Supporting Information

Copper-catalyzed four-component reaction of alkenes, Togni's reagent, amines and CO_2: stereoselective synthesis of (*Z*)-enol carbamates

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A. General methods

^{1}H and ^{13}C NMR spectra were recorded by using 400 MHz or 500 MHz NMR spectrometer using $CDCl_3$ as solvent and TMS as an internal standard. The chemical shifts are referenced to signals at 7.26 and 77.0 ppm, respectively. Mass spectra were recorded on a gas chromatograph-mass spectrometer. The data of HRMS was carried out on a high-resolution mass spectrometer (LCMS-IT-TOF). IR spectra were obtained either as potassium bromide plates or as liquid films between two potassium bromide plates with an infrared spectrometer. Melting points were determined with a digital melting point measuring instrument. Substrates and other reagents were commercially purchased and used without further purification.

B. General procedure for the preparation of carbamates 4

To a dried 15 mL polyterafluoroethylene (PTFE) reaction vessel was added the mixture of alkene **1** (0.1 mmol), $Cu(OAc)_2$ (0.01 mmol), Togni's reagent **3a** (0.12 mmol), anhydrous DMSO (2 mL), and amine **2** (0.5 mmol) successively. The vessel was fixed into a stainless steel autoclave with a pressure-regulating system. Then the autoclave was charged with a pressure of CO_2 without air purge and sealed. The reaction was carried out at the selected temperature under magnetic stirring for 8 h. After the reaction was completed, the vessel was cooled with an ice bath and the pressure was released slowly to atmospheric pressure. Then reaction mixture was diluted with H_2O (20 mL) and extracted with EtOAc (15 mL×3). The combined organic layers were dried over anhydrous Na_2SO_4 and then filtered. The volatile compounds were removed under vacuum and the crude residue was separated by column chromatography on a silica gel column using petroleum ether/ethyl acetate as eluent to give the desired product **4**.

C. X-ray crystal structure and data for compound 4fa

Single-crystal X-ray diffraction data for **4fa** was collected on an X-ray diffractometer operated at 90 kV and 50 mA using CuKα radiation (λ= 1.54184 Å) at 100 K. All empirical absorption corrections were performed using the CrystalClear program. The structure was solved by a direct method and refined on F^2 by the full-matrix least squares technique using the SHELXTL-97 program package. All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms attached to carbon were placed in geometrically idealized positions and refined

using a riding model. The X-ray crystal structure of compound **4fa** is shown in **Figure S1**, and the crystallographic data for compound **4fa** is given in **Table S1**.

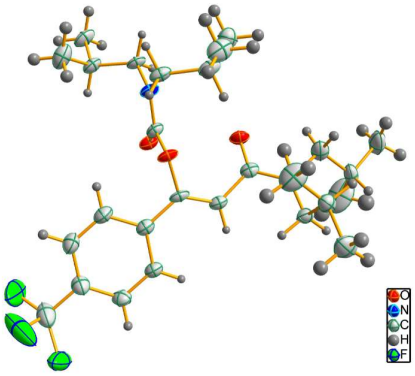


Figure S1. X-ray crystal structures of compound **4fa**. Ellipses are drawn at the 50% probability level.

Table S1. Crystal data and structure refinements for **4fa**

Compound	**4fa**
Empirical formula	$C_{27}H_{41}F_3N_2O_3$
Formula weight	498.31
Temperature (K)	100.00(10)
Wavelength (Å)	1.54184
Crystal system	monoclinic
Space group	$P2_1/n$
	a = 13.2194(4)Å α = 90°
	b = 11.2130(3)Å β = 102.554(3)°
	c = 19.9692(6)Å γ = 90°
Volume (Å^3)	2889.25(15)
Z	4
Density (calcd g cm^{-3})	1.143
Absorption coeff. (mm^{-1})	0.721
F(000)	1067.0
Crystal size (mm^3)	0.13 × 0.12 × 0.11
2θ range for data collection (°)	7.348 to 147.254
Limiting indices	-16 ≤ h ≤ 15, -11 ≤ k ≤ 13, -23 ≤ l ≤ 24
Reflections collected	11090
Unique	5674 [R_{int} = 0.0420, R_{sigma} = 0.0498]
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	5674/0/365
Goodness-of-fit on F^2	1.044
Final R indexes [I>=2σ (I)]	R_1 = 0.0596, wR_2 = 0.1492
R indexes (all data)	R_1 = 0.0748, wR_2 = 0.1619

