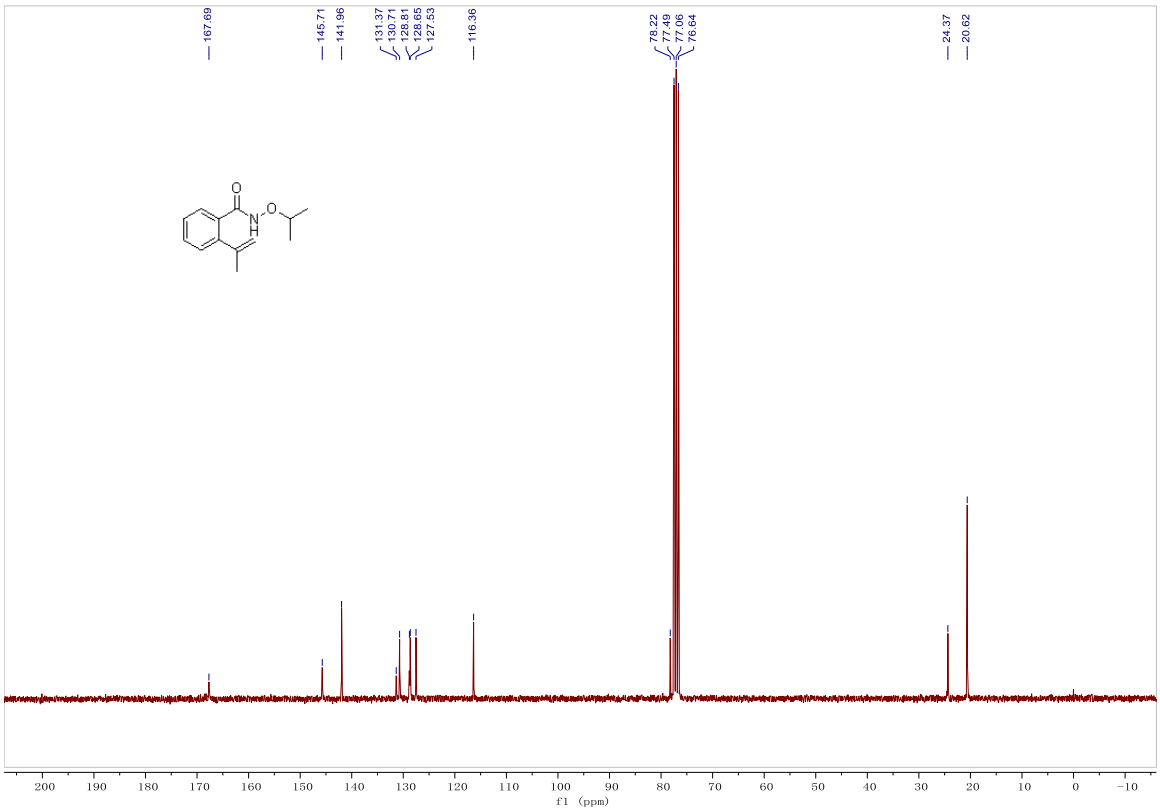
1.03
1.01
1.00
1.01
1.00
3.06
6.05
f1 (ppm)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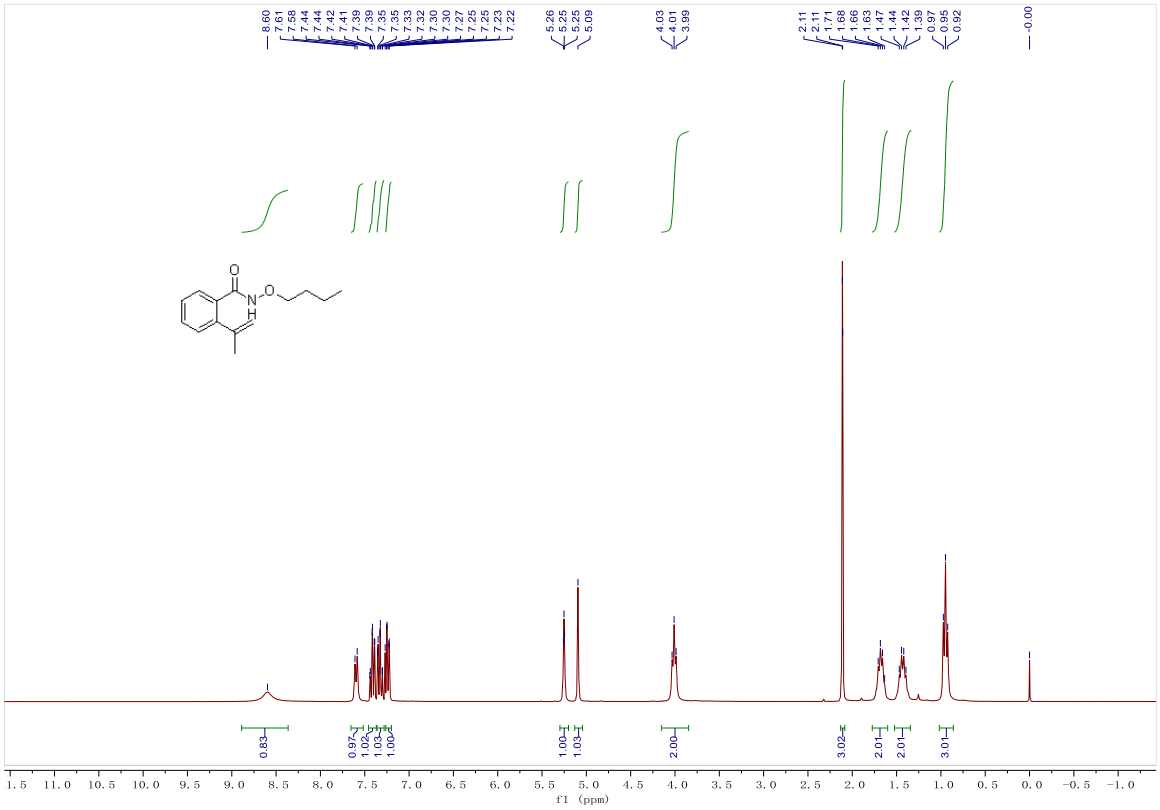
f1 (ppm)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7.39
7.35
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7.32
7.30
7.30
7.27
7.25
7.25
7.23
7.22
5.26
5.25
5.25
5.09
4.03
4.01
3.99
2.11
2.11
1.71
1.68
1.66
1.63
1.47
1.44
1.42
1.39
0.97
0.95
0.92
-0.00
0.83
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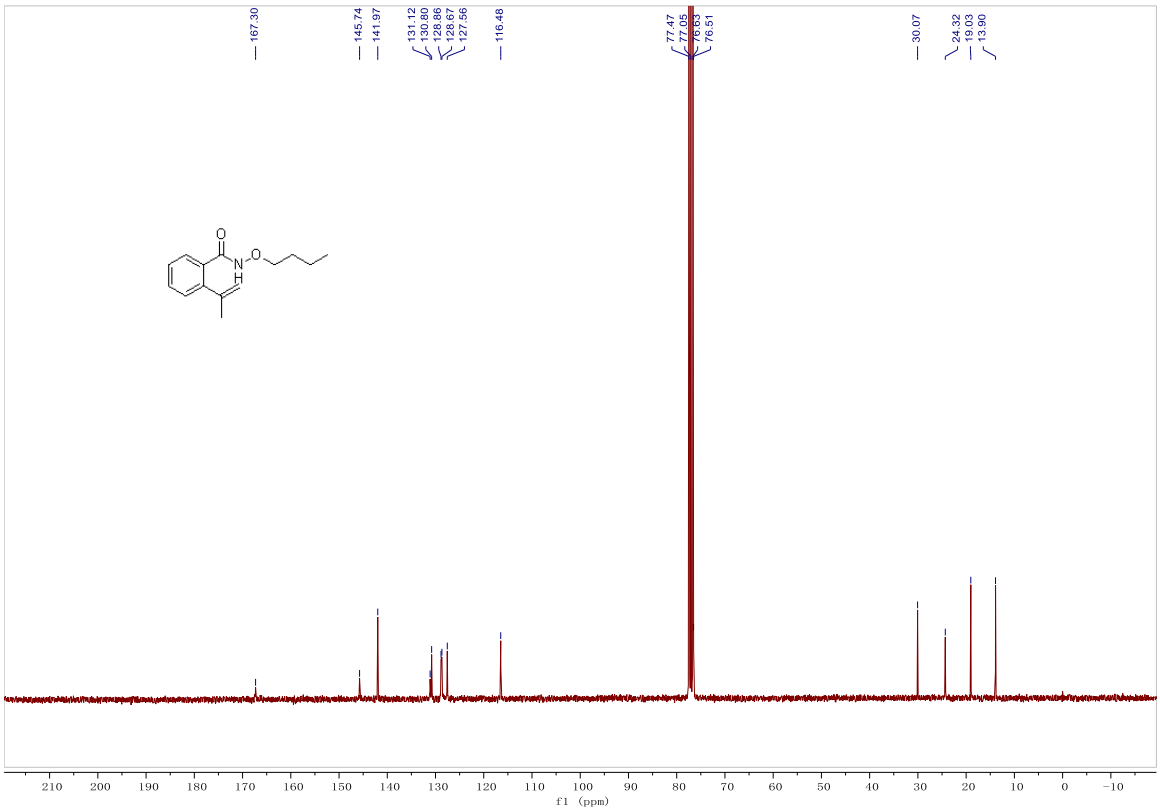
1.02
1.03
1.00
1.00
1.03
2.00
3.02
2.01
2.01
3.01
f1 (ppm)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127.56
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77.05
76.63
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30.07
24.32
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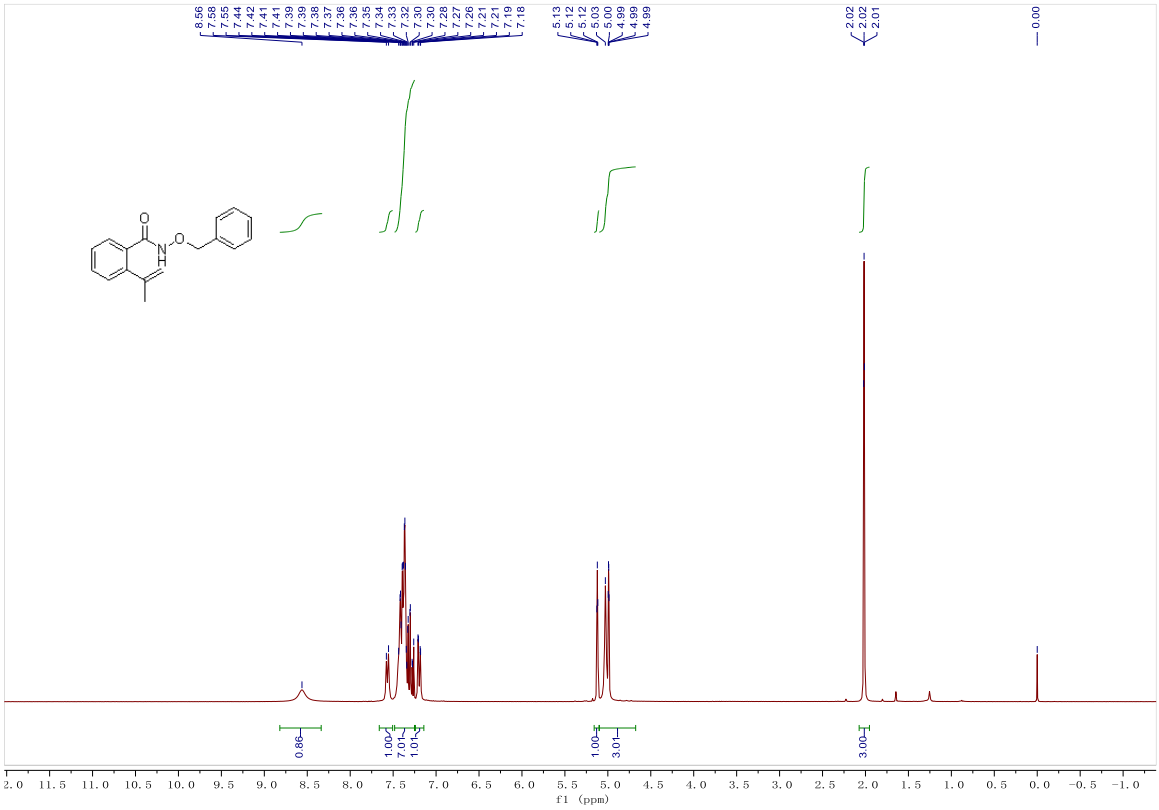
13.90
f1 (ppm)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7.34
7.33
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7.30
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7.27
7.26
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7.21
7.19
7.18
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5.12
5.12
5.03
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4.99
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2.02
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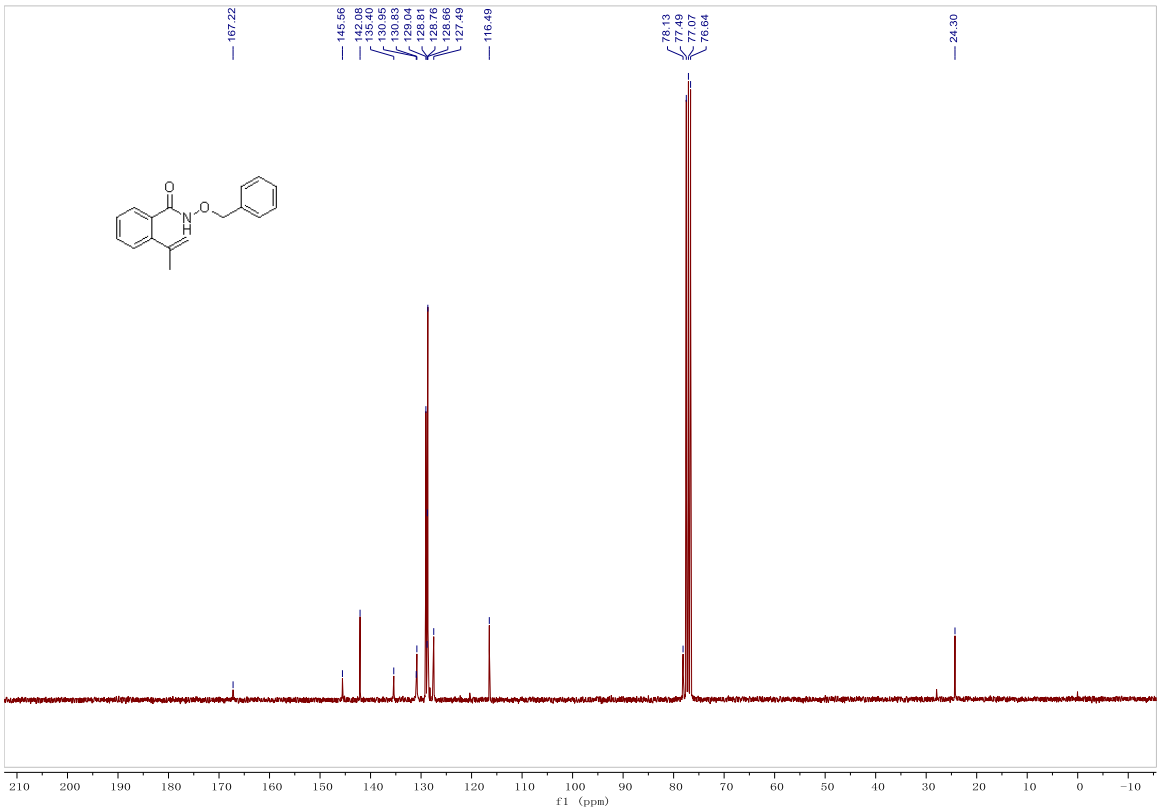
3.00
f1 (ppm)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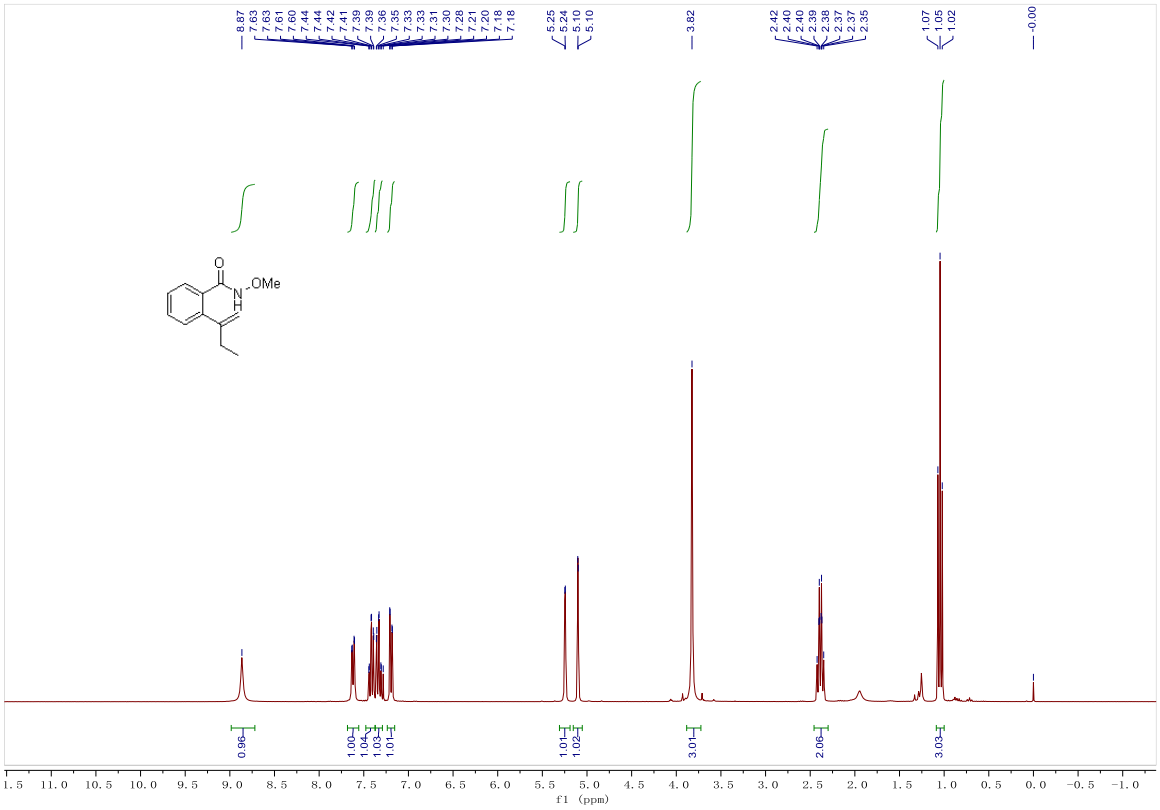
77.07
76.64
24.30
f1 (ppm)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7.31
7.30
7.28
7.21
7.20
7.18
7.18
5.25
5.24
5.10
5.10
3.82
2.42
2.40
2.40
2.39
2.38
2.37
2.37
2.35
1.07
1.05
1.02
-0.00
O
N
H
OMe
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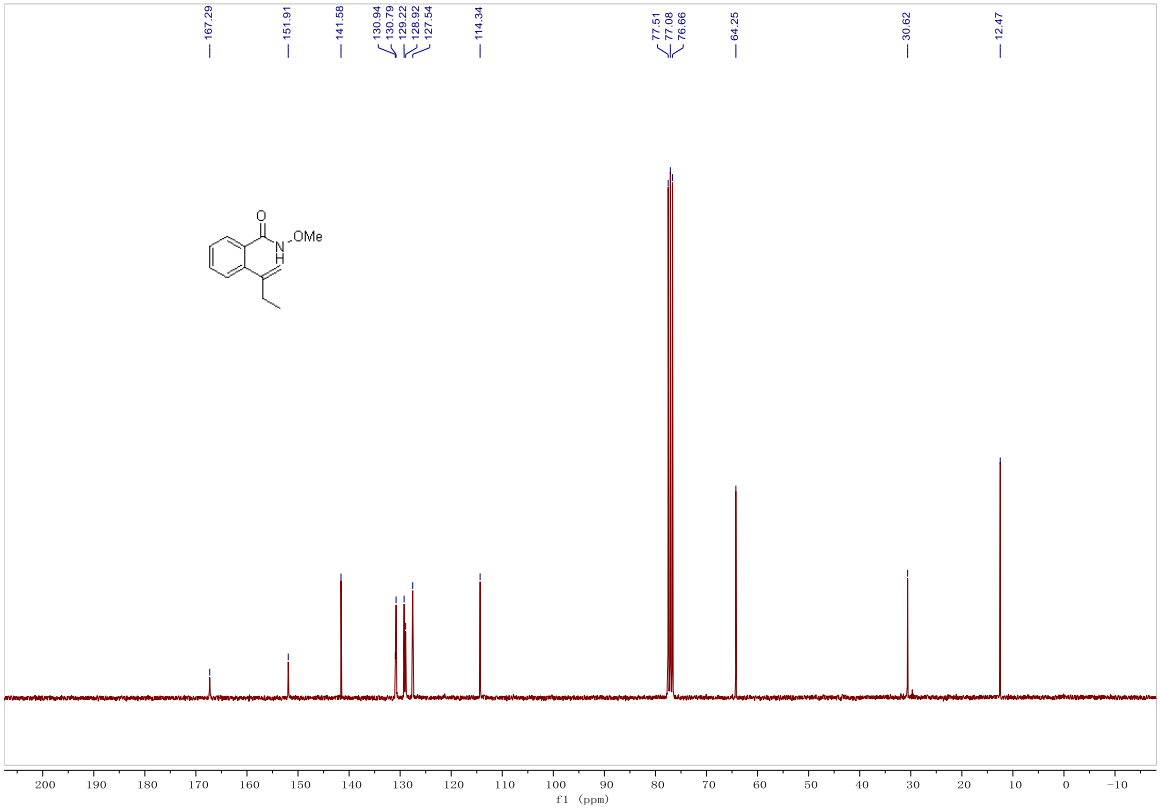
1.04
1.03
1.01
1.01
1.02
3.01
2.06
3.03
f1 (ppm)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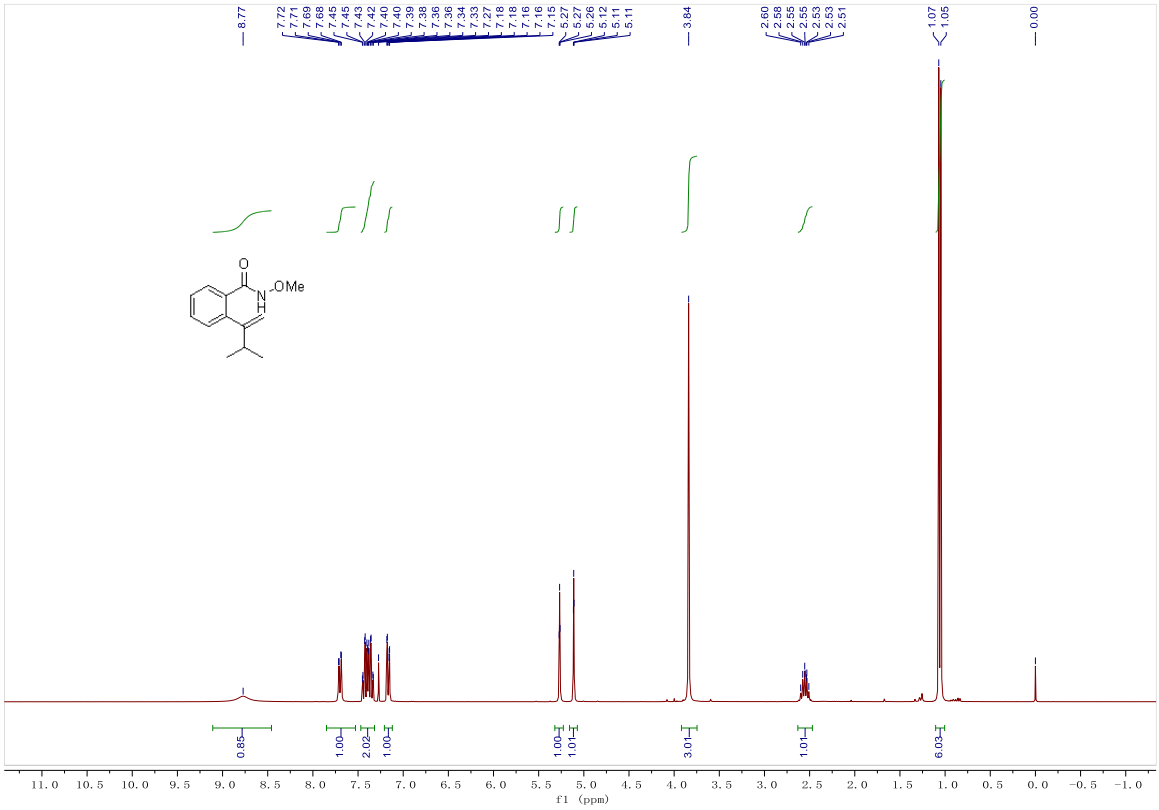
64.25
30.62
12.47
O
N
H
OMe
f1 (ppm)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7.34
7.33
7.27
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7.18
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5.27
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2.53
2.51
1.07
1.05
0.00
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OMe
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3.01
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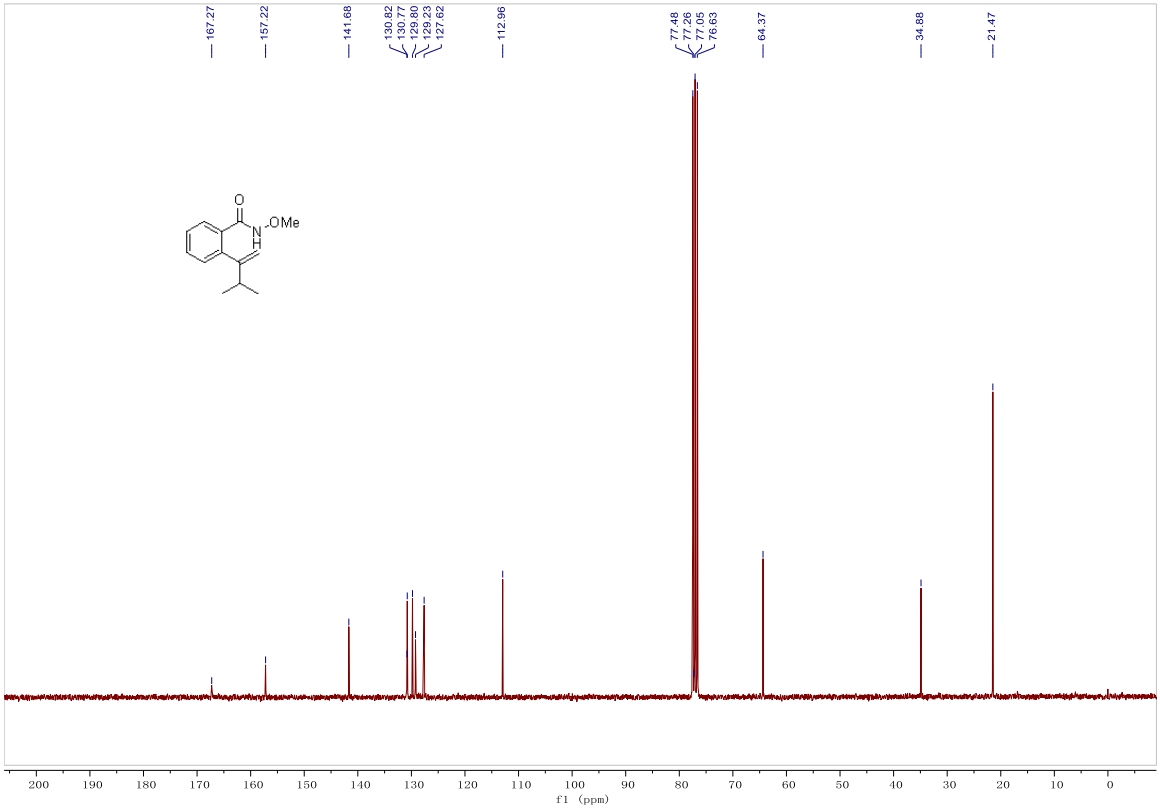
6.03
f1 (ppm)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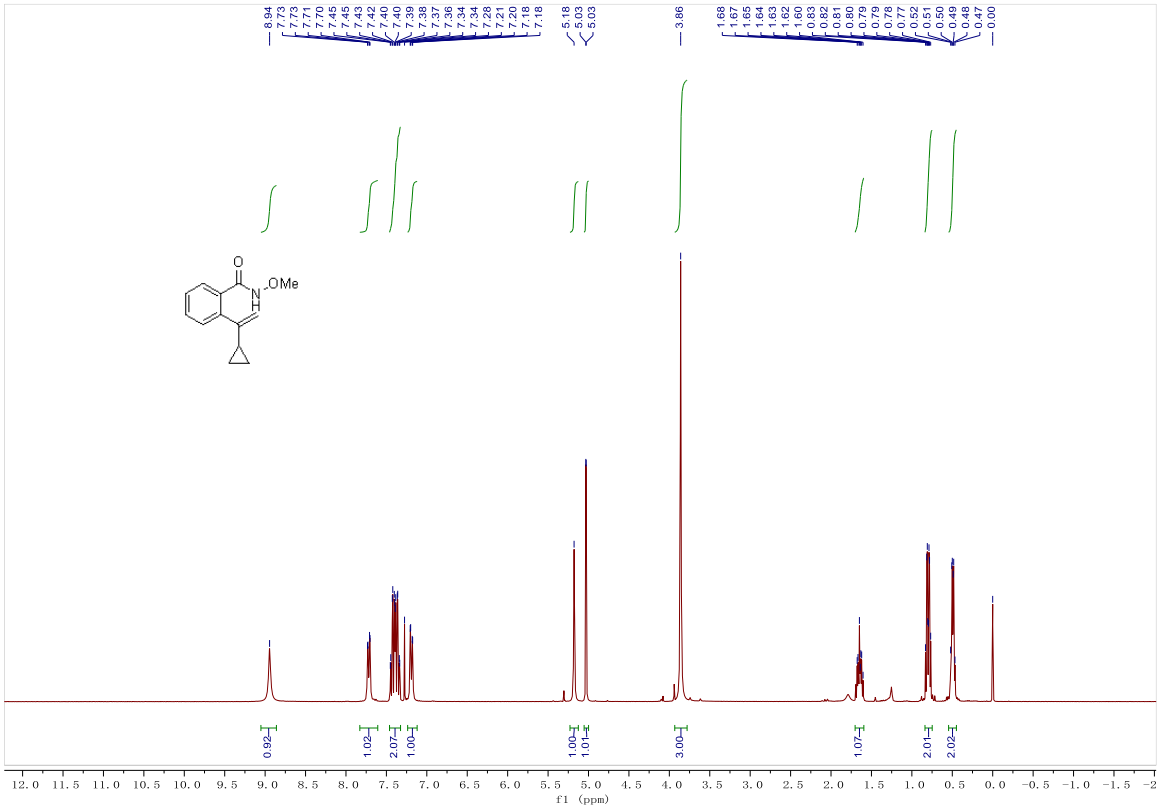
O
N
H
OMe
f1 (ppm)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7.18
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5.03
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0.79
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0.51
0.50
0.49
0.48
0.47
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O
N
H
OMe
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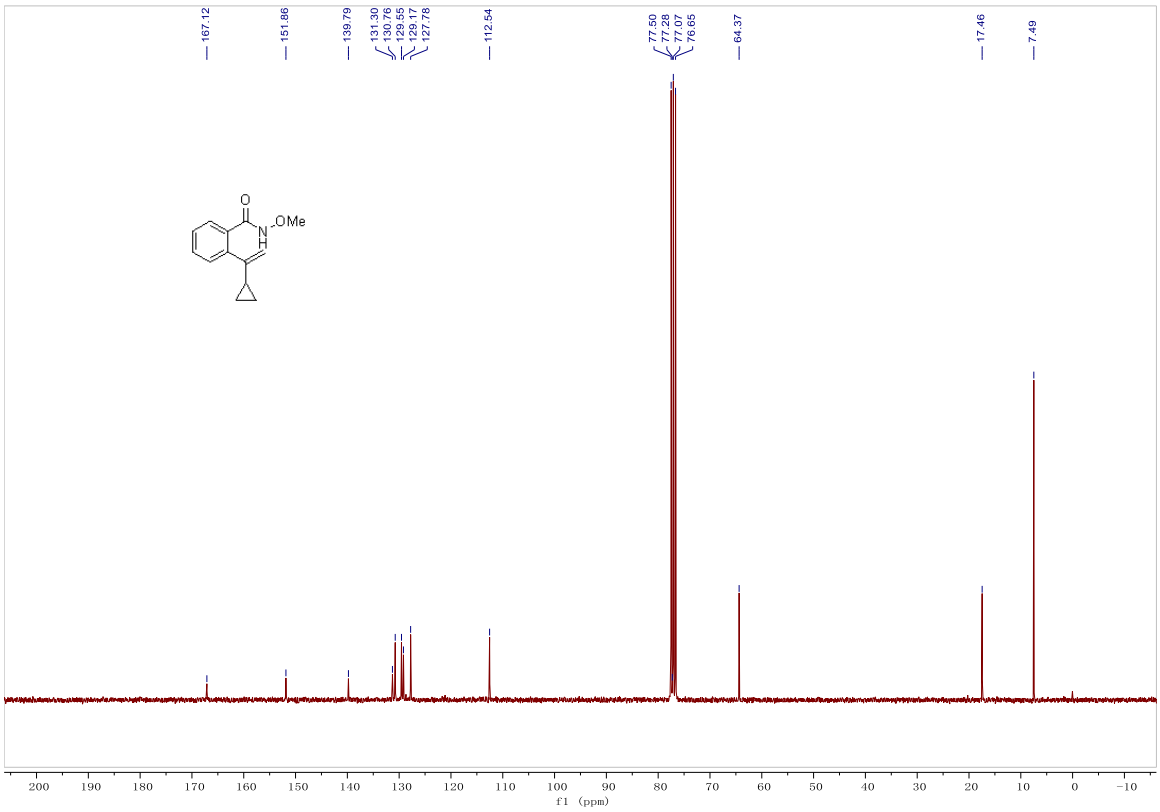
1.00
1.00
1.01
3.00
1.07
2.01
2.02
f1 (ppm)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129.17
127.78
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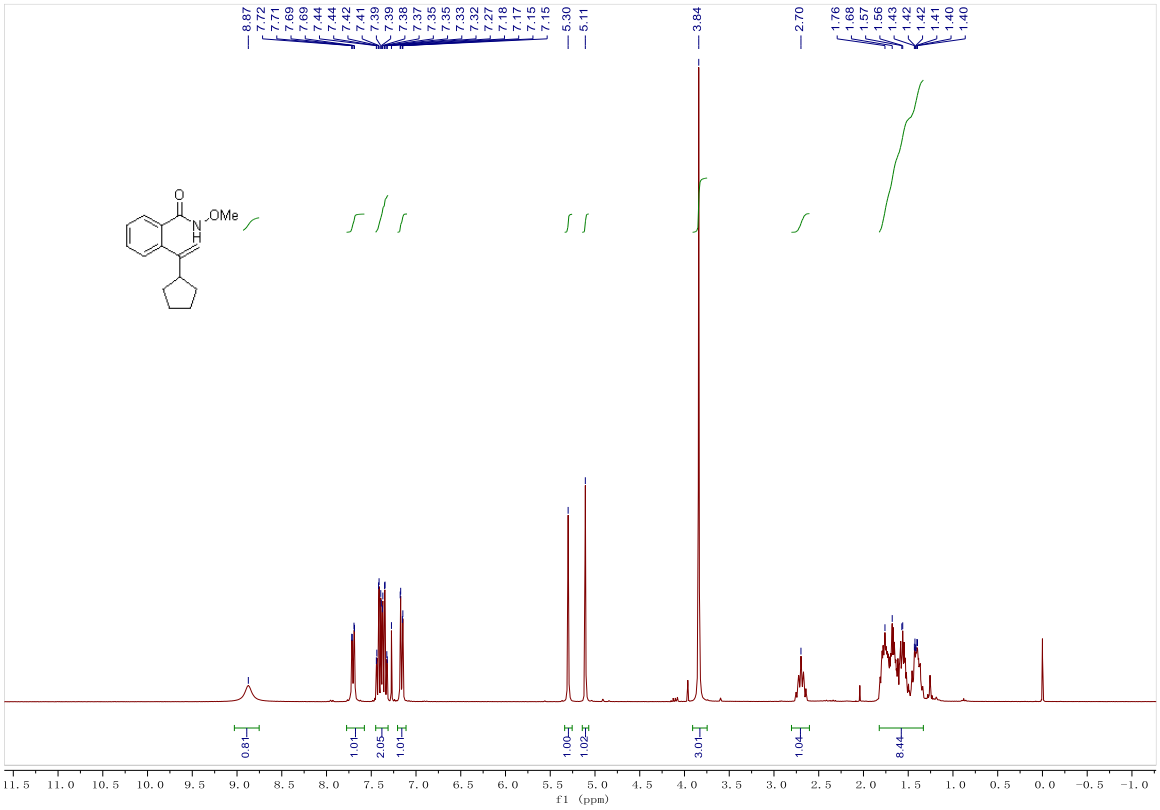
77.07
76.65
64.37
17.46
7.49
O
N
H
OMe
f1 (ppm)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7.71
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7.44
7.42
7.41
7.39
7.39
7.38
7.37
7.35
7.35
7.33
7.32
7.27
7.18
7.17
7.15
7.15
5.30
5.11
3.84
2.70
1.76
1.68
1.57
1.56
1.43
1.42
1.42
1.41
1.40
1.40
OMe
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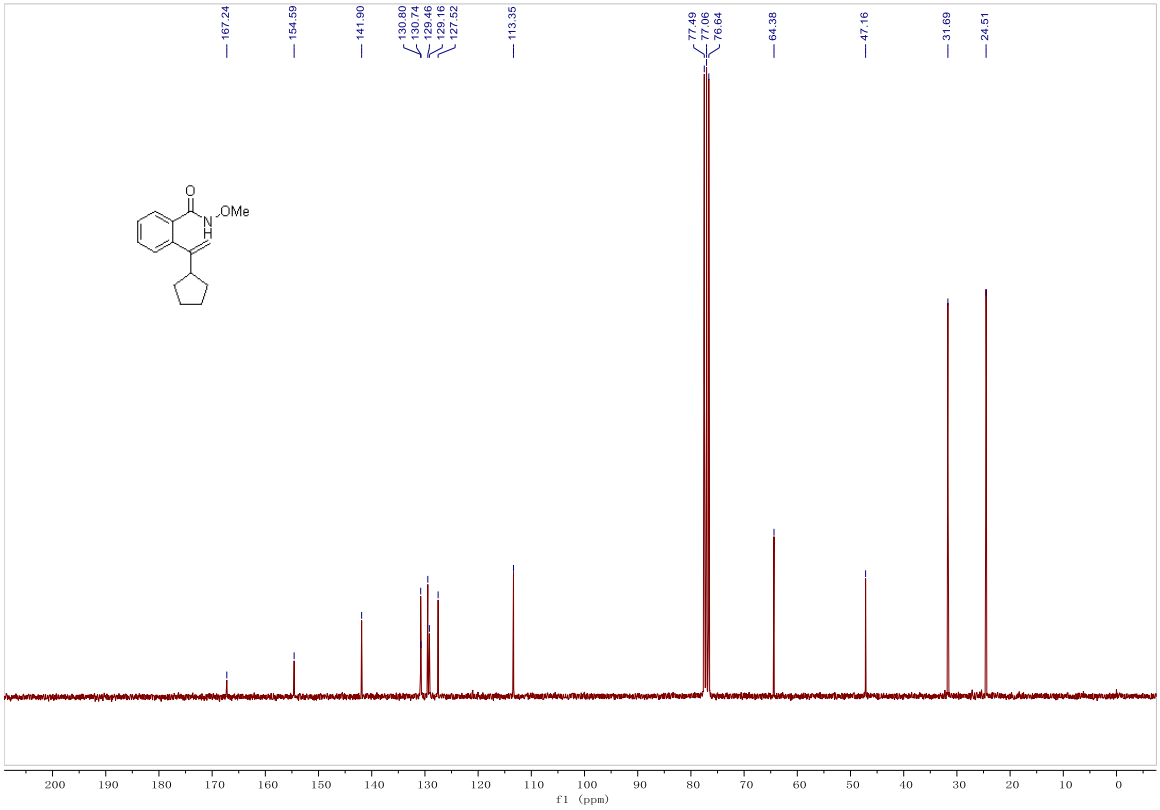
1.01
2.05
1.01
1.00
1.02
3.01
1.04
8.44
f1 (ppm)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154.59
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129.46
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127.52
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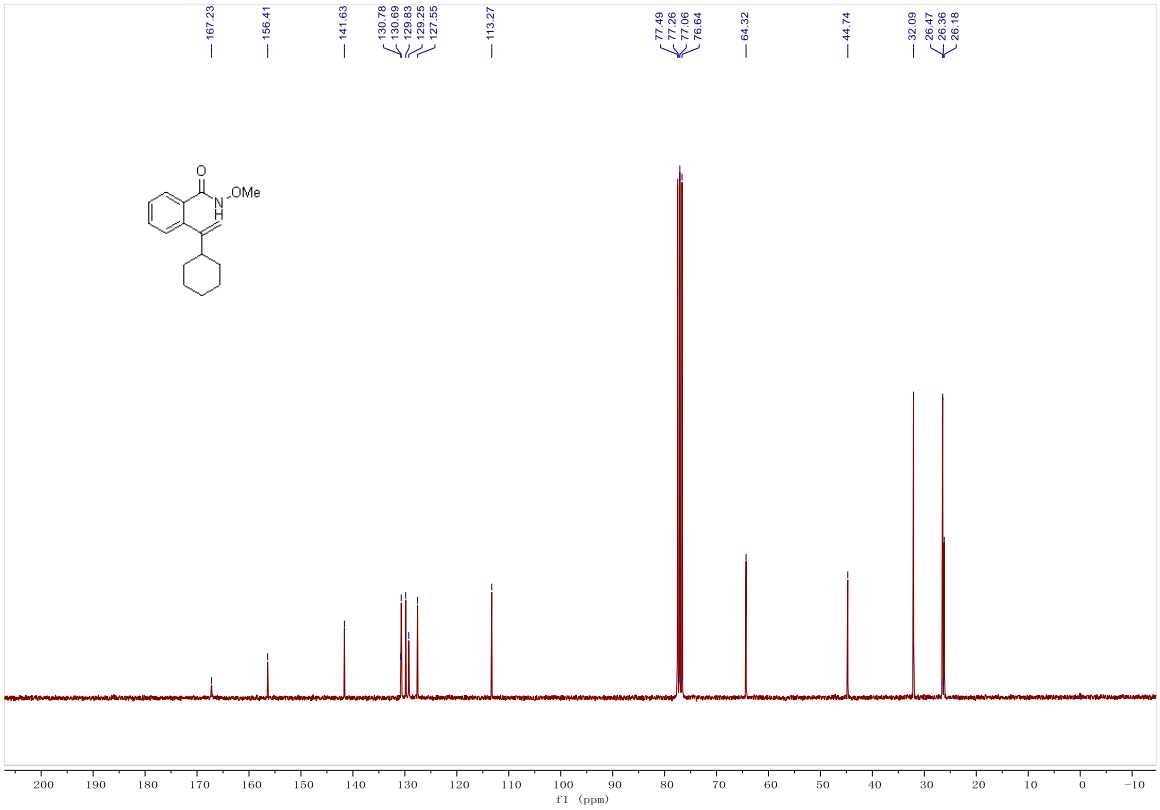
77.06
76.64
64.38
47.16
31.69
24.51
OMe
f1 (ppm)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127.55
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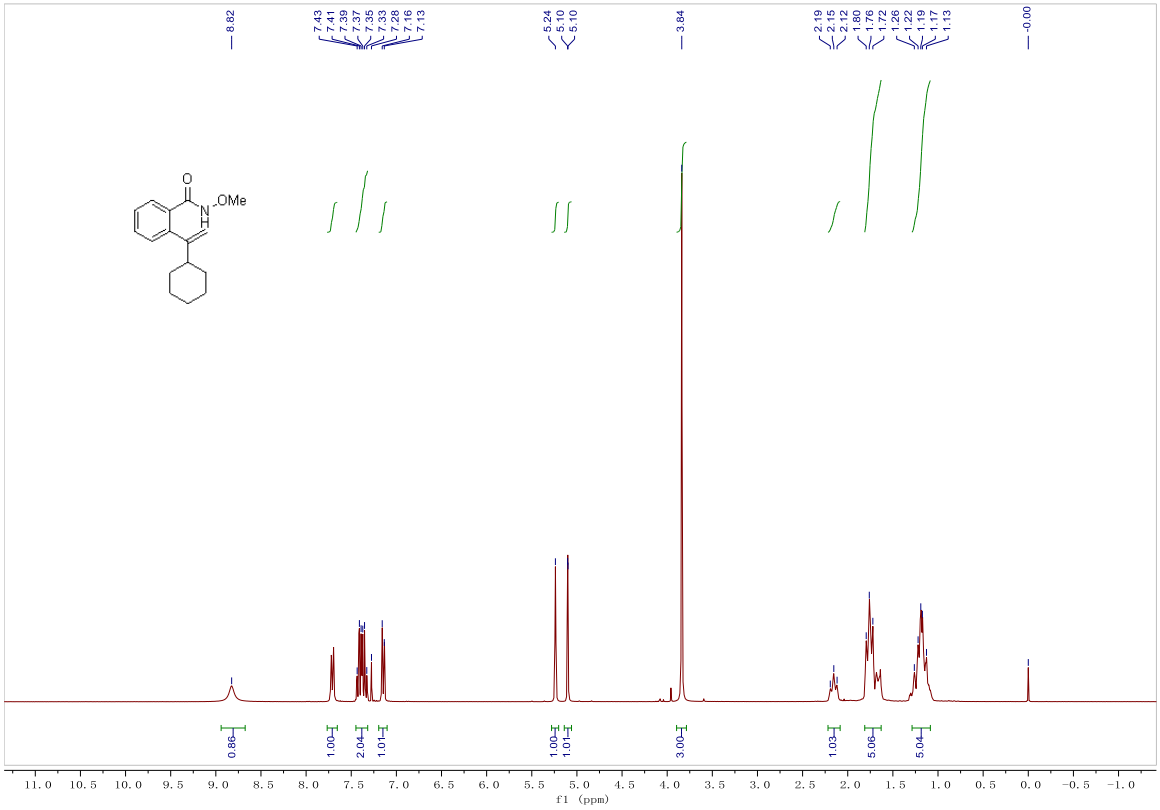
77.49
77.26
77.06
76.64
64.32
44.74
32.09
26.47
26.36
26.18
O
N
H
OMe
f1 (ppm)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7.28
7.16
7.13
5.24
5.10
5.10
3.84
2.19
2.15
2.12
1.80
1.75
1.72
1.26
1.22
1.19
1.17
1.13
0.00
0.86
1.00
2.04
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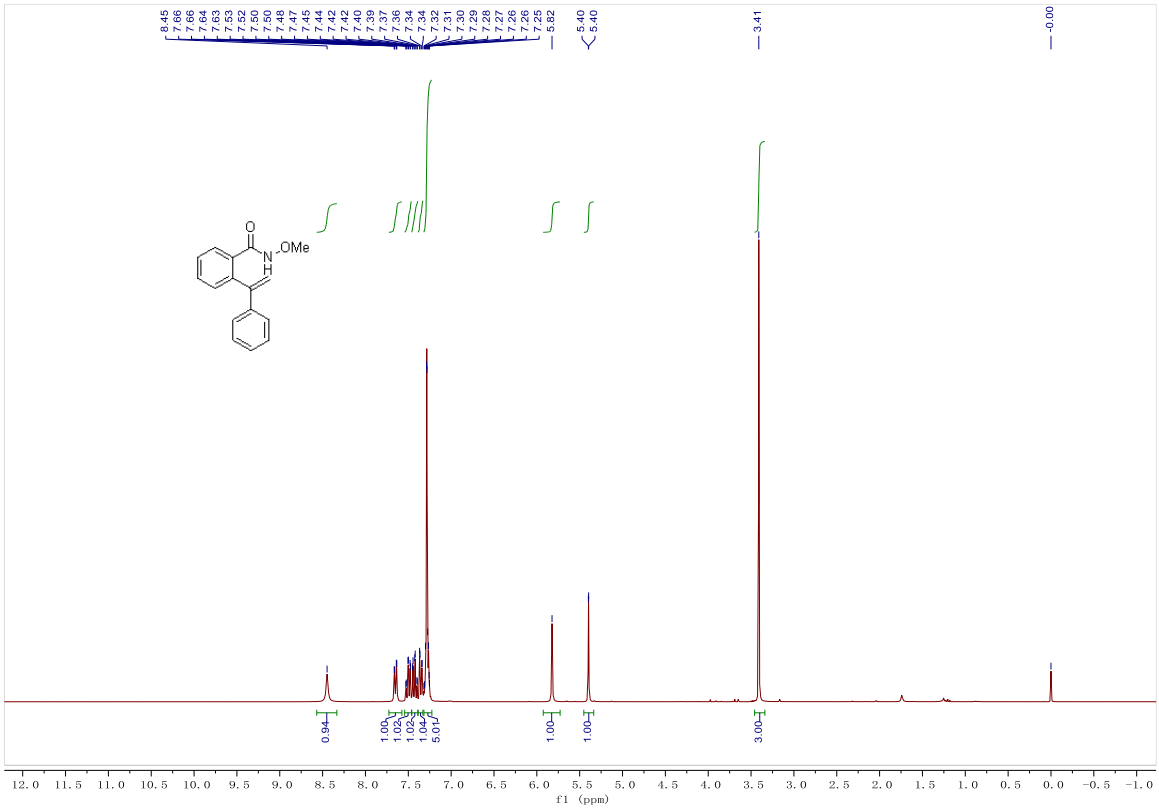
1.00
1.01
3.00
1.03
5.06
5.04
O
N
H
OMe
f1 (ppm)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7.66
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7.50
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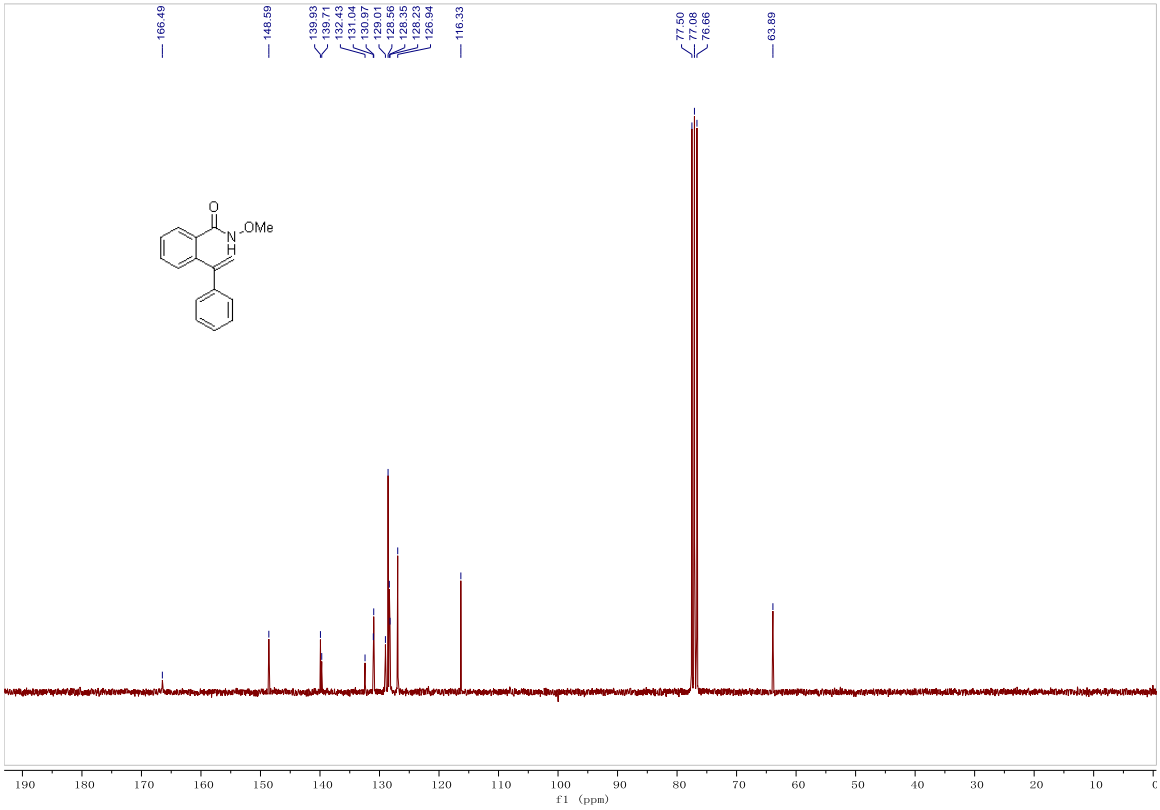
7.47
7.45
7.44
7.42
7.42
7.40
7.39
7.37
7.36
7.34
7.34
7.32
7.31
7.30
7.29
7.28
7.27
7.26
7.26
7.25
5.82
5.40
5.40
3.41
-0.00
O
N
H
OMe
0.94
1.00
1.02
1.02
1.04
5.01
1.00
1.00
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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130.97
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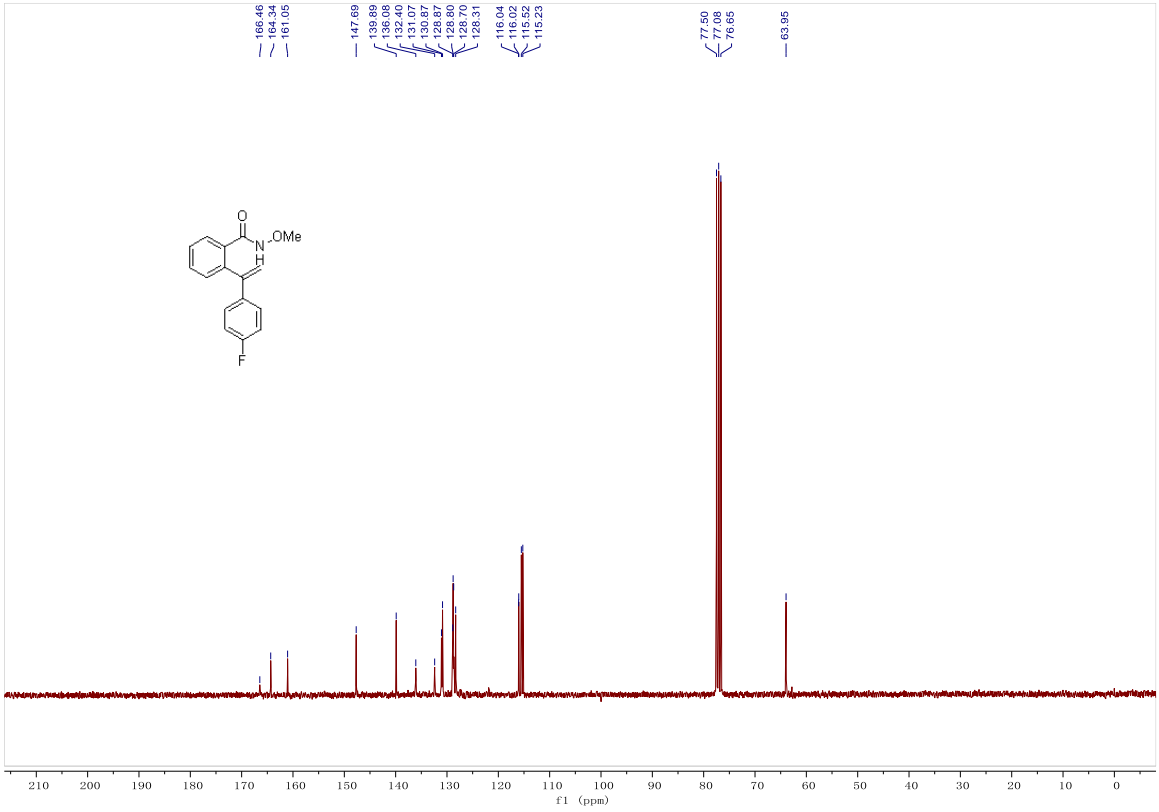
128.56
128.35
128.23
126.94
116.33
77.50
77.08
76.66
63.89
O
N
H
OMe
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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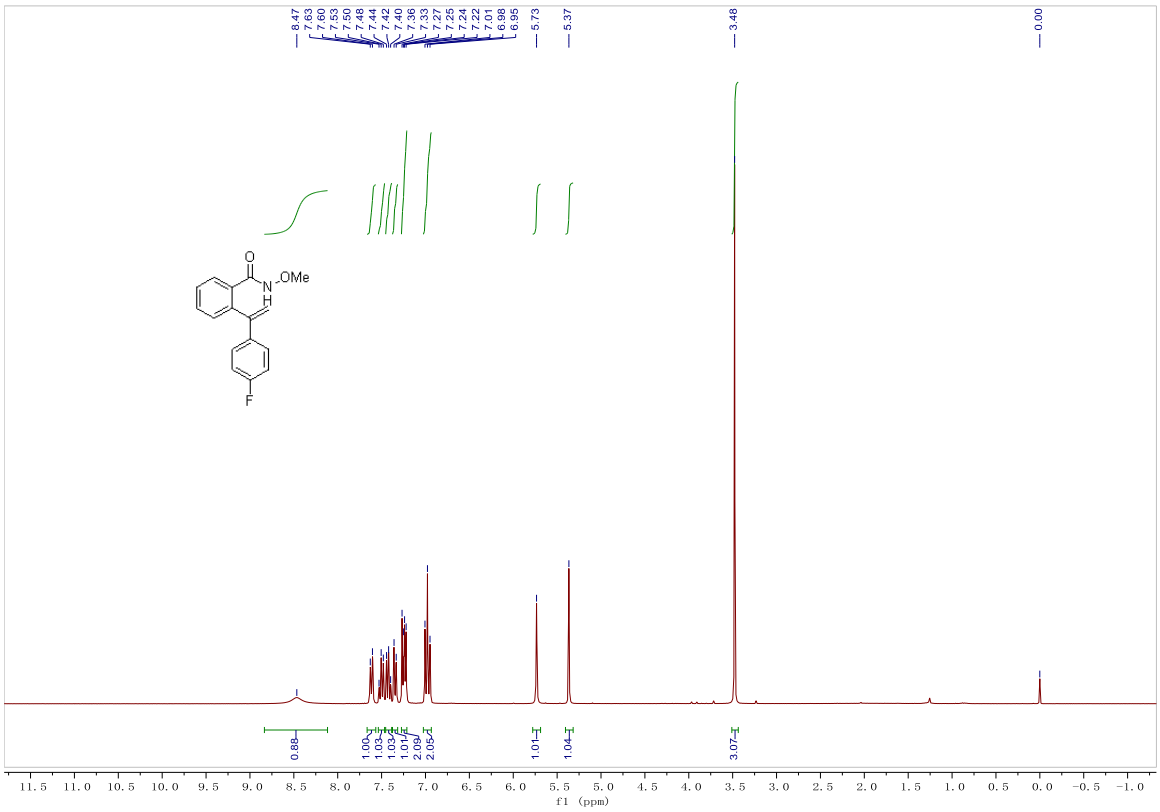
164.34
161.05
147.69
139.89
136.08
132.40
131.07
130.87
128.87
128.60
128.70
128.31
116.04
116.02
115.52
115.23
77.50
77.08
76.65
63.95
O
N
H
OMe
F
f1 (ppm)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7.53
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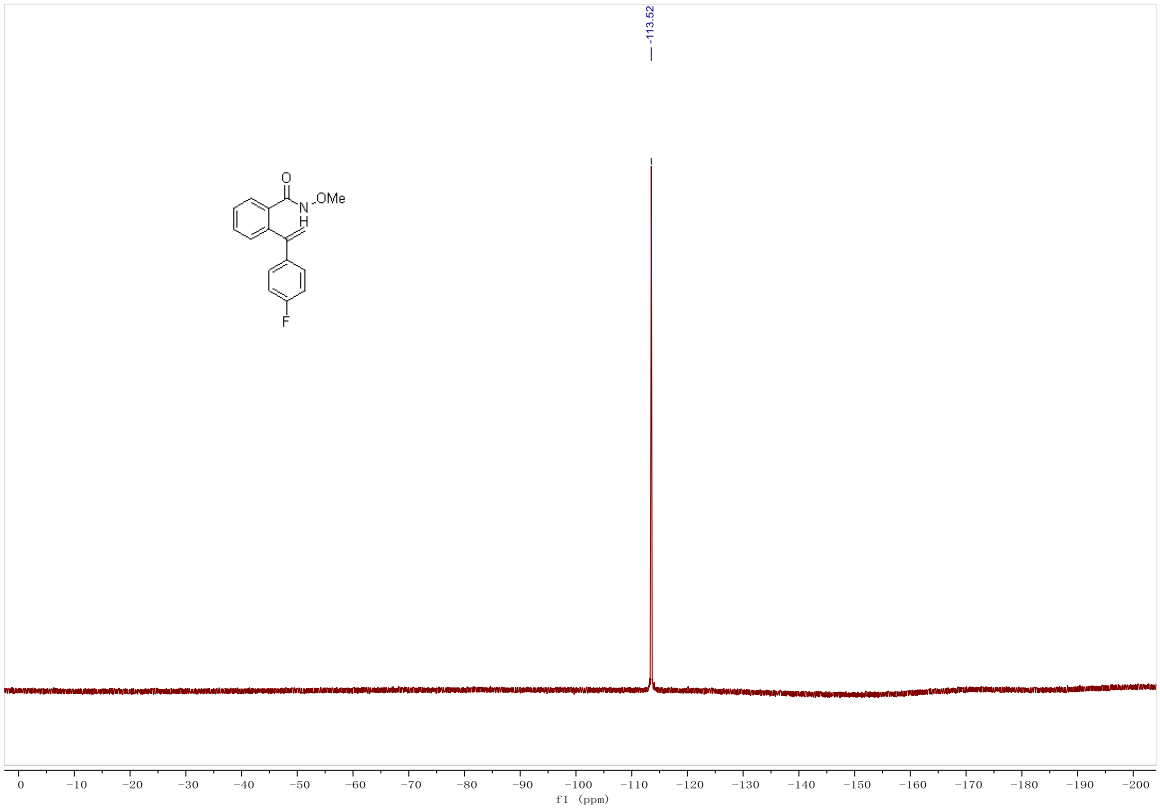
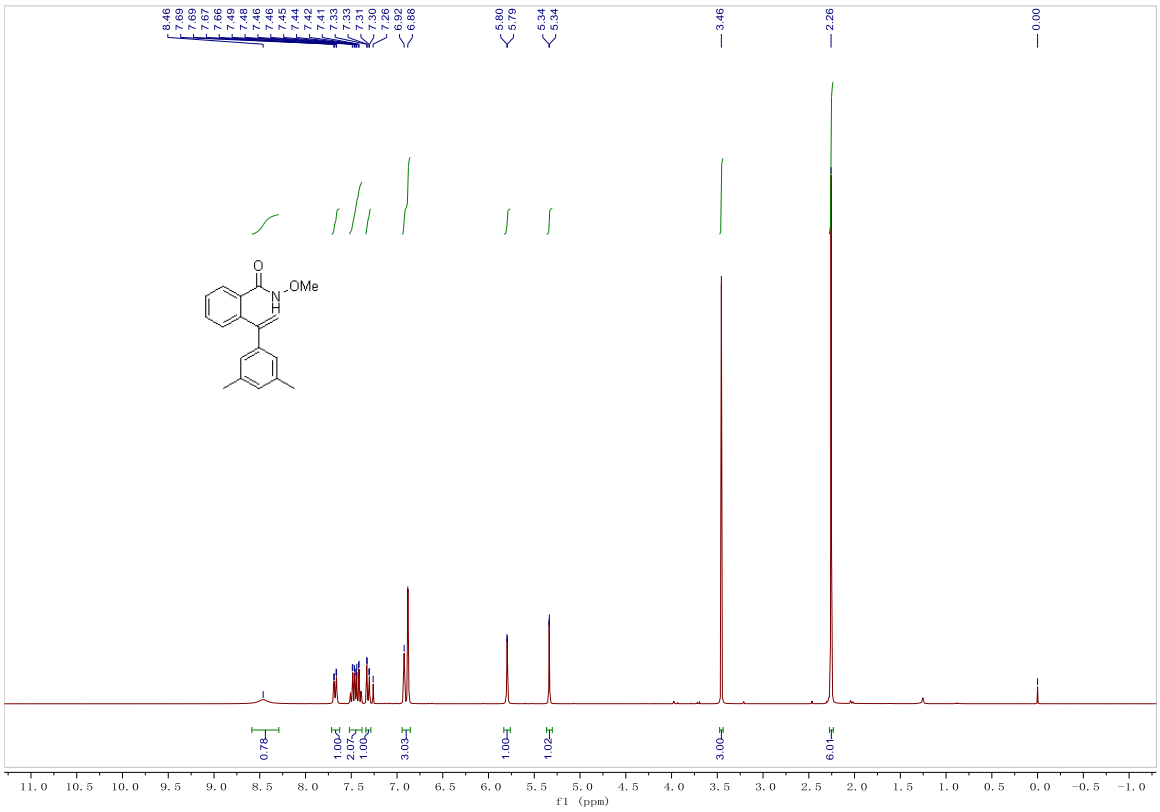
7.48
7.44
7.42
7.40
7.36
7.33
7.27
7.25
7.24
7.22
7.01
6.98
6.95
5.73
5.37
3.48
0.00
O
N
H
OMe
F
0.88
1.00
1.03
1.03
1.01
2.09
2.05
1.01
1.04
3.07
f1 (ppm)