D. Computational Details

All calculations were carried out with Gaussian 16 program.[1] The geometry optimizations were performed at the M06-2X[2]/6-31+G(d,p) level. Each optimized structure was subsequently analyzed by harmonic vibration frequencies at the same level to characterize a minimum without imaginary frequency (Nimag = 0) or a transition state with only one imaginary frequency (Nimag = 1) and to obtain the thermodynamic corrections to Gibbs free energy. The connection of transition states was confirmed via intrinsic reaction coordinate (IRC) calculations. All the structures were optimized without any symmetry restrictions. The subsequent single-point calculations were carried out at the level of M06-2X/6-311+G(2d,p) together with SMD model[3] for considering the dimethylsulfoxide (DMSO) solvation effect. Gibbs free energies in solution described in the study were obtained from such single-point energy calculations, including gas-phase free energy corrections. The corresponding relative enthalpies (ΔH, kcal mol^{-1}) were also provided for the estimation of entropy effects.

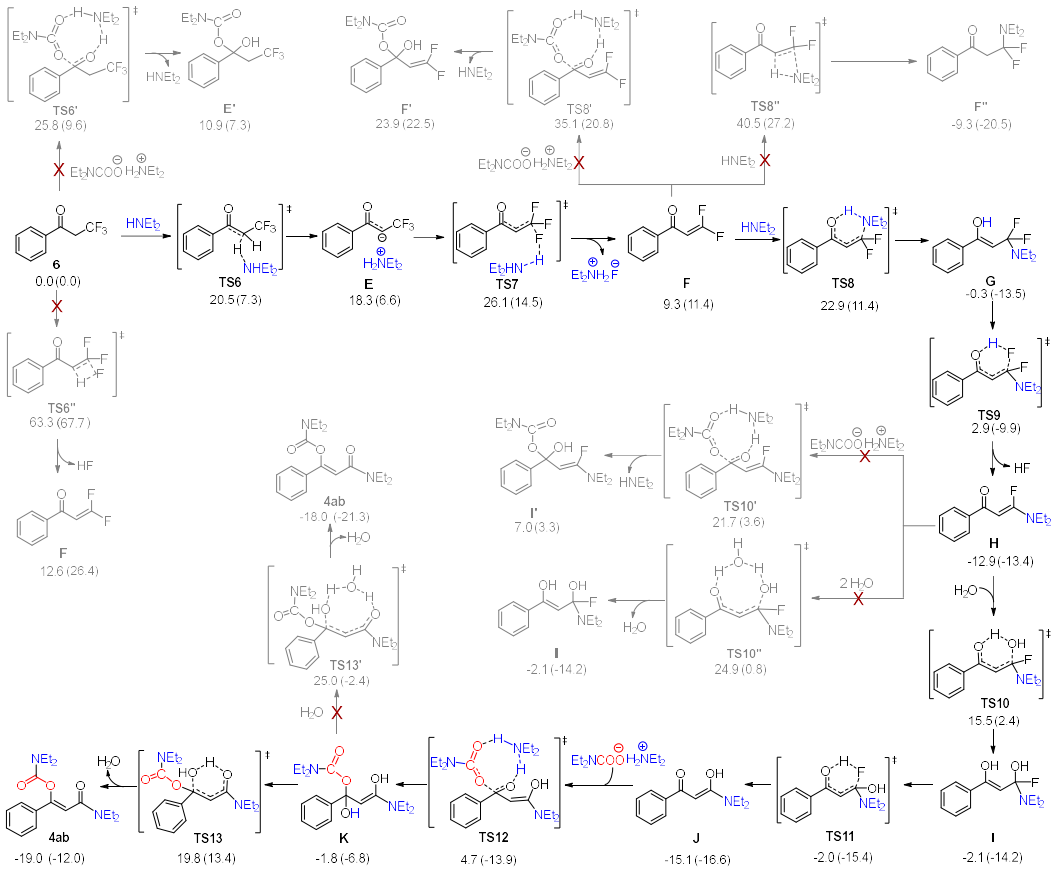


Figure S2. Computational analysis of the possible mechanisms of the transformation of **6** to **4ab**. The structure with square bracket means transition state. The relative free energies and enthalpies (in parentheses) shown below the structures are given in kcal mol^{-1}.

The cartesian coordinates of all stationary points and the imaginary frequencies (IF) of transition states calculated at the M06-2X/6-31+G(d,p) level are as follows:

$CF_3^{\bullet}$

C	0.000000000	0.000000000	0.330853000
F	0.000000000	1.255387000	−0.073523000
F	−1.087197000	−0.627693000	−0.073523000
F	1.087197000	−0.627693000	−0.073523000

styrene

C	−1.864991000	1.671479000	0.328786000
C	−0.479490000	1.576909000	0.218672000
C	0.292727000	2.682257000	−0.159438000
C	−0.361932000	3.897253000	−0.408329000
C	−1.744357000	3.994654000	−0.298893000
C	−2.503121000	2.881519000	0.067887000
H	−2.444219000	0.800697000	0.619682000
H	0.015282000	0.630765000	0.422974000
H	0.215232000	4.776824000	−0.676585000
H	−2.233338000	4.944307000	−0.492962000
H	−3.582002000	2.961213000	0.155159000
C	1.755372000	2.527014000	−0.275941000
C	2.606232000	3.393067000	−0.832572000
H	2.151768000	1.596738000	0.129016000
H	3.669208000	3.181866000	−0.867198000
H	2.278272000	4.327948000	−1.277209000

TS1, IF = -288.23 cm^{-1}

C	−2.438741000	1.442956000	0.424930000
C	−1.282303000	0.715945000	0.680787000
C	−1.172665000	−0.621941000	0.268750000
C	−2.250152000	−1.198307000	−0.419548000
C	−3.409453000	−0.471528000	−0.674060000
C	−3.508464000	0.852271000	−0.250375000
H	−2.504901000	2.477580000	0.746458000
H	−0.452705000	1.196864000	1.189808000
H	−2.173900000	−2.230254000	−0.752368000
H	−4.233647000	−0.937491000	−1.204784000
H	−4.409207000	1.423808000	−0.450017000
C	0.023001000	−1.432465000	0.523933000
C	1.067599000	−1.091887000	1.308389000
H	0.060619000	−2.386430000	0.000739000

H	1.882324000	-1.789251000	1.472416000
H	1.052763000	-0.205034000	1.935619000
C	2.493089000	0.205358000	-0.208823000
F	2.370175000	-0.282348000	-1.432494000
F	2.048362000	1.455272000	-0.169211000
F	3.764484000	0.165721000	0.172620000

A

C	-2.521712000	1.447930000	0.126848000
C	-1.270543000	0.910841000	0.388933000
C	-1.044811000	-0.486408000	0.293140000
C	-2.141280000	-1.303020000	-0.090338000
C	-3.386370000	-0.757029000	-0.351031000
C	-3.587998000	0.623075000	-0.241911000
H	-2.669375000	2.520625000	0.203333000
H	-0.453275000	1.574873000	0.650210000
H	-1.988769000	-2.375619000	-0.175077000
H	-4.208037000	-1.404242000	-0.641266000
H	-4.563826000	1.050711000	-0.446697000
C	0.210077000	-1.090728000	0.565400000
C	1.427502000	-0.360529000	1.033017000
H	0.302062000	-2.161324000	0.414207000
H	2.050941000	-1.006092000	1.658813000
H	1.180219000	0.530495000	1.618026000
C	2.311946000	0.098945000	-0.109015000
F	3.416154000	0.719656000	0.347863000
F	2.723095000	-0.931056000	-0.869043000
F	1.679550000	0.963858000	-0.920132000

TS2, IF = -299.84 cm^{-1}

C	-2.732220000	-1.182806000	-1.140958000
C	-1.437354000	-0.719942000	-0.947165000
C	-1.108190000	0.027907000	0.201707000
C	-2.127055000	0.291647000	1.141603000
C	-3.420118000	-0.169196000	0.940785000
C	-3.728963000	-0.908958000	-0.202644000
H	-2.966586000	-1.764438000	-2.026679000
H	-0.675580000	-0.959165000	-1.681648000
H	-1.885959000	0.868520000	2.030496000
H	-4.189947000	0.045573000	1.674867000
H	-4.738920000	-1.273354000	-0.359680000
C	0.203473000	0.566981000	0.441111000

C	1.392350000	0.342237000	-0.425653000
H	0.408432000	0.926007000	1.445567000
H	2.004504000	1.254417000	-0.453302000
H	1.121898000	0.095879000	-1.455047000
C	2.283197000	-0.767264000	0.087328000
F	3.383568000	-0.900216000	-0.672697000
F	2.694064000	-0.536611000	1.347186000
F	1.654269000	-1.955485000	0.086676000
O	0.833700000	3.189642000	-0.622894000
O	-0.160660000	2.617073000	-0.202324000