-113.52
O
N
OMe
H
F
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)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7.69
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7.49
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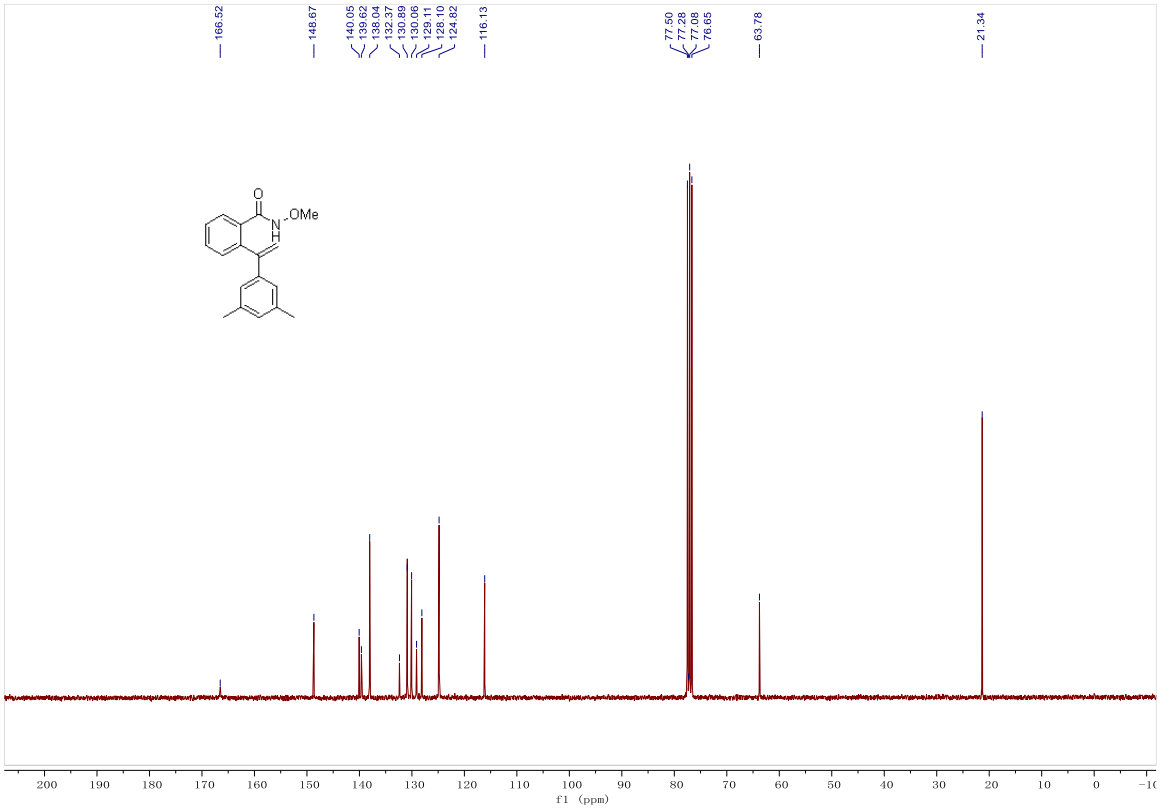
7.46
7.46
7.45
7.44
7.42
7.41
7.33
7.33
7.31
7.30
7.26
6.92
6.88
5.80
5.79
5.34
5.34
3.46
2.26
0.00
O
N
OMe
H
0.78
1.00
2.07
1.00
3.03
1.00
1.02
3.00
6.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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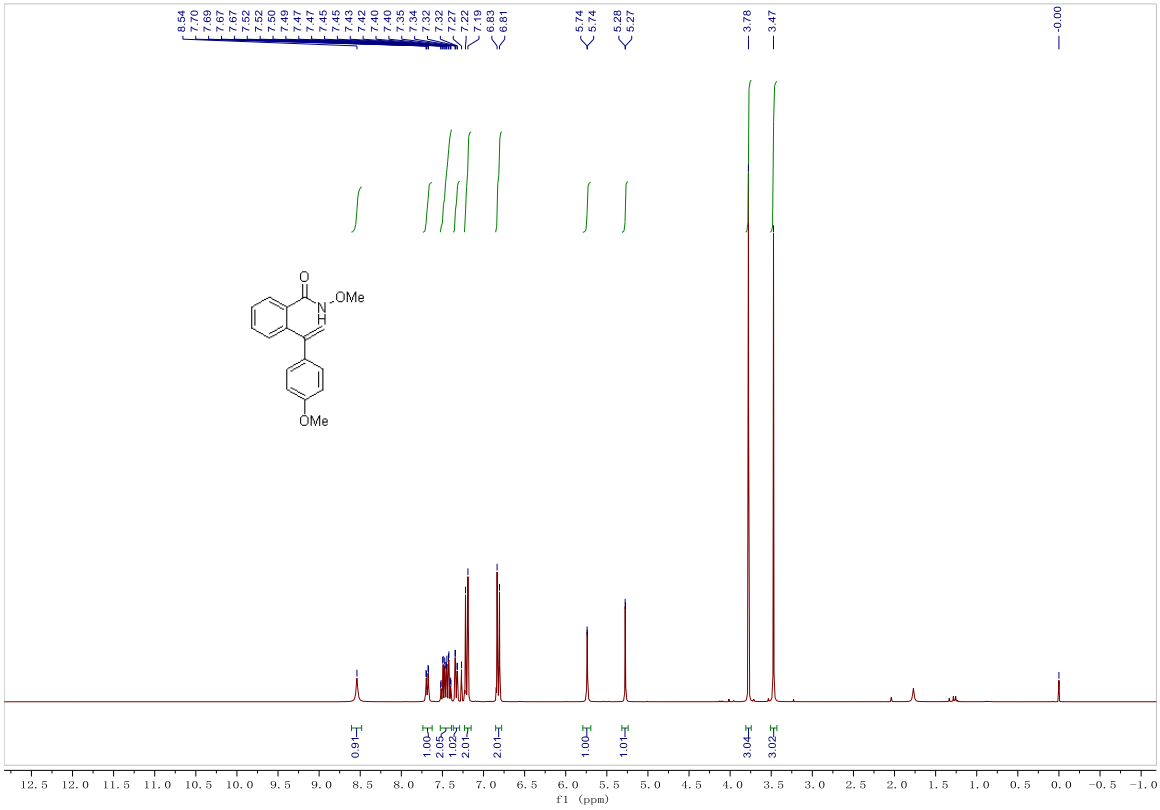
148.67
140.05
139.62
138.04
132.37
130.89
130.06
129.11
128.10
124.82
116.13
77.50
77.28
77.08
76.65
63.78
21.34
OMe
f1 (ppm)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7.52
7.52
7.50
7.49
7.47
7.47
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7.45
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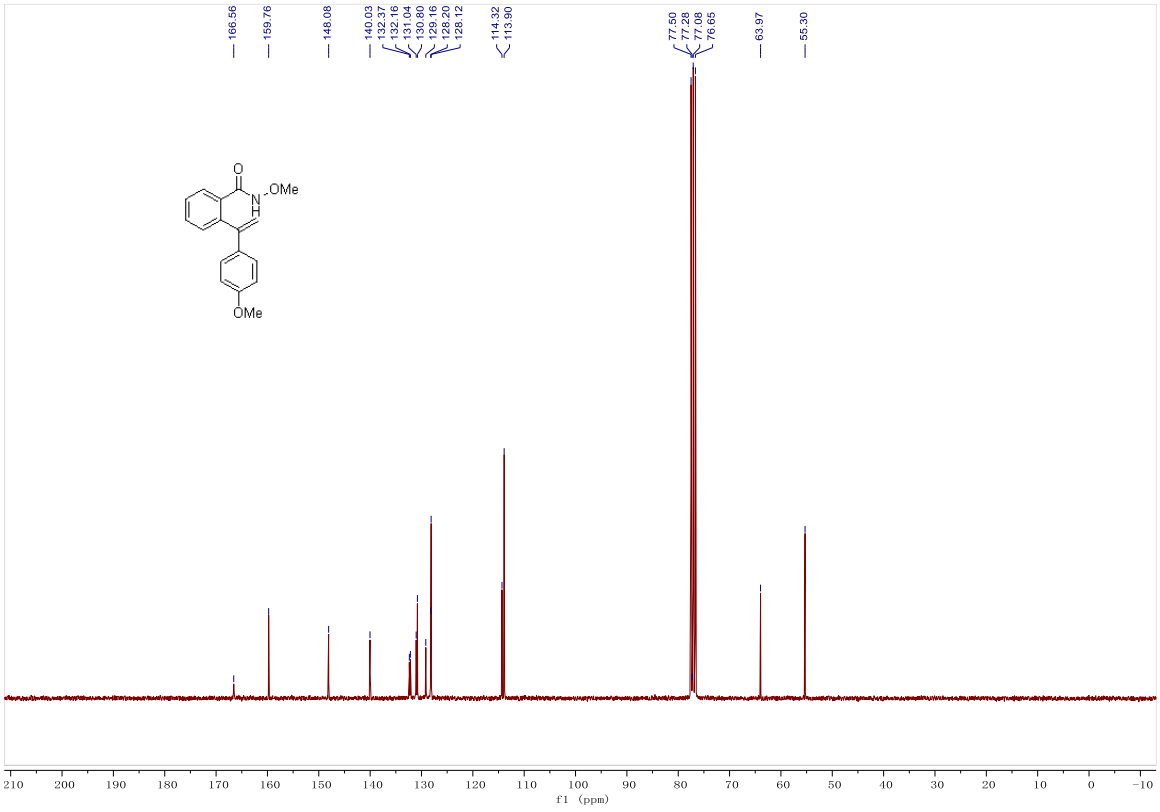
7.42
7.40
7.40
7.35
7.34
7.32
7.32
7.27
7.22
7.19
6.83
6.81
5.74
5.74
5.28
5.27
3.78
3.47
-0.00
OMe
OMe
0.91
1.00
2.05
1.02
2.01
2.01
1.00
1.01
3.04
3.02
f1 (ppm)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128.20
128.12
114.32
113.90
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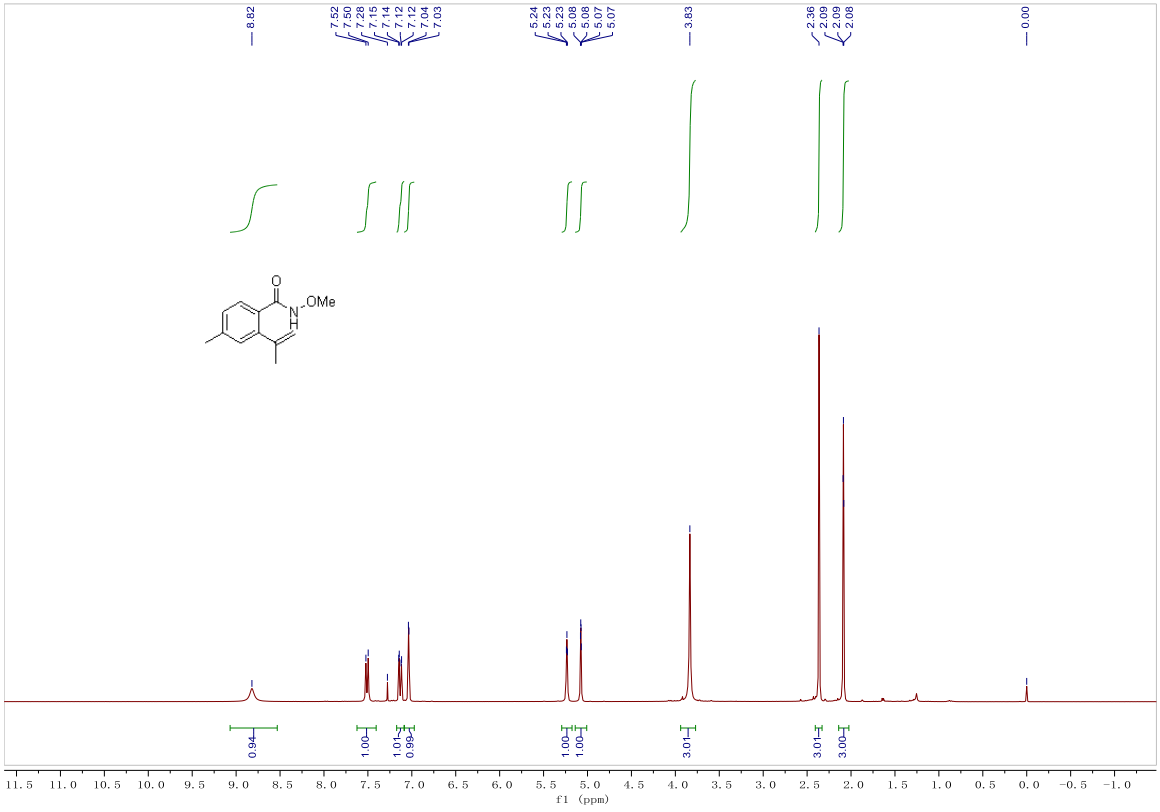
77.28
77.08
76.65
63.97
55.30
O
N
H
OMe
OMe
f1 (ppm)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7.52
7.50
7.28
7.15
7.14
7.12
7.12
7.04
7.03
5.24
5.23
5.23
5.08
5.08
5.07
5.07
3.83
2.36
2.09
2.09
2.08
0.00
O
N
H
OMe
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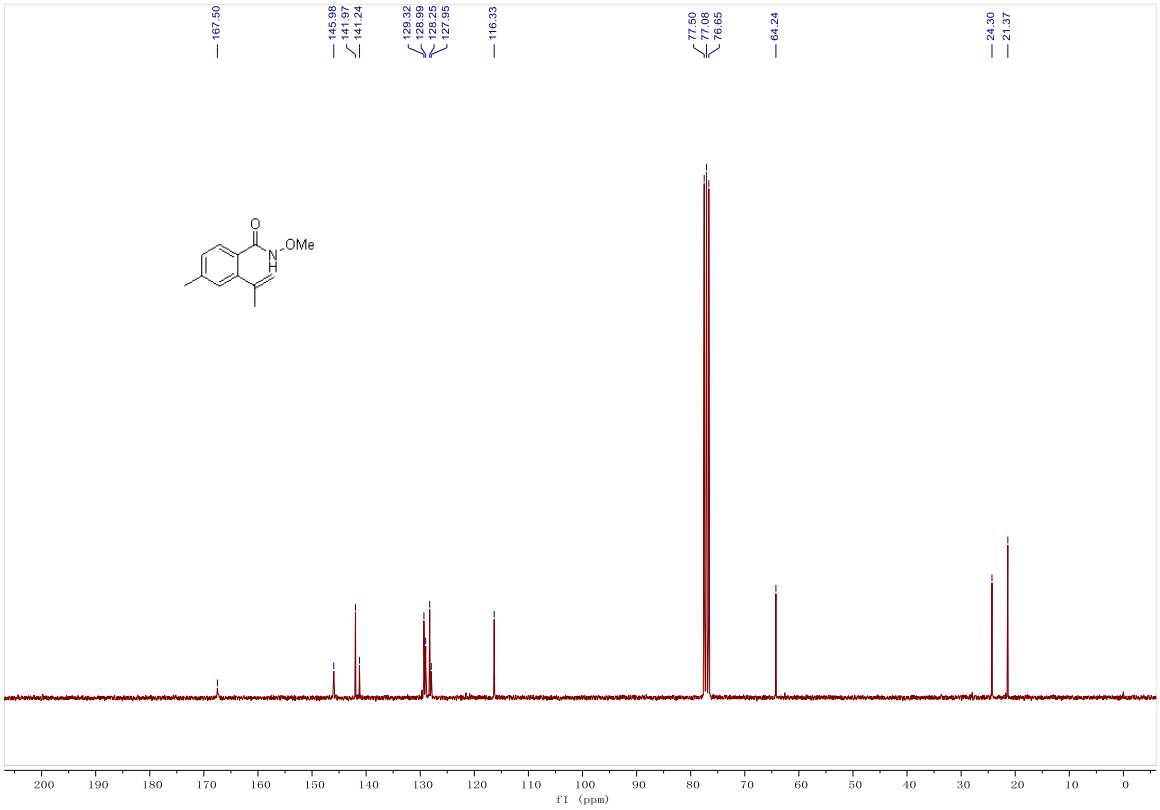
1.00
1.01
0.99
1.00
1.00
3.01
3.01
3.00
f1 (ppm)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128.25
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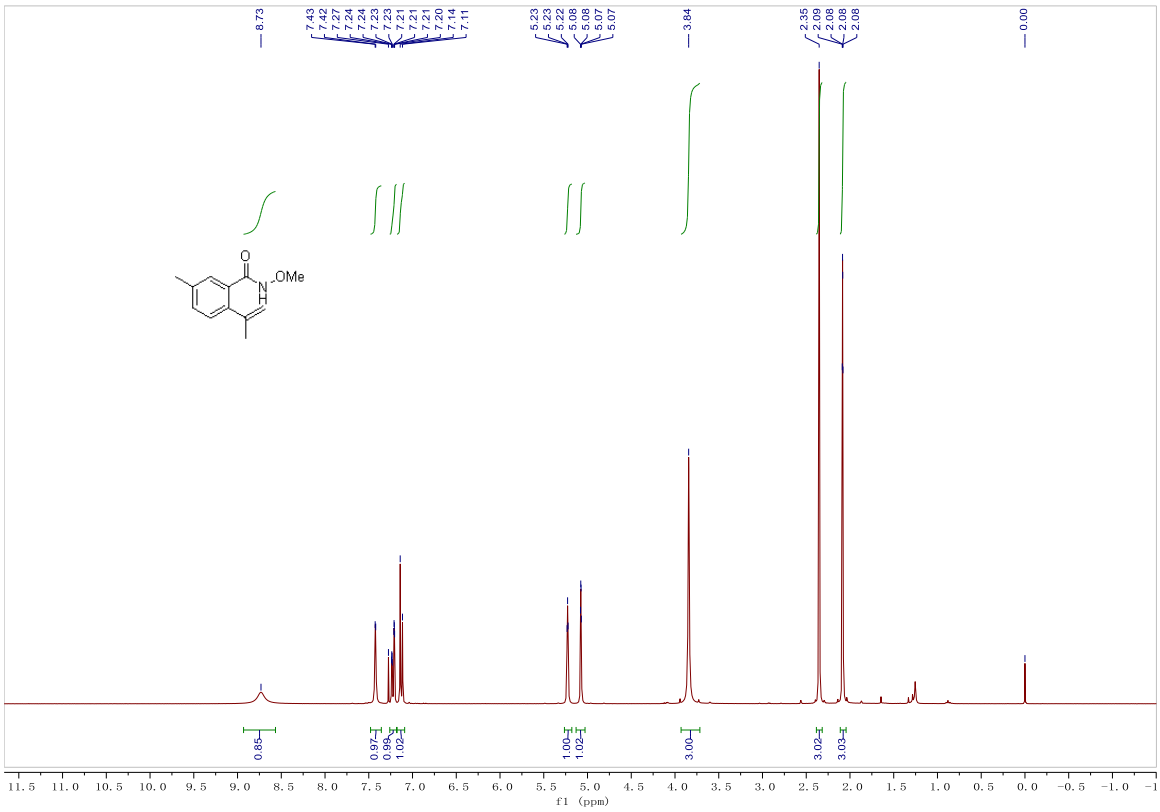
77.08
76.65
64.24
24.30
21.37
O
N
OMe
H
f1 (ppm)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7.24
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7.21
7.21
7.21
7.20
7.14
7.11
5.23
5.23
5.22
5.08
5.08
5.07
5.07
3.84
2.35
2.09
2.08
2.08
2.08
0.00
O
N
OMe
H
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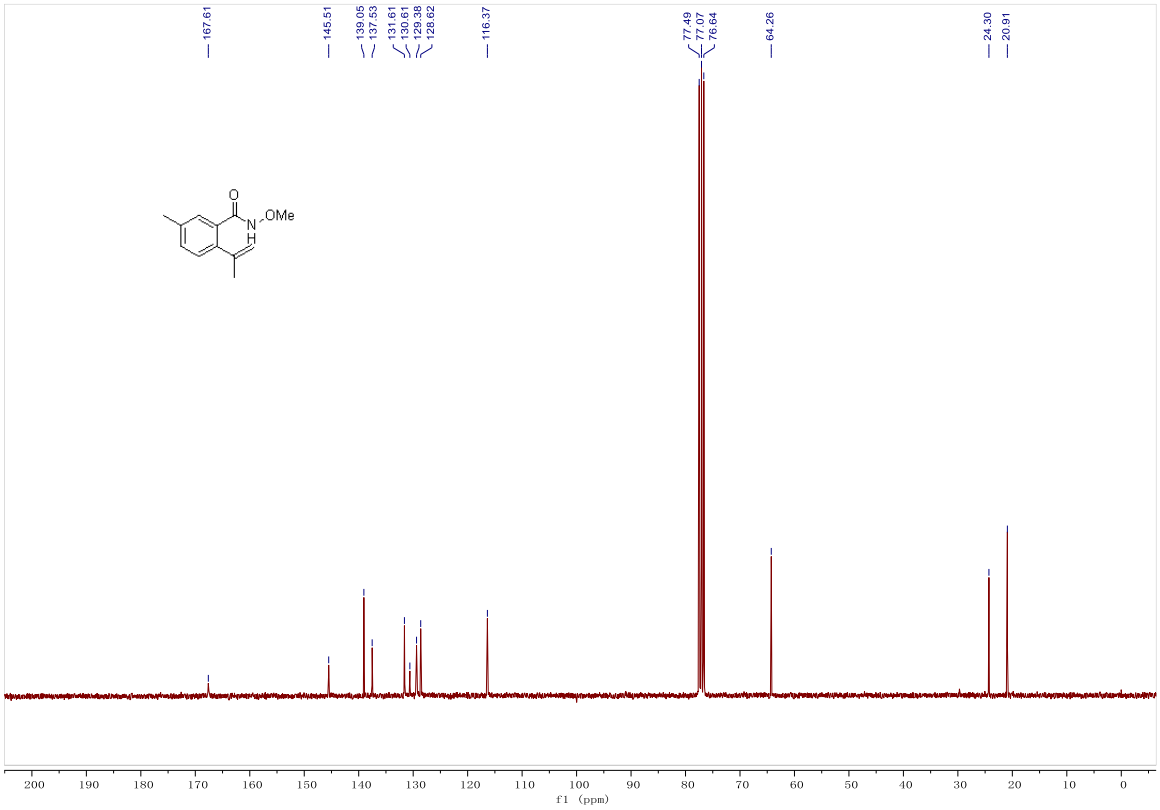
0.97
0.99
1.02
1.00
1.02
3.00
3.02
3.03
f1 (ppm)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129.38
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77.07
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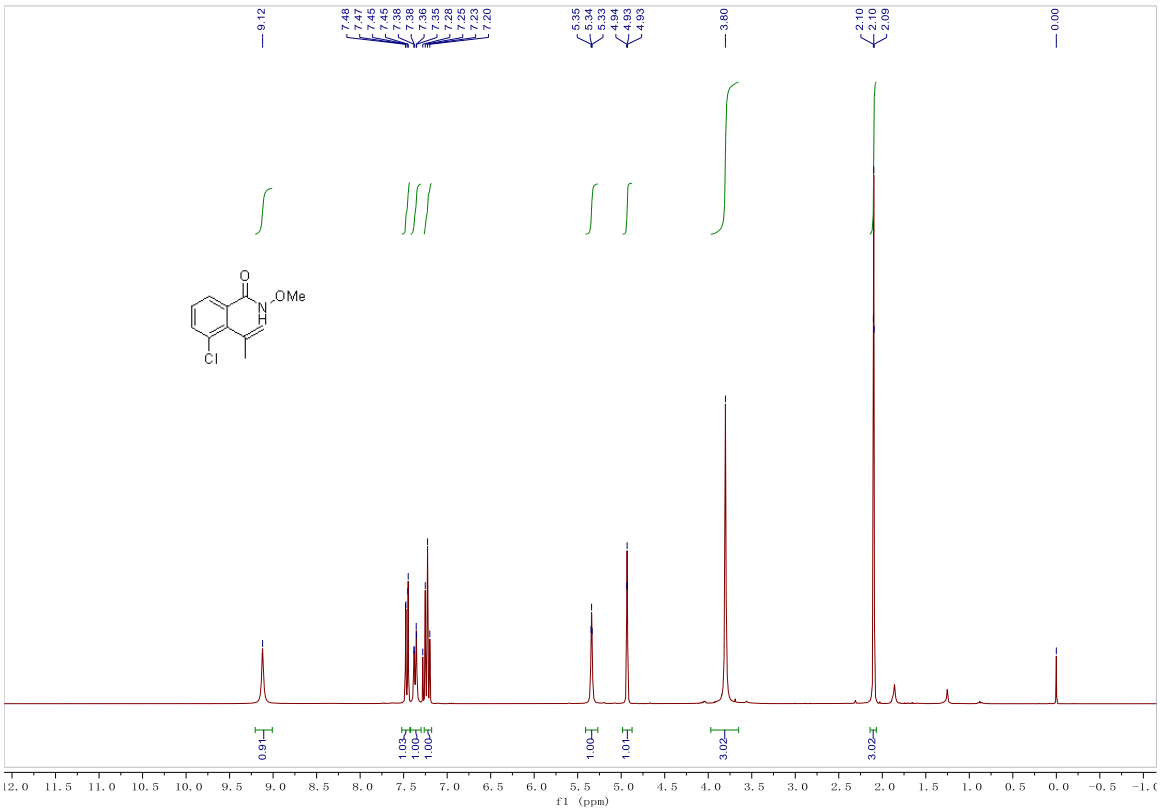
64.26
24.30
20.91
O
N
OMe
H
f1 (ppm)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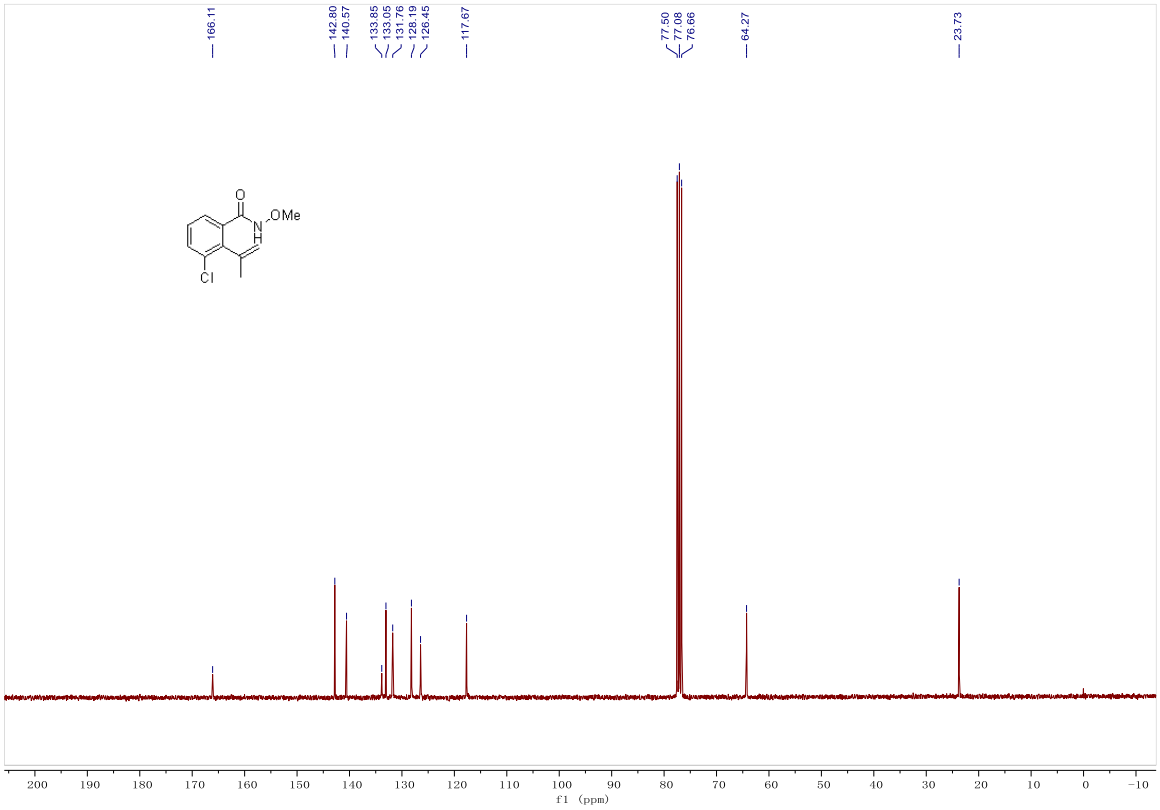
7.45
7.45
7.38
7.38
7.36
7.35
7.28
7.25
7.23
7.20
5.35
5.34
5.33
4.94
4.93
4.93
3.80
2.10
2.10
2.09
0.00
O
N
OMe
H
Cl
0.91
1.03
1.00
1.00
1.00
1.01
3.02
3.02
f1 (ppm)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140.57
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131.76
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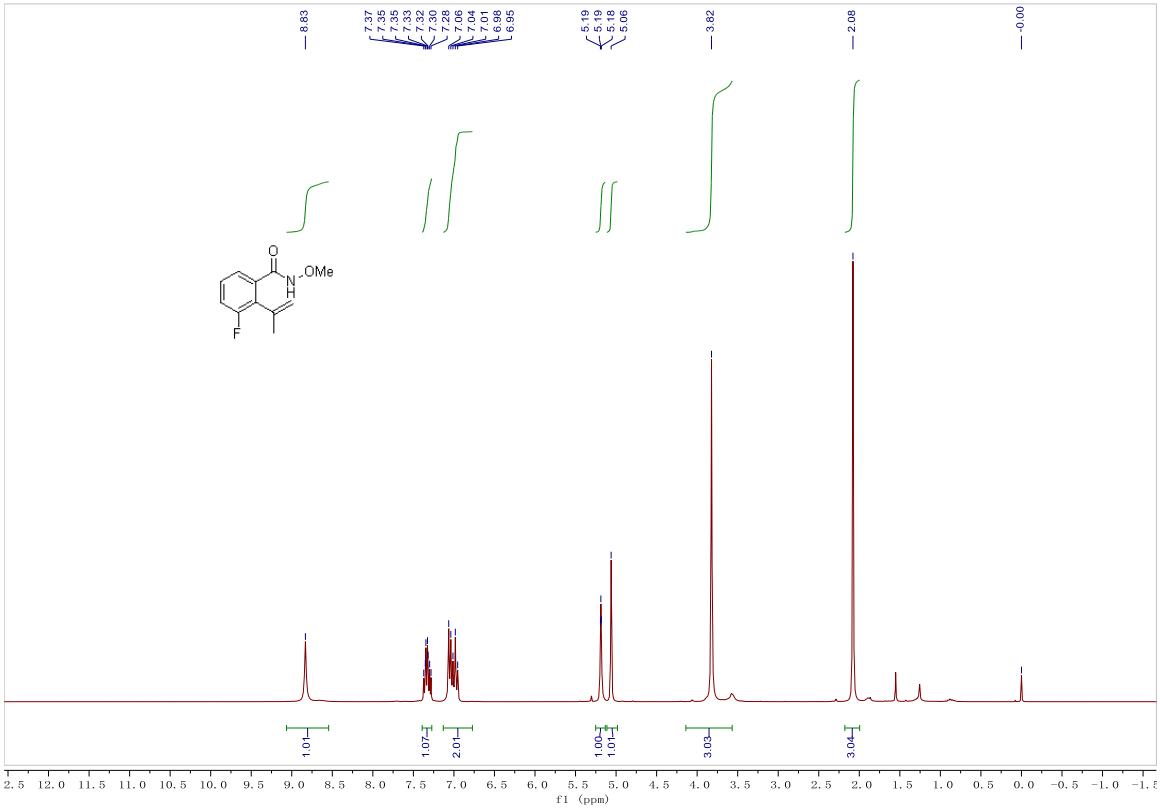
77.50
77.08
76.66
64.27
23.73
O
N
OMe
H
Cl
f1 (ppm)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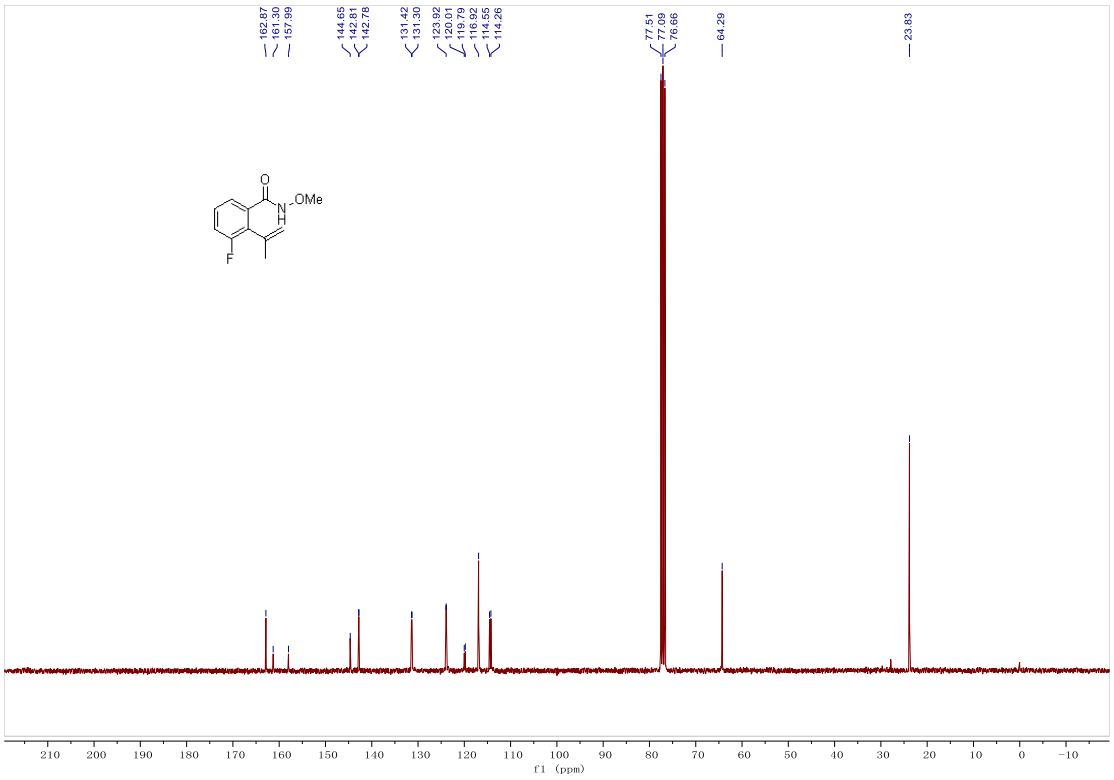
7.30
7.28
7.06
7.04
7.01
6.98
6.95
5.19
5.19
5.18
5.06
3.82
2.08
-0.00
O
N
OMe
H
F
1.01
1.07
2.01
1.00
1.01
3.03
3.04
f1 (ppm)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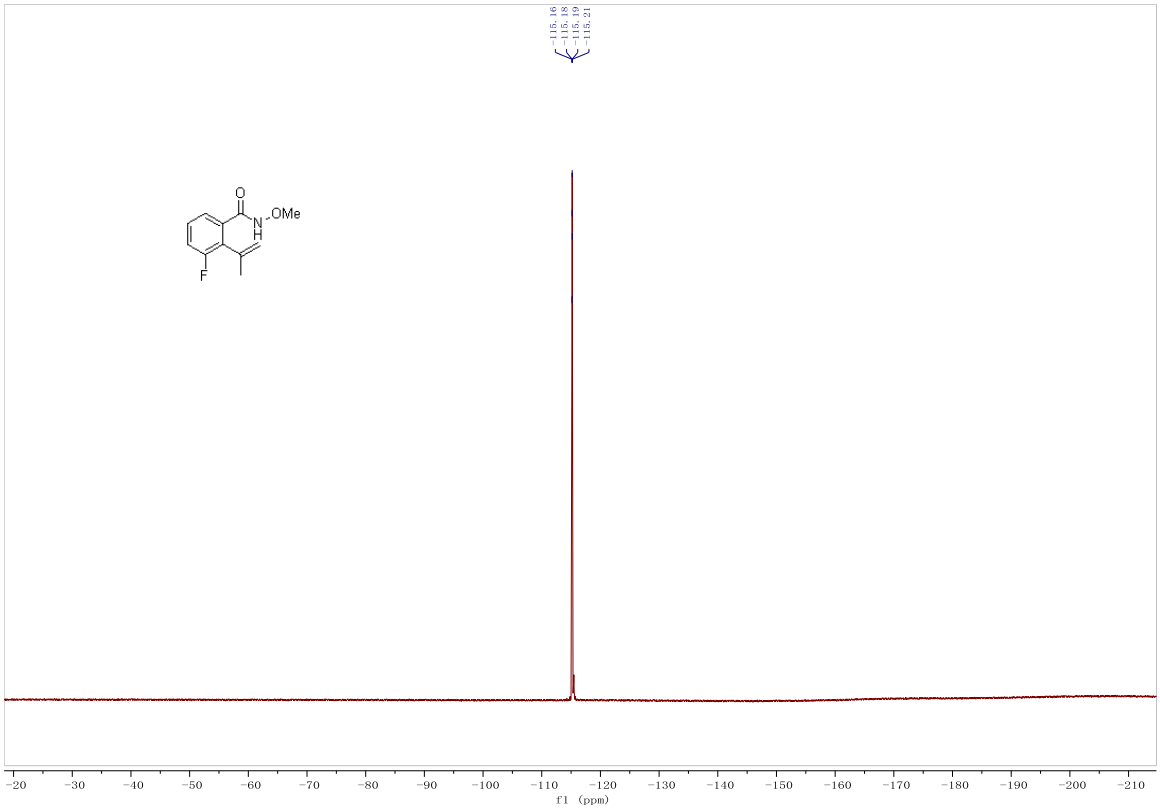
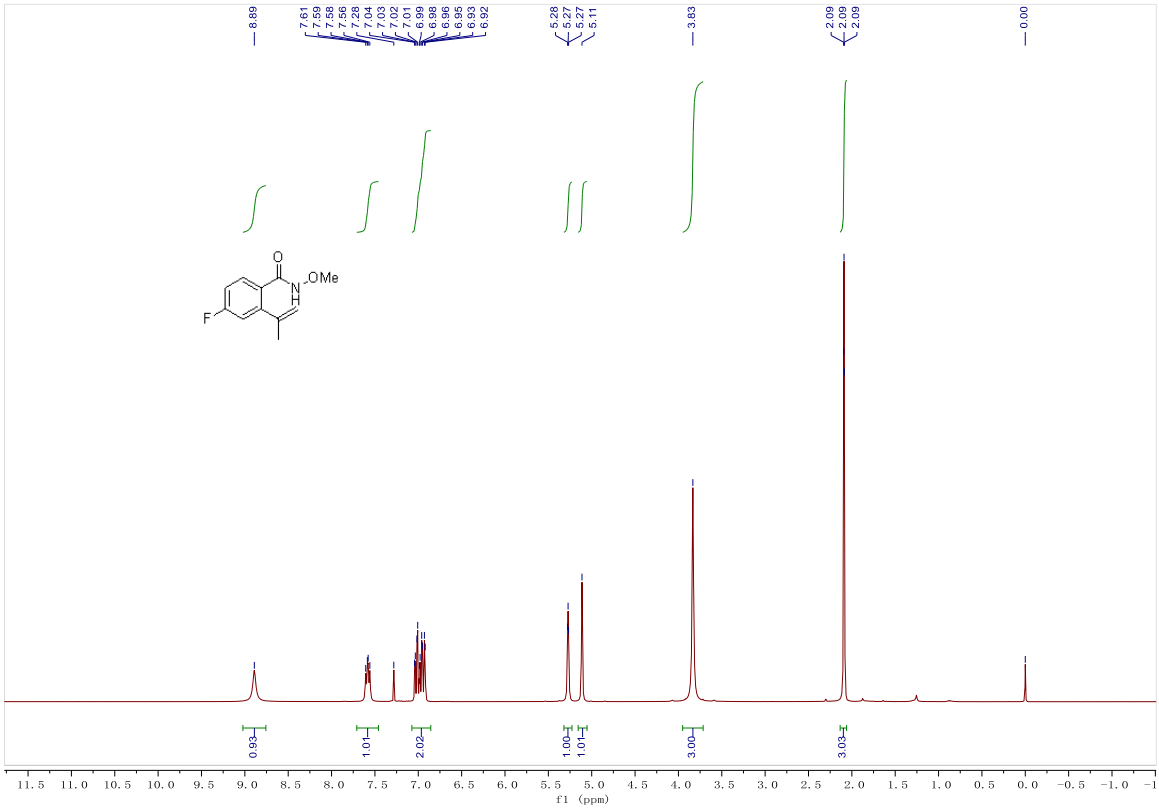
131.42
131.30
123.92
120.01
119.79
116.92
114.55
114.26
77.51
77.09
76.66
64.29
23.83
O
N
OMe
H
F
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