B

C	3.307362000	-1.035299000	-0.928255000
C	1.971157000	-0.688165000	-1.123078000
C	1.278457000	0.014255000	-0.138088000
C	1.931482000	0.379026000	1.042082000
C	3.267725000	0.039175000	1.232498000
C	3.956396000	-0.672082000	0.249419000
H	3.841801000	-1.579246000	-1.700390000
H	1.467837000	-0.958515000	-2.047795000
H	1.398959000	0.945862000	1.801253000
H	3.773379000	0.331994000	2.147015000
H	4.998380000	-0.935721000	0.399444000
C	-0.184577000	0.331980000	-0.329644000
C	-1.076673000	-0.553243000	0.535248000
H	-0.459533000	0.260667000	-1.386576000
H	-0.996083000	-0.258013000	1.585816000
H	-0.744489000	-1.590628000	0.447398000
C	-2.533181000	-0.518239000	0.136425000
F	-3.255311000	-1.360377000	0.895820000
F	-3.078389000	0.699094000	0.257173000
F	-2.696284000	-0.900173000	-1.146066000
O	0.026081000	2.559353000	-0.756930000
O	-0.465990000	1.697177000	0.085911000

TS3', IF = -1751.31 cm^{-1}

C	-2.555848000	-1.804620000	-0.026109000
C	-1.296932000	-1.229106000	-0.172558000
C	-1.155742000	0.164343000	-0.153316000
C	-2.288207000	0.970444000	0.031989000
C	-3.541832000	0.388699000	0.179491000
C	-3.679948000	-0.999449000	0.149857000

H	-2.657059000	-2.884749000	-0.049446000
H	-0.431019000	-1.869721000	-0.298281000
H	-2.168914000	2.048233000	0.052944000
H	-4.413779000	1.019604000	0.317990000
H	-4.659718000	-1.451861000	0.264739000
C	0.172361000	0.818553000	-0.293555000
C	1.349954000	0.095873000	-0.939065000
H	0.565358000	1.237437000	0.861114000
H	1.955057000	0.843642000	-1.456238000
H	1.005895000	-0.641886000	-1.670867000
C	2.265444000	-0.609422000	0.035416000
F	3.260475000	-1.233514000	-0.615245000
F	2.824876000	0.245220000	0.904822000
F	1.622031000	-1.541120000	0.765223000
O	0.626754000	2.552004000	0.626609000
O	0.101027000	2.159513000	-0.675116000

B2

C	-2.816344000	3.014945000	-0.171831000
C	-2.293442000	1.745972000	0.065431000
C	-2.261078000	0.797993000	-0.956960000
C	-2.749080000	1.124142000	-2.223171000
C	-3.268238000	2.395581000	-2.459914000
C	-3.305517000	3.341387000	-1.435814000
H	-2.831058000	3.749033000	0.628299000
H	-1.895089000	1.492158000	1.046155000
H	-2.706902000	0.392724000	-3.025012000
H	-3.640846000	2.648600000	-3.447380000
H	-3.708807000	4.331177000	-1.624870000
C	-1.742139000	-0.582854000	-0.636390000
C	-2.856222000	-1.526417000	-0.192433000
H	-0.950762000	-0.528478000	0.118385000
H	-3.422492000	-1.876229000	-1.061113000
H	-3.541224000	-0.991186000	0.469490000
C	-2.346768000	-2.724307000	0.572879000
F	-3.365907000	-3.519662000	0.948030000
F	-1.494343000	-3.470787000	-0.137460000
F	-1.708070000	-2.344285000	1.697979000
O	-0.058243000	-0.599507000	-2.170988000
O	-1.154194000	-1.201287000	-1.811939000
C	0.374663000	3.103882000	1.746365000
C	1.068860000	2.243338000	0.901698000

C	1.222599000	0.893062000	1.233802000
C	0.640402000	0.404440000	2.404744000
C	-0.064338000	1.268354000	3.245709000
C	-0.189482000	2.618596000	2.926626000
H	0.264500000	4.149346000	1.476030000
H	1.486998000	2.622616000	-0.028288000
H	0.732680000	-0.645139000	2.664303000
H	-0.510428000	0.879620000	4.155609000
H	-0.730230000	3.287694000	3.588526000
C	2.046900000	0.016042000	0.310144000
C	3.521795000	0.411837000	0.314279000
H	1.624877000	0.028005000	-0.701114000
H	4.004568000	0.027846000	1.217932000
H	3.618441000	1.499622000	0.313594000
C	4.272867000	-0.098623000	-0.892285000
F	5.568700000	0.255937000	-0.832953000
F	4.224457000	-1.432081000	-1.006818000
F	3.770987000	0.417356000	-2.030605000
O	0.898801000	-1.949456000	0.471911000
O	2.027478000	-1.363491000	0.754593000