−115.16
−115.18
−115.19
−115.21
O
N
OMe
H
F
−20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)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7.02
7.01
6.99
6.98
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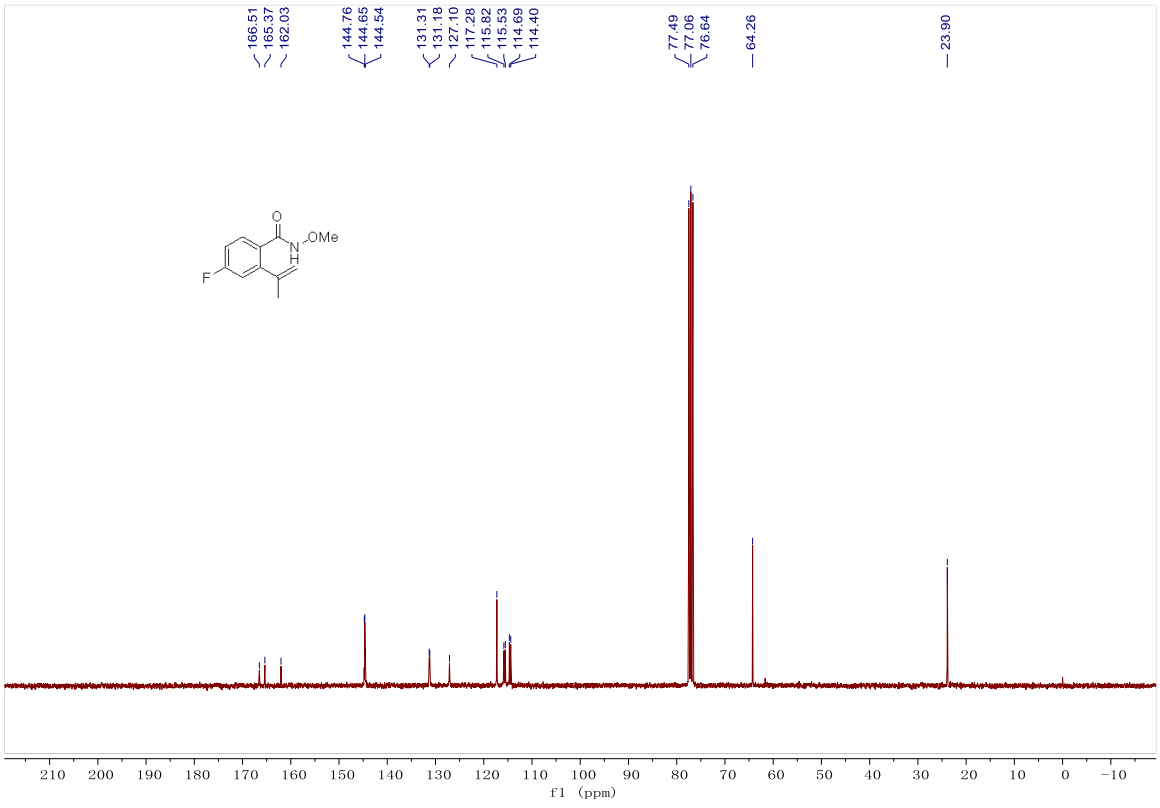
6.95
6.93
6.92
5.28
5.27
5.27
5.11
3.83
2.09
2.09
2.09
0.00
O
N
OMe
H
F
0.93
1.01
2.02
1.00
1.01
3.00
3.03
f1 (ppm)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144.54
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131.18
127.10
117.28
115.82
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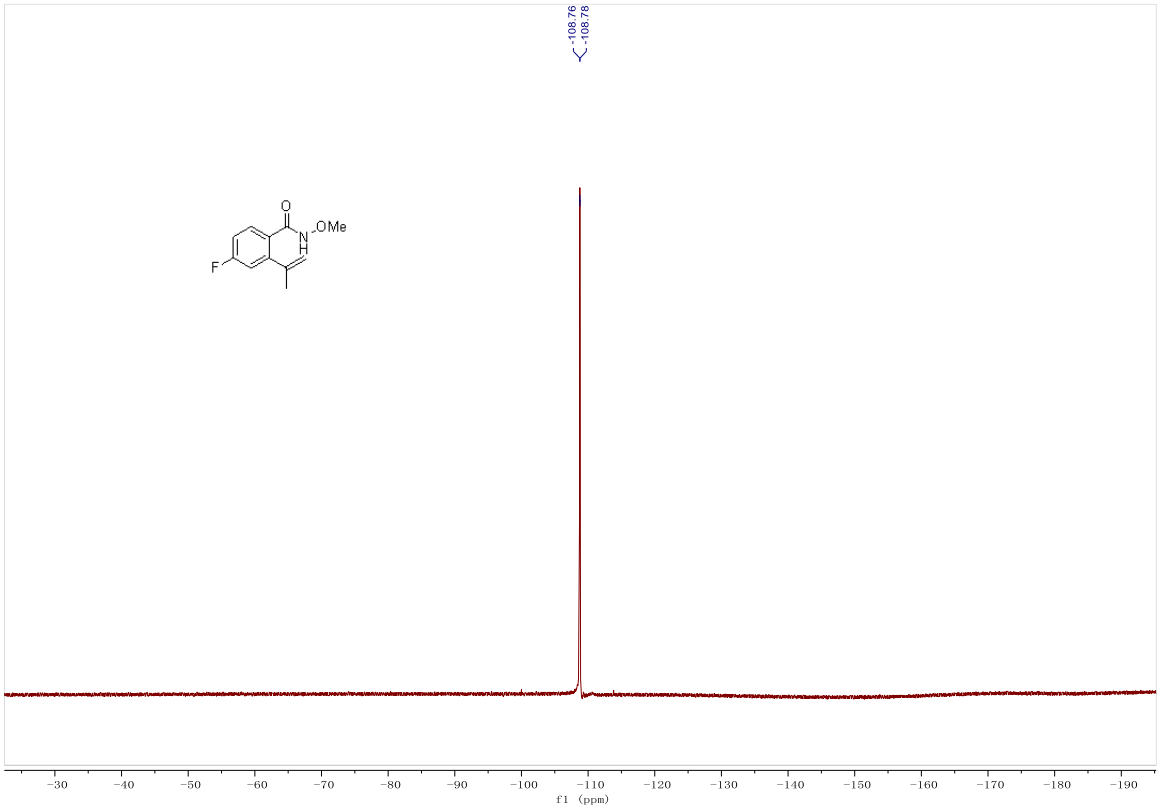
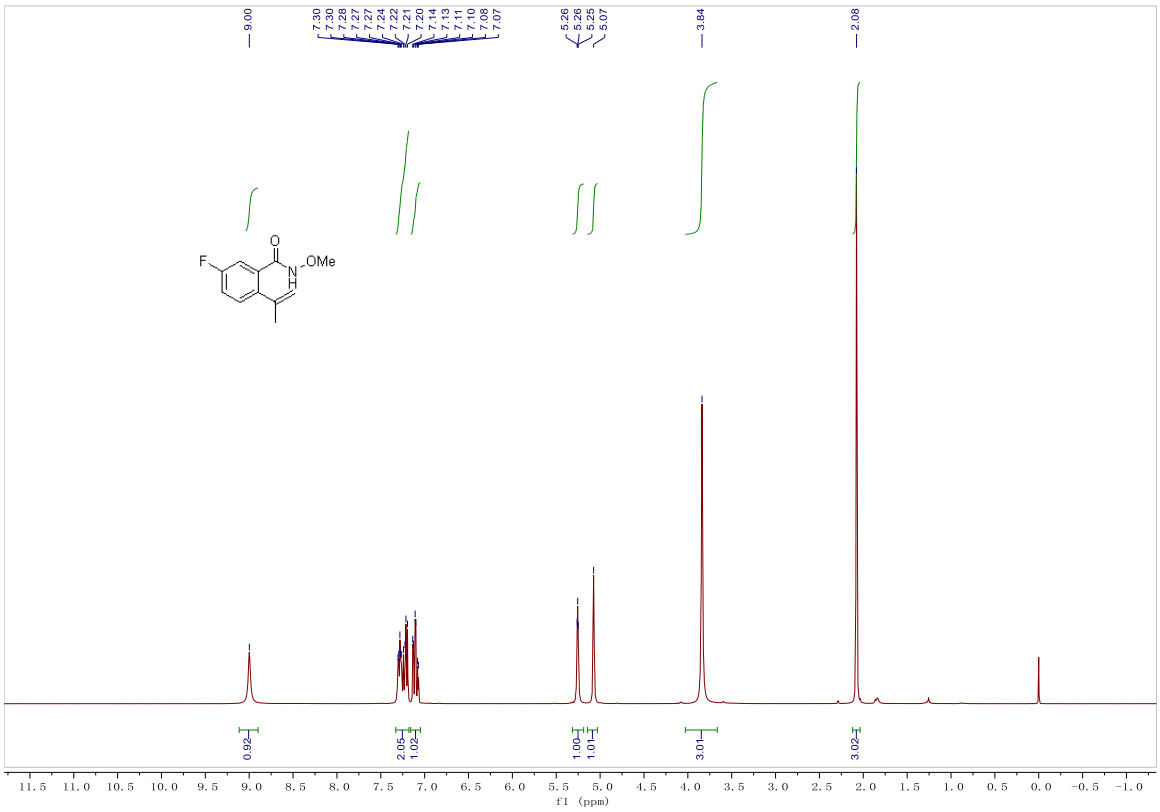
77.49
77.06
76.64
64.26
23.90
O
N
OMe
H
F
f1 (ppm)


-108.76
-108.78
O
N
OMe
H
F
-30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm)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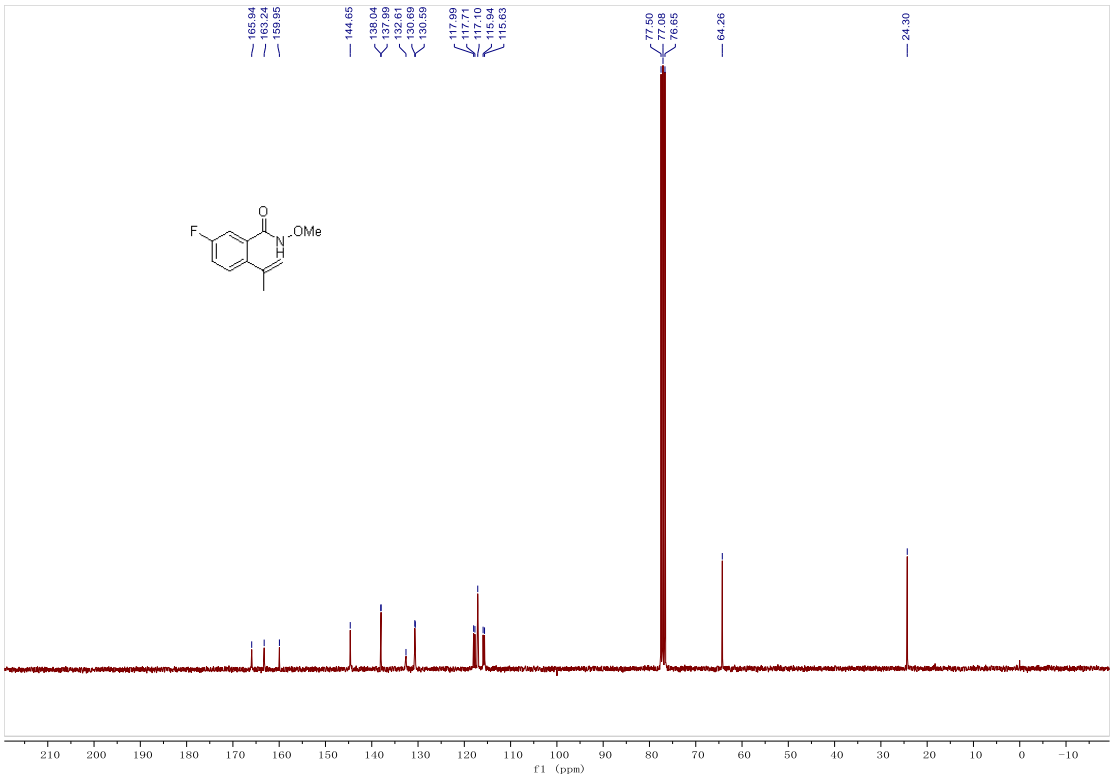
7.27
7.24
7.22
7.21
7.20
7.14
7.13
7.11
7.10
7.08
7.07
5.26
5.26
5.25
5.07
3.84
2.08
O
N
OMe
H
F
0.92
2.05
1.02
1.00
1.01
3.01
3.02
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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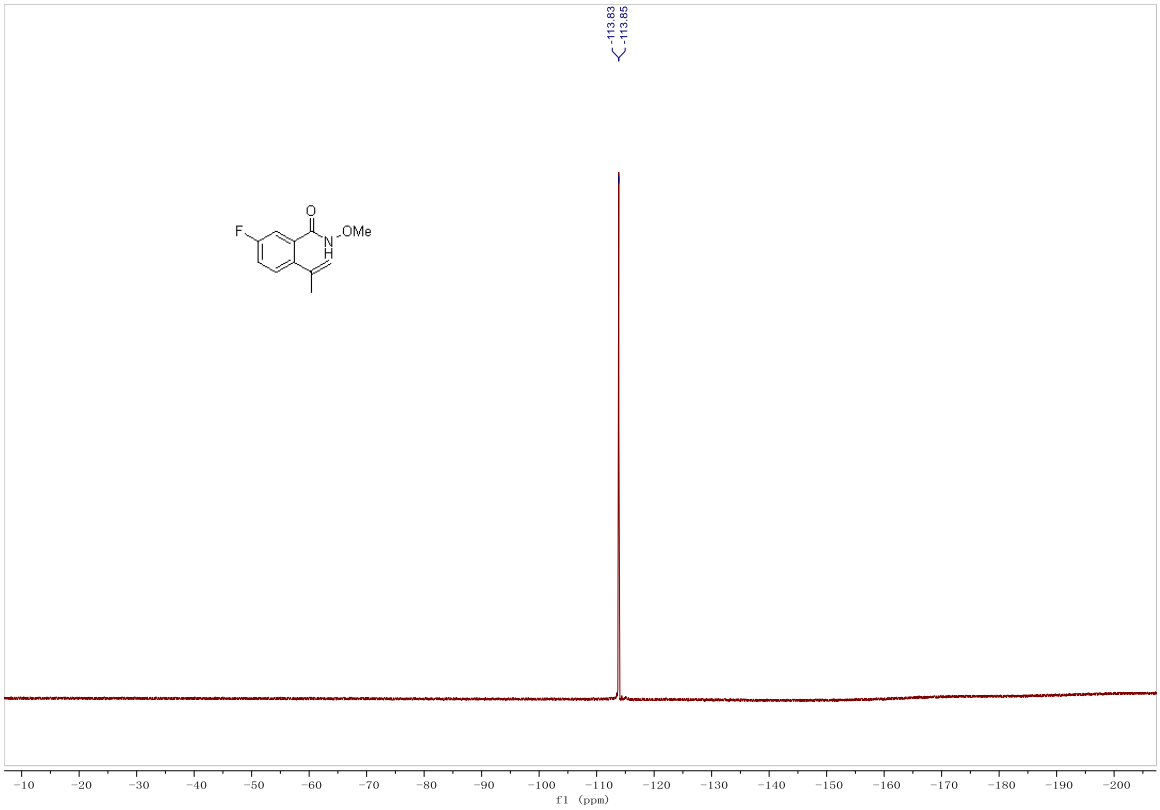
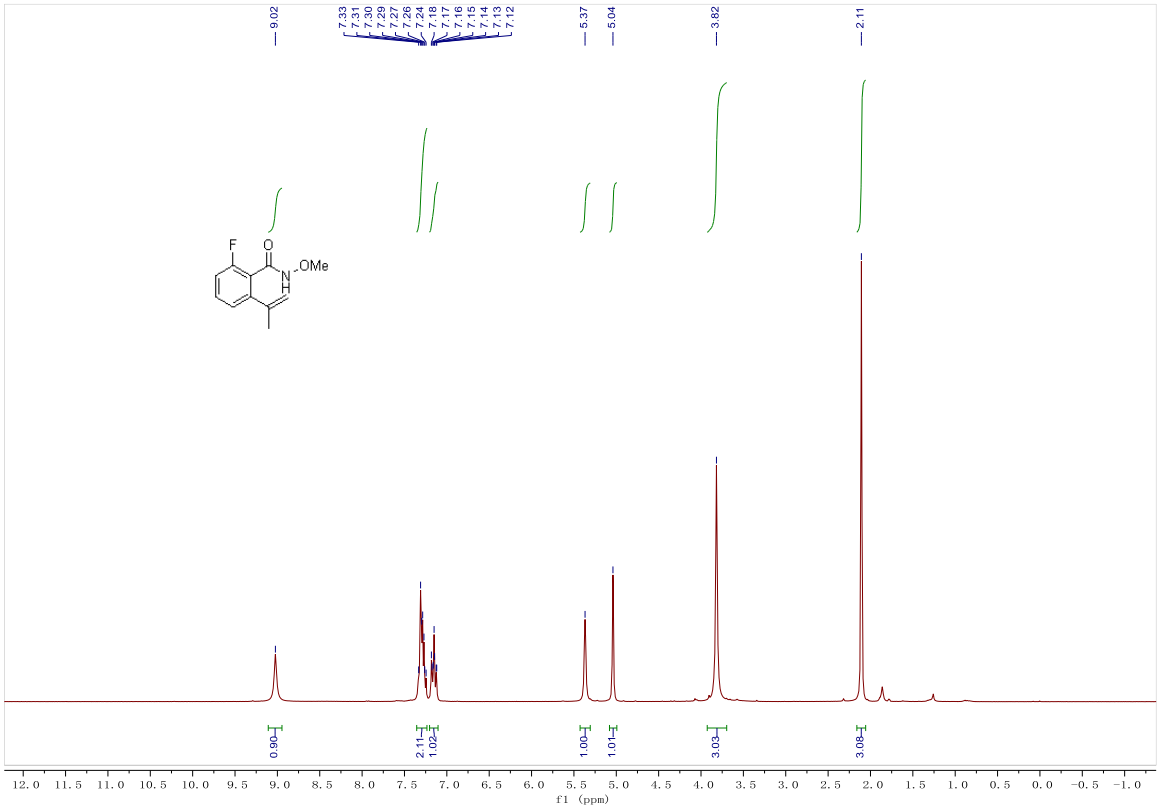
117.99
117.71
117.10
115.94
115.63
77.50
77.08
76.65
64.26
24.30
F
O
N
H
OMe
f1 (ppm)


-113.83
-113.85
F
O
N
H
OMe
f1 (ppm)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7.33
7.31
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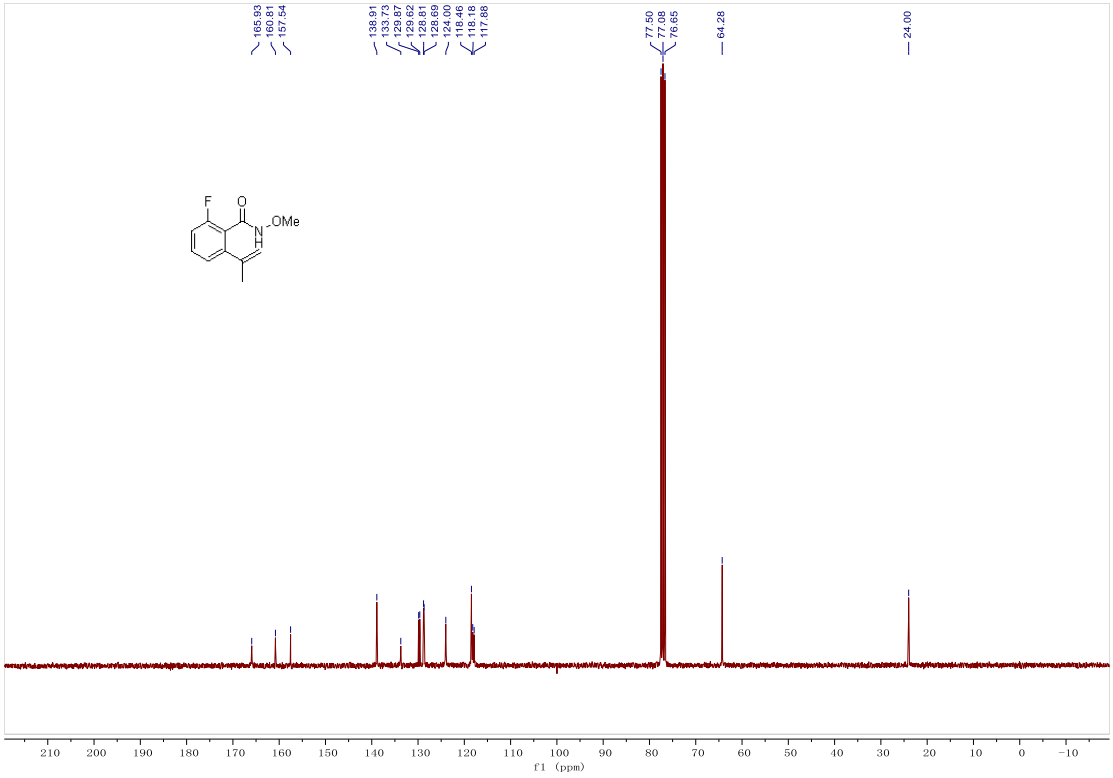
7.27
7.26
7.24
7.18
7.17
7.16
7.15
7.14
7.13
7.12
5.37
5.04
3.82
2.11
F
O
N
H
OMe
0.90
2.11
1.02
1.00
1.01
3.03
3.08
f1 (ppm)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160.81
157.54
138.91
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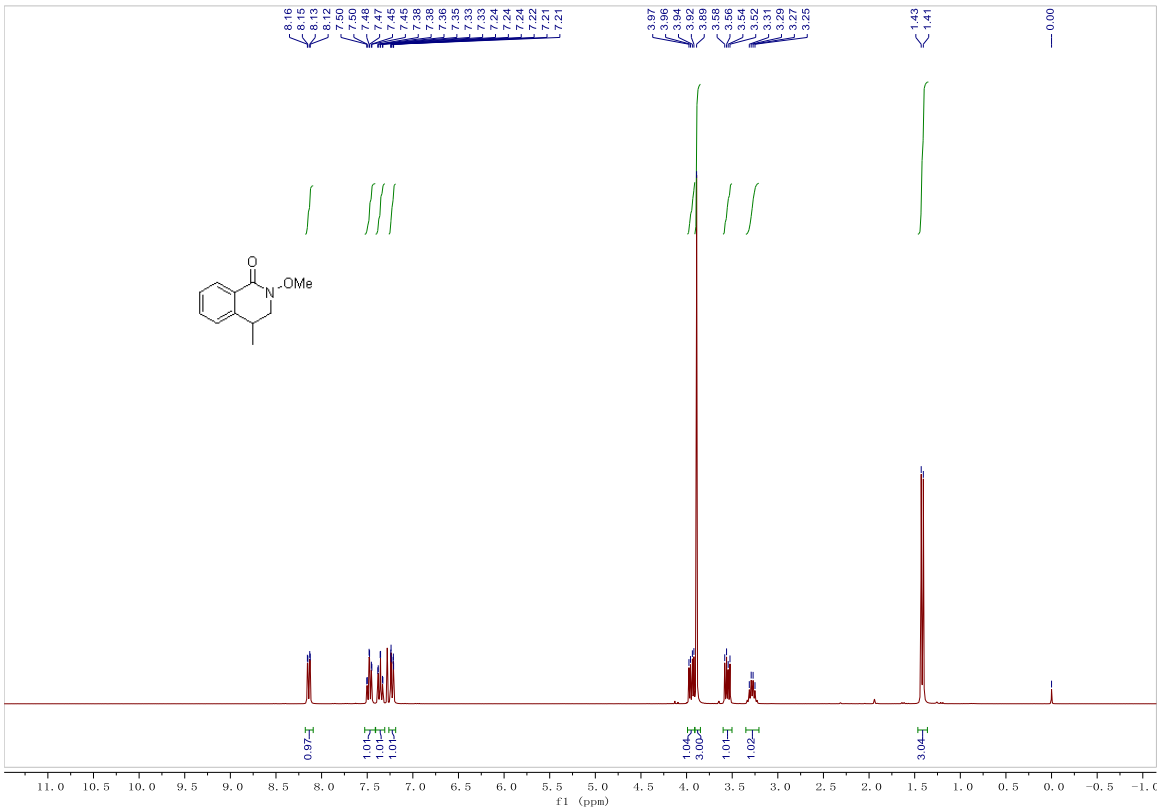
129.87
129.62
128.81
128.69
124.00
118.46
118.18
117.88
77.50
77.08
76.65
64.28
24.00
F
O
N
H
OMe
f1 (ppm)


-114.27
-114.28
-114.30
-114.32
F
O
N
H
OMe
f1 (ppm)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8.15
8.13
8.12
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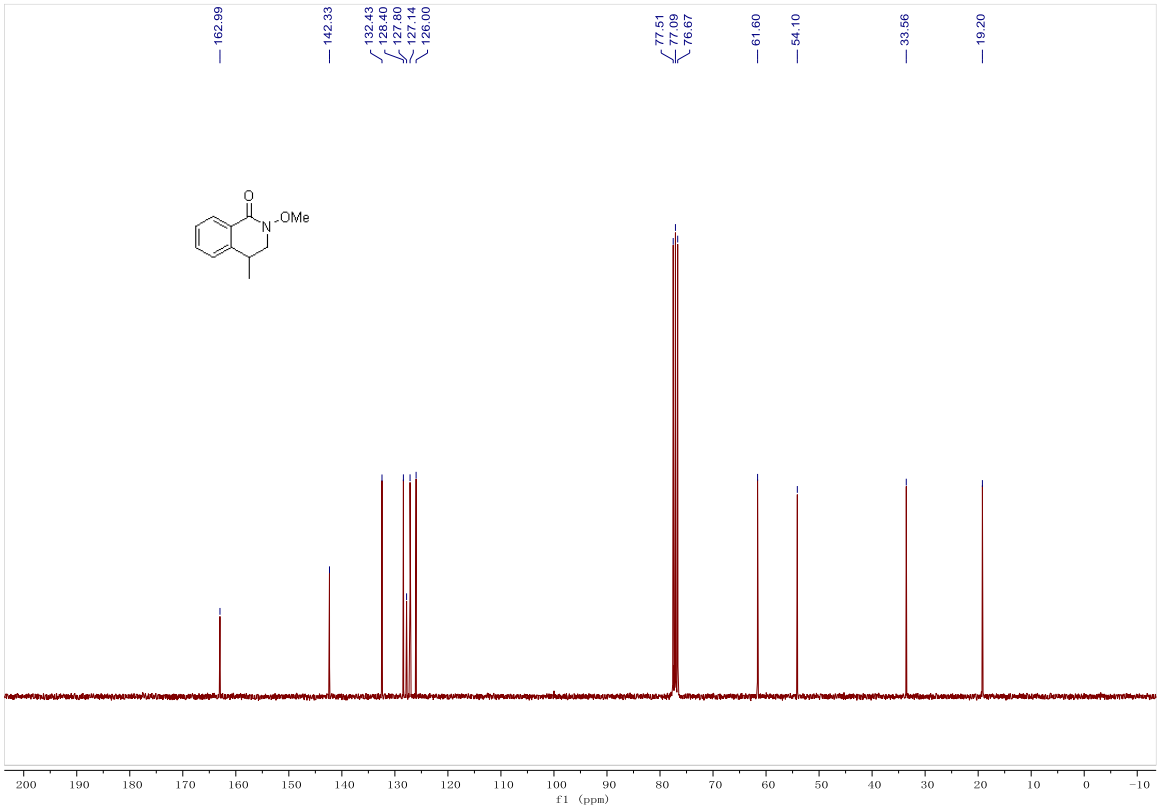
7.50
7.48
7.47
7.45
7.45
7.38
7.38
7.36
7.35
7.33
7.33
7.24
7.24
7.24
7.22
7.21
7.21
3.97
3.96
3.94
3.92
3.89
3.88
3.56
3.54
3.52
3.31
3.29
3.27
3.25
1.43
1.41
0.00
O
N
OMe
0.97
1.01
1.01
1.01
1.04
3.00
1.01
1.02
3.04
f1 (ppm)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142.33
132.43
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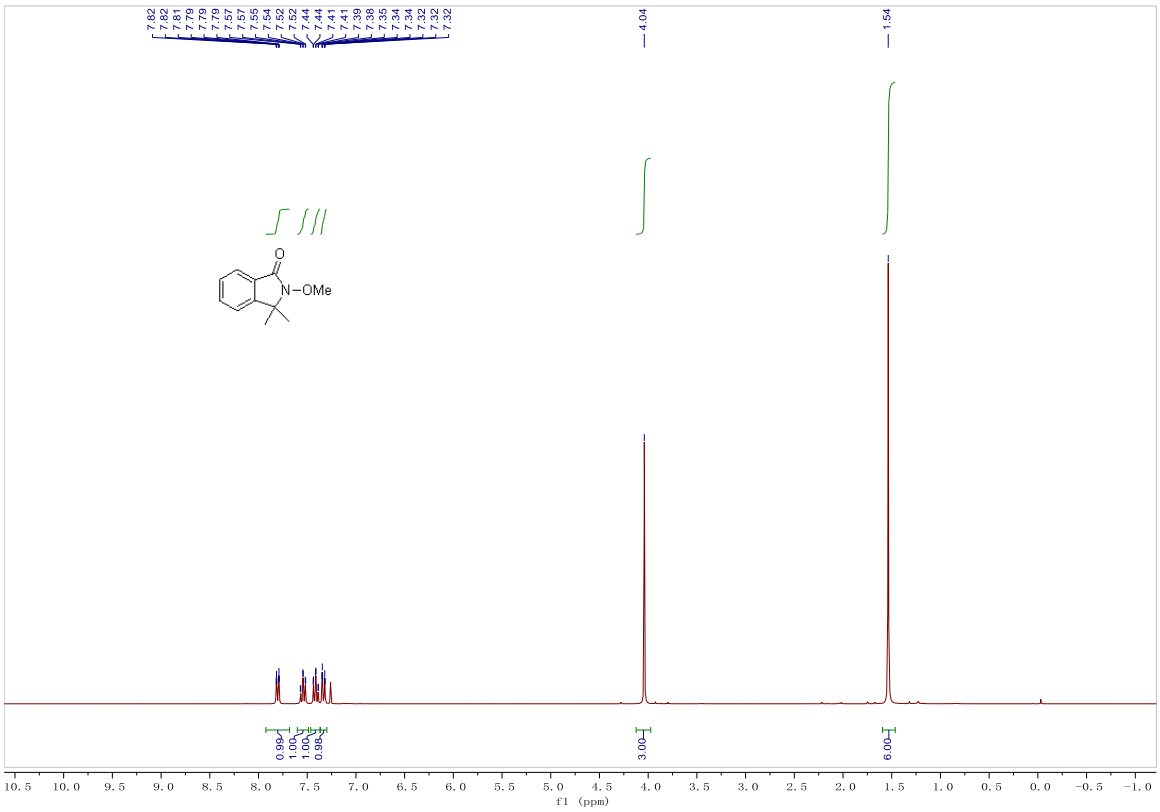
76.67
61.60
54.10
33.56
19.20
O
N
OMe
f1 (ppm)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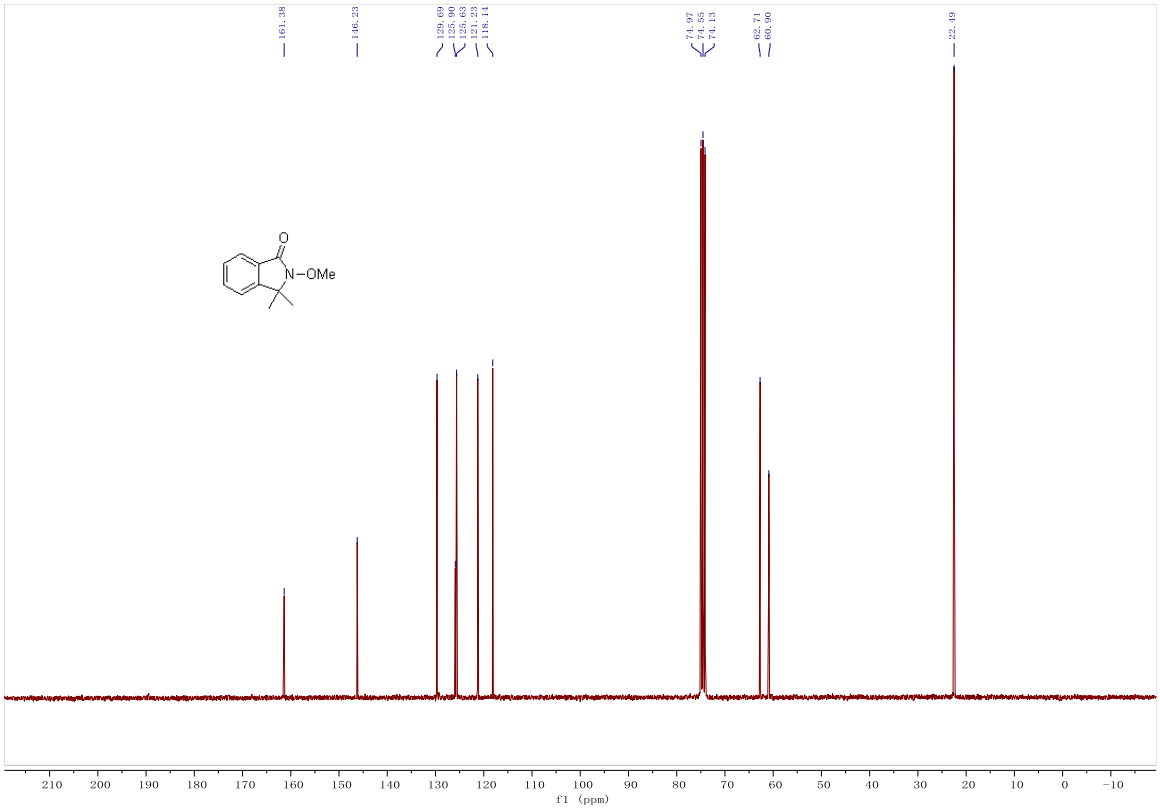
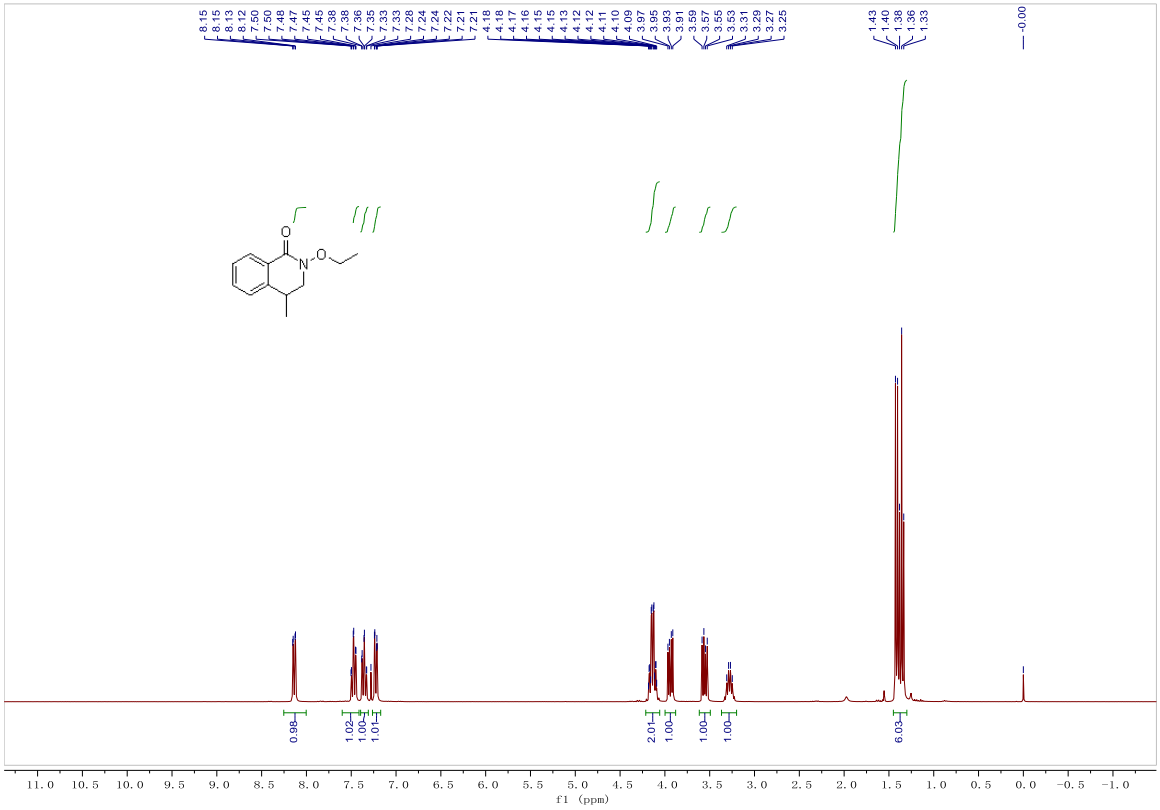
7.79
7.79
7.57
7.57
7.55
7.54
7.52
7.52
7.44
7.44
7.41
7.41
7.39
7.38
7.35
7.34
7.34
7.32
7.32
7.32
4.04
1.54
O
N–OMe
0.98
1.00
1.00
3.00
6.00
f1 (ppm)


161.38
146.23
129.69
125.90
125.65
121.25
118.14
74.97
74.55
74.13
62.71
60.90
22.49
O
N–OMe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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7.47
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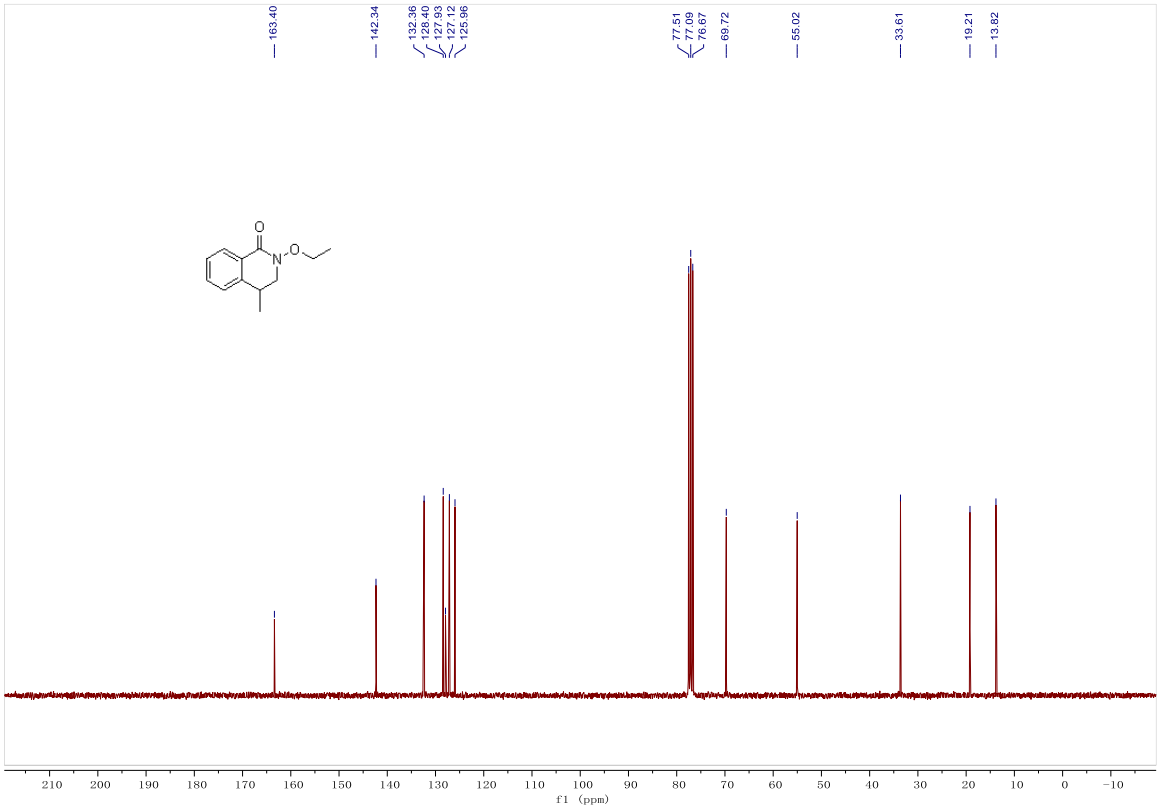
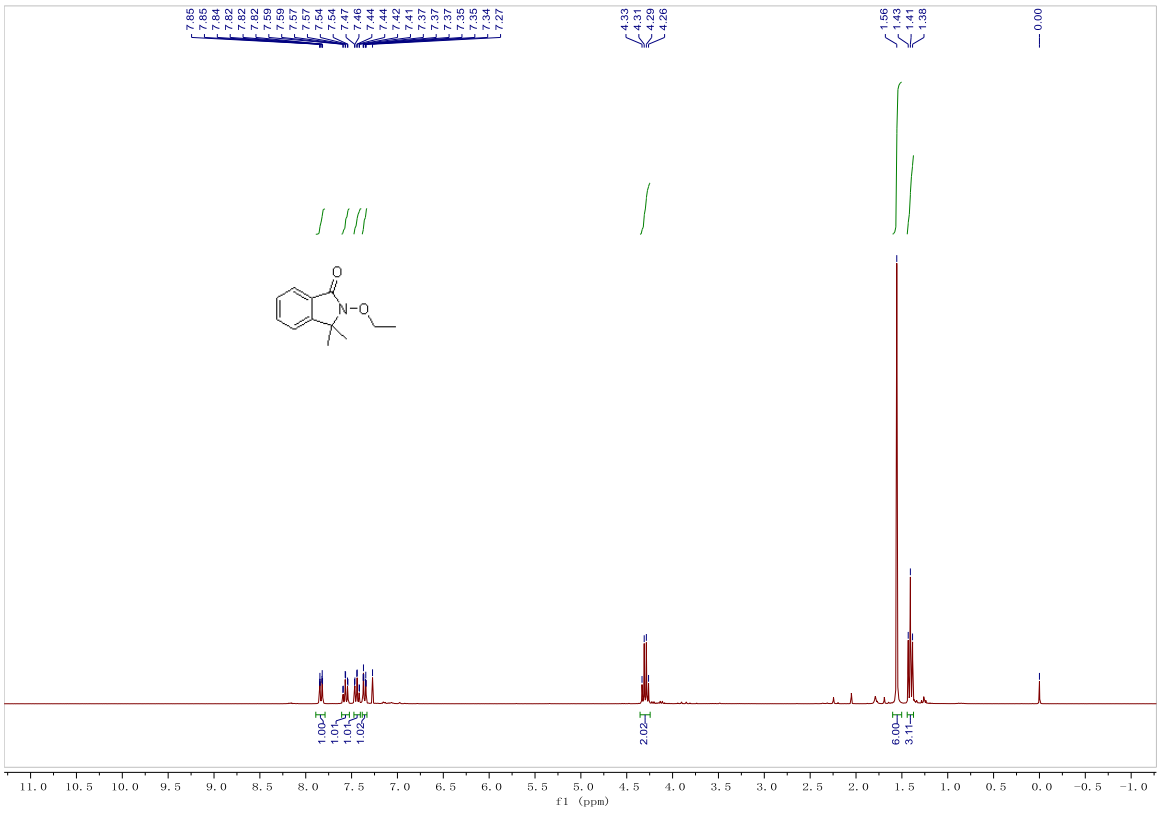
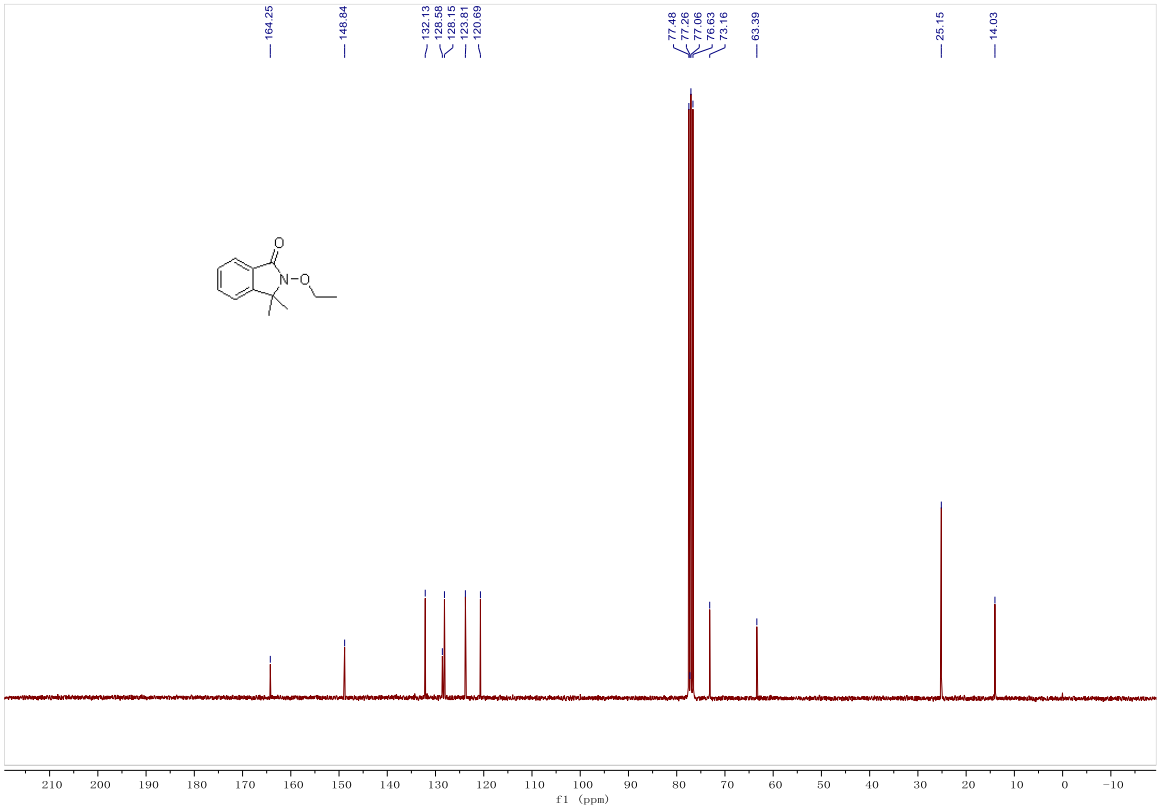
7.45
7.38
7.38
7.36
7.35
7.33
7.33
7.28
7.24
7.22
7.21
4.18
4.18
4.17
4.16
4.15
4.15
4.13
4.12
4.12
4.11
4.10
4.09
3.97
3.95
3.93
3.91
3.59
3.57
3.55
3.53
3.31
3.29
3.27
3.25
1.43
1.40
1.38
1.36
1.33
-0.00
O
N
O
0.98
1.02
1.00
1.01
2.01
1.00
1.00
1.00
6.03
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0
f1 (ppm)


163.40
142.34
132.36
128.40
127.93
127.12
125.96
77.51
77.09
76.67
69.72
55.02
33.61
19.21
13.82
O
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


7.85
7.85
7.84
7.82
7.82
7.82
7.59
7.59
7.57
7.57
7.54
7.54
7.47
7.46
7.44
7.44
7.42
7.41
7.37
7.37
7.37
7.35
7.35
7.34
7.27
4.33
4.31
4.29
4.26
1.56
1.43
1.41
1.38
0.00
O
N
O
1.00
1.01
1.01
1.02
2.02
6.00
3.11
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0
f1 (ppm)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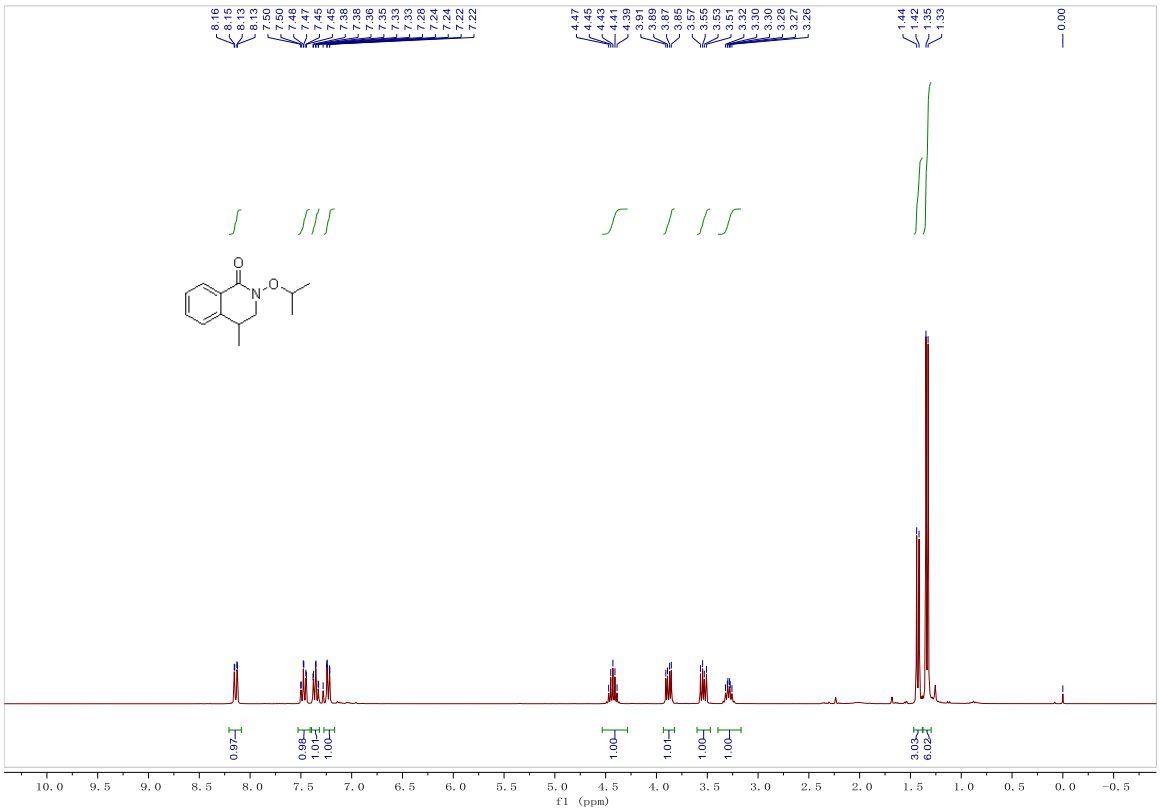
148.84
132.13
128.58
128.15
123.81
120.69
77.48
77.26
77.06
76.63
73.16
63.39
25.15
14.03
O
N-O
f1 (ppm)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8.15
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8.13
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7.47
7.45
7.45
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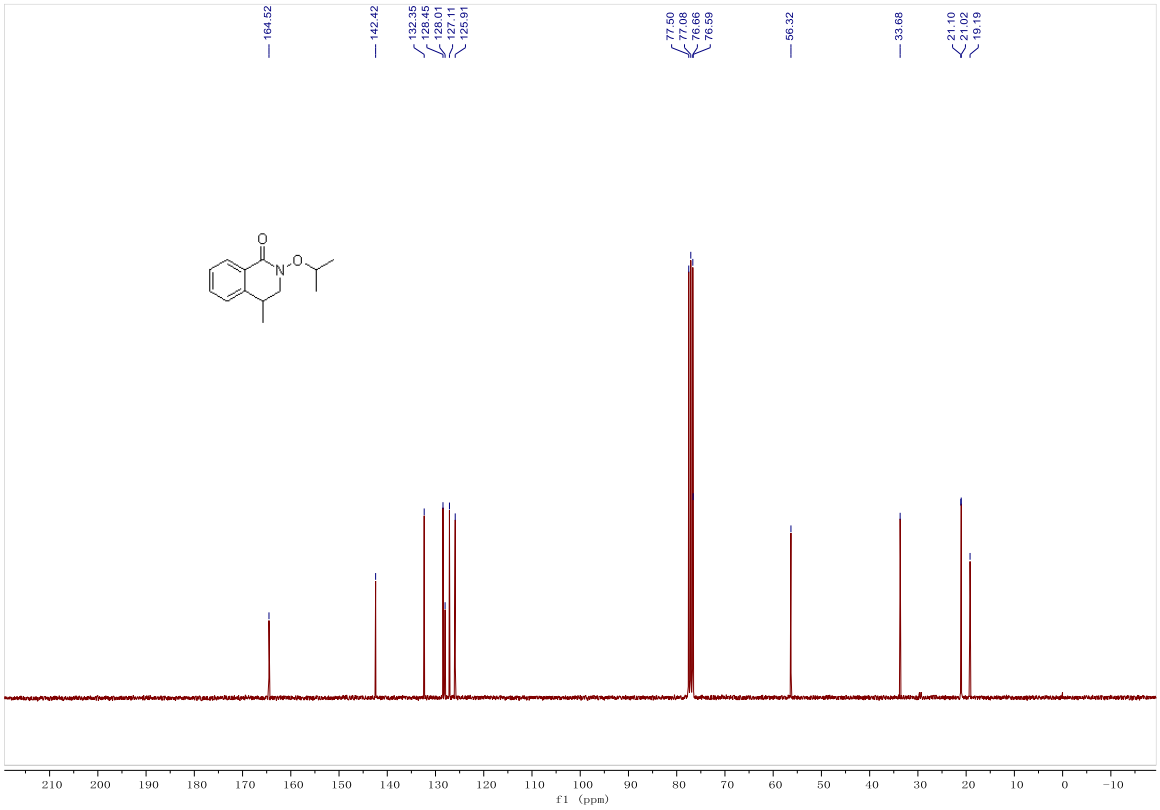
7.36
7.35
7.33
7.33
7.28
7.24
7.22
7.22
4.47
4.45
4.43
4.41
4.39
3.91
3.89
3.87
3.85
3.57
3.55
3.53
3.51
3.32
3.30
3.30
3.28
3.27
3.26
1.44
1.42
1.35
1.33
0.00
O
N-O
0.97
0.98
1.01
1.00
1.00
1.01
1.00
1.00
3.03
6.02
f1 (ppm)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142.42
132.35
128.45
128.01
127.11
125.91
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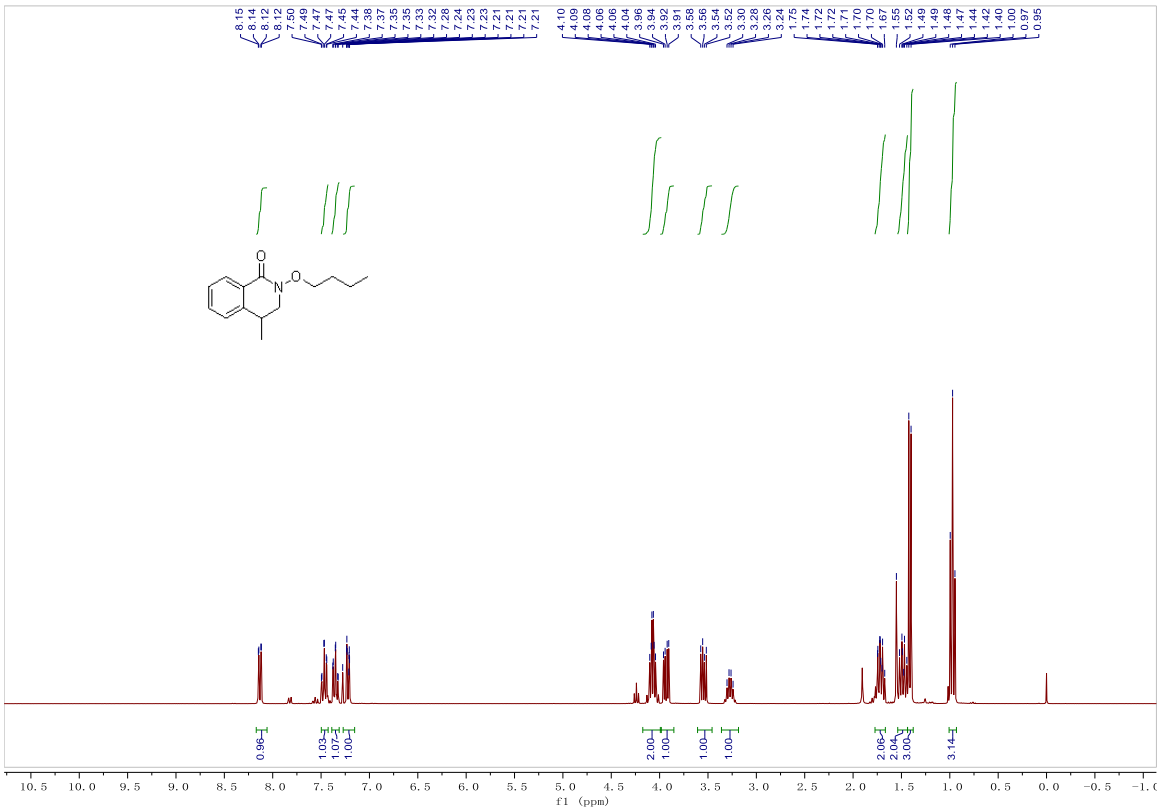
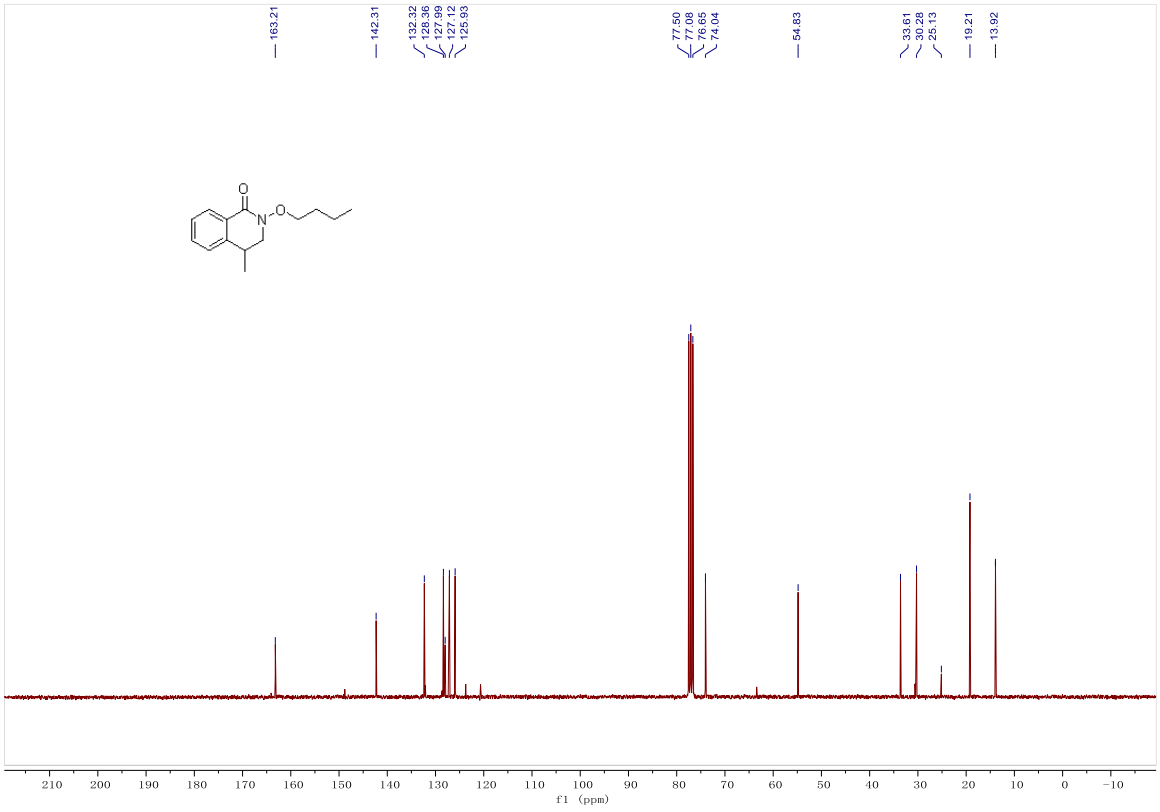
77.08
76.66
76.59
56.32
33.68
21.10
21.02
19.19
f1 (ppm)


f1 (ppm)


163.21
142.31
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127.12
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77.50
77.08
76.65
74.04
54.83
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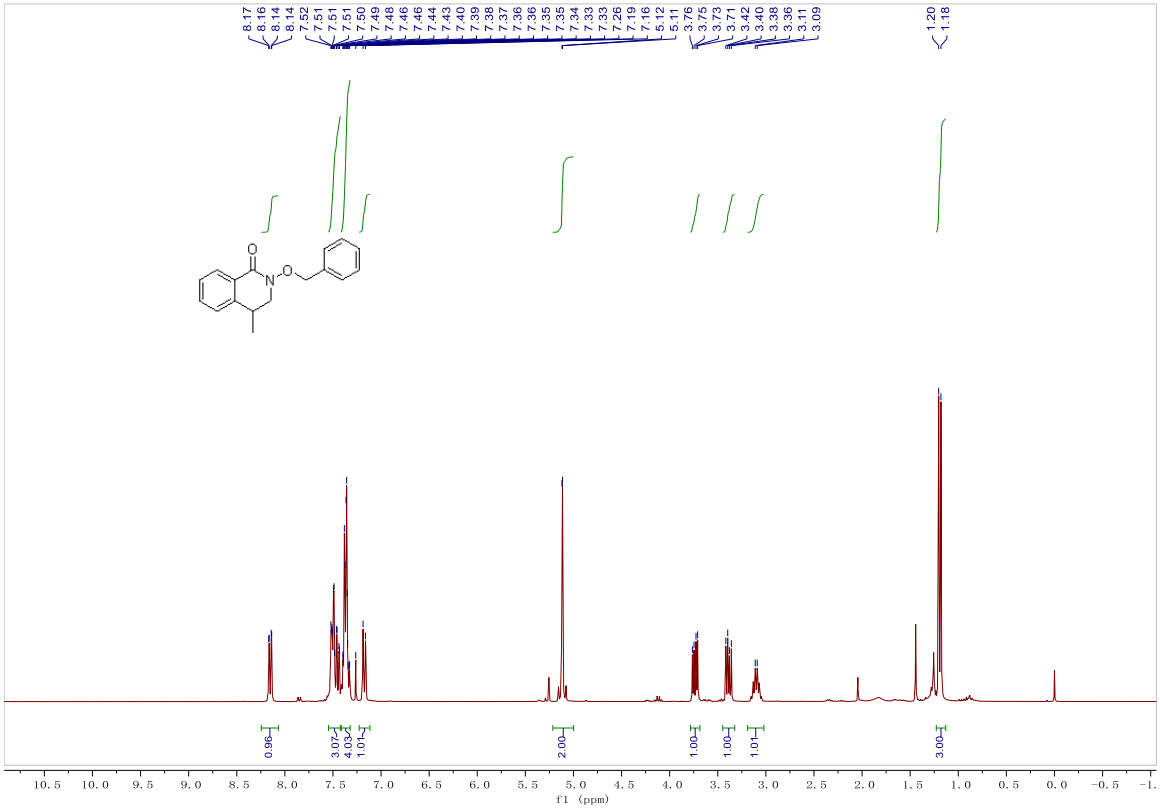
30.28
25.13
19.21
13.92
f1 (ppm)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8.14
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7.50
7.49
7.48
7.46
7.46
7.44
7.43
7.40
7.39
7.38
7.37
7.36
7.36
7.35
7.35
7.34
7.33
7.33
7.26
7.19
7.16
7.12
5.11
3.76
3.75
3.73
3.71
3.42
3.40
3.38
3.36
3.11
3.09
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1.18
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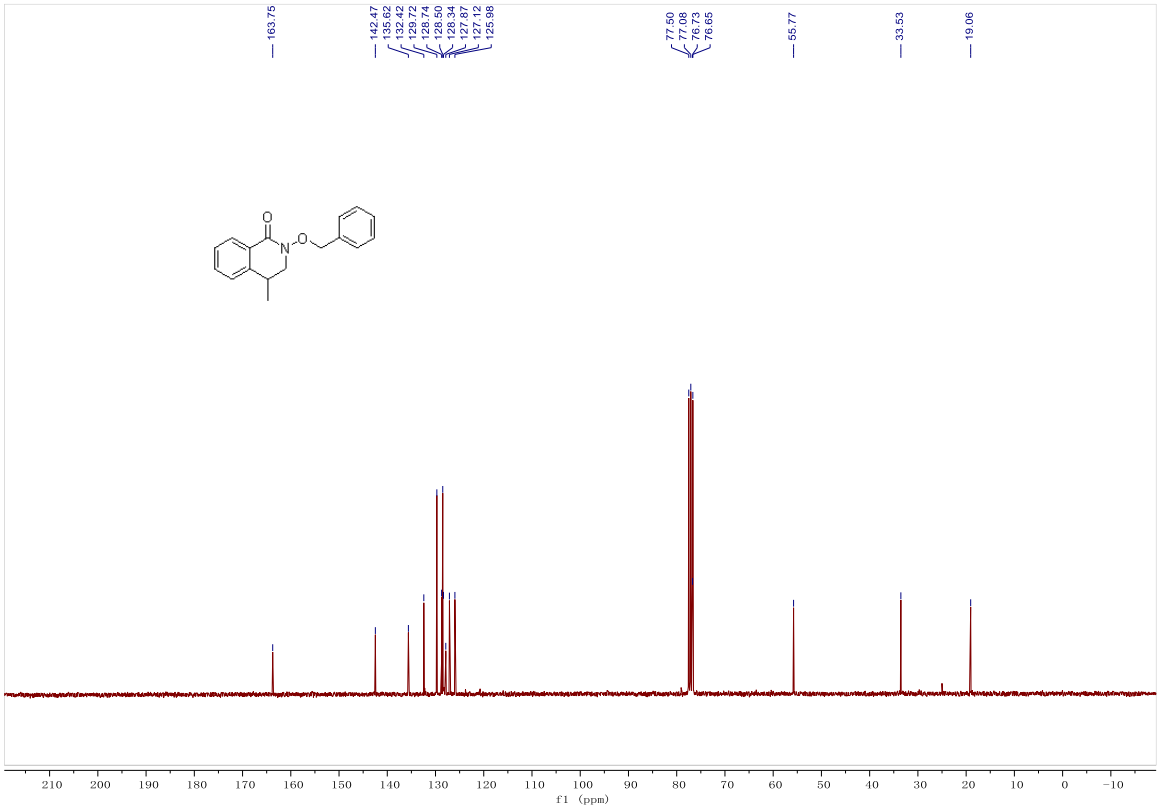
3.07
4.03
1.01
2.00
1.00
1.00
1.01
3.00
f1 (ppm)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128.34
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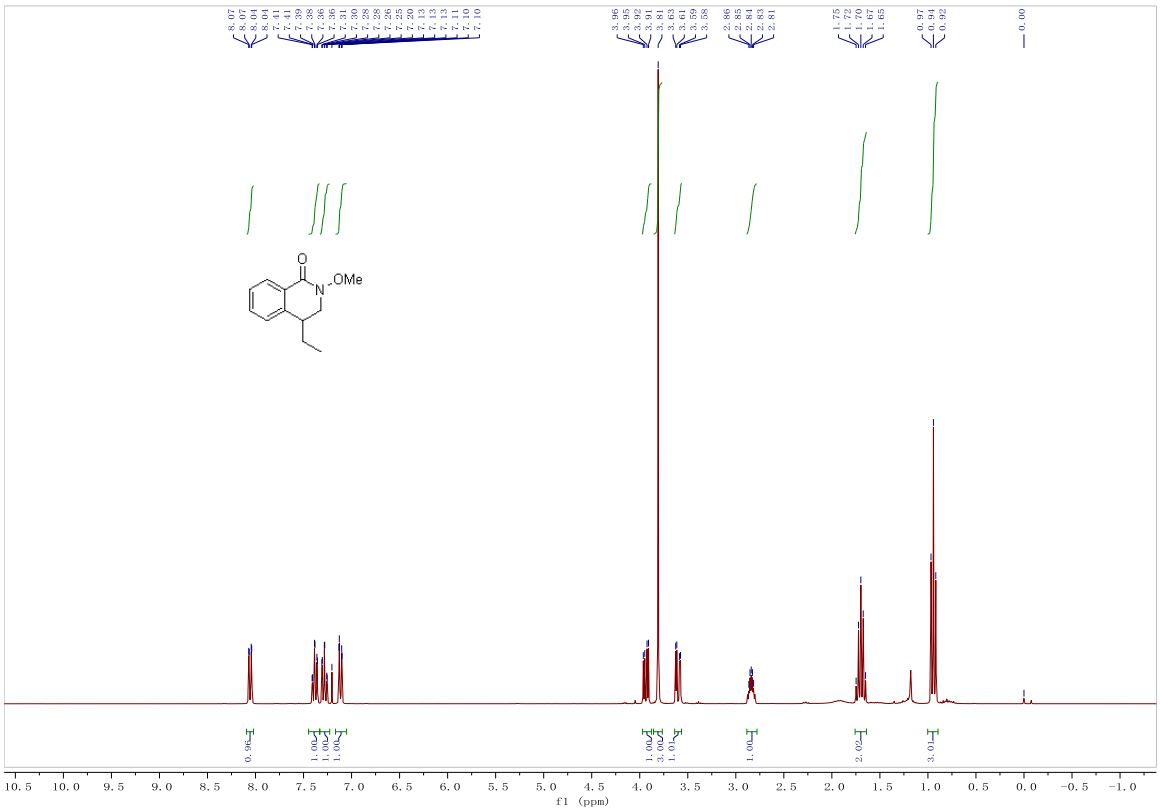
76.65
55.77
33.53
19.06
O
N
O
f1 (ppm)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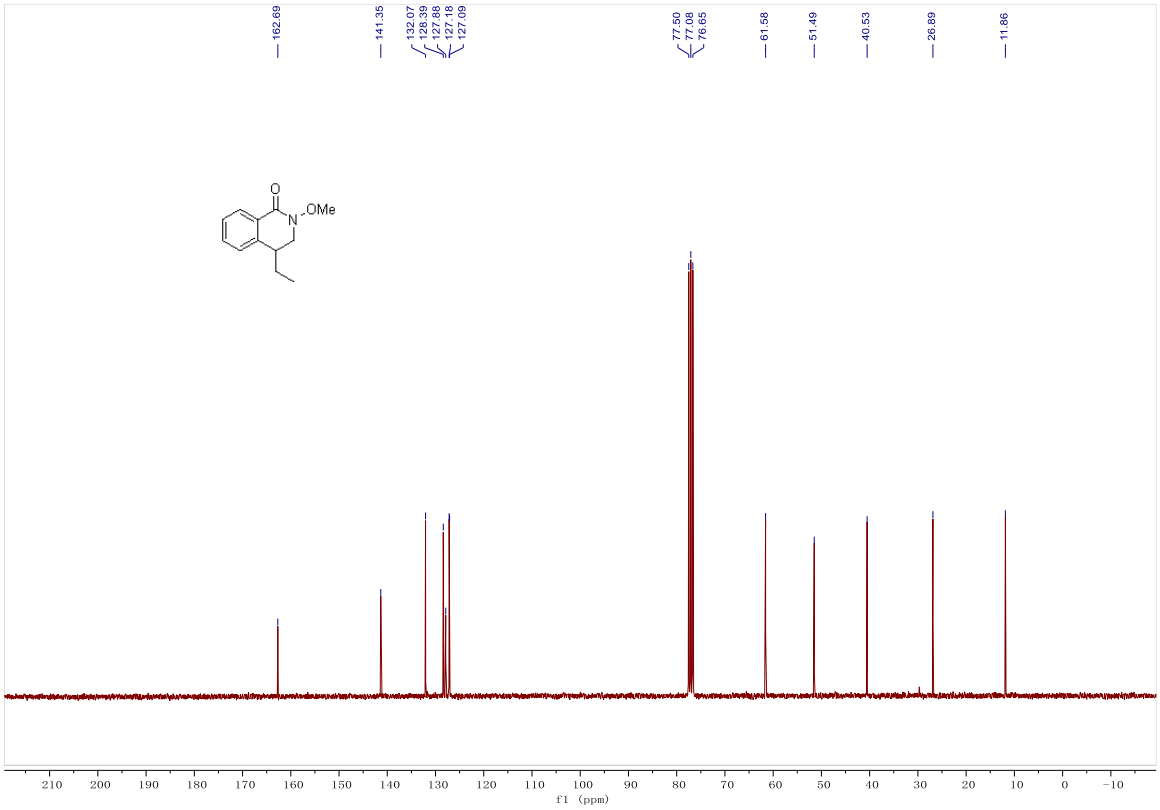
7.30
7.28
7.26
7.25
7.20
7.13
7.11
7.10
3.96
3.95
3.92
3.91
3.61
3.59
3.58
2.86
2.85
2.84
2.83
2.81
1.75
1.72
1.70
1.67
1.65
0.97
0.94
0.92
0.00
O
N
OMe
0.96
1.00
1.00
1.00
1.00
1.00
3.01
1.00
2.03
3.01
f1 (ppm)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127.16
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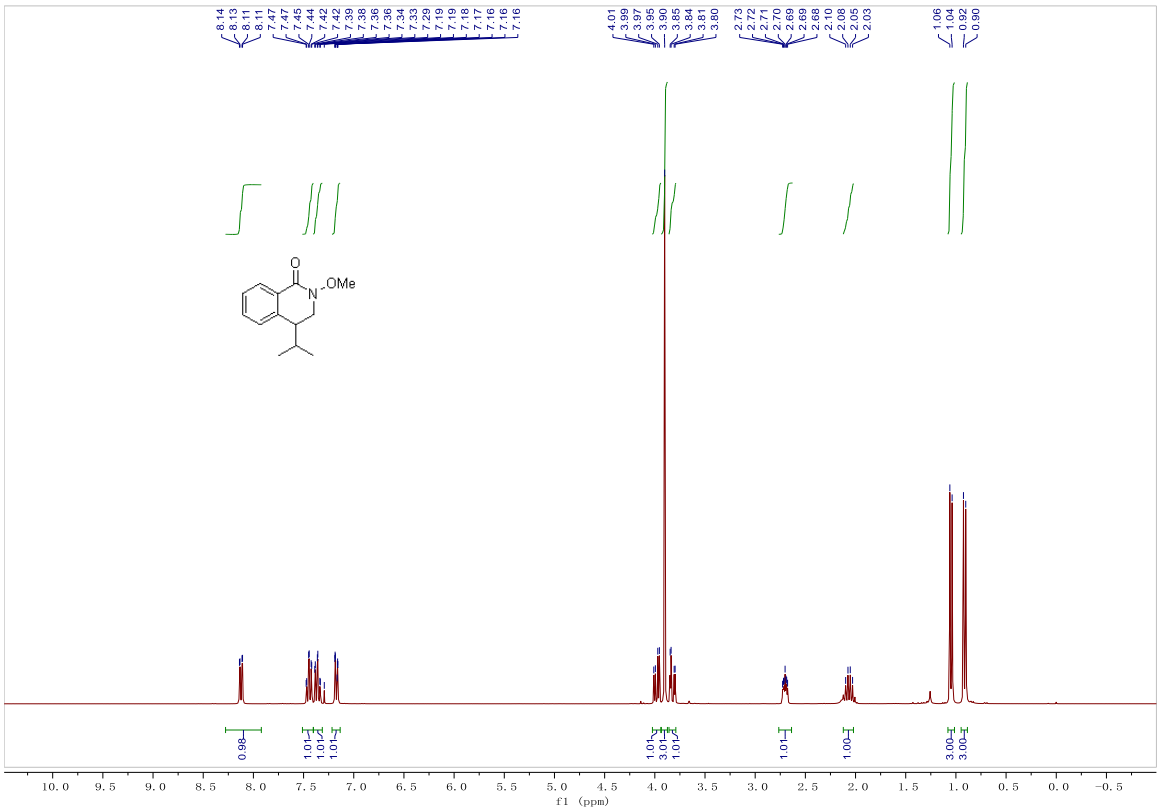
77.08
76.65
61.58
51.49
40.53
26.89
11.86
O
N
OMe
f1 (ppm)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8.11
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7.47
7.45
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7.42
7.42
7.39
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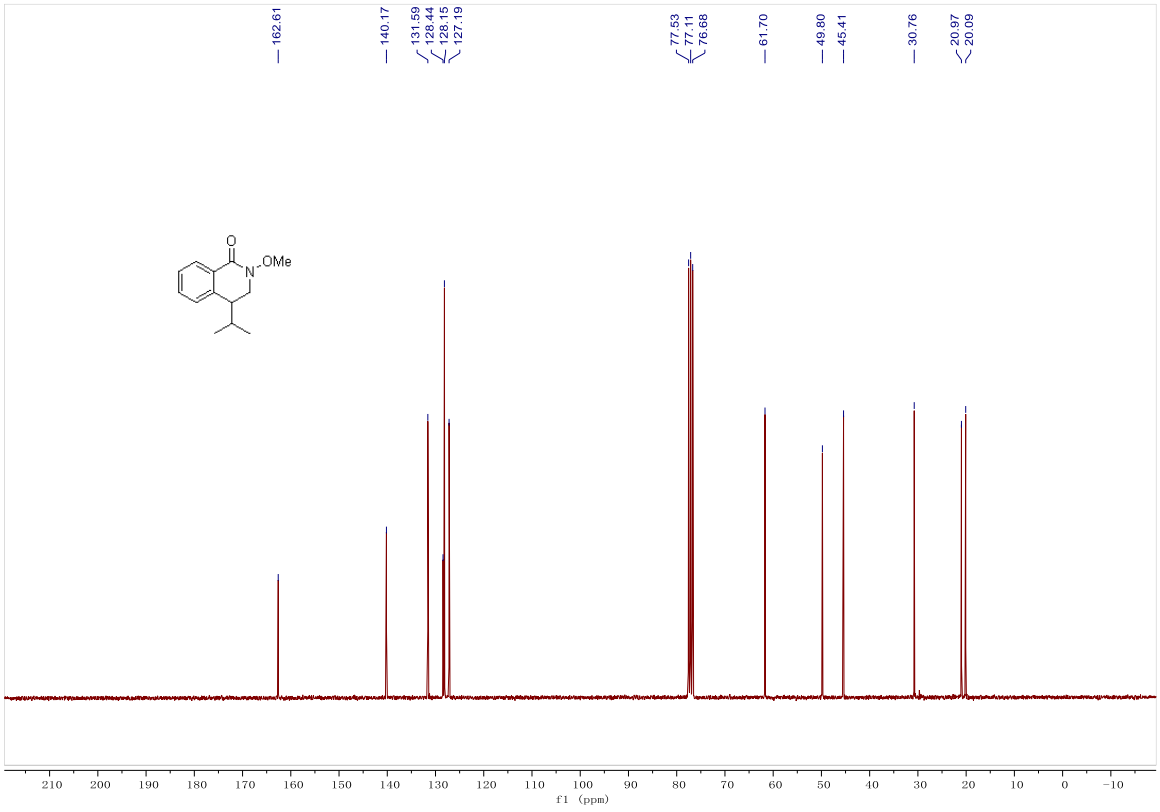
7.36
7.36
7.34
7.33
7.29
7.19
7.19
7.18
7.18
7.17
7.16
7.16
7.16
4.01
3.99
3.97
3.95
3.90
3.85
3.84
3.81
3.80
2.73
2.72
2.71
2.70
2.69
2.69
2.68
2.10
2.08
2.05
2.03
1.06
1.04
0.92
0.90
0.98
1.01
1.01
1.01
1.01
3.01
1.01
1.01
1.00
3.00
3.00
O
N
OMe
f1 (ppm)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128.15
127.19
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77.11
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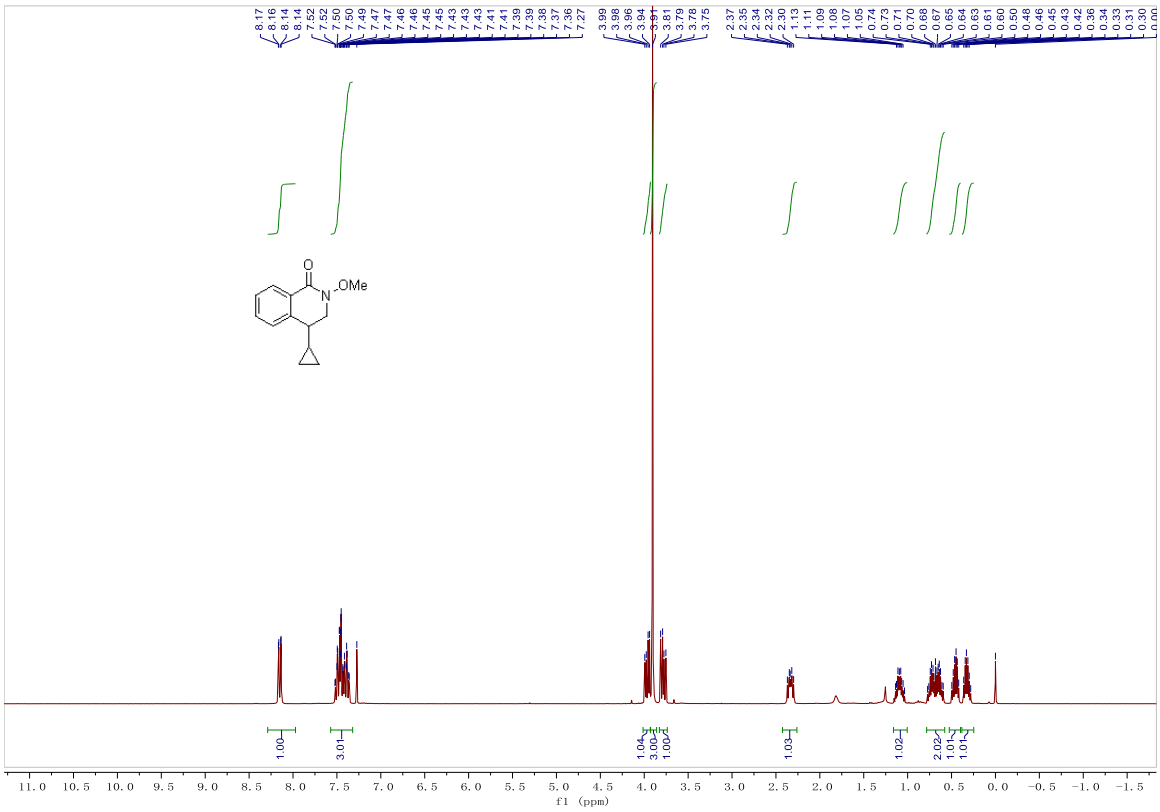
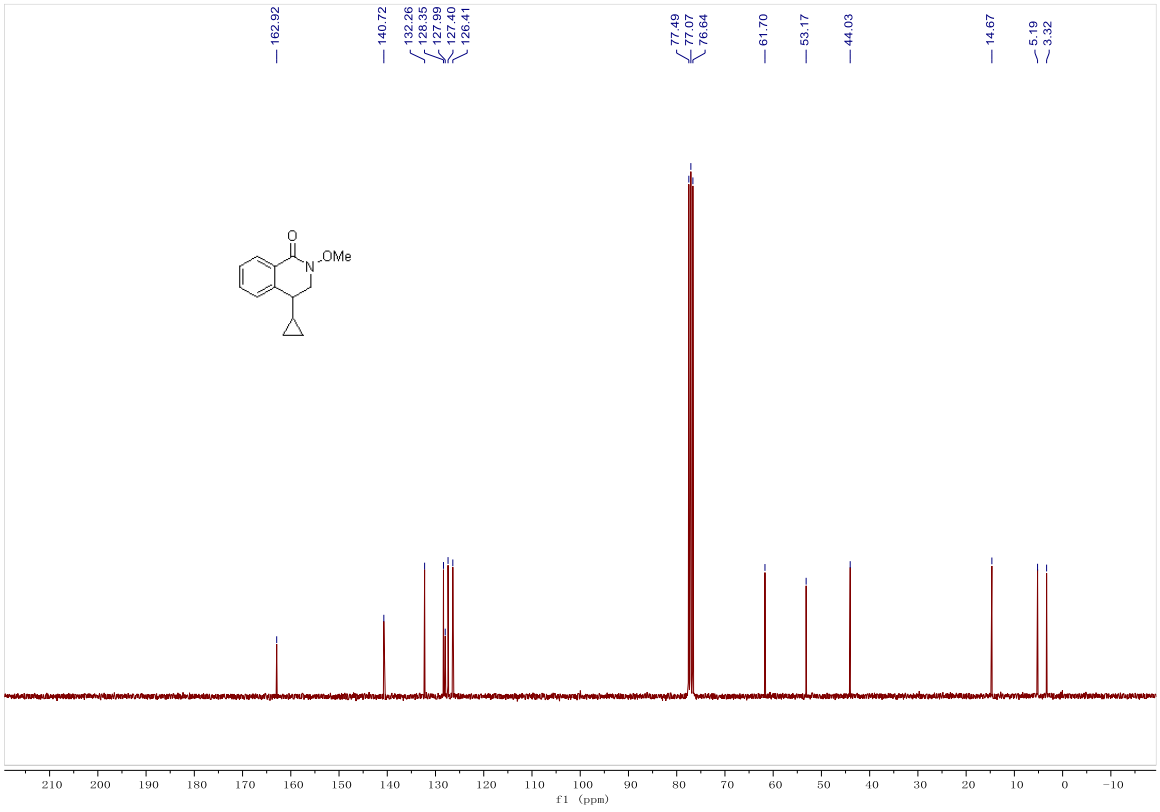
61.70
49.80
45.41
30.76
20.97
20.09
O
N
OMe
f1 (ppm)


O
N
OMe
1.00
3.01
1.04
3.00
1.00
1.03
1.02
2.02
1.01
1.01
f1 (ppm)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127.40
126.41
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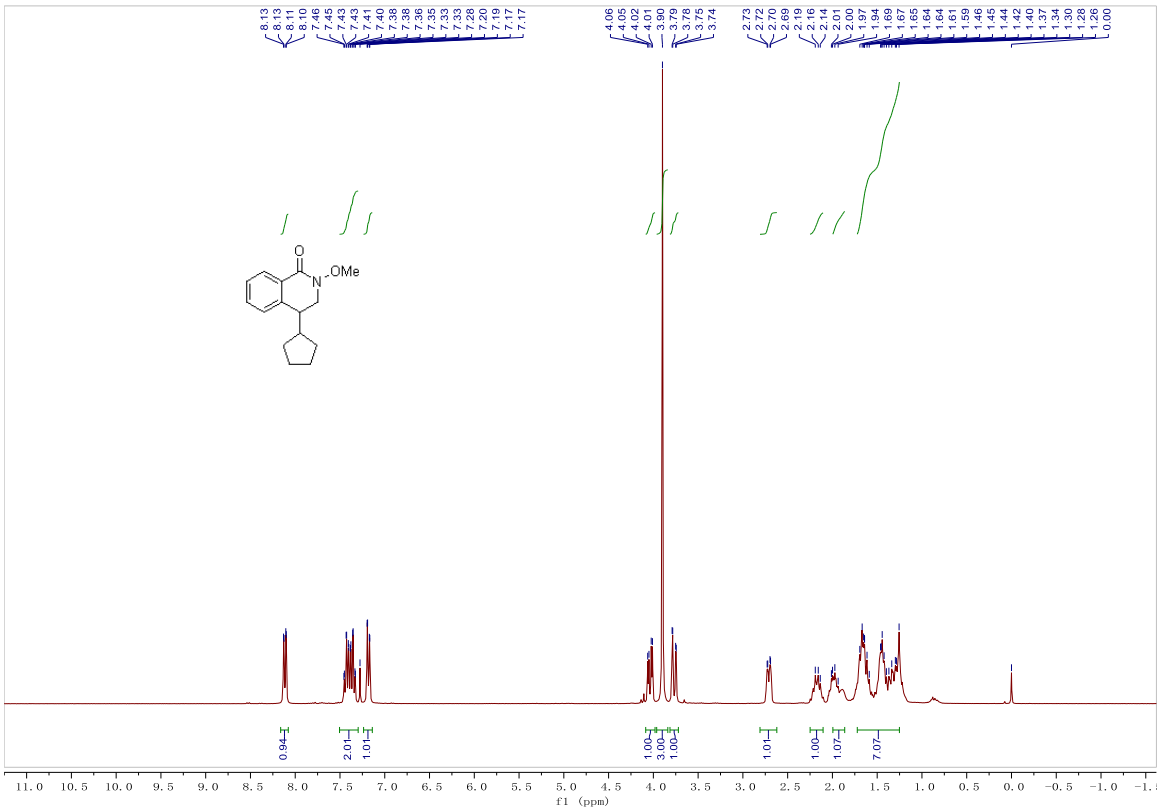
61.70
53.17
44.03
14.67
5.19
3.32
O
N
OMe
f1 (ppm)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7.45
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7.43
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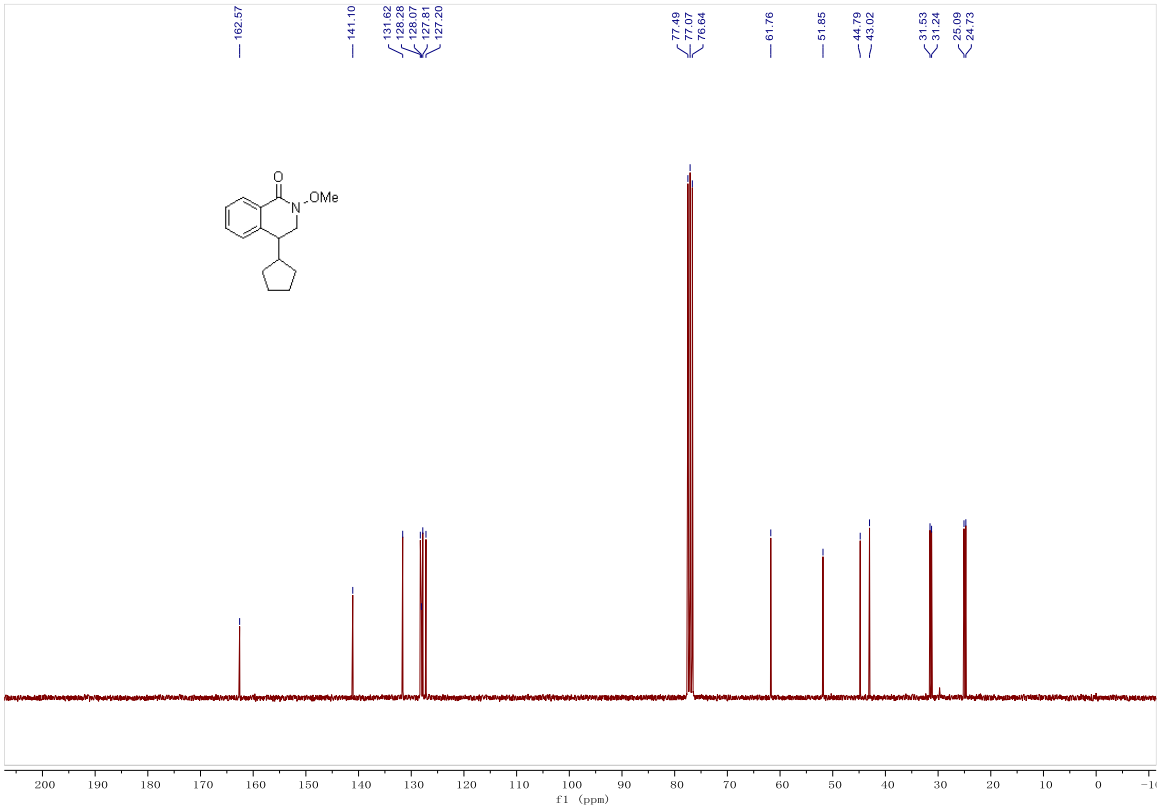
7.40
7.38
7.38
7.36
7.35
7.33
7.33
7.28
7.20
7.19
7.17
7.17
4.06
4.05
4.02
4.01
3.90
3.79
3.78
3.75
3.74
2.73
2.72
2.69
2.68
2.19
2.16
2.14
2.01
2.00
1.97
1.94
1.69
1.67
1.65
1.64
1.64
1.61
1.59
1.46
1.45
1.44
1.42
1.40
1.37
1.34
1.30
1.28
1.26
0.00
O
N
OMe
0.94
2.01
1.01
1.00
3.00
1.00
1.01
1.00
1.07
7.07
f1 (ppm)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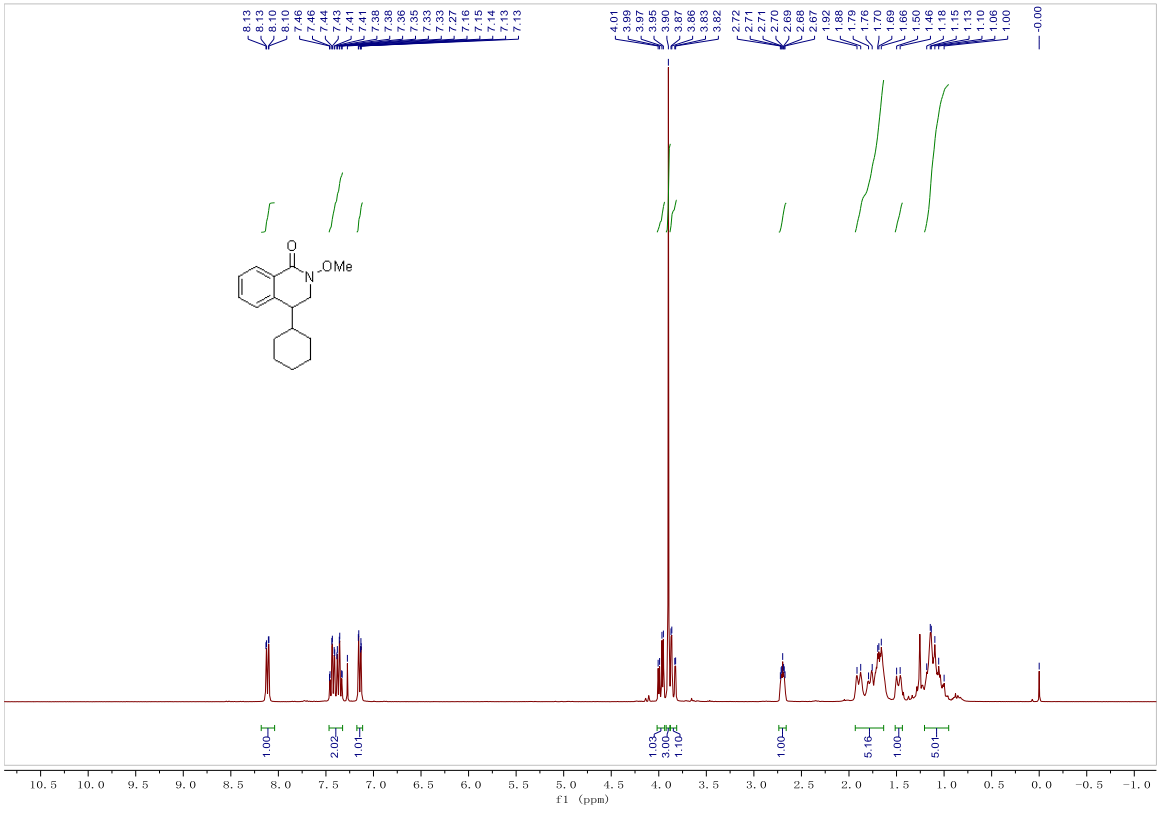
127.81
127.20
77.49
77.07
76.64
61.76
51.85
44.79
43.02
31.53
31.24
25.09
24.73
OMe
f1 (ppm)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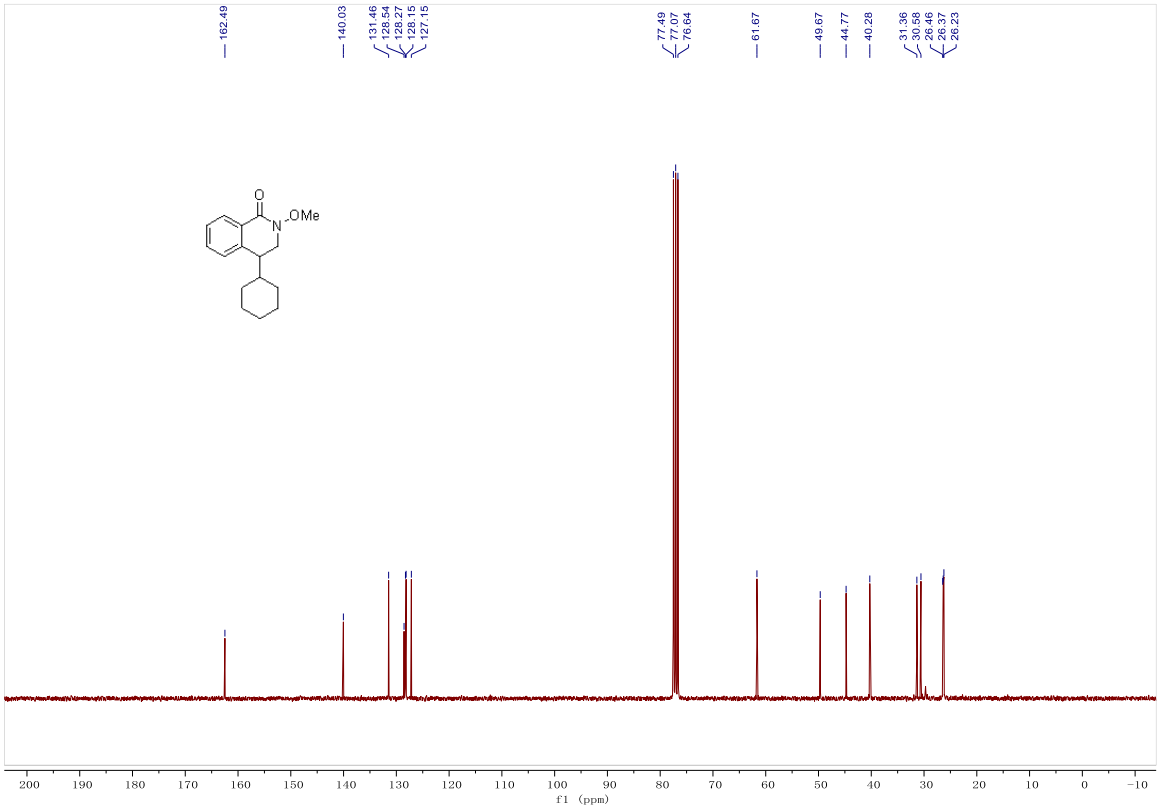
8.13
8.10
8.10
7.46
7.46
7.44
7.43
7.41
7.41
7.38
7.38
7.36
7.35
7.33
7.33
7.27
7.16
7.15
7.14
7.13
7.13
4.01
3.99
3.97
3.95
3.90
3.87
3.86
3.83
3.82
2.72
2.71
2.71
2.70
2.69
2.68
2.67
1.92
1.88
1.79
1.76
1.70
1.69
1.66
1.50
1.46
1.18
1.15
1.13
1.10
1.06
1.00
-0.00
OMe
1.00
2.02
1.01
1.03
3.00
1.10
1.00
5.16
1.00
5.01
f1 (ppm)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128.54
128.27
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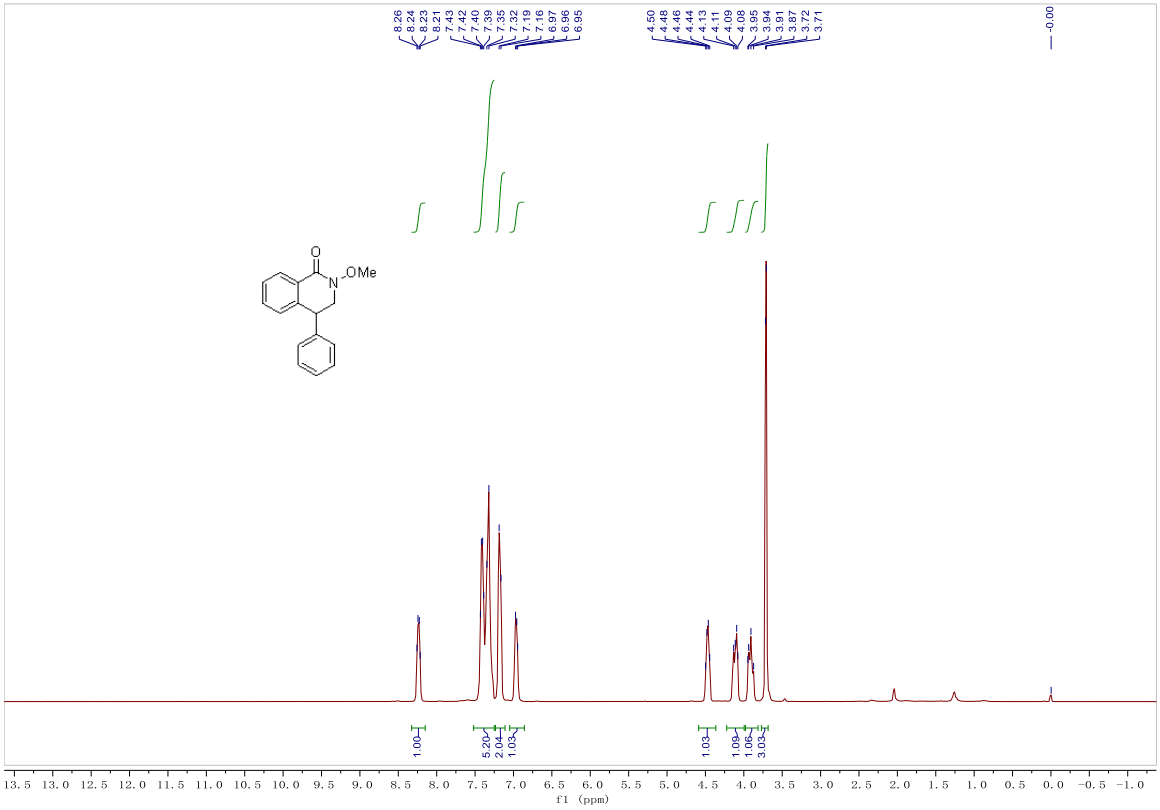
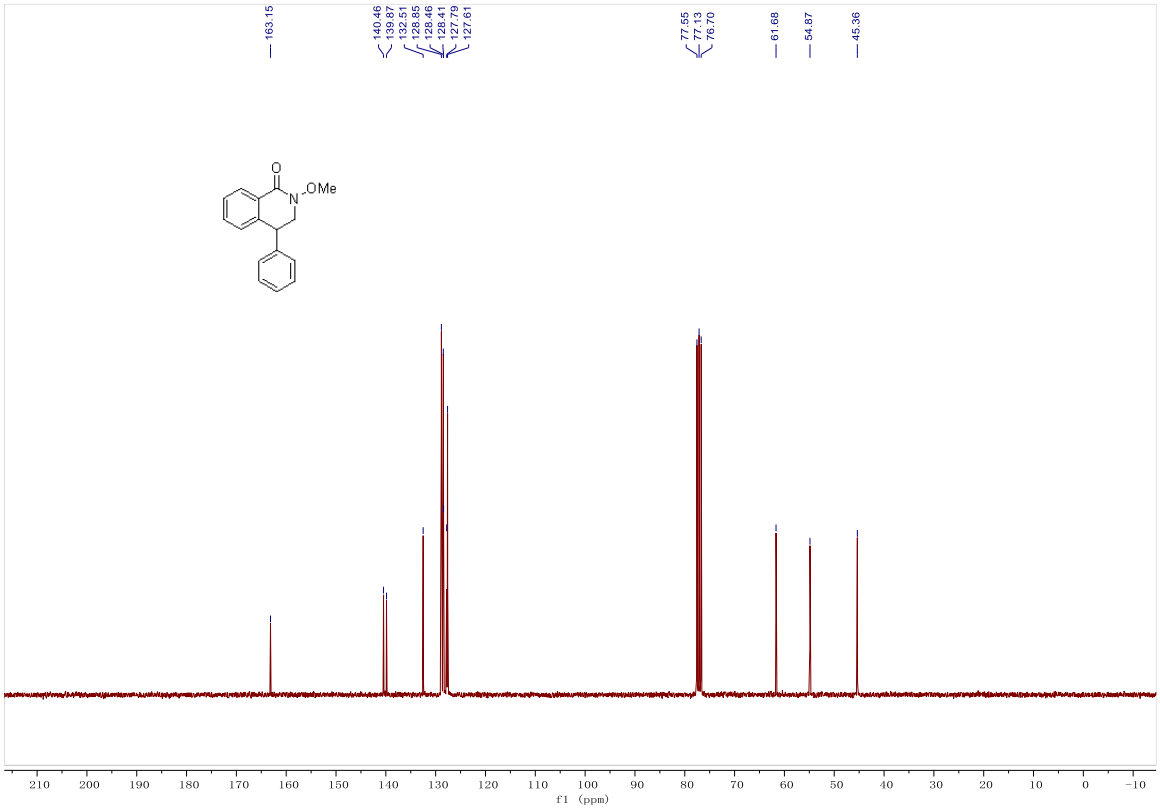
127.15
77.49
77.07
76.64
61.67
49.67
44.77
40.28
31.36
30.58
26.46
26.37
26.23
O
N
OMe
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


8.26
8.24
8.23
8.21
7.43
7.42
7.40
7.39
7.35
7.32
7.19
7.16
6.97
6.96
6.95
4.50
4.48
4.46
4.44
4.13
4.11
4.09
4.08
3.95
3.94
3.91
3.87
3.72
3.71
-0.00
O
N
OMe
1.00
5.20
2.04
1.03
1.03
1.09
1.06
3.03
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0
f1 (ppm)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140.46
139.87
132.51
128.85
128.46
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127.79
127.61
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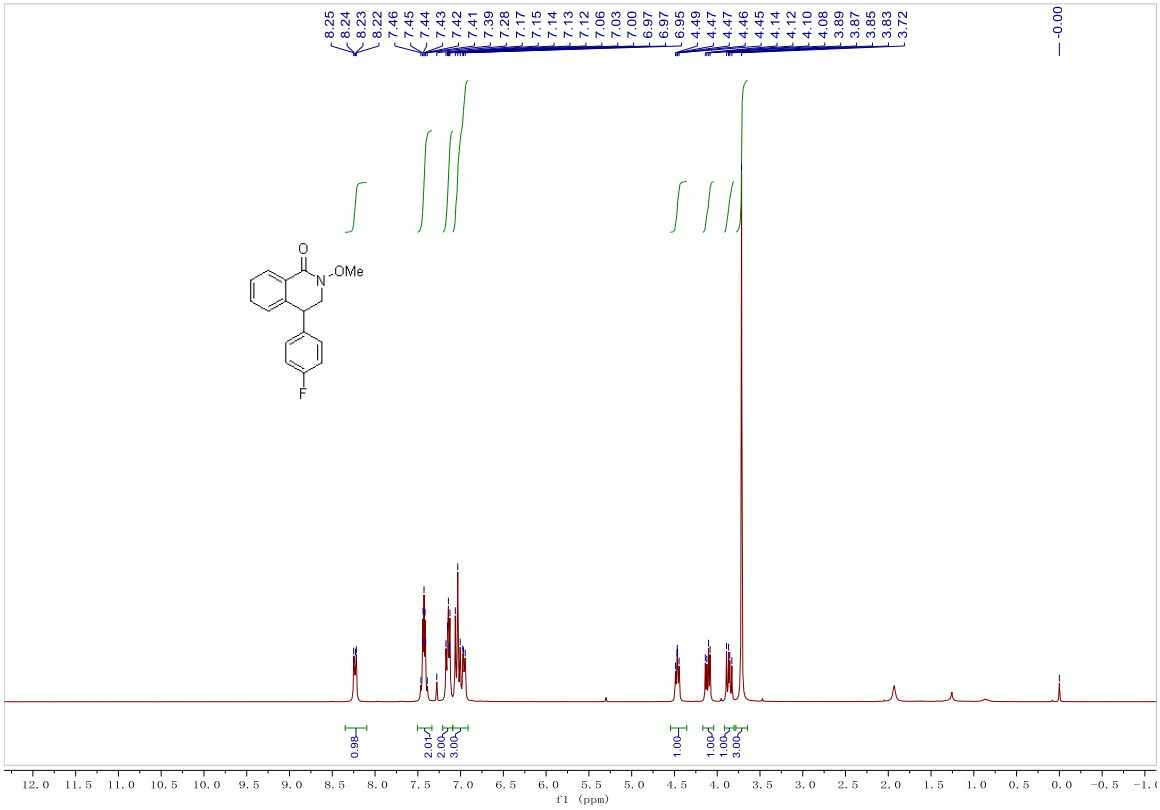
77.13
76.70
61.68
54.87
45.36
O
N
OMe
f1 (ppm)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7.45
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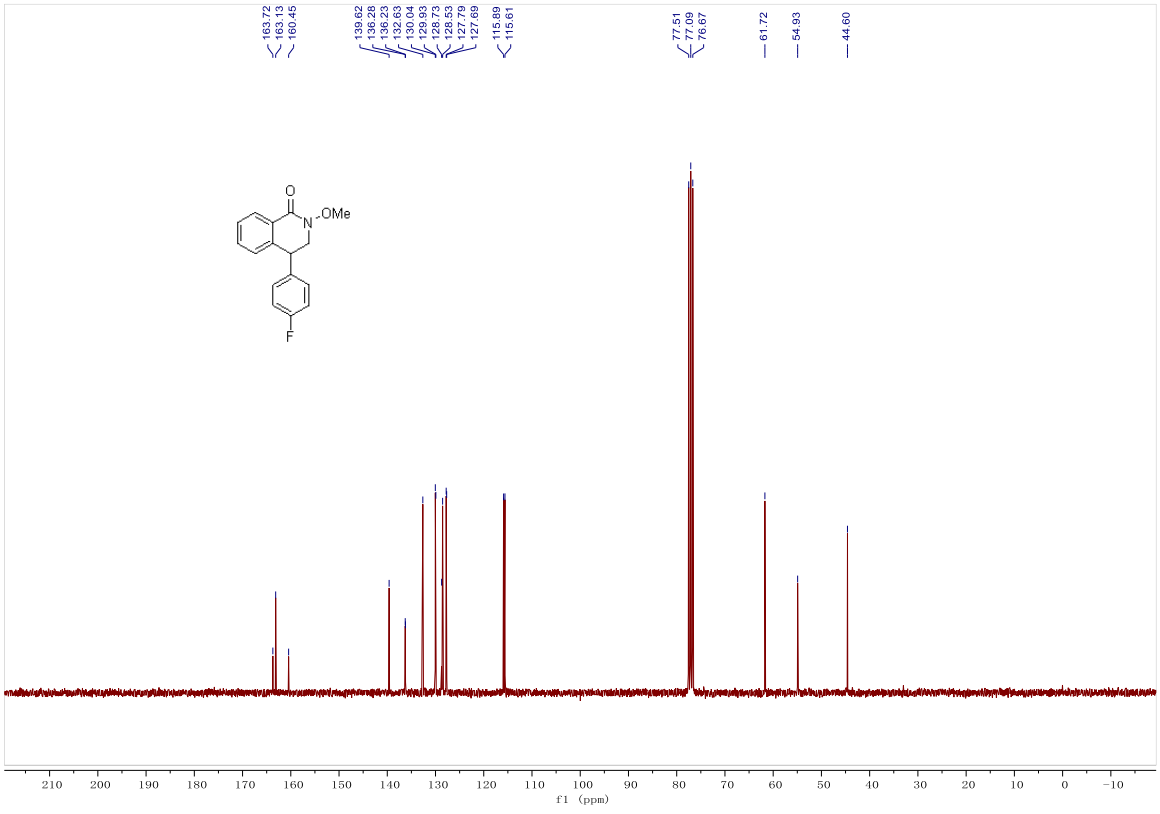
7.43
7.42
7.41
7.39
7.28
7.17
7.15
7.14
7.13
7.12
7.06
7.03
7.00
6.97
6.97
6.95
4.49
4.47
4.47
4.46
4.45
4.14
4.12
4.10
4.08
3.89
3.87
3.85
3.83
3.72
-0.00
O
N
OMe
F
0.98
2.01
2.00
3.00
1.00
1.00
1.00
3.00
f1 (ppm)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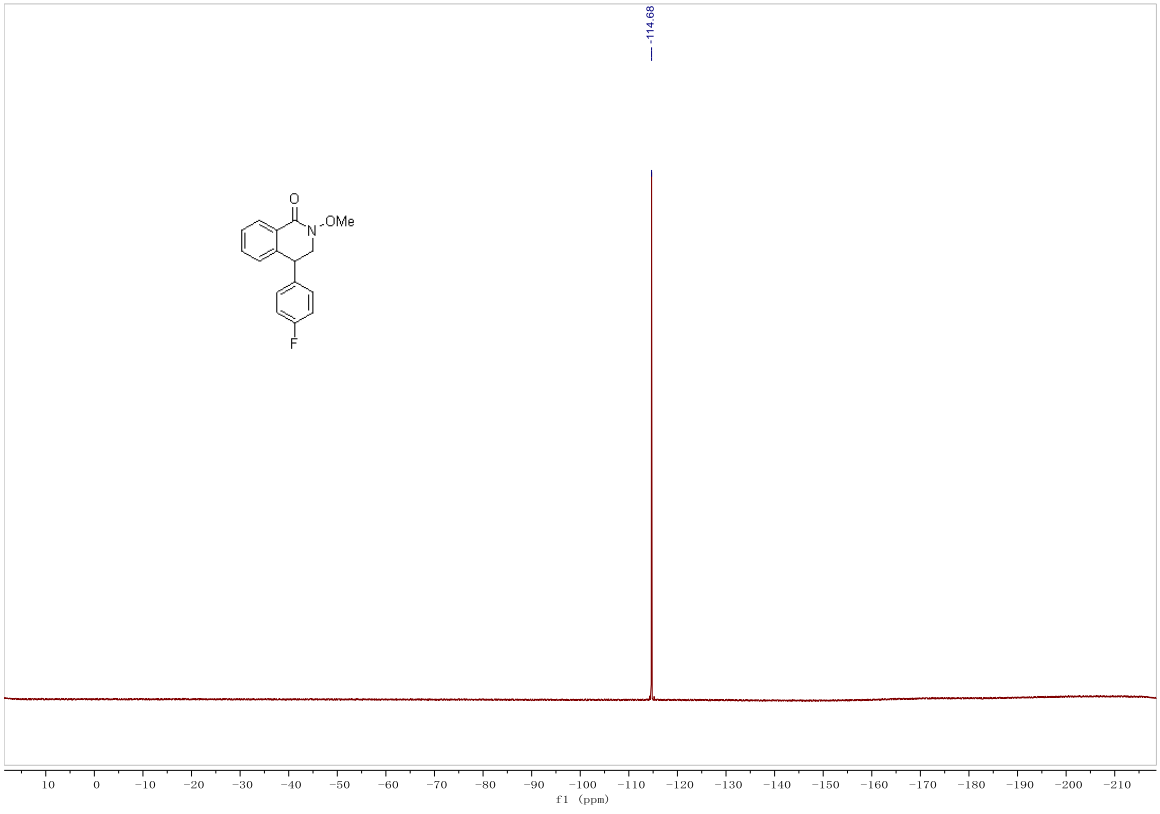
163.13
160.45
139.62
136.28
136.23
132.63
130.04
129.93
129.73
128.53
127.79
127.69
115.89
115.61
77.51
77.09
76.67
61.72
54.93
44.60
O
N
OMe
F
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


-114.68
O
N
OMe
F
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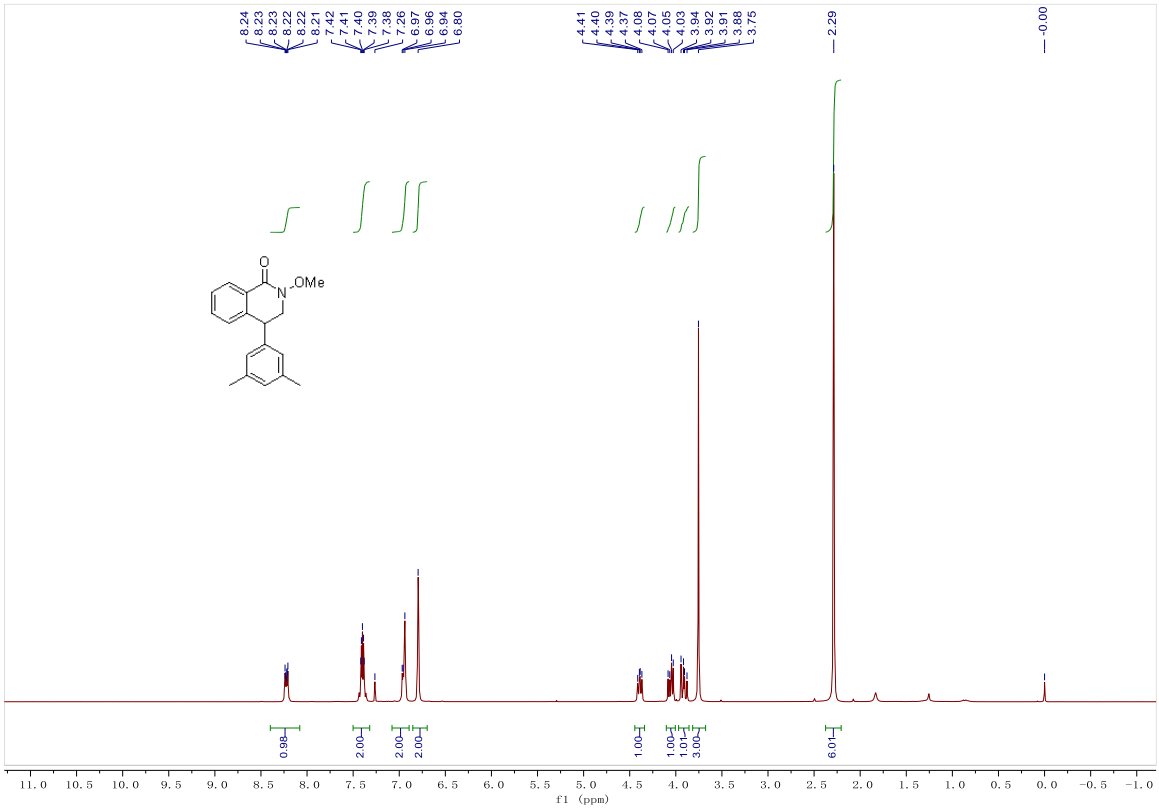
f1 (ppm)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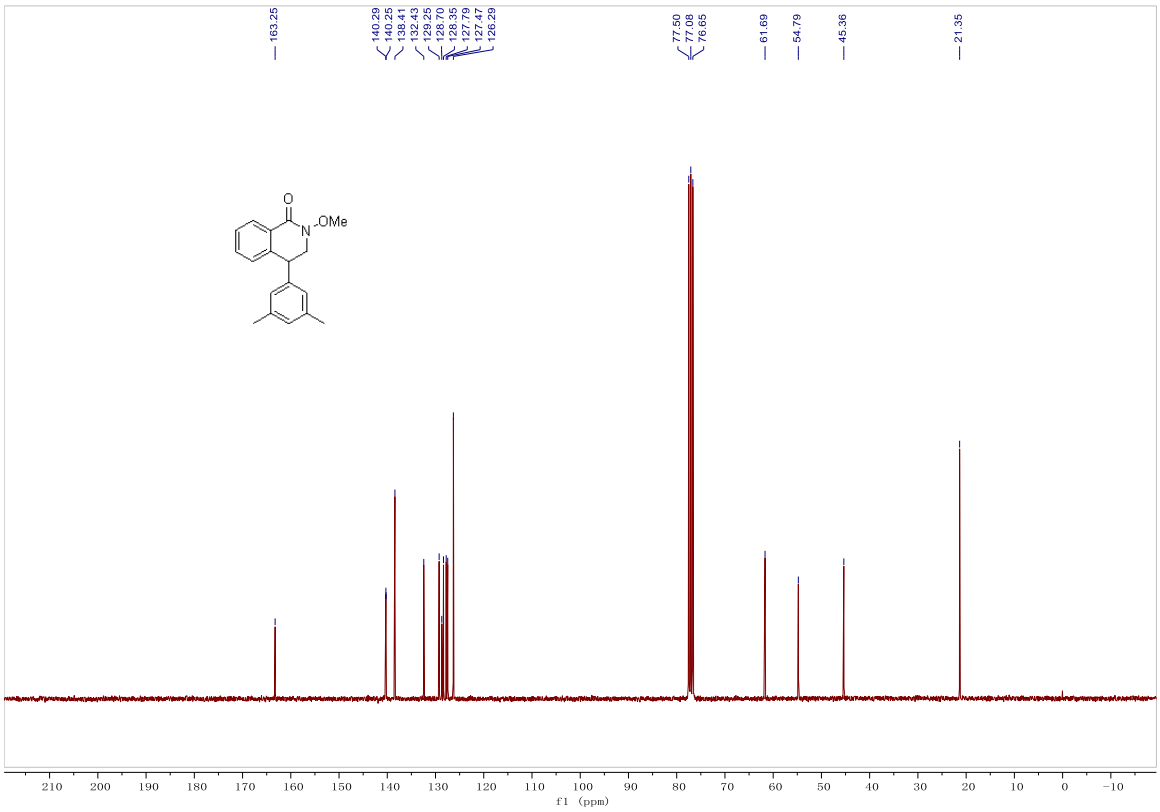
8.23
8.23
8.22
8.22
8.21
7.42
7.41
7.40
7.39
7.38
7.26
6.97
6.96
6.94
6.80
4.41
4.40
4.39
4.37
4.08
4.07
4.05
4.03
3.94
3.92
3.91
3.88
3.75
2.29
-0.00
O
N
OMe
0.98
2.00
2.00
2.00
1.00
1.00
1.01
3.00
6.01
f1 (ppm)


163.25
140.29
140.25
138.41
132.43
129.25
128.70
128.35
127.79
127.47
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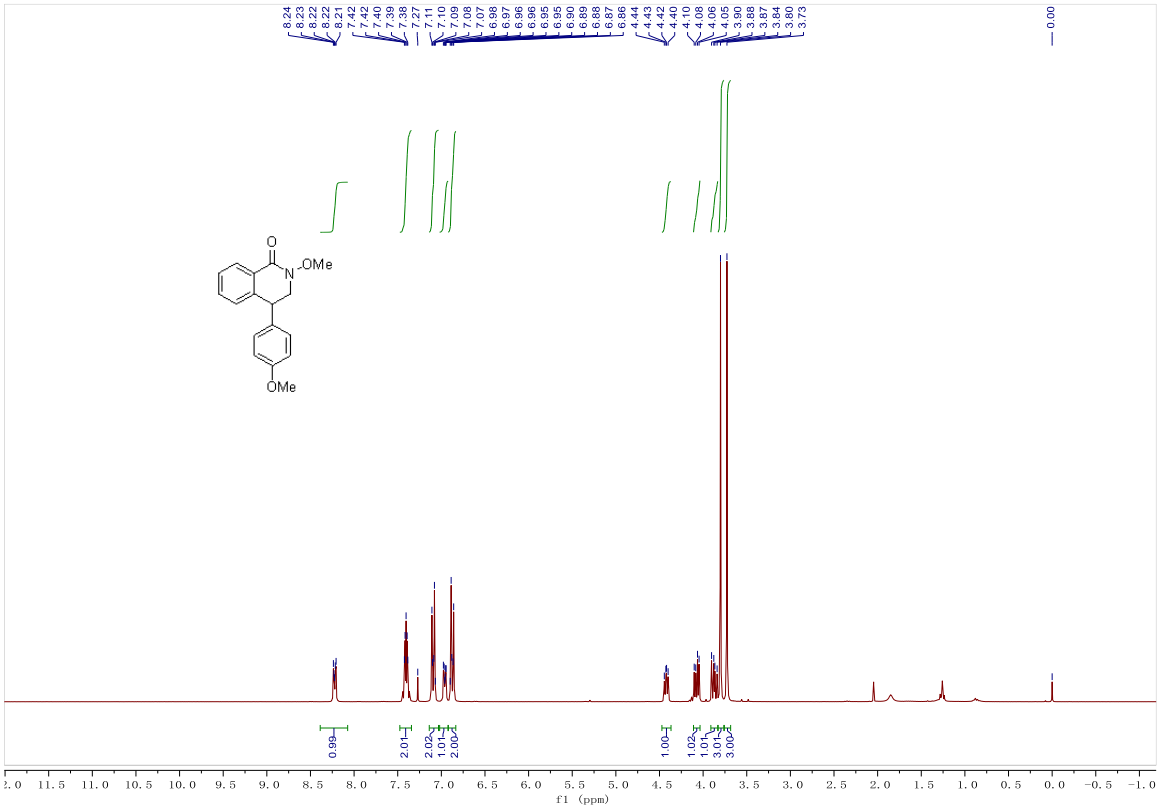
77.50
77.08
76.65
61.69
54.79
45.36
21.35
O
N
OMe
f1 (ppm)


8.24
8.23
8.22
8.22
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7.42
7.40
7.39
7.38
7.27
7.11
7.10
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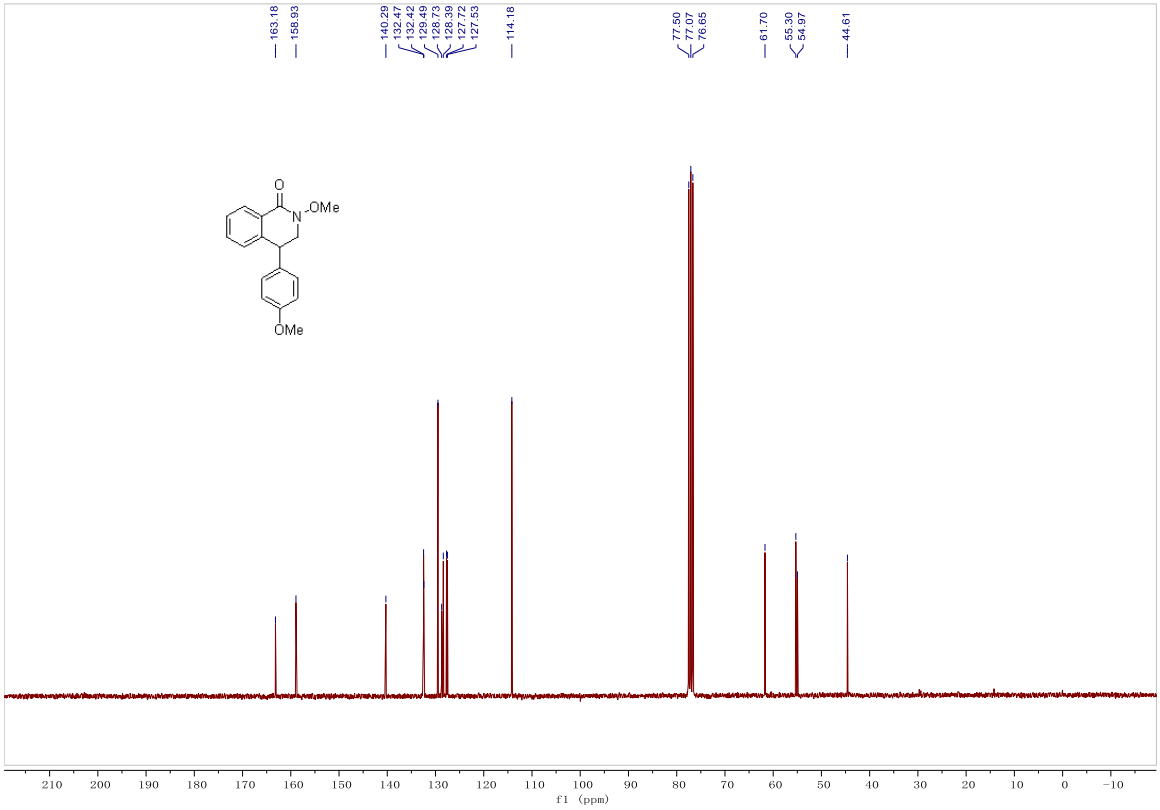
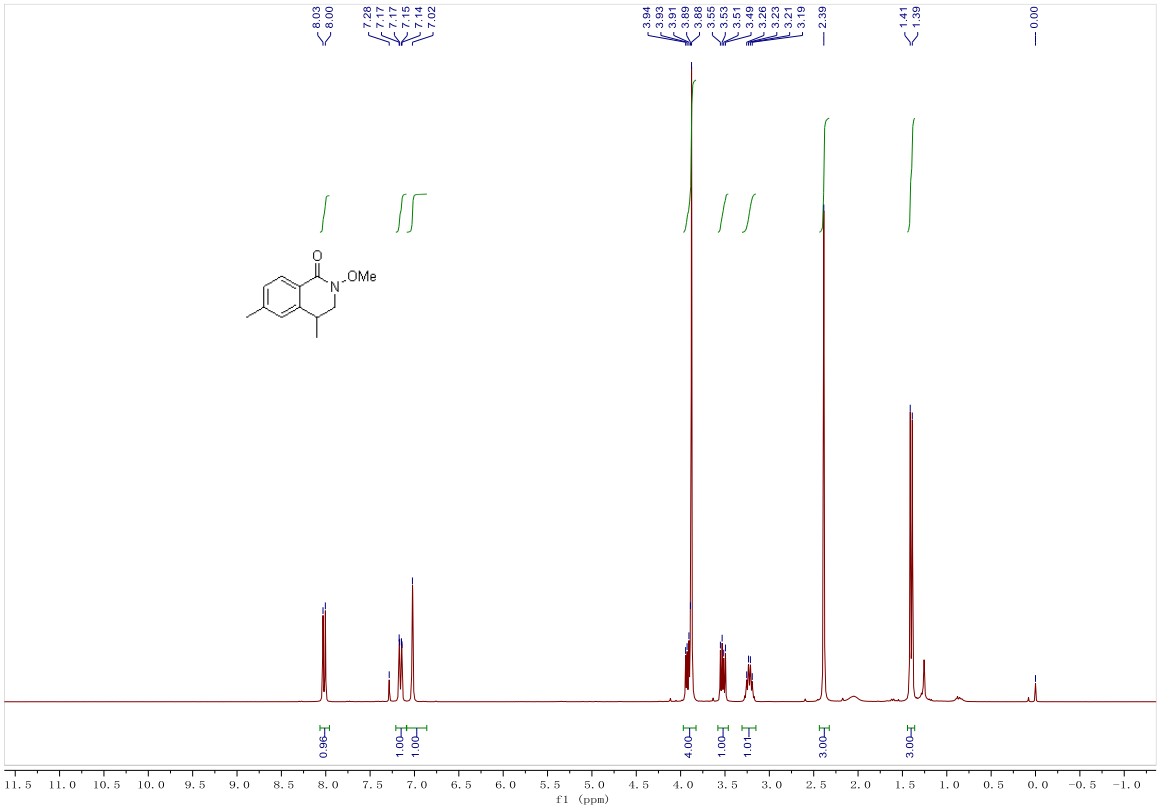
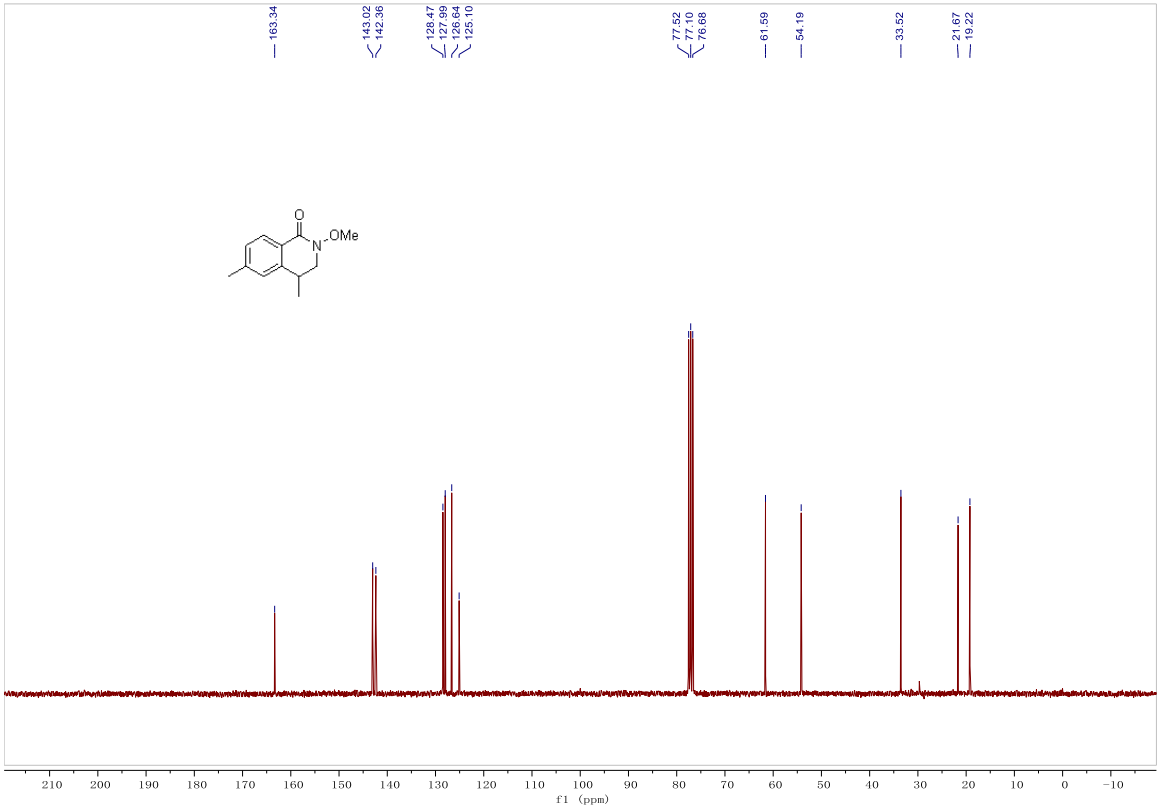
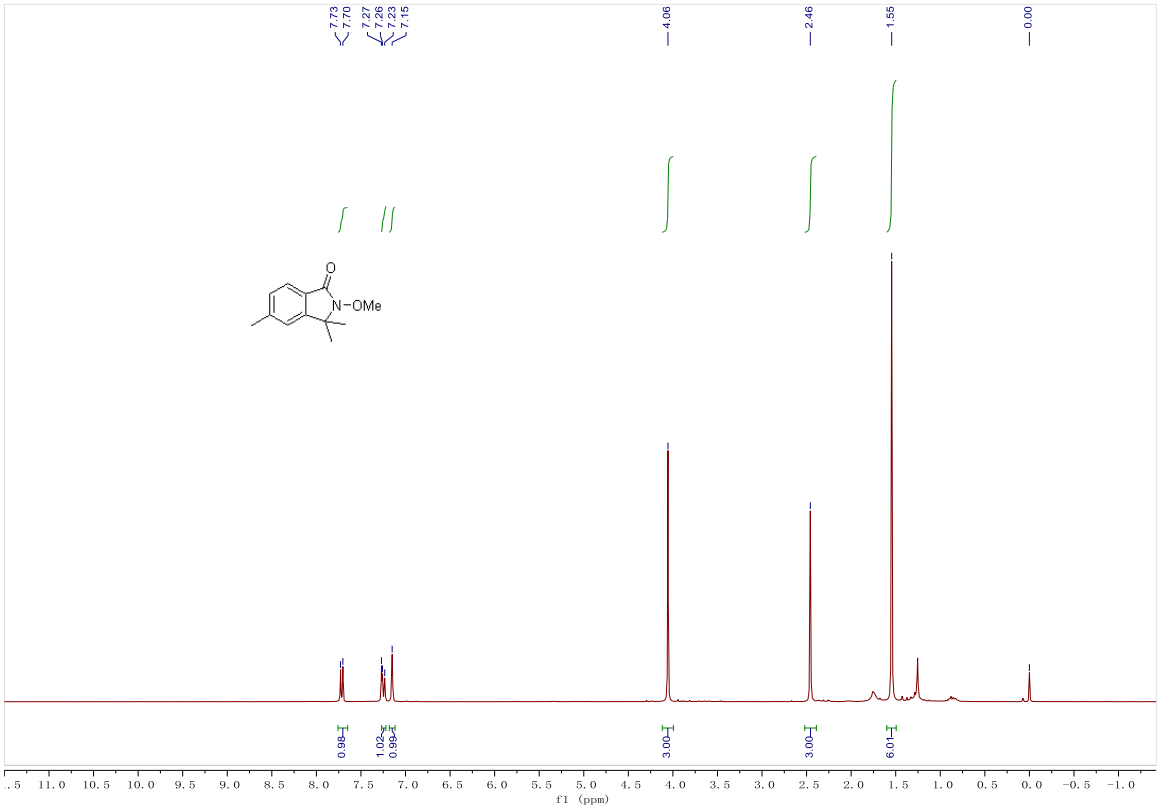
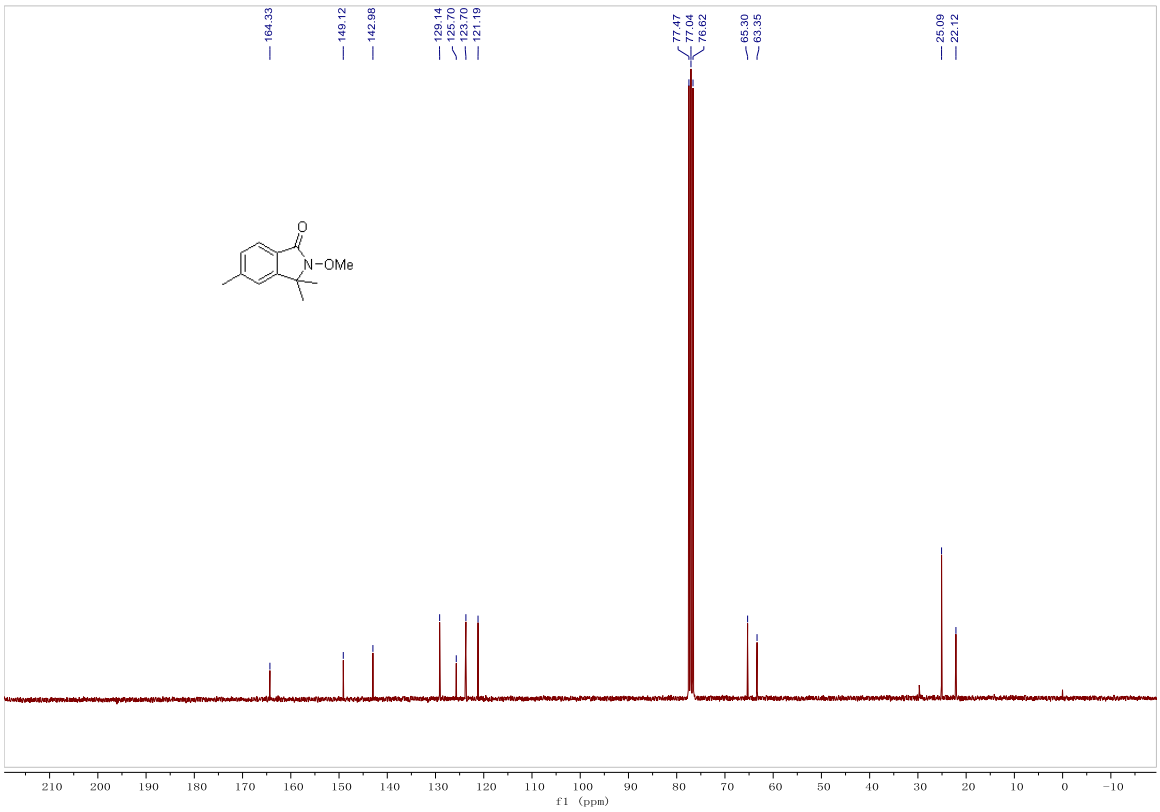
7.08
7.07
6.98
6.97
6.96
6.95
6.95
6.90
6.89
6.88
6.87
6.86
4.44
4.43
4.42
4.40
4.10
4.08
4.06
4.05
3.90
3.88
3.87
3.84
3.80
3.73
0.00
O
N
OMe
OMe
0.99
2.01
2.02
1.01
2.00
1.00
1.02
1.01
3.01
3.00
f1 (ppm)

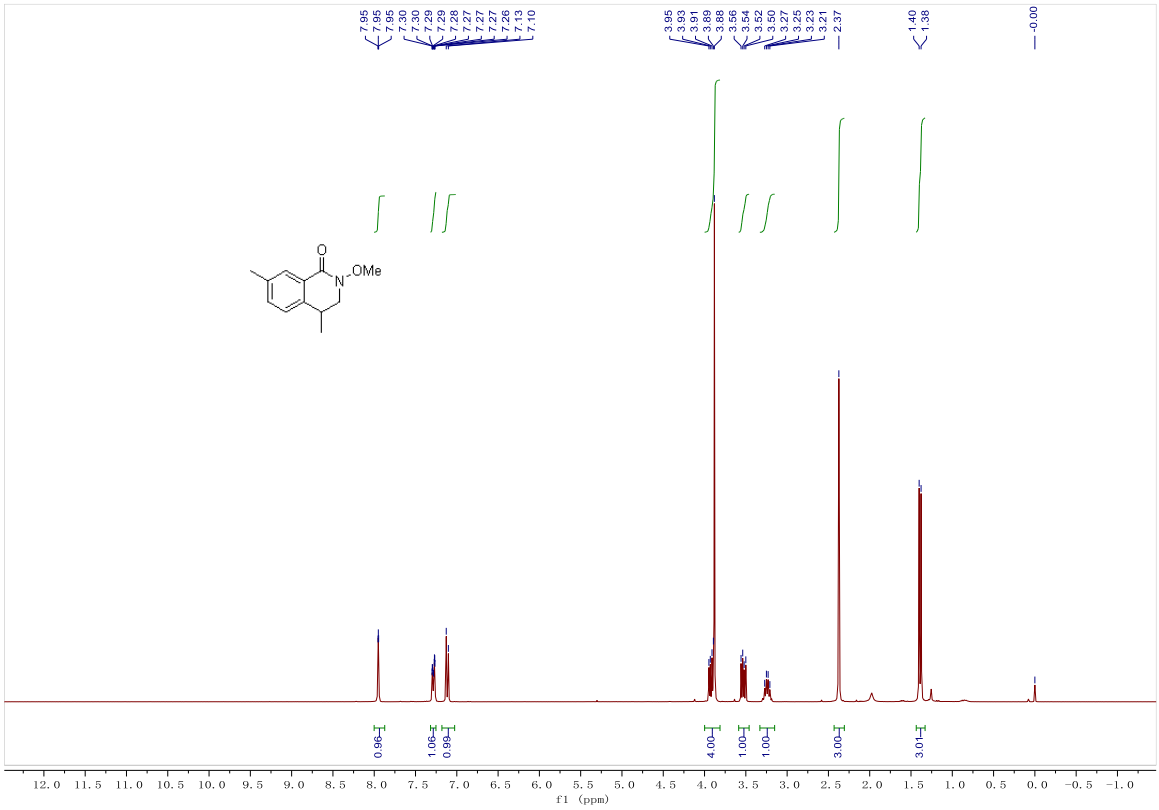

163.18
158.93
140.29
132.47
132.42
129.49
128.73
128.39
127.72
127.53
114.18
77.50
77.07
76.65
61.70
55.30
54.97
44.61
O
N
OMe
OMe
f1 (ppm)

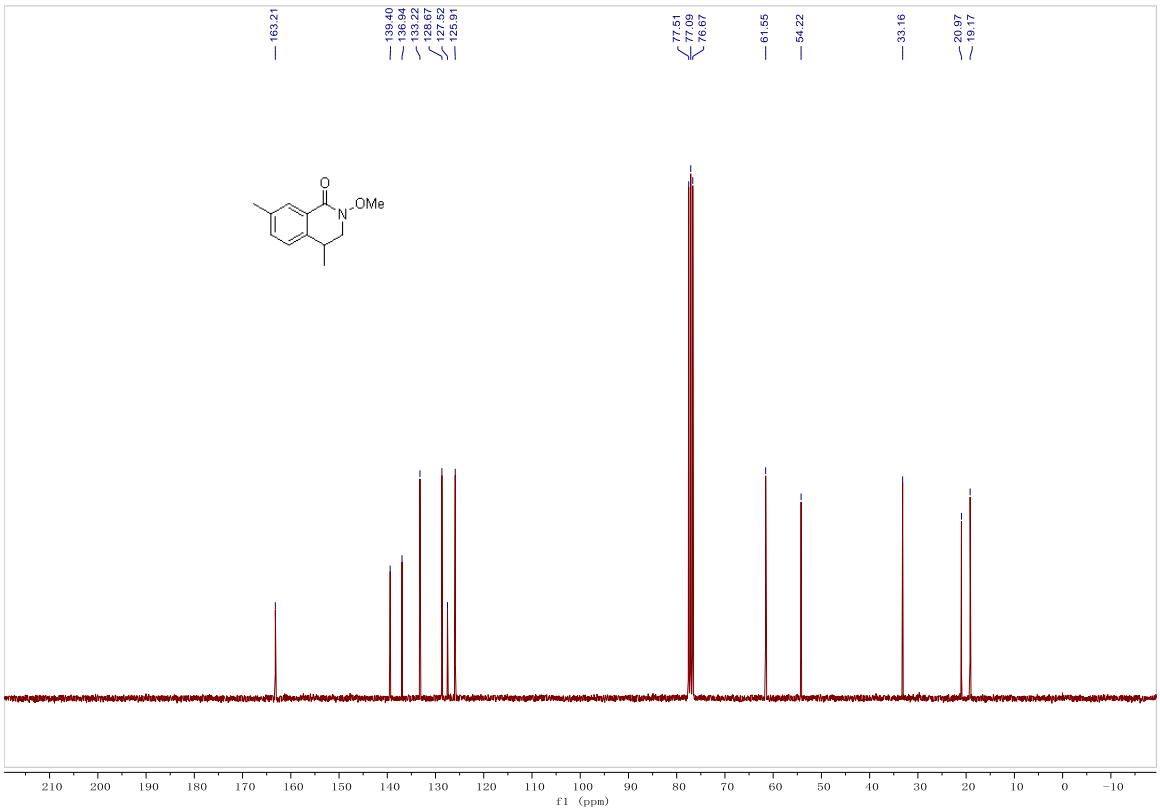

8.03
8.00
7.28
7.17
7.17
7.15
7.14
7.02
3.94
3.93
3.91
3.89
3.88
3.55
3.53
3.51
3.49
3.26
3.23
3.21
3.19
2.39
1.41
1.39
0.00
O
N
OMe
0.96
1.00
1.00
4.00
1.00
1.01
3.00
3.00
f1 (ppm)

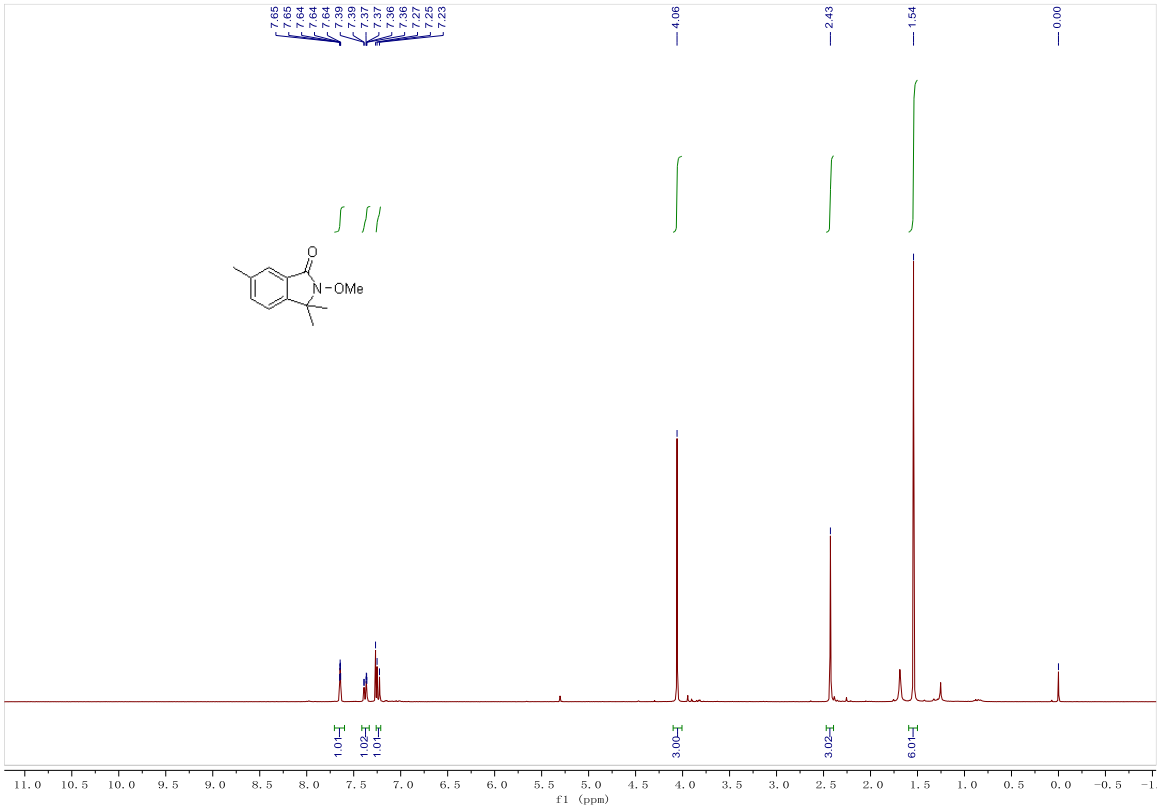

163.34
143.02
142.36
128.47
127.99
126.64
125.10
77.52
77.10
76.68
61.59
54.19
33.52
21.67
19.22
O
N
OMe
f1 (ppm)


7.73
7.70
7.27
7.26
7.23
7.15
4.06
2.46
1.55
0.00
O
N−OMe
0.98
1.02
0.99
3.00
3.00
6.01
f1 (ppm)


164.33
149.12
142.98
129.14
125.70
123.70
121.19
77.47
77.04
76.62
65.30
63.35
25.09
22.12
O
N−OMe
f1 (ppm)


7.95
7.95
7.95
7.30
7.29
7.29
7.28
7.27
7.27
7.27
7.26
7.13
7.10
3.95
3.93
3.91
3.89
3.88
3.56
3.54
3.52
3.50
3.27
3.25
3.23
3.21
2.37
1.40
1.38
-0.00
OMe
0.96
1.06
0.99
4.00
1.00
1.00
3.00
3.01
f1 (ppm)


163.21
139.40
136.94
133.22
128.67
127.52
125.91
77.51
77.09
76.67
61.55
54.22
33.16
20.97
19.17
OMe
f1 (ppm)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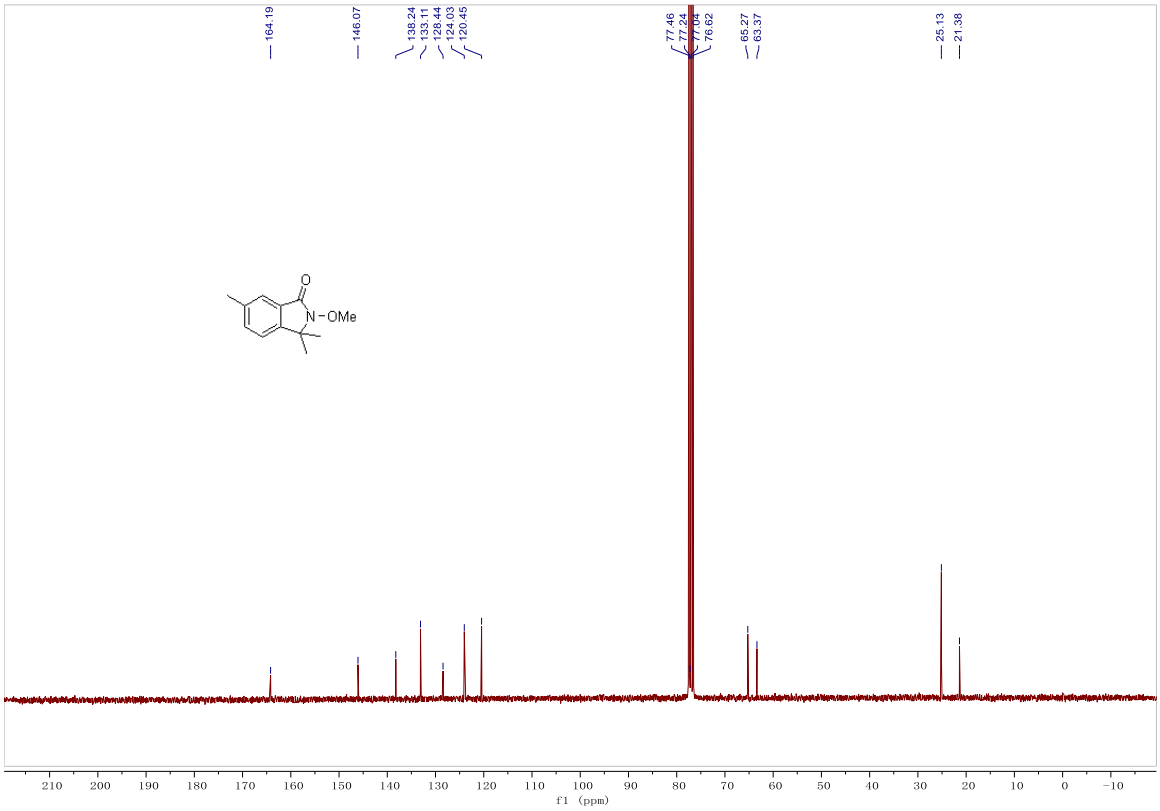
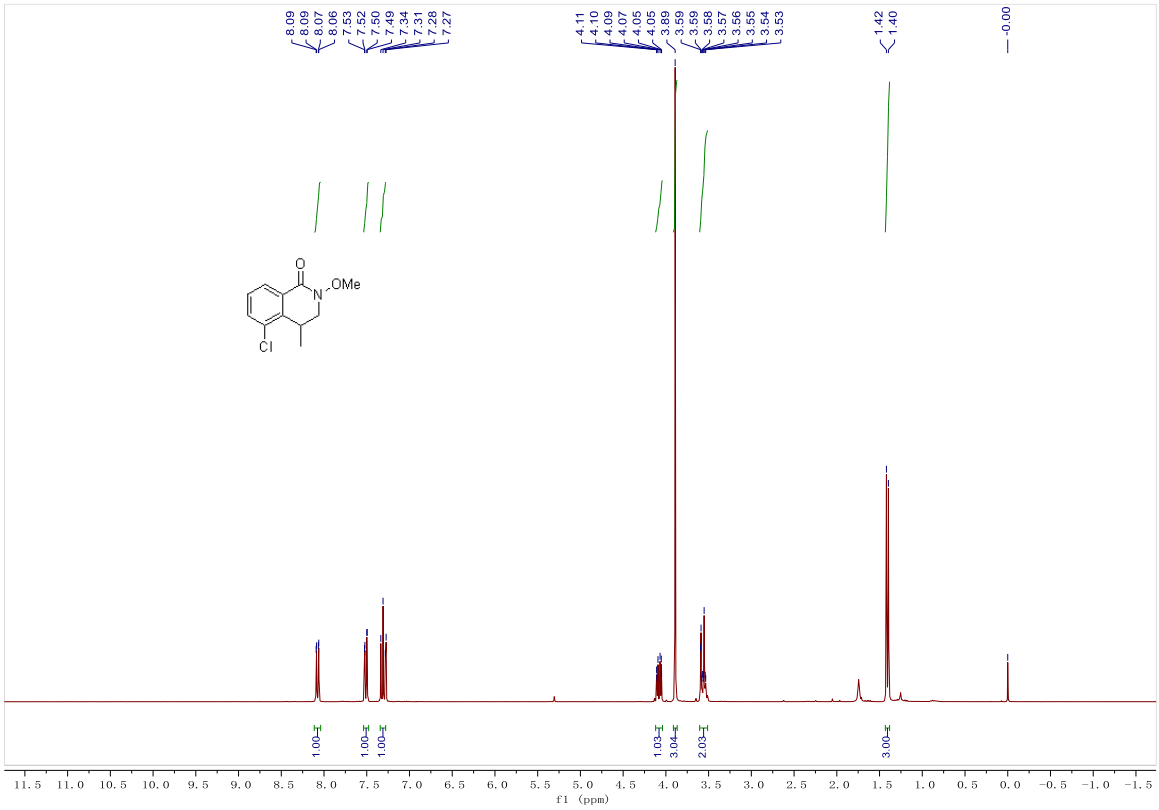
7.65
7.64
7.64
7.64
7.39
7.39
7.37
7.37
7.36
7.36
7.27
7.25
7.23
4.06
2.43
1.54
0.00
O
N-OMe
1.01
1.02
1.01
3.00
3.02
6.01
f1 (ppm)


164.19
146.07
138.24
133.11
128.44
124.03
120.45
77.46
77.24
77.04
76.62
65.27
63.37
25.13
21.38
O
N-OMe
f1 (ppm)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8.09
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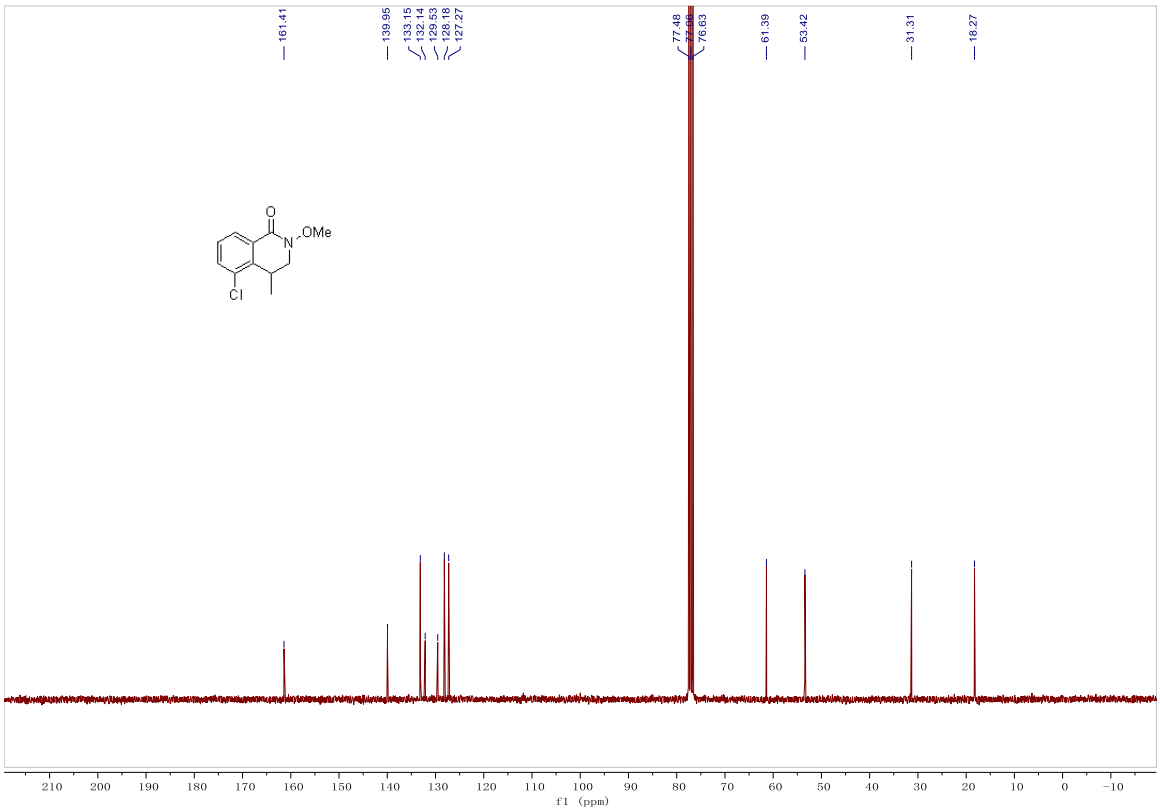
8.06
7.53
7.52
7.50
7.49
7.34
7.31
7.28
7.27
4.11
4.10
4.09
4.07
4.05
4.05
3.89
3.59
3.59
3.58
3.57
3.56
3.55
3.54
3.53
1.42
1.40
-0.00
O
N
OMe
Cl
1.00
1.00
1.00
1.03
3.04
2.03
3.00
f1 (ppm)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139.95
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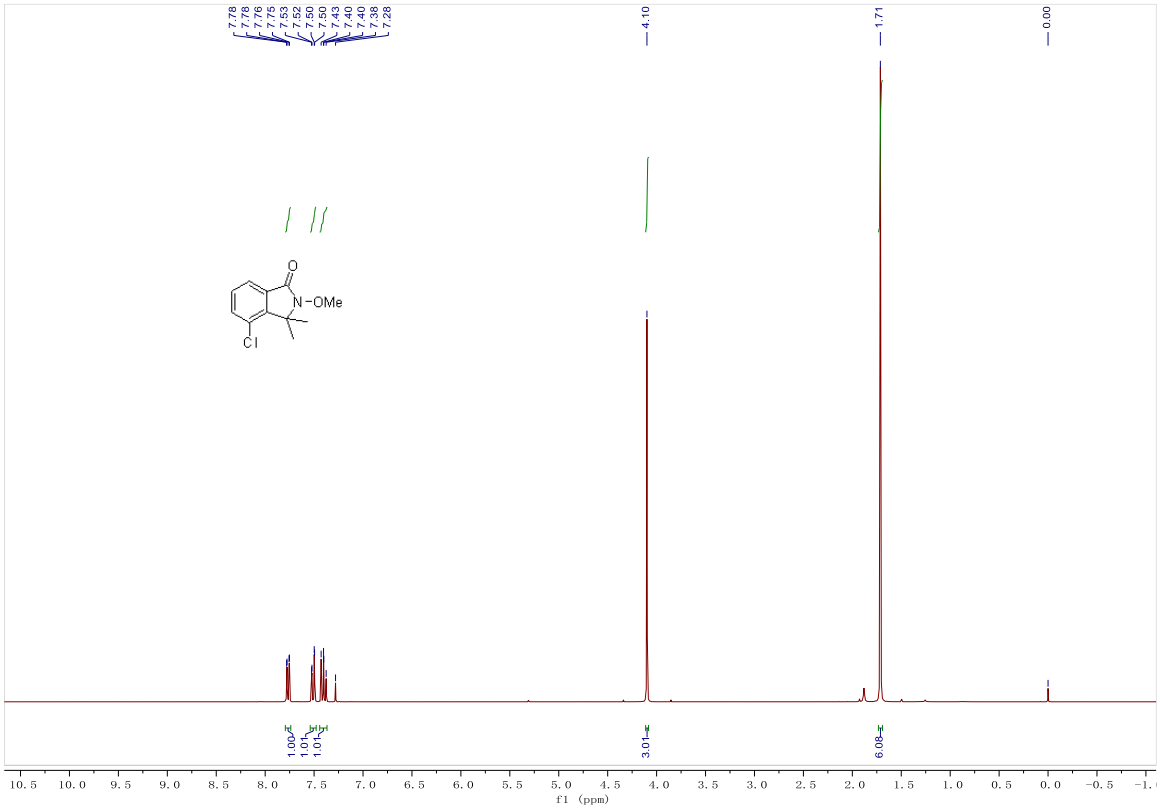
132.14
129.53
128.18
127.27
77.48
77.06
76.63
61.39
53.42
31.31
18.27
O
N
OMe
Cl
f1 (ppm)


7.78
7.78
7.76
7.75
7.53
7.52
7.50
7.50
7.43
7.40
7.40
7.38
7.28
4.10
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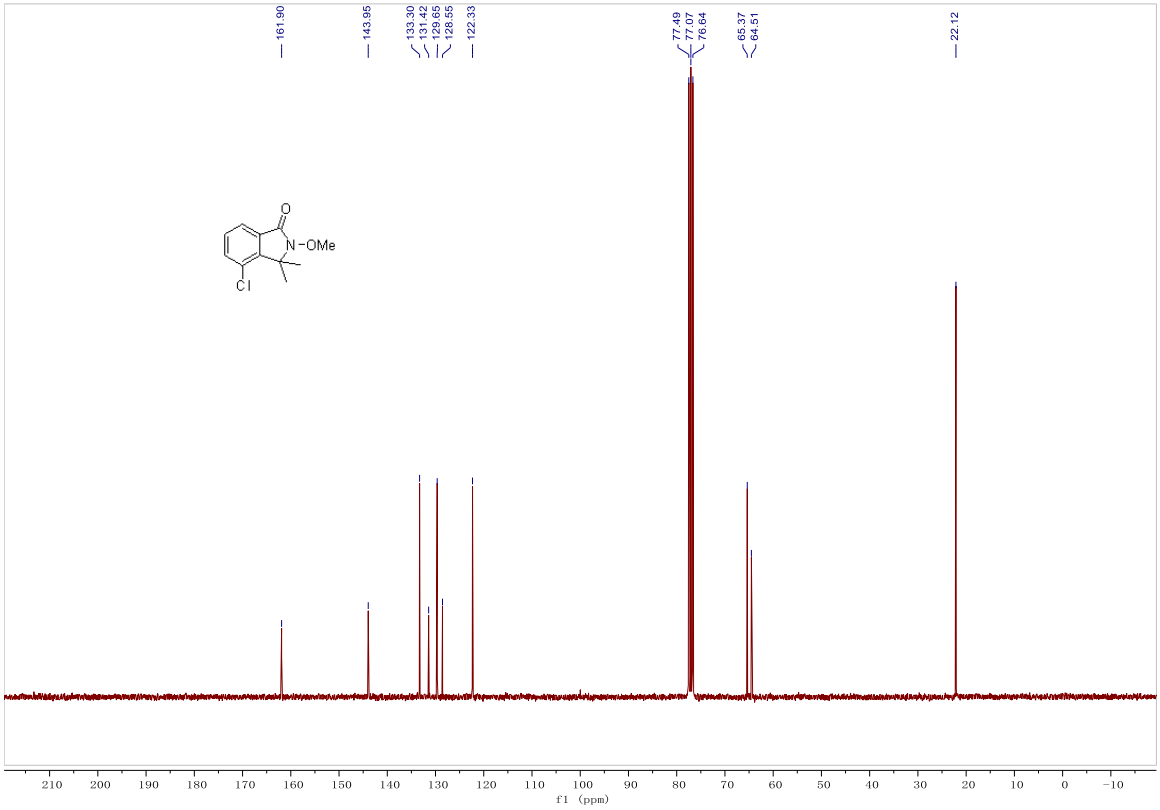
0.00
O
N-OMe
Cl
1.00
1.01
1.01
3.01
6.08
f1 (ppm)


161.90
143.95
133.30
131.42
129.65
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77.07
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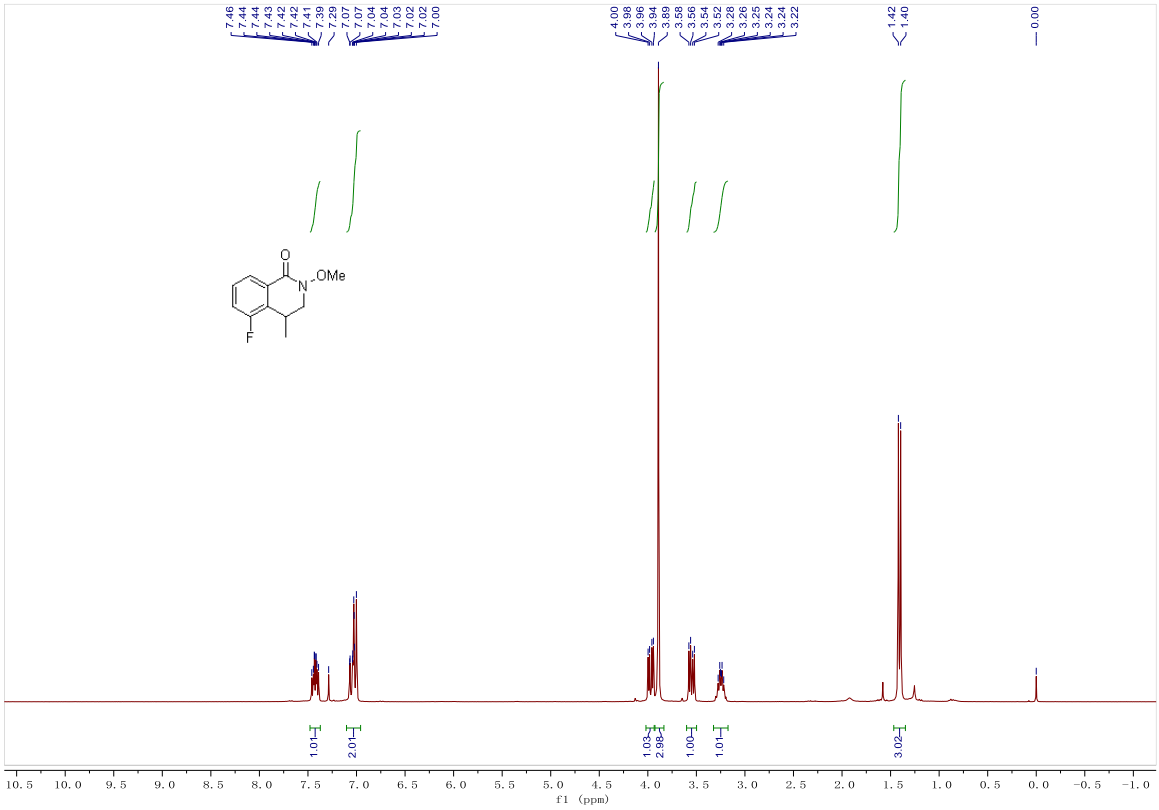
64.51
22.12
O
N-OMe
Cl
f1 (ppm)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7.44
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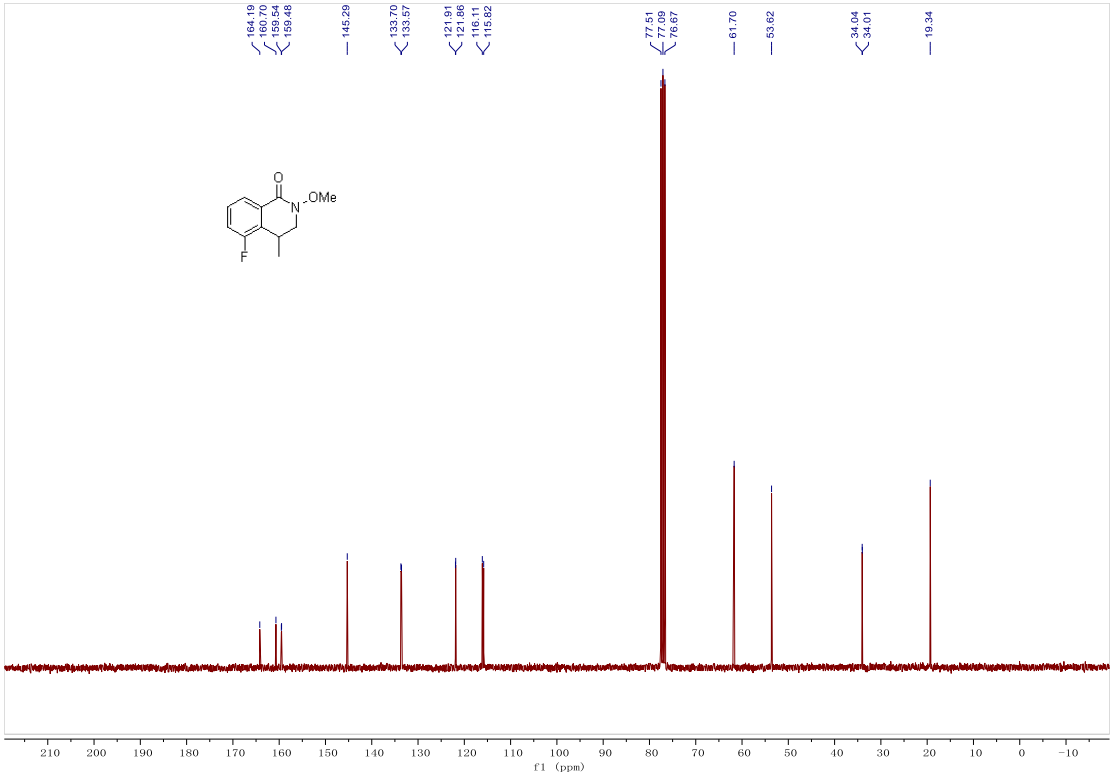
7.42
7.41
7.39
7.29
7.07
7.07
7.04
7.04
7.03
7.02
7.02
7.00
4.00
3.98
3.96
3.94
3.89
3.58
3.56
3.54
3.52
3.28
3.26
3.25
3.24
3.24
3.22
1.42
1.40
0.00
O
N
OMe
F
1.01
2.01
1.03
2.96
1.00
1.01
3.02
f1 (ppm)


164.19
160.70
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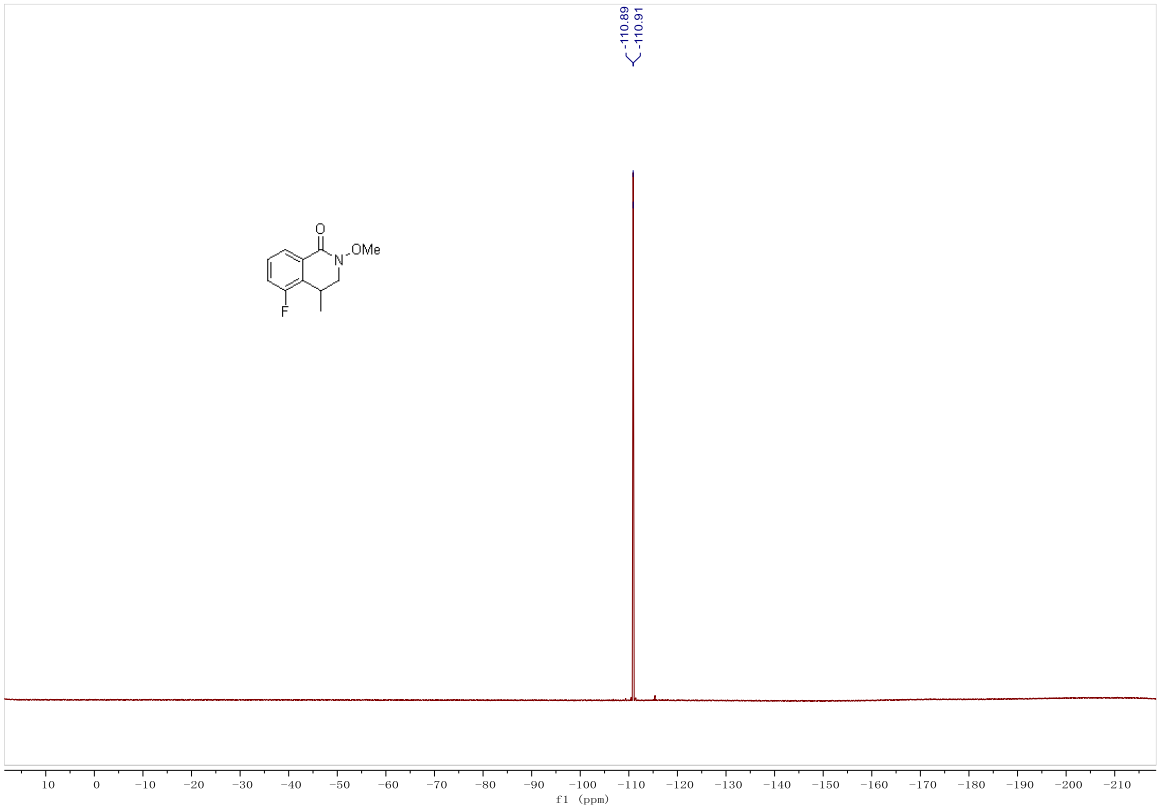
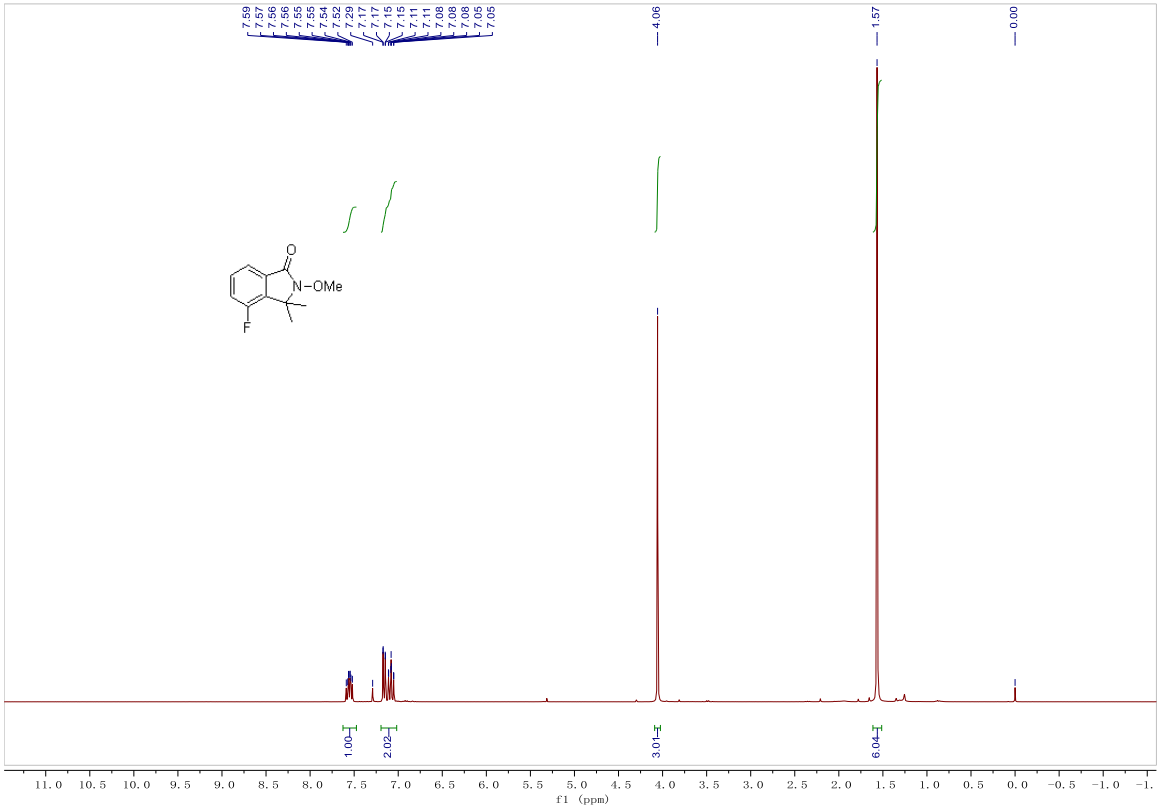
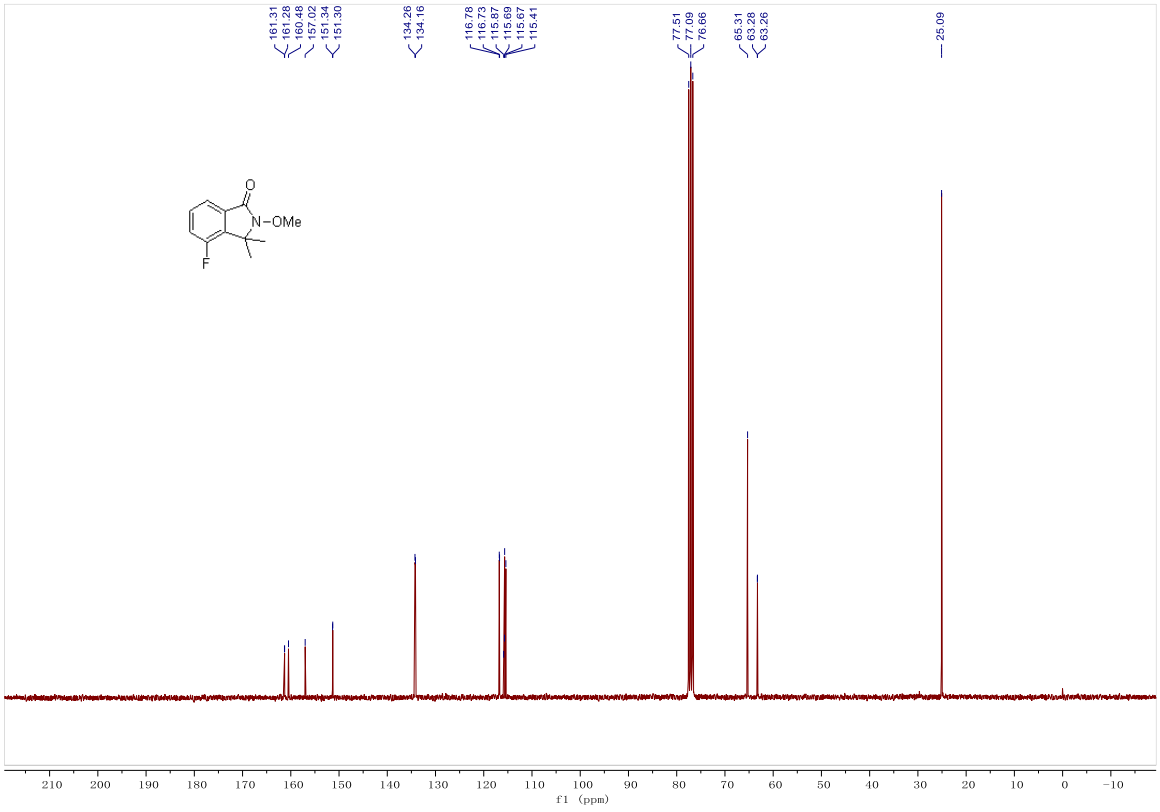
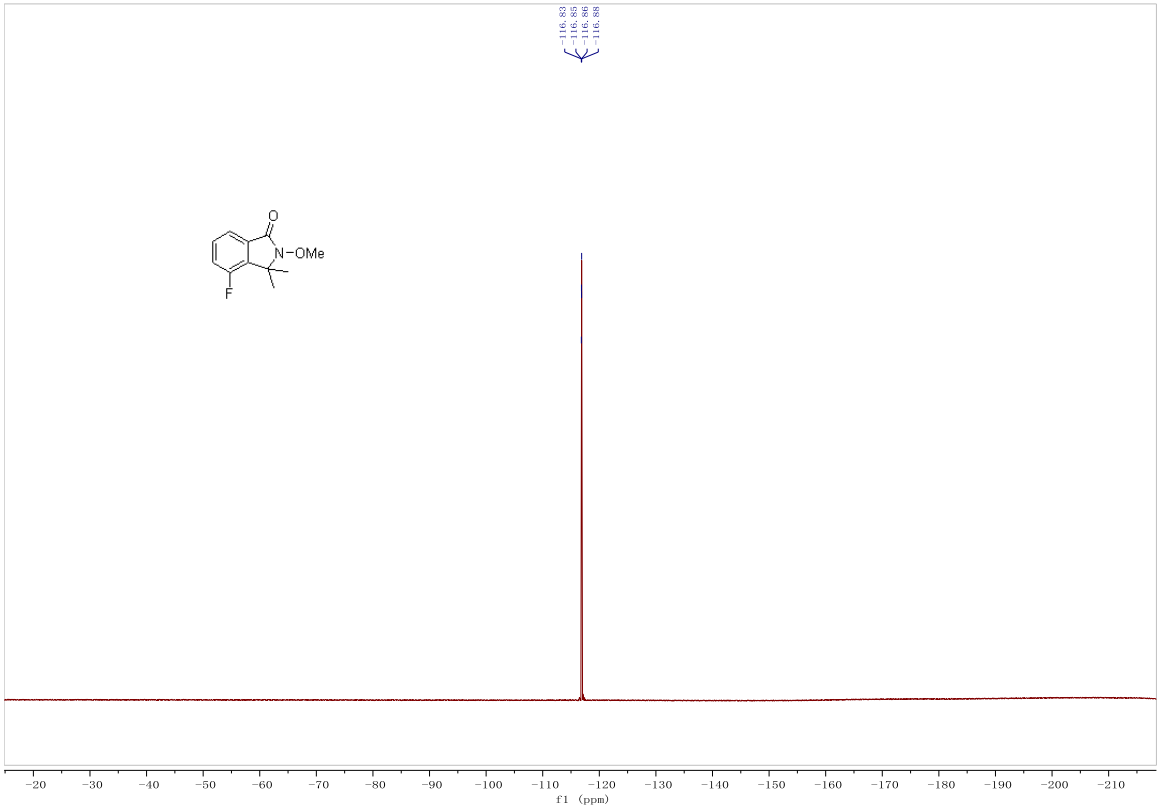
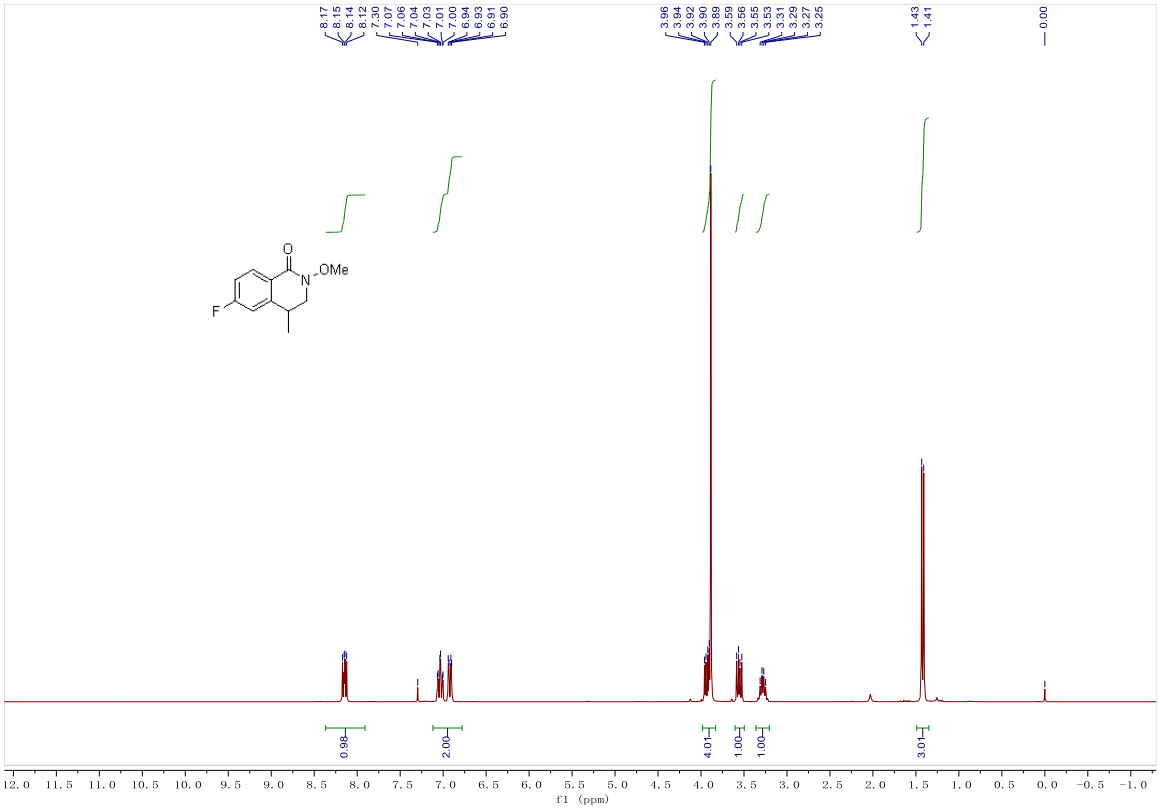
159.48
145.29
133.70
133.57
121.91
121.86
116.11
115.82
77.51
77.09
76.67
61.70
53.62
34.04
34.01
19.34
O
N
OMe
F
f1 (ppm)


-110.89
-110.91
O
N
OMe
F
10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)


7.59
7.57
7.56
7.56
7.55
7.55
7.54
7.52
7.29
7.17
7.17
7.15
7.15
7.11
7.11
7.08
7.08
7.08
7.05
7.05
4.06
1.57
0.00
O
N
OMe
F
1.00
2.02
3.01
6.04
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0 −1.
f1 (ppm)


161.31
161.28
160.48
157.02
151.34
151.30
134.26
134.16
116.78
116.73
115.87
115.69
115.67
115.41
77.51
77.09
76.66
65.31
63.28
63.26
25.09
O
N–OMe
F
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


−116.83
−116.85
−116.86
−116.88
O
N–OMe
F
−20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)


8.17
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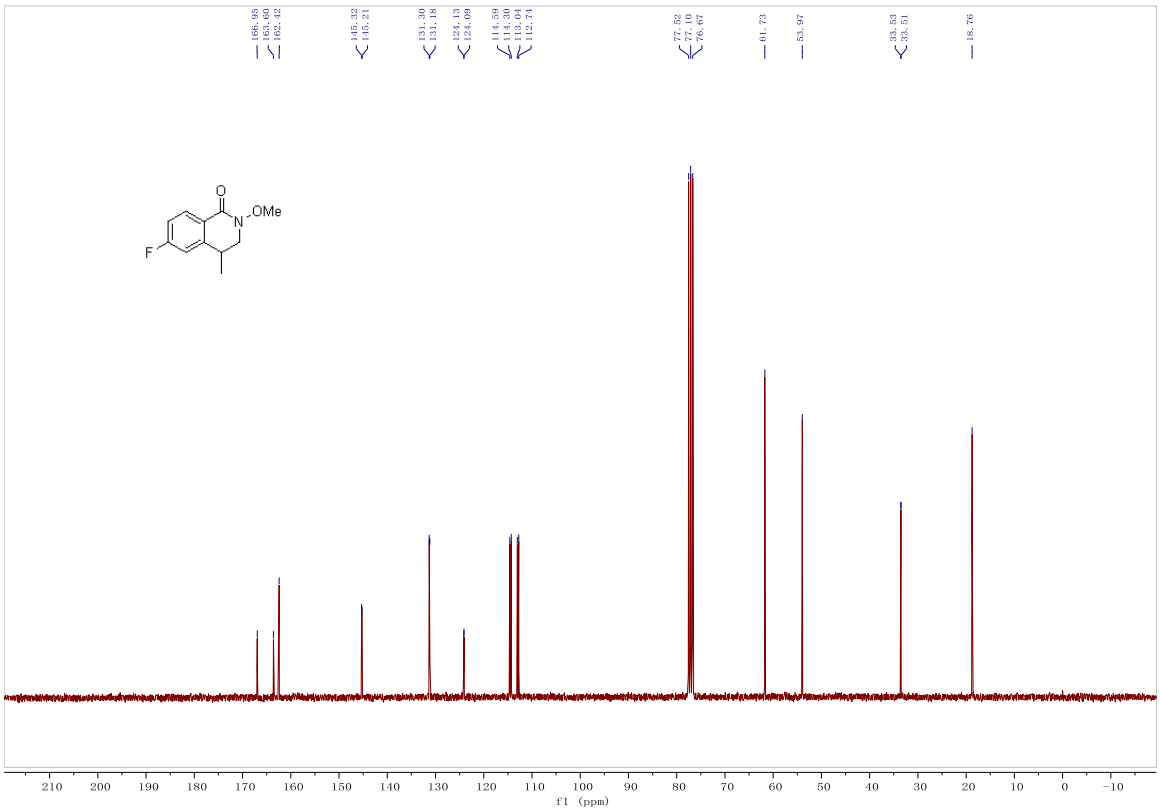
8.14
8.12
7.30
7.07
7.06
7.04
7.03
7.01
7.00
6.94
6.93
6.91
6.90
3.96
3.94
3.92
3.90
3.89
3.59
3.56
3.55
3.53
3.31
3.29
3.27
3.25
1.43
1.41
0.00
O
N
OMe
F
0.98
2.00
4.01
1.00
1.00
3.01
f1 (ppm)


166.95
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131.30
131.18
124.13
124.09
114.59
114.50
113.84
112.74
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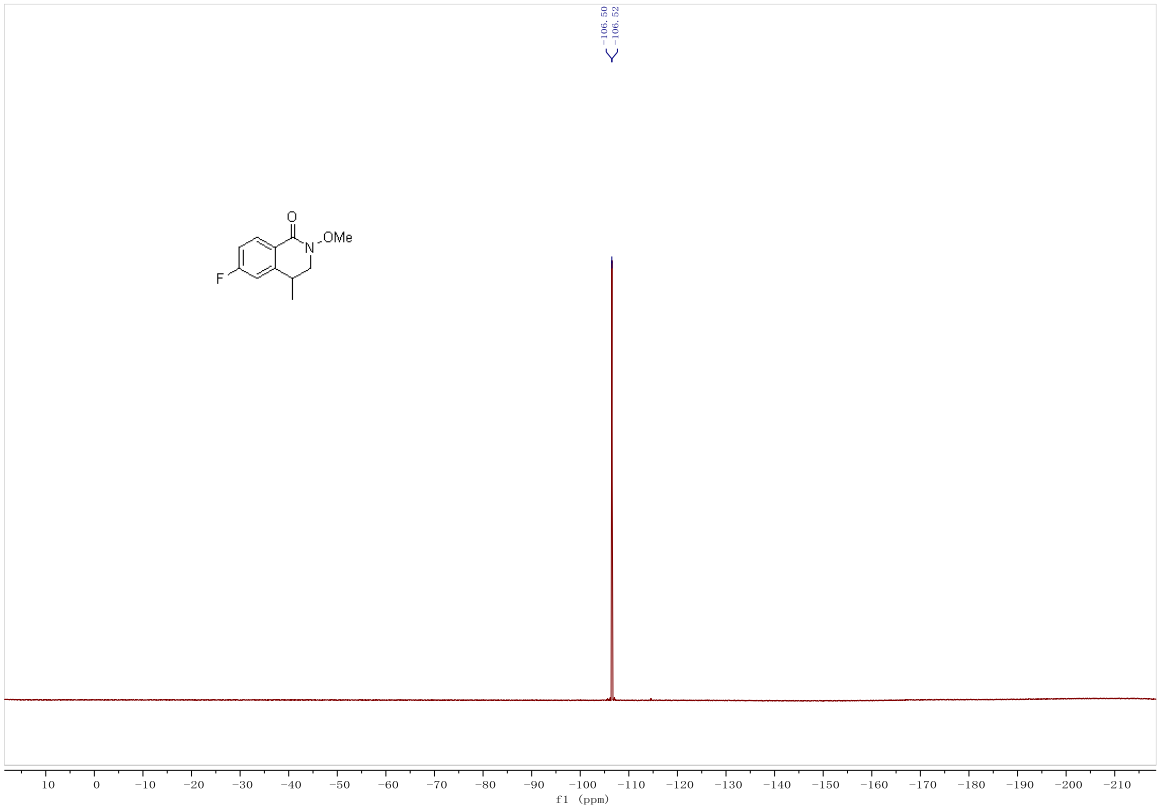
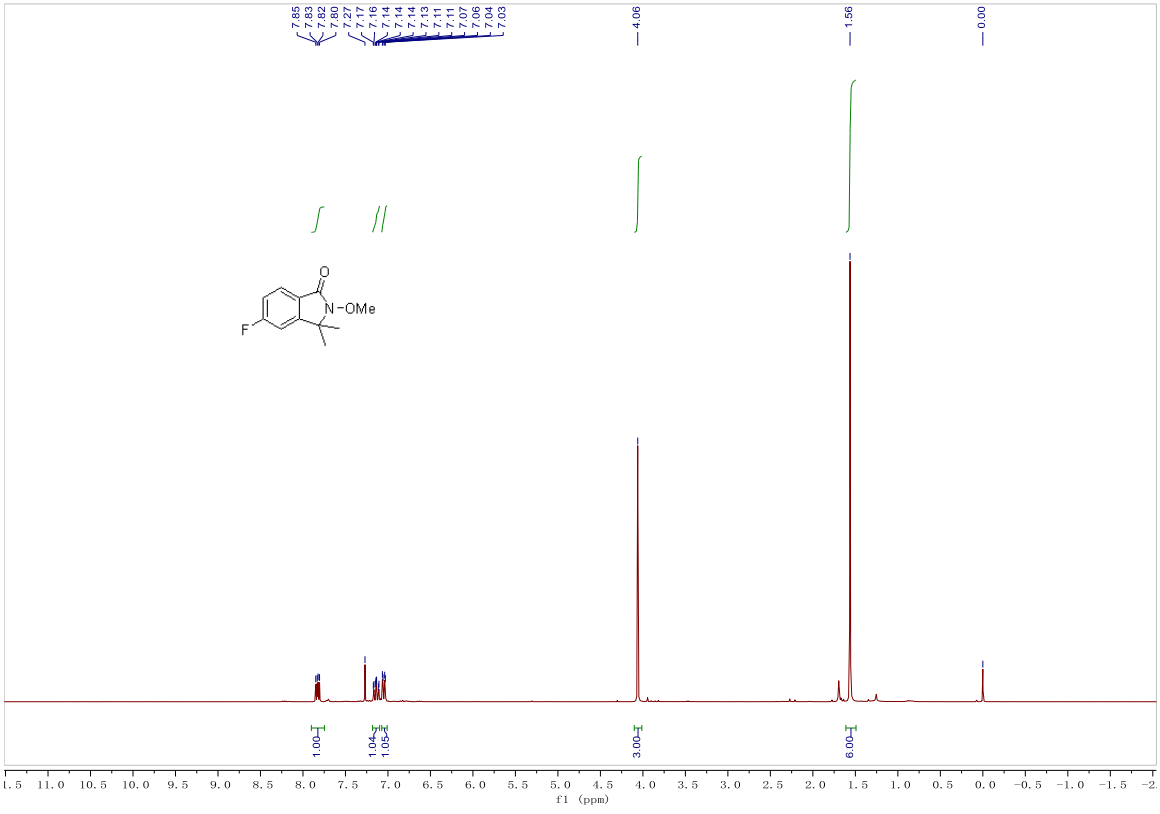
33.51
18.76
O
N
OMe
F
f1 (ppm)


-106.50
-106.52
O
N
OMe
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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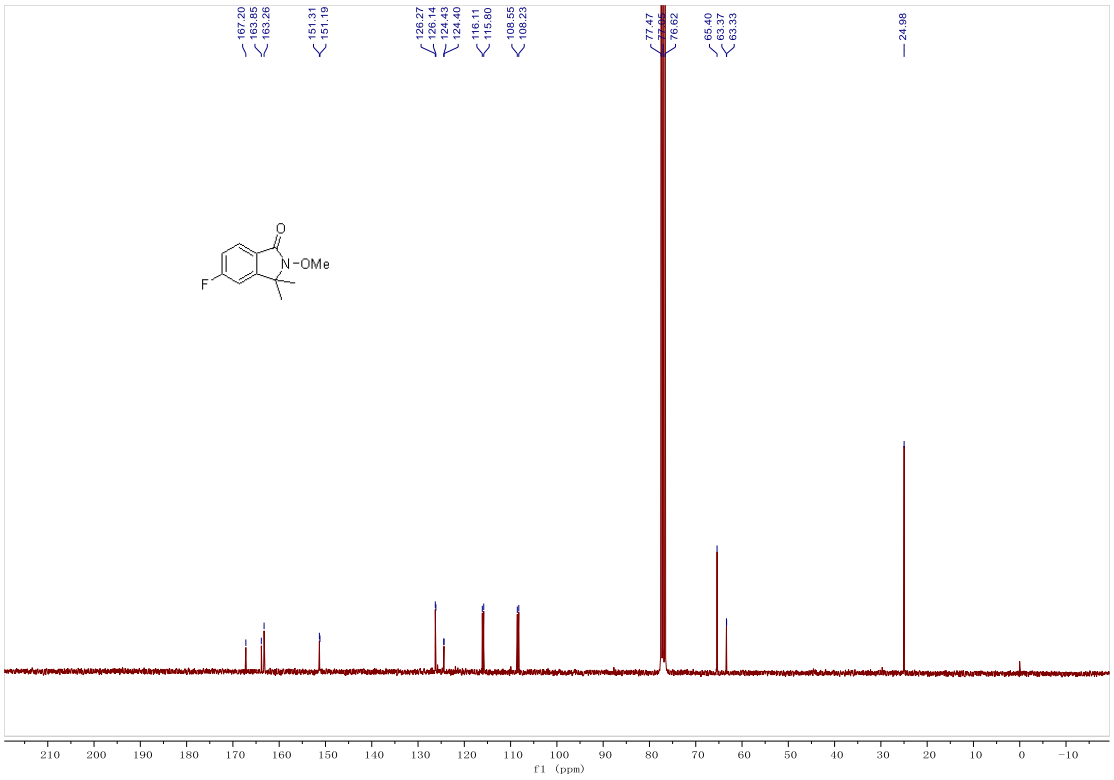
7.14
7.14
7.14
7.13
7.11
7.11
7.07
7.06
7.04
7.03
4.06
1.56
0.00
O
N
OMe
F
1.00
1.04
1.05
3.00
6.00
f1 (ppm)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124.43
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116.11
115.80
108.55
108.23
77.47
77.05
76.62
65.40
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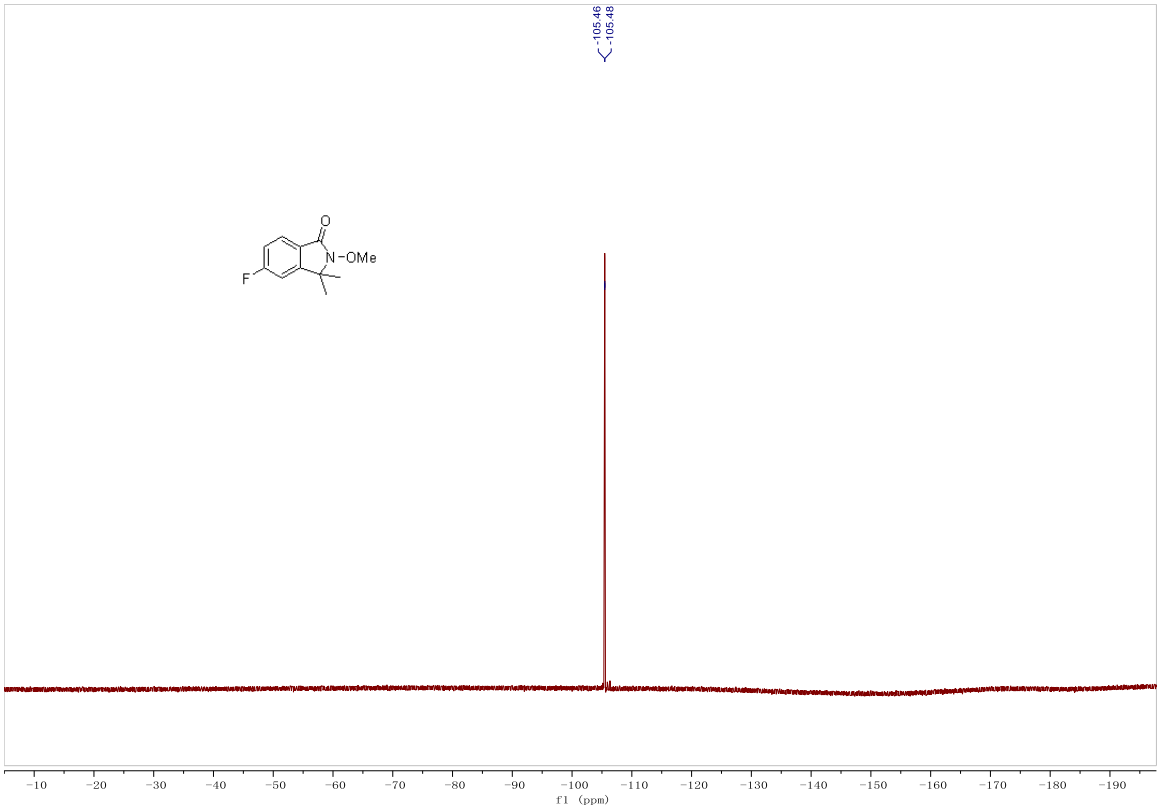
63.33
24.98
O
N-OMe
F
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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-105.48
O
N-OMe
F
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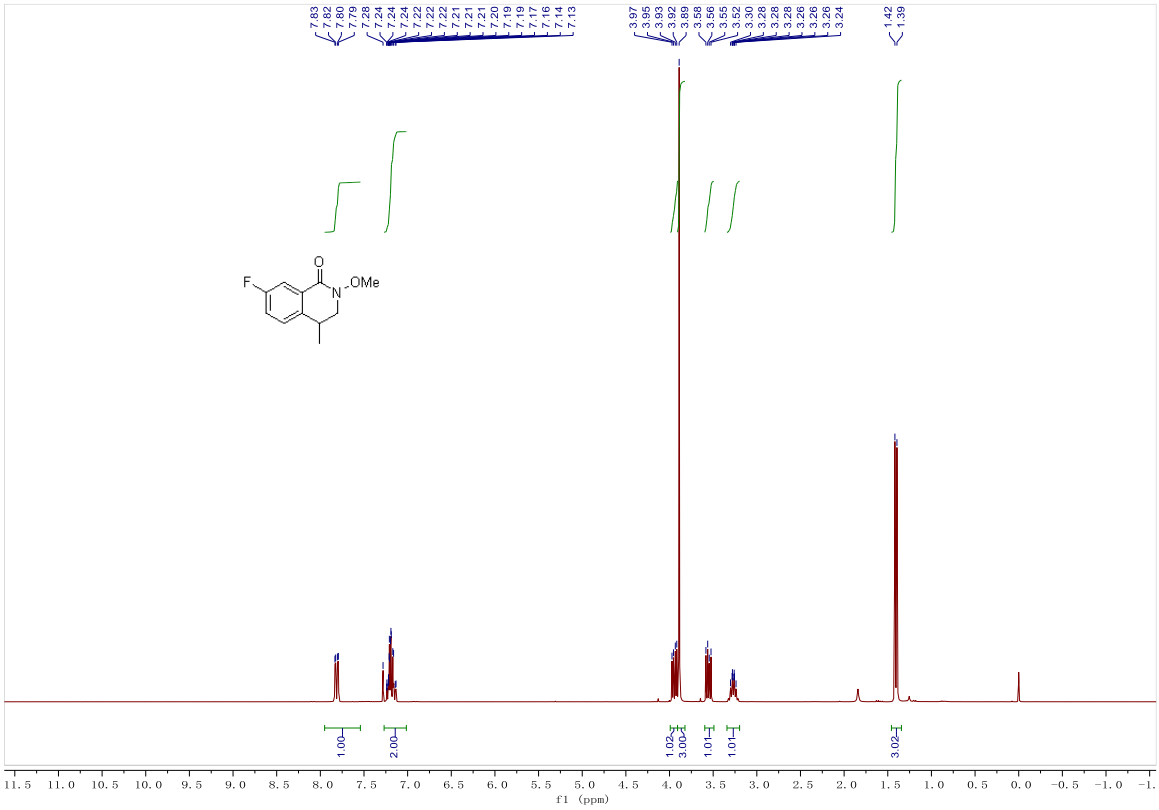
f1 (ppm)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7.80
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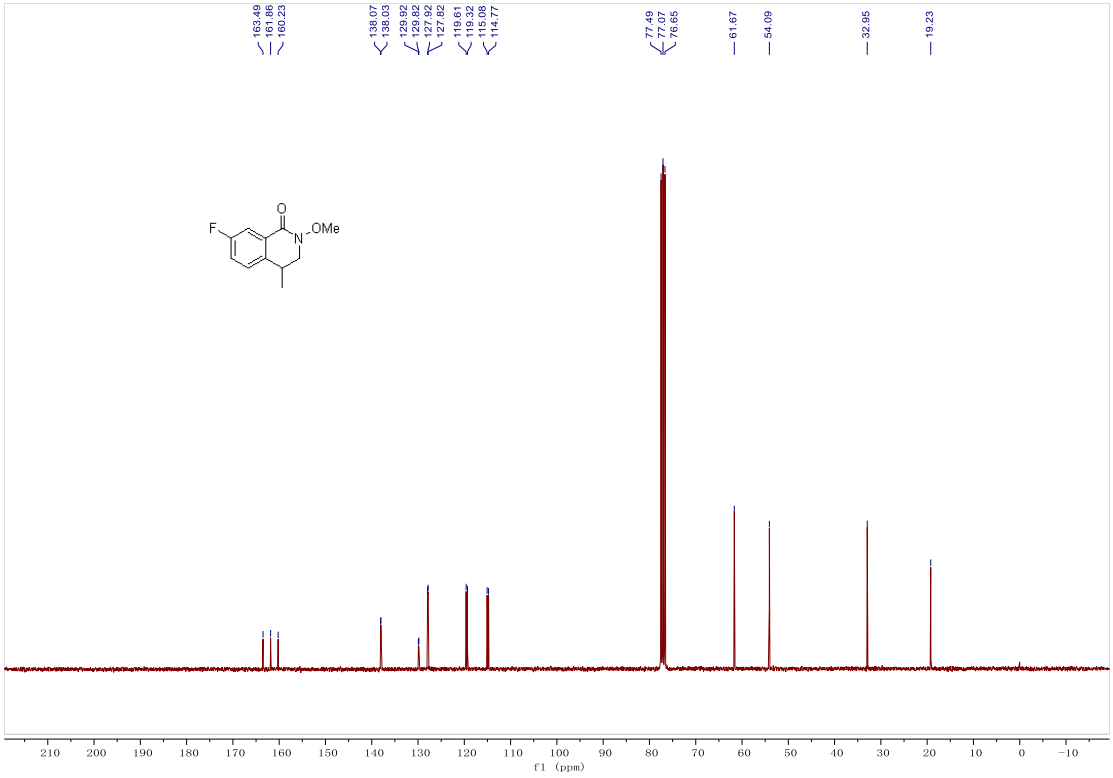
7.21
7.20
7.19
7.19
7.17
7.16
7.14
7.13
3.97
3.95
3.93
3.92
3.89
3.58
3.56
3.55
3.52
3.30
3.28
3.28
3.26
3.26
3.26
3.24
1.42
1.39
F
O
N
OMe
1.00
2.00
1.02
3.00
1.01
1.01
3.02
f1 (ppm)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138.03
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129.82
127.92
127.82
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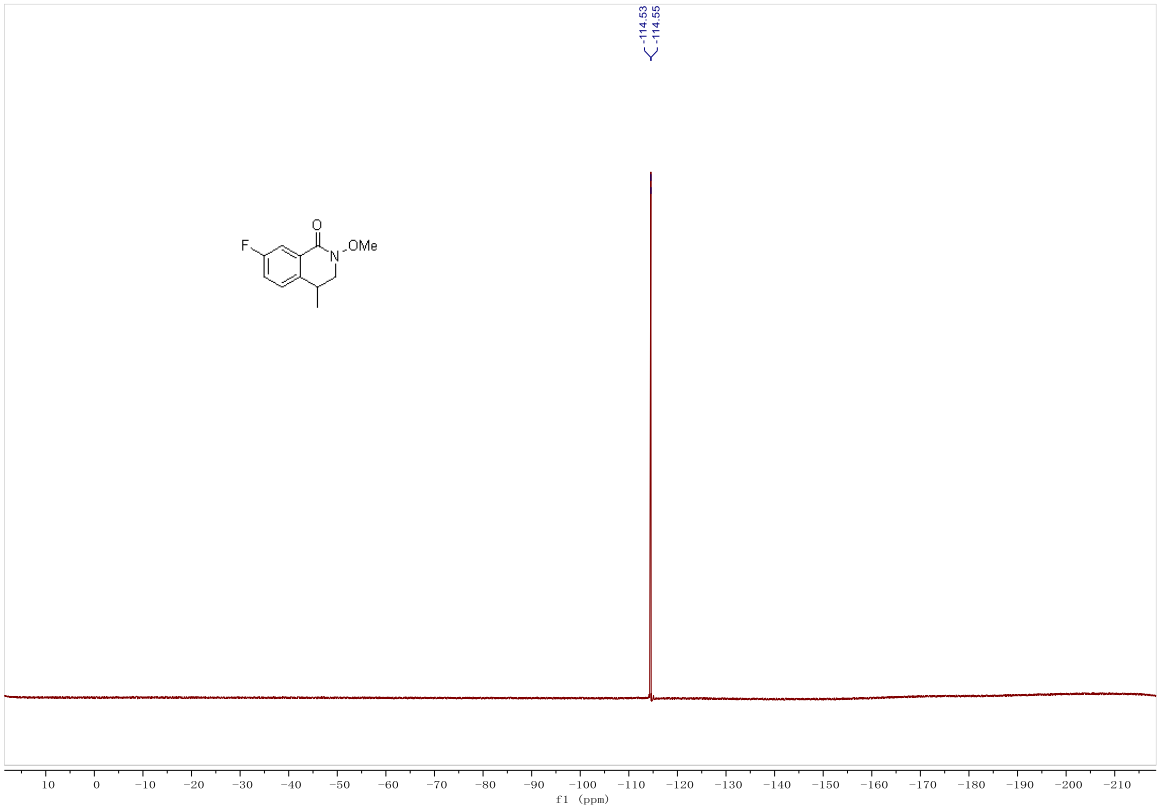
119.32
115.08
114.77
77.49
77.07
76.65
61.67
54.09
32.95
19.23
F
O
N
OMe
f1 (ppm)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-114.55
F
O
N
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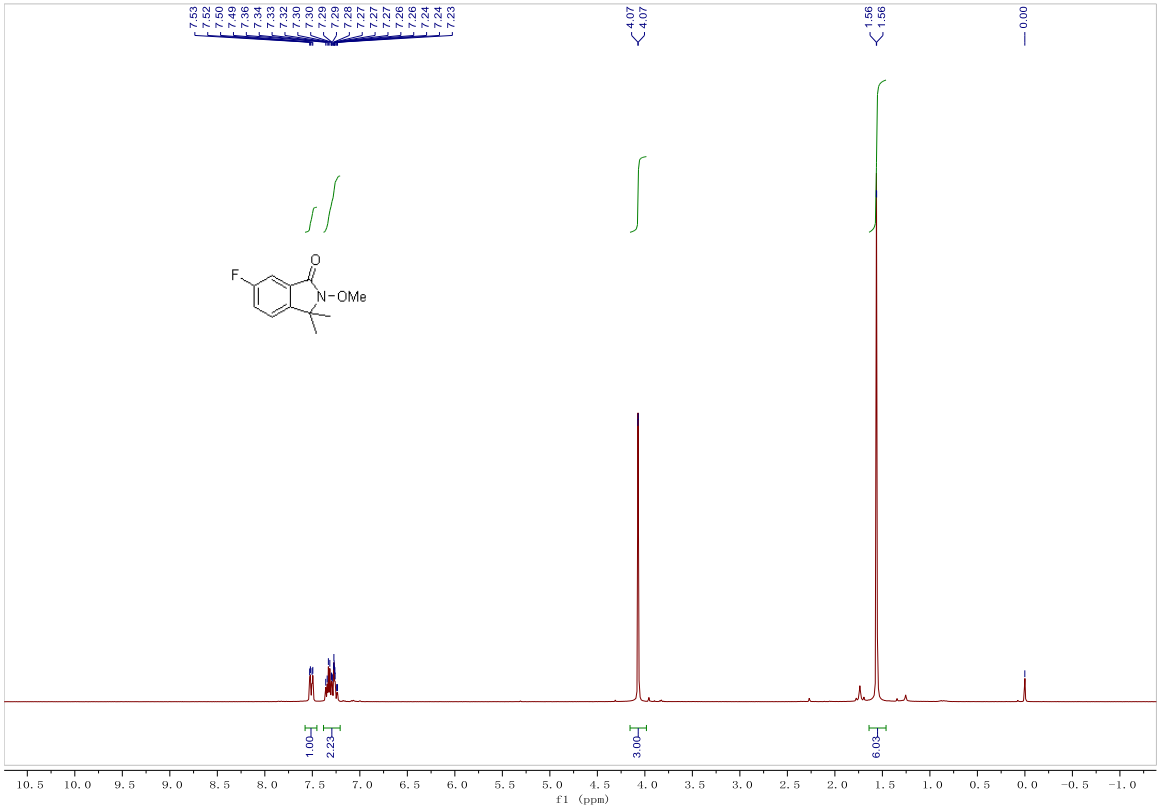
f1 (ppm)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7.36
7.34
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7.32
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7.30
7.29
7.29
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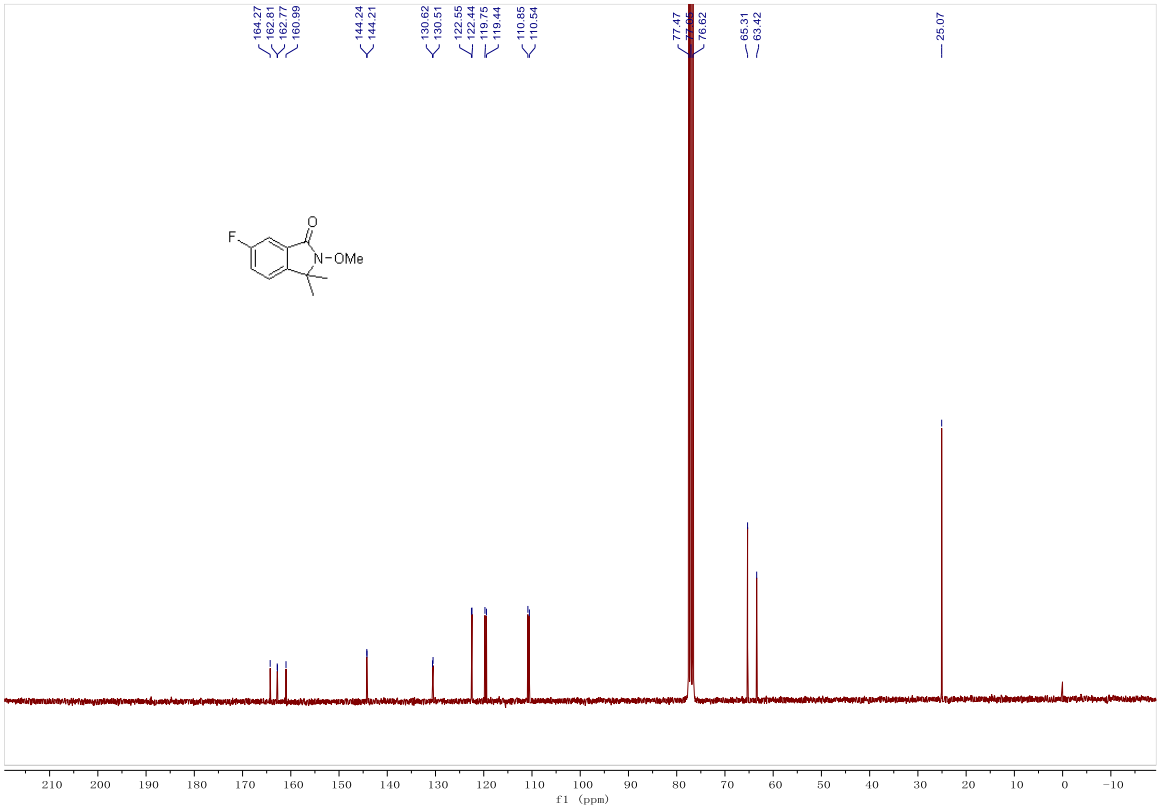
7.27
7.27
7.27
7.26
7.26
7.24
7.24
7.23
4.07
4.07
1.56
1.56
0.00
F
O
N-OMe
1.00
2.23
3.00
6.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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162.77
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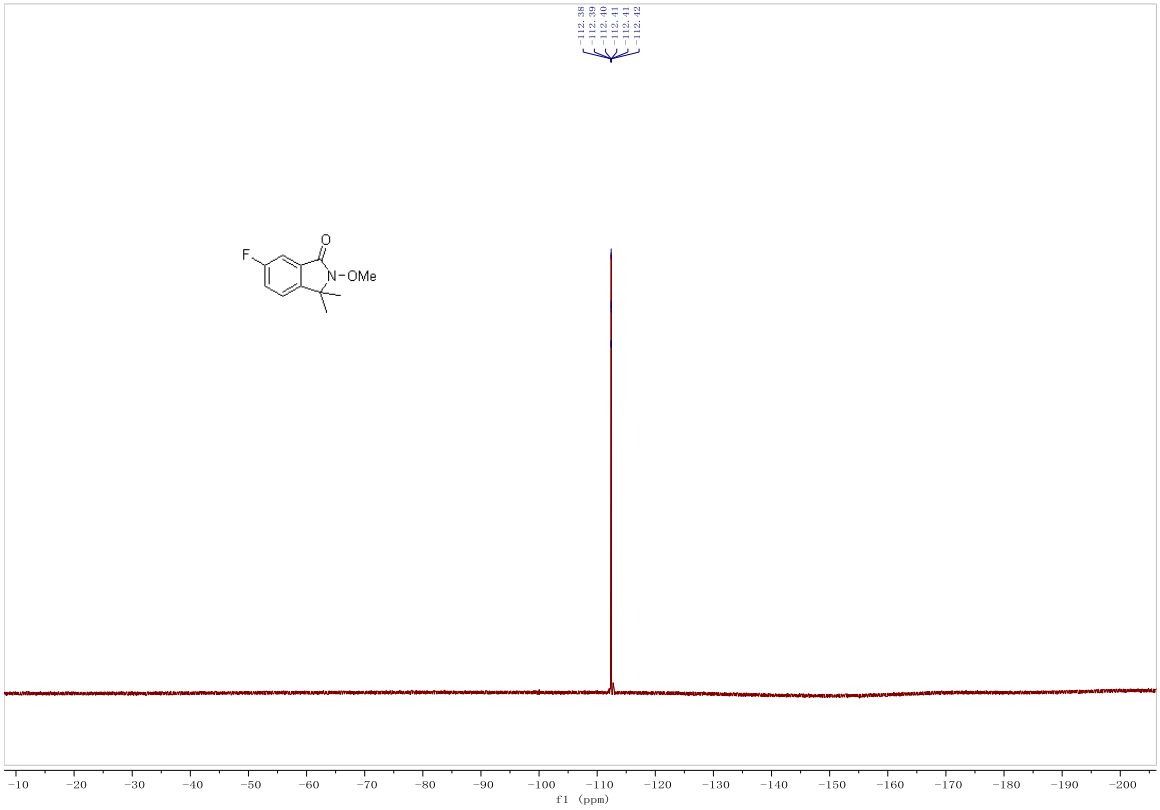
144.21
130.62
130.51
122.55
122.44
119.75
119.44
110.85
110.54
77.47
77.05
76.62
65.31
63.42
25.07
F
O
N−OMe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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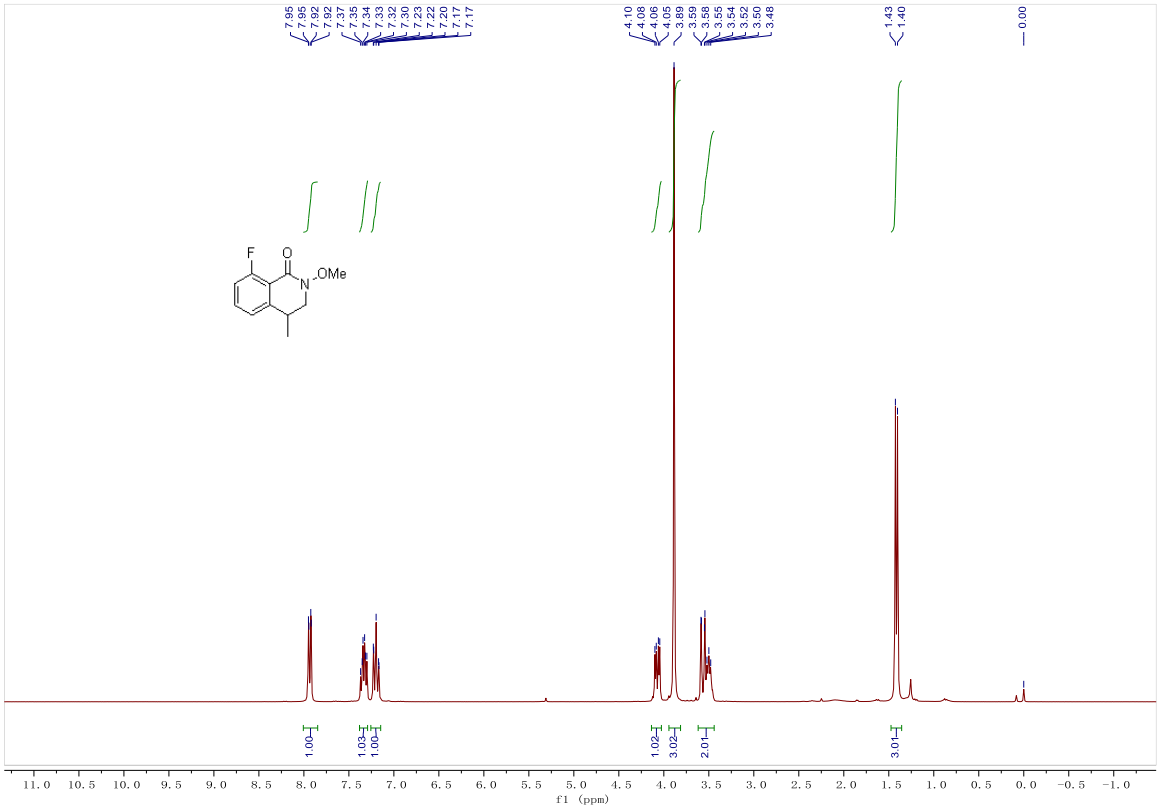
−112.39
−112.40
−112.41
−112.41
−112.42
F
O
N−OMe
−10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200
f1 (ppm)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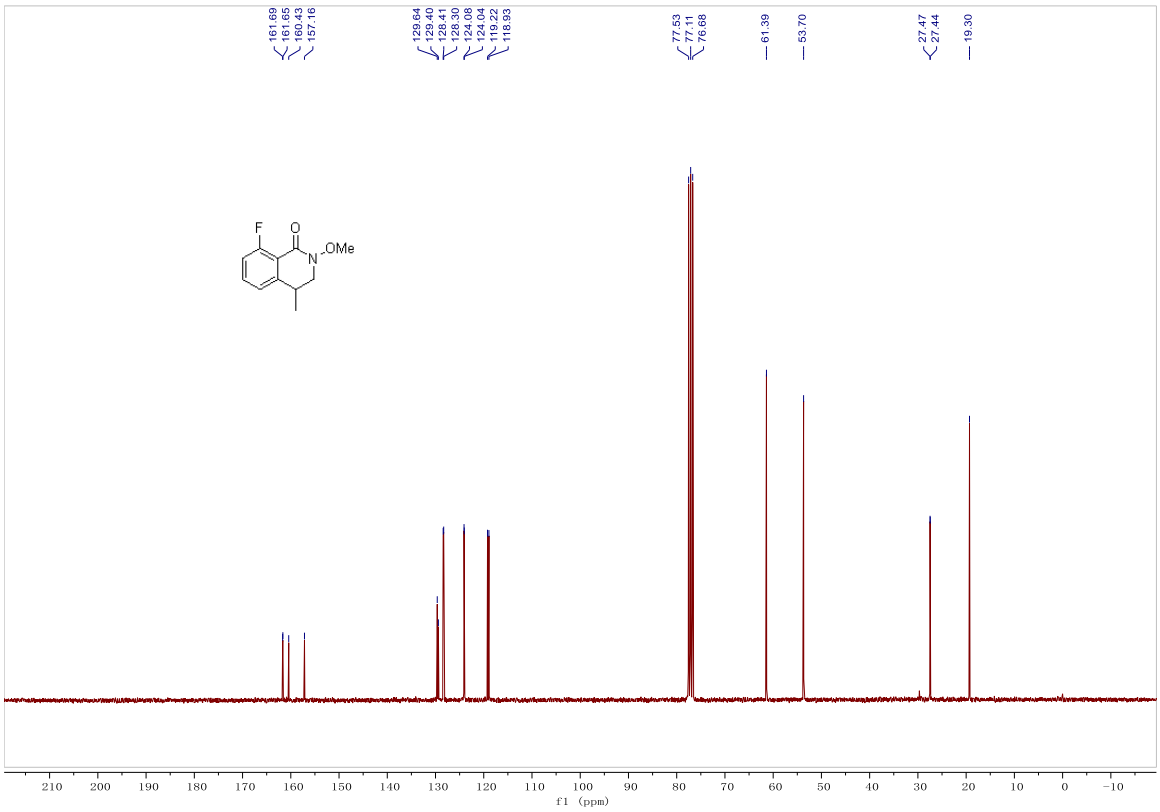
7.95
7.92
7.92
7.37
7.35
7.34
7.33
7.32
7.30
7.23
7.22
7.20
7.17
7.17
4.10
4.08
4.06
4.05
3.89
3.59
3.58
3.55
3.54
3.52
3.50
3.48
1.43
1.40
0.00
F
O
N
OMe
1.00
1.03
1.00
1.02
3.02
2.01
3.01
f1 (ppm)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161.65
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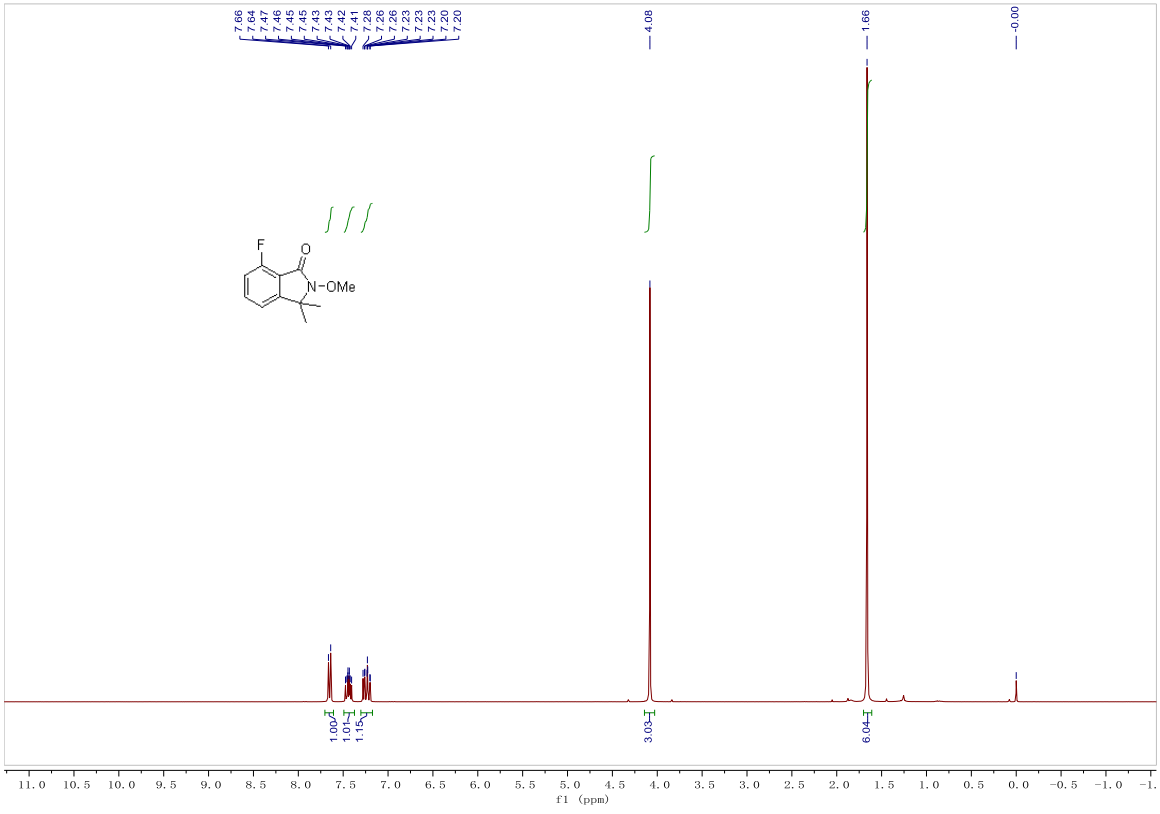
129.40
128.41
128.30
124.08
124.04
119.22
118.93
77.53
77.11
76.68
61.39
53.70
27.47
27.44
19.30
F
O
N
OMe
f1 (ppm)


-121.25
-121.27
-121.29
-121.31
F
O
N
OMe
-20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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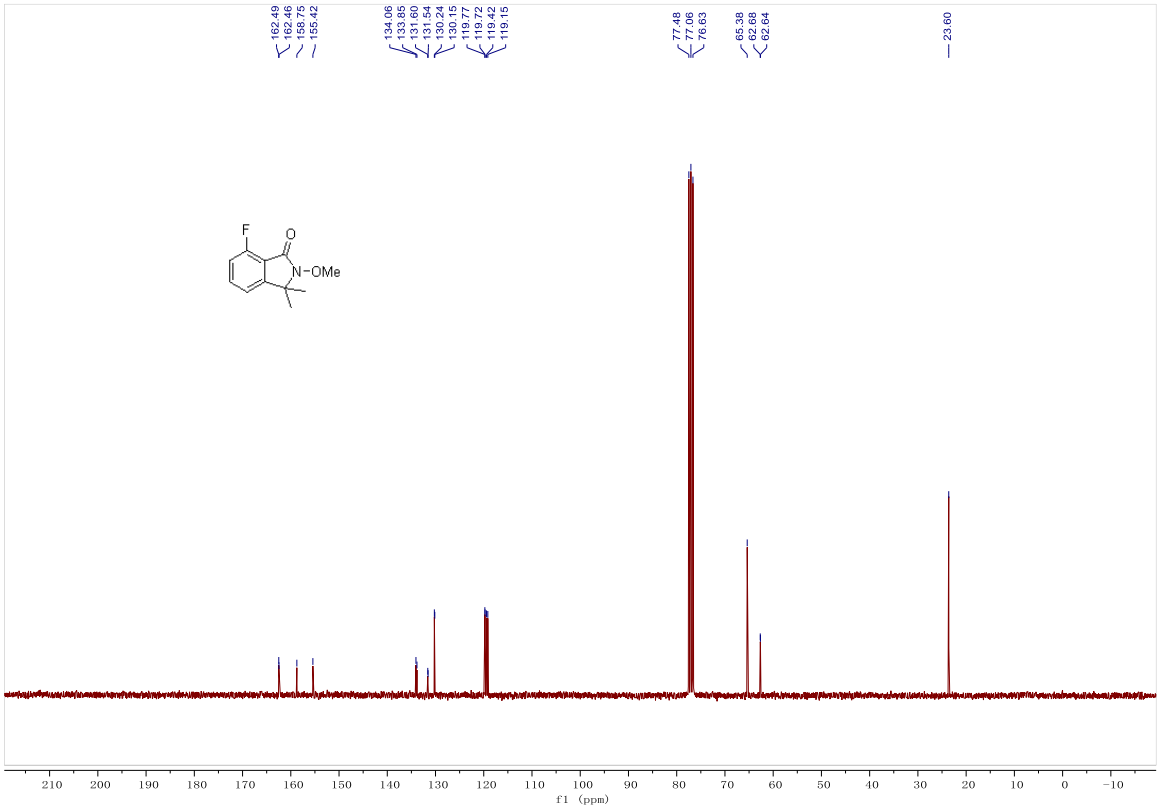
7.45
7.45
7.43
7.43
7.42
7.41
7.28
7.26
7.26
7.23
7.23
7.23
7.20
7.20
4.08
1.66
0.00
F
O
N-OMe
1.00
1.01
1.15
3.03
6.04
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.
f1 (ppm)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162.46
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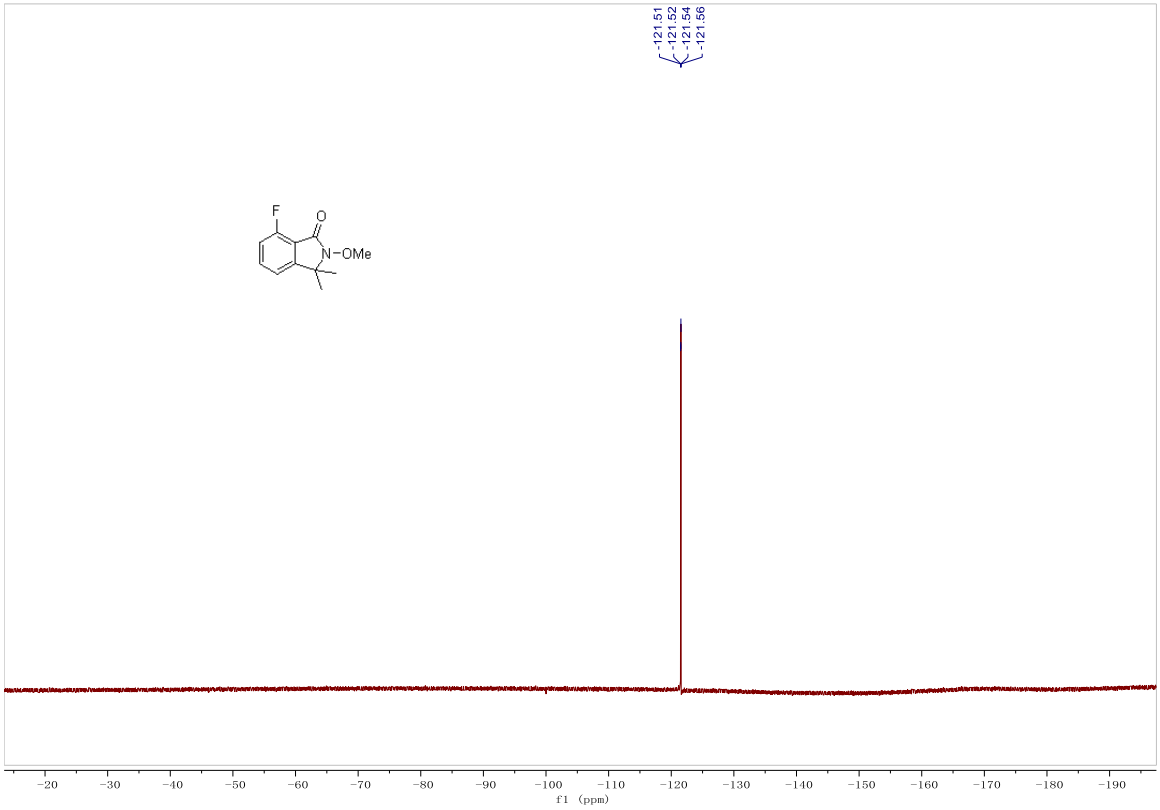
134.06
133.85
131.60
131.54
130.24
130.15
119.77
119.72
119.42
119.15
77.48
77.06
76.63
65.38
62.68
62.64
23.60
F
O
N-OMe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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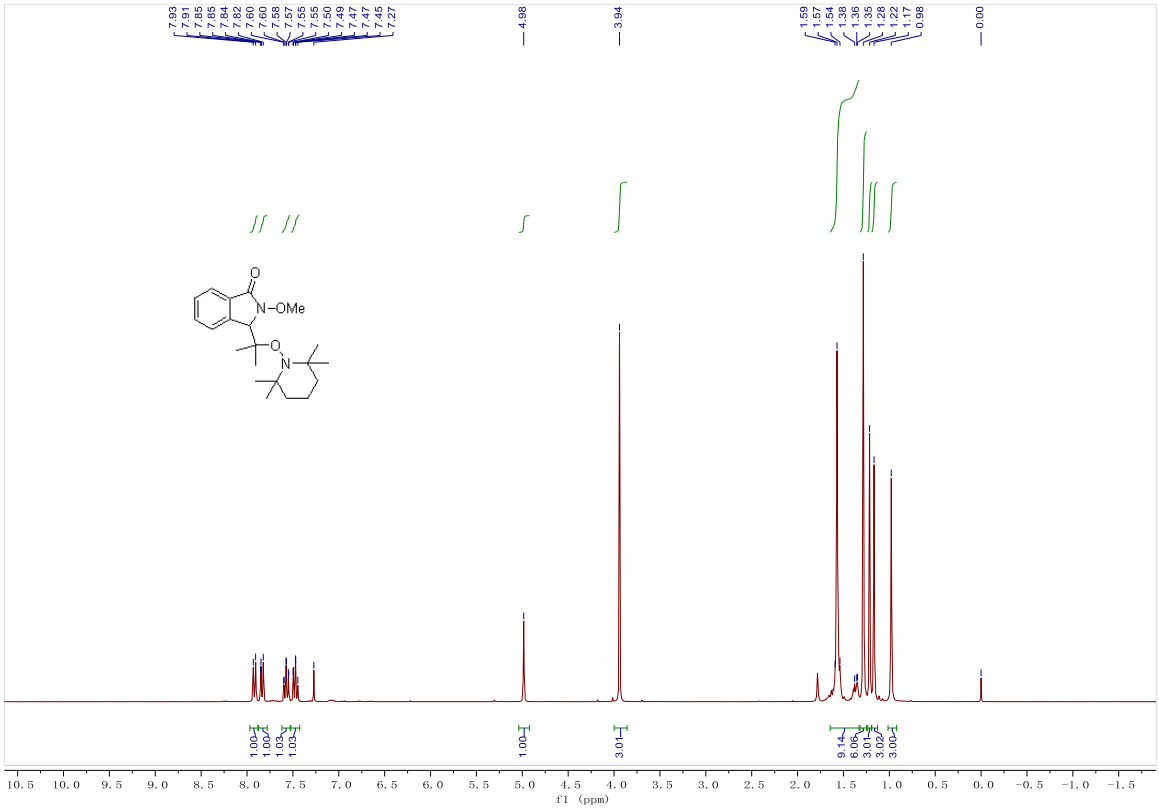
-121.52
-121.54
-121.56
F
O
N-OMe
-20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm)


7.93
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7.85
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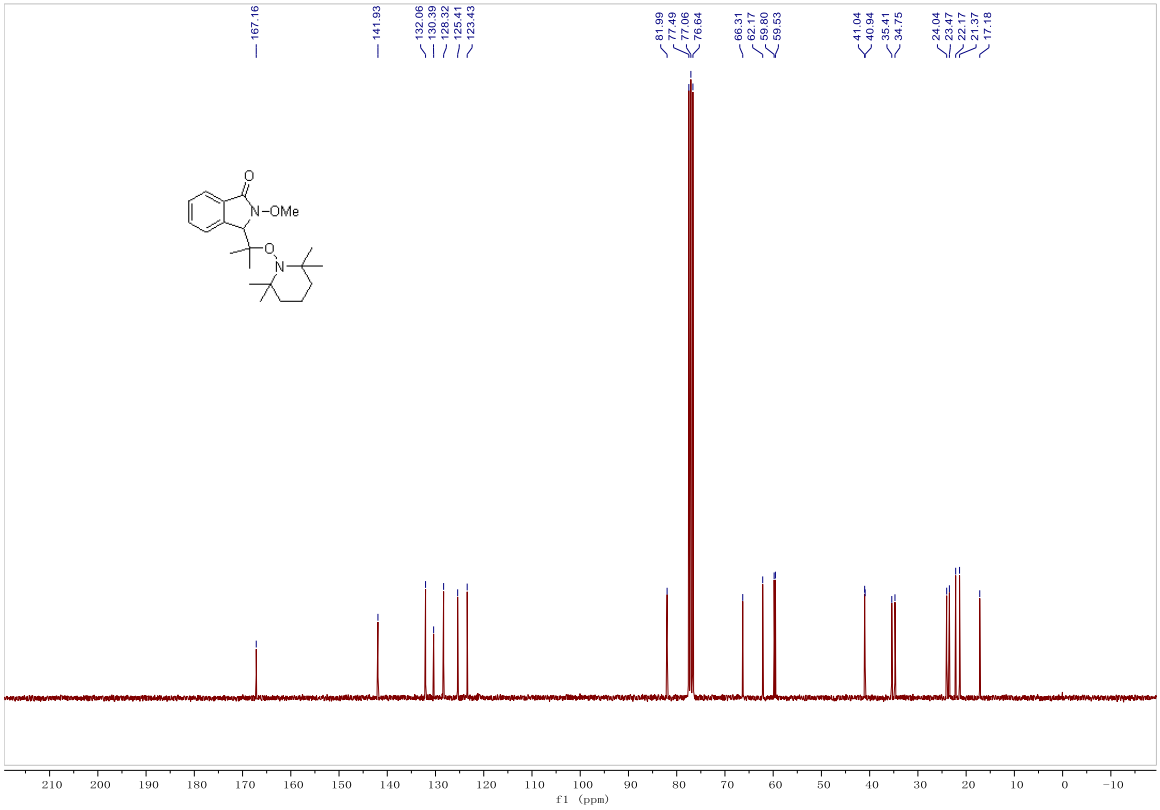
7.60
7.58
7.57
7.55
7.55
7.50
7.49
7.47
7.47
7.45
7.27
4.98
3.94
1.59
1.57
1.54
1.38
1.36
1.35
1.28
1.22
1.17
0.98
0.00
N–OMe
O
N
1.00
1.00
1.03
1.03
1.00
3.01
9.14
6.06
3.01
3.02
3.00
f1 (ppm)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141.93
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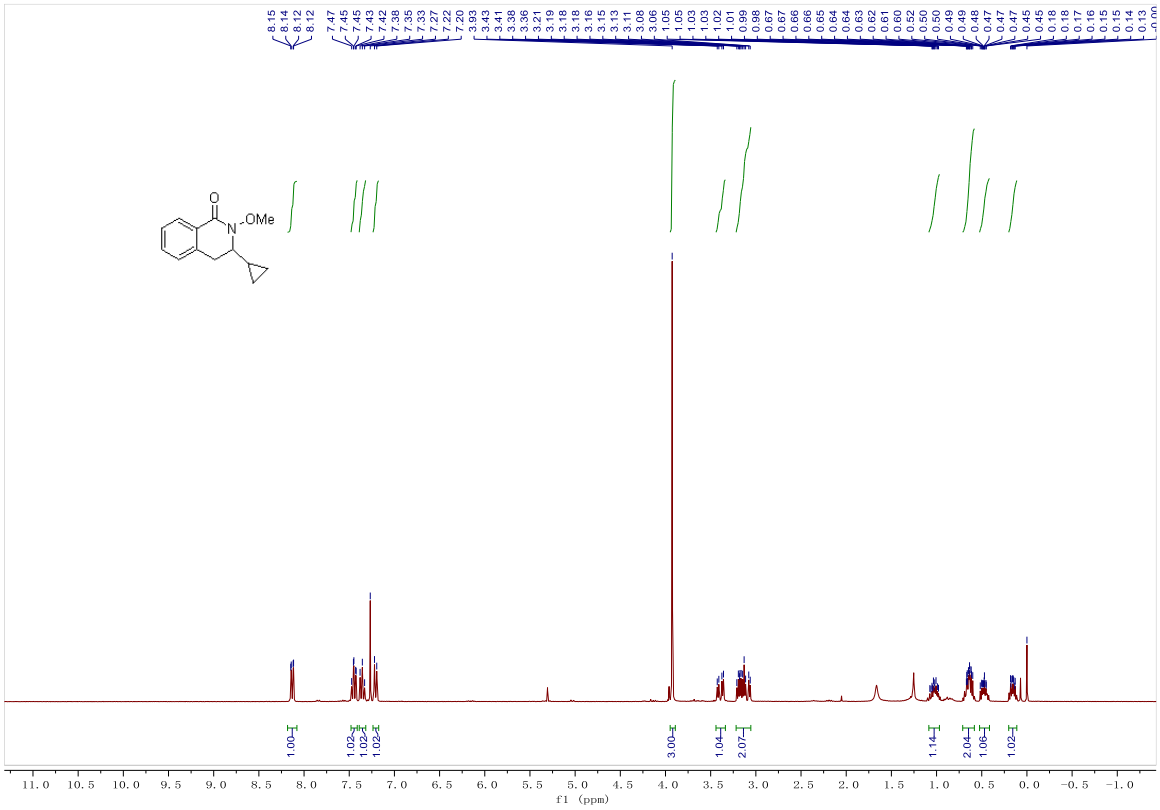
130.39
128.32
125.41
123.43
81.99
77.49
77.06
76.64
66.31
62.17
59.80
59.53
41.04
40.94
35.41
34.75
24.04
23.47
22.17
21.37
17.18
N–OMe
O
N
f1 (ppm)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8.12
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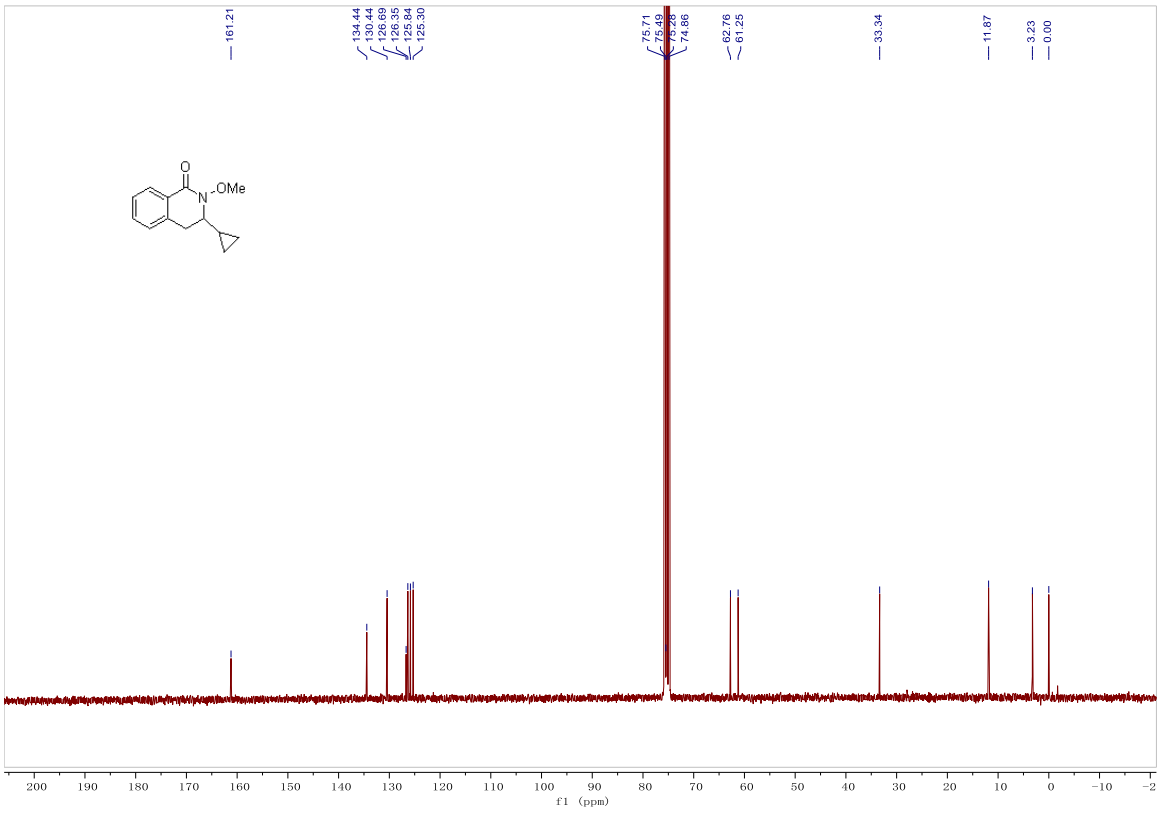
7.42
7.38
7.35
7.33
7.27
7.22
7.20
3.93
3.43
3.41
3.38
3.36
3.21
3.19
3.18
3.18
3.16
3.15
3.13
3.11
3.08
3.06
1.05
1.05
1.03
1.03
1.02
1.01
1.01
0.99
0.98
0.67
0.67
0.66
0.66
0.65
0.64
0.64
0.63
0.62
0.61
0.60
0.52
0.50
0.50
0.49
0.49
0.48
0.47
0.47
0.47
0.45
0.45
0.18
0.18
0.17
0.16
0.15
0.15
0.14
0.13
O
N
OMe
1.00
1.02
1.02
1.02
3.00
1.04
2.07
1.14
2.04
1.06
1.02
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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130.44
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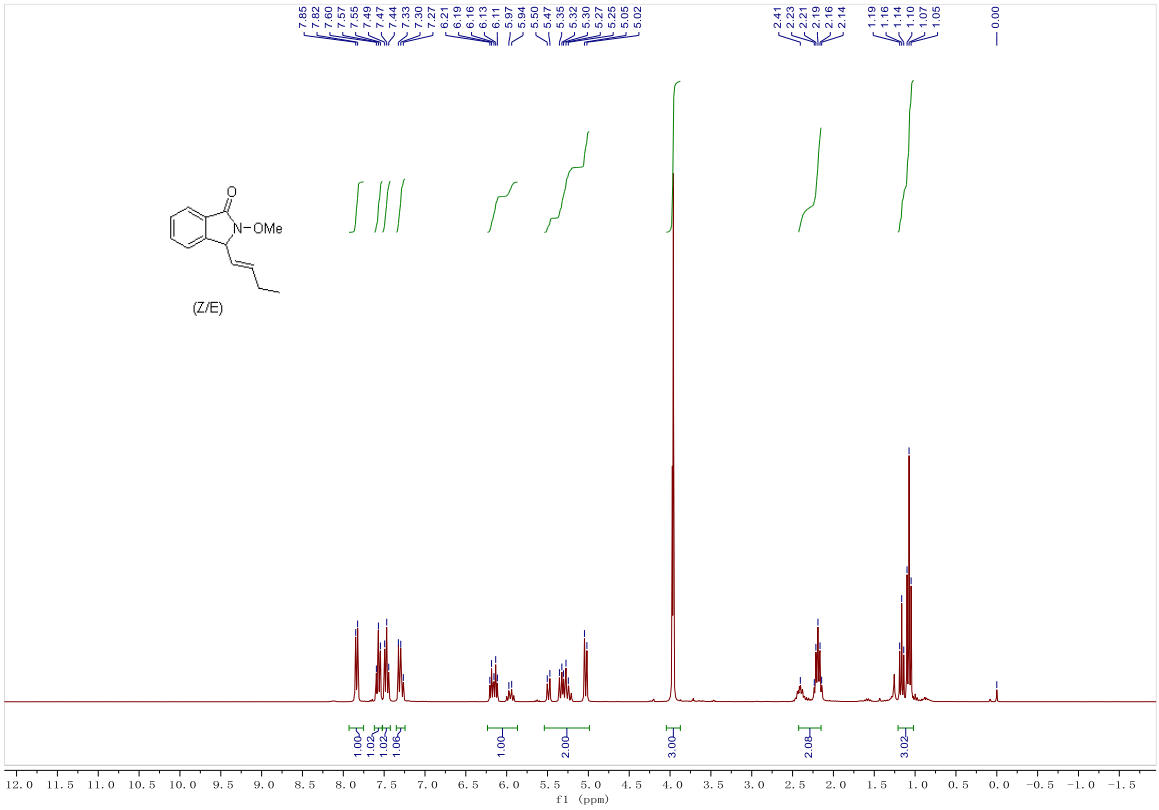
126.35
125.54
125.30
75.71
75.49
75.28
74.86
62.76
61.25
33.34
11.87
3.23
0.00
O
N
OMe
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (ppm)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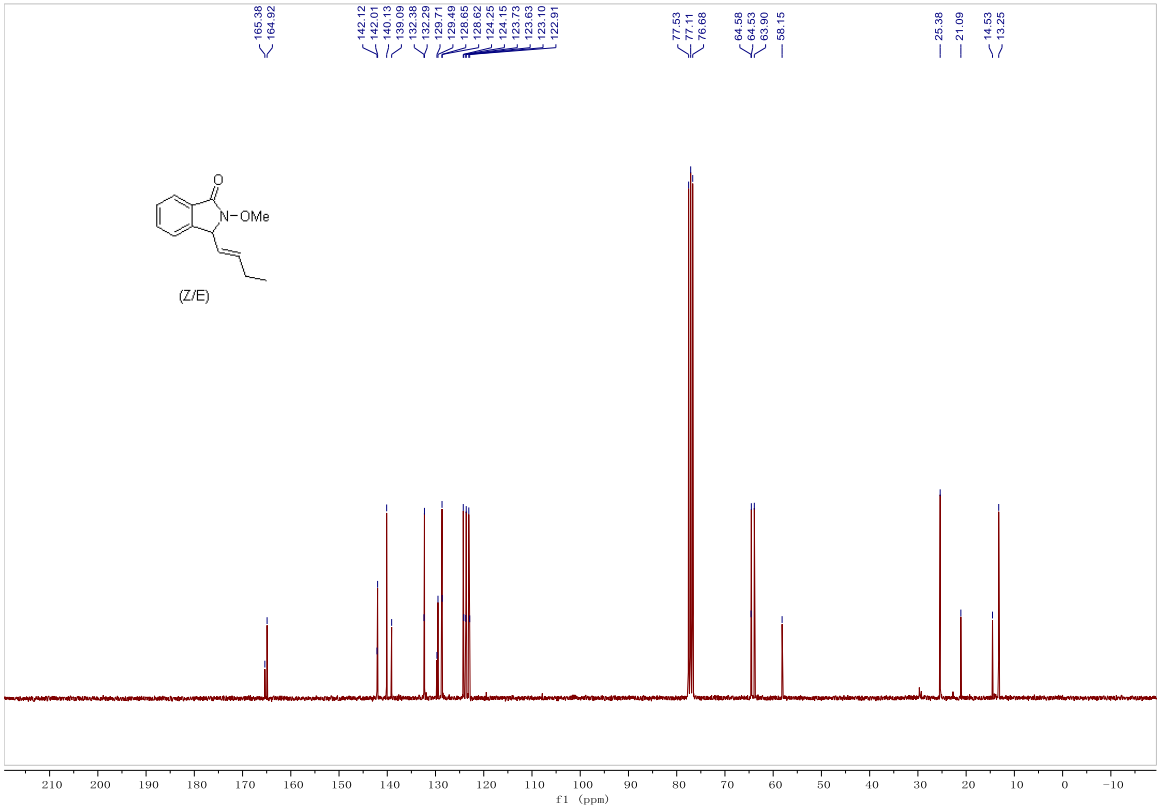
7.82
7.60
7.57
7.55
7.49
7.47
7.44
7.33
7.30
7.27
6.21
6.19
6.16
6.13
6.11
5.97
5.94
5.50
5.47
5.35
5.32
5.30
5.27
5.25
5.05
5.02
2.41
2.23
2.21
2.19
2.16
2.14
1.19
1.16
1.14
1.10
1.07
1.05
0.00
O
N−OMe
(Z/E)
1.00
1.02
1.02
1.06
1.00
2.00
3.00
2.08
3.02
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0 −1.5
f1 (ppm)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140.13
139.09
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132.29
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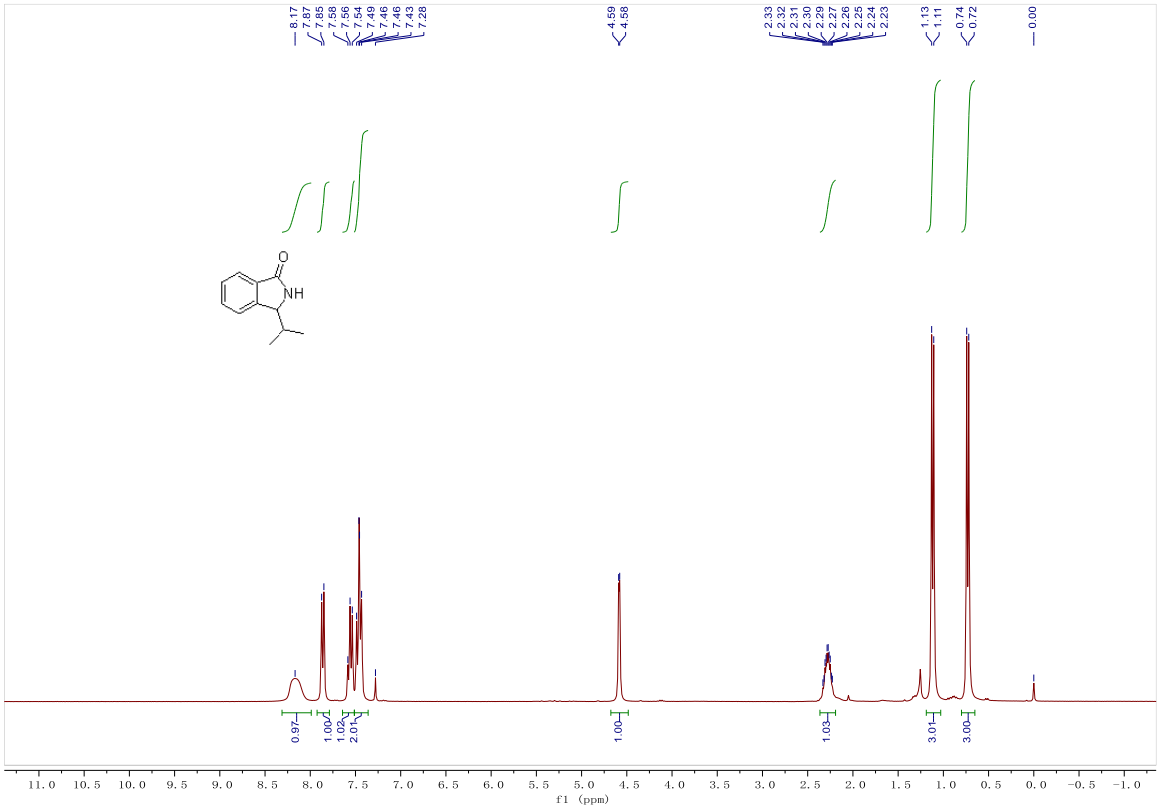
128.65
128.62
124.25
124.15
123.73
123.63
123.10
122.91
77.53
77.11
76.68
64.58
64.53
63.90
58.15
25.38
21.09
14.53
13.25
O
N−OMe
(Z/E)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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7.46
7.43
7.28
4.59
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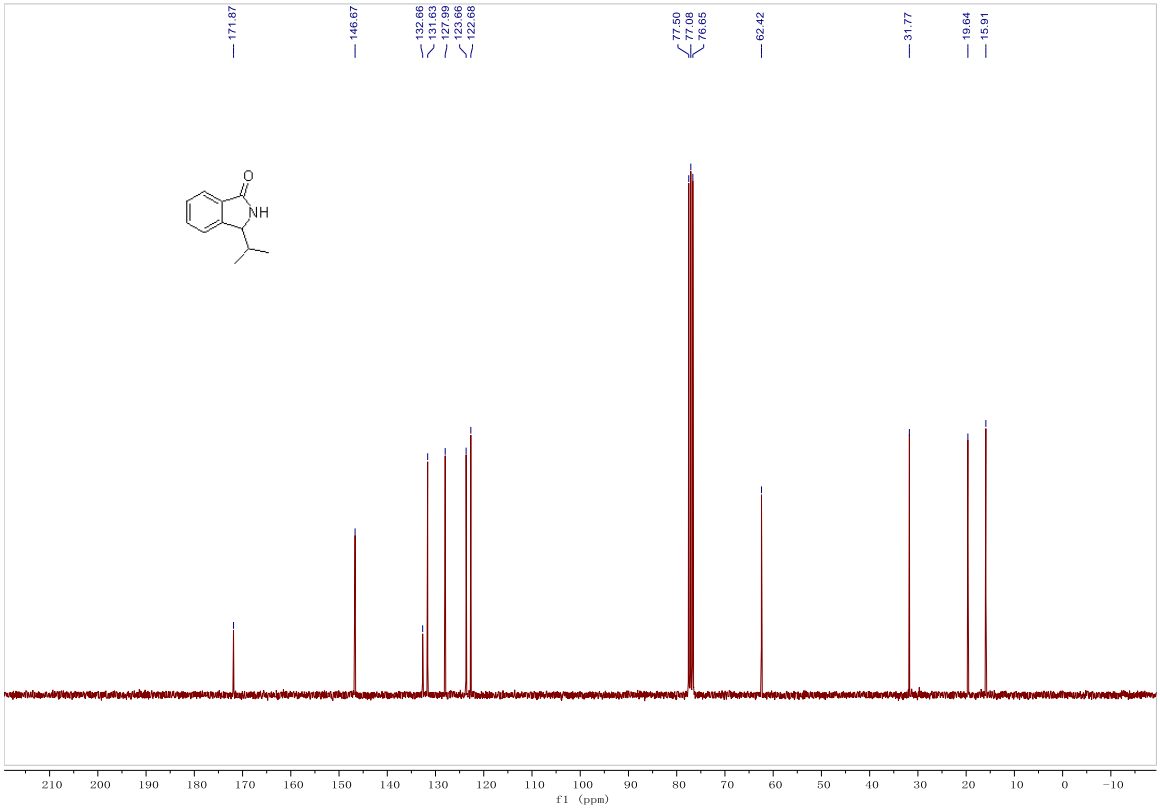
2.33
2.32
2.31
2.30
2.29
2.27
2.26
2.25
2.24
2.23
1.13
1.11
0.74
0.72
0.00
O
NH
0.97
1.00
1.02
2.01
1.00
1.03
3.01
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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123.66
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77.50
77.08
76.65
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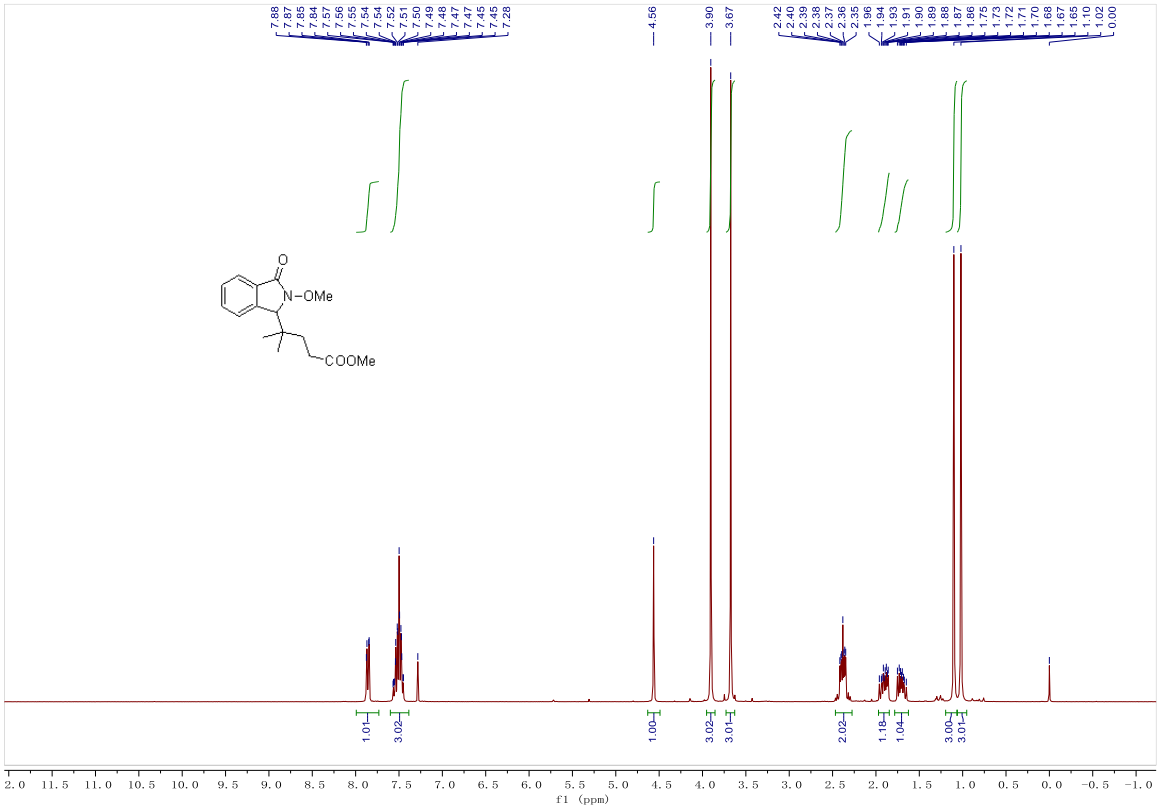
31.77
19.64
15.91
O
NH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.54
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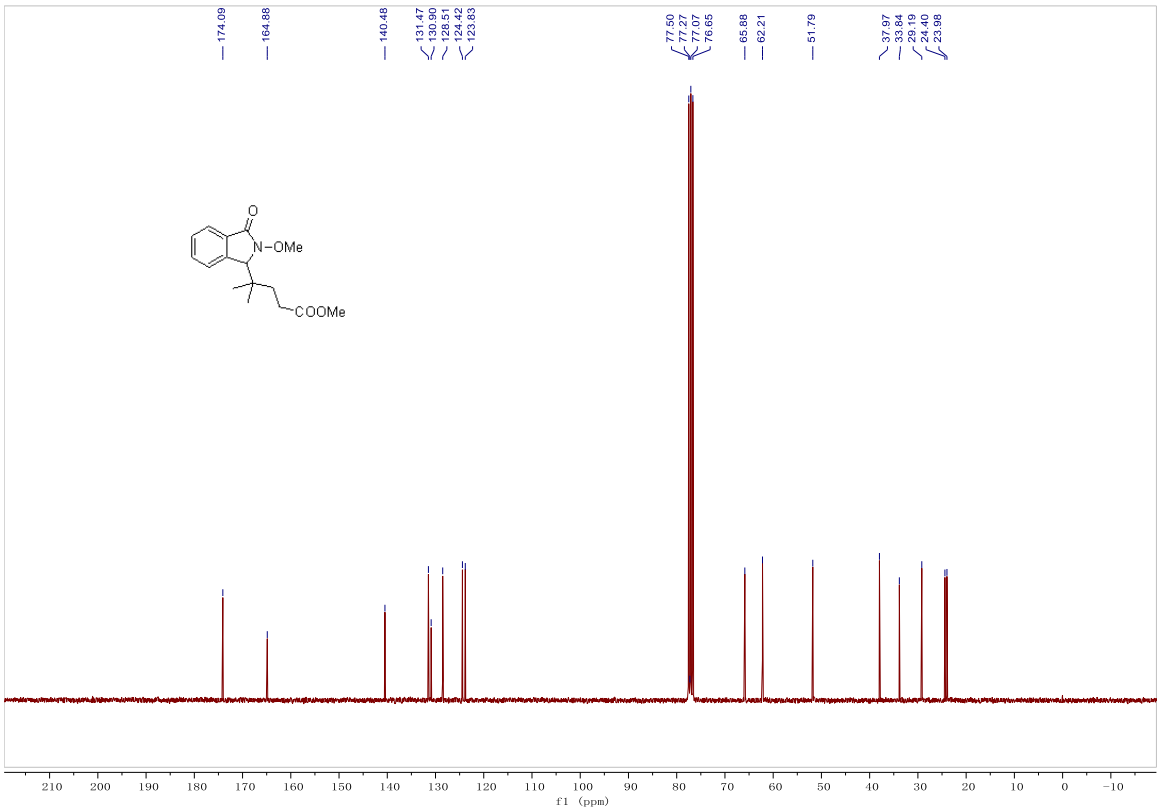
7.50
7.49
7.48
7.47
7.47
7.45
7.45
7.28
4.56
3.90
3.67
2.42
2.40
2.39
2.38
2.37
2.36
2.35
1.96
1.94
1.93
1.91
1.90
1.89
1.88
1.87
1.86
1.75
1.73
1.72
1.71
1.70
1.68
1.67
1.65
1.10
1.02
0.00
O
N–OMe
COOMe
1.01
3.02
1.00
3.02
3.01
2.02
1.18
1.04
3.00
3.01
f1 (ppm)


174.09
164.88
140.48
131.47
130.90
128.51
124.42
123.83
77.50
77.27
77.07
76.65
65.88
62.21
51.79
37.97
33.84
30.19
24.40
23.98
O
N–OMe
COOMe
f1 (ppm)

9. References

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