TS3, IF = -2056.06 cm^{-1}

C	-2.630482000	3.135853000	-0.500358000
C	-2.176793000	1.895811000	-0.051097000
C	-1.981727000	0.851091000	-0.951845000
C	-2.229916000	1.052664000	-2.311410000
C	-2.678487000	2.291105000	-2.761083000
C	-2.883269000	3.334045000	-1.855677000
H	-2.776342000	3.946254000	0.207657000
H	-1.957087000	1.742891000	1.004177000
H	-2.047036000	0.245027000	-3.015395000
H	-2.864076000	2.446281000	-3.819209000
H	-3.232281000	4.299215000	-2.209131000
C	-1.535284000	-0.497179000	-0.438387000
C	-2.681468000	-1.506777000	-0.429387000
H	-1.125308000	-0.390531000	0.574364000
H	-2.907041000	-1.829743000	-1.450232000
H	-3.572814000	-1.028305000	-0.015909000
C	-2.414225000	-2.732242000	0.412195000
F	-3.501251000	-3.529262000	0.439489000
F	-1.393293000	-3.470280000	-0.035441000
F	-2.141214000	-2.399205000	1.689892000

O	0.505846000	-0.202337000	-1.449375000
O	-0.523472000	-1.086794000	-1.266543000
C	0.596862000	3.258631000	1.583122000
C	1.226219000	2.228360000	0.895715000
C	1.262161000	0.931854000	1.433969000
C	0.627751000	0.679410000	2.658773000
C	-0.001944000	1.717407000	3.341765000
C	-0.015616000	3.007368000	2.811867000
H	0.570383000	4.254088000	1.151935000
H	1.668271000	2.419750000	-0.079385000
H	0.635436000	-0.319475000	3.081677000
H	-0.479023000	1.515593000	4.295408000
H	-0.506067000	3.811816000	3.350687000
C	1.936002000	-0.132915000	0.652494000
C	3.378647000	0.100996000	0.247504000
H	1.168769000	-0.235861000	-0.488126000
H	4.028308000	-0.412168000	0.966083000
H	3.620889000	1.164782000	0.271244000
C	3.725230000	-0.410117000	-1.133819000
F	5.054776000	-0.361002000	-1.332831000
F	3.333145000	-1.675727000	-1.320500000
F	3.153492000	0.341831000	-2.088449000
O	0.652960000	-1.908775000	1.264242000
O	1.874934000	-1.429469000	1.249008000

C

C	0.922062000	3.393350000	1.740280000
C	-0.022316000	2.454385000	1.331696000
C	-0.137137000	2.108234000	-0.017478000
C	0.698435000	2.711370000	-0.956705000
C	1.642035000	3.652916000	-0.547343000
C	1.759602000	3.993937000	0.799082000
H	1.008102000	3.650803000	2.791373000
H	-0.660948000	1.972604000	2.069304000
H	0.622826000	2.420389000	-1.999514000
H	2.293680000	4.114351000	-1.283455000
H	2.498056000	4.724334000	1.115248000
C	-1.179209000	1.088930000	-0.435464000
C	-2.580932000	1.702021000	-0.462201000
H	-1.156259000	0.237734000	0.258917000
H	-2.710030000	2.289656000	-1.376154000
H	-2.710304000	2.367216000	0.394947000

C	-3.682408000	0.673311000	-0.385818000
F	-4.892353000	1.265456000	-0.407766000
F	-3.654519000	-0.208274000	-1.395356000
F	-3.612042000	-0.034986000	0.758678000
O	0.255163000	-0.114086000	-1.757616000
O	-0.967681000	0.616836000	-1.758150000
C	3.804232000	-1.338589000	-1.523318000
C	2.830191000	-1.819919000	-0.666301000
C	2.293180000	-0.990070000	0.354001000
C	2.788921000	0.335172000	0.475515000
C	3.762771000	0.797607000	-0.392588000
C	4.276641000	-0.028179000	-1.396213000
H	4.200760000	-1.986021000	-2.298791000
H	2.472498000	-2.836840000	-0.785020000
H	2.385257000	0.993456000	1.237725000
H	4.117934000	1.818135000	-0.290897000
H	5.037581000	0.344054000	-2.074023000
C	1.287396000	-1.473530000	1.219665000
C	0.668950000	-2.830769000	1.254884000
H	-0.062988000	-1.024141000	-1.869385000
H	0.215570000	-3.000786000	2.234688000
H	1.415183000	-3.615560000	1.086144000
C	-0.427743000	-3.055990000	0.227299000
F	0.050965000	-2.987859000	-1.039410000
F	-0.961567000	-4.277662000	0.372033000
F	-1.418920000	-2.164285000	0.306873000
O	-0.346611000	-0.496675000	2.424963000
O	0.959255000	-0.636828000	2.305737000

TS4, IF = -1733.63 cm^{-1}

C	0.555083000	-3.749284000	-1.355330000
C	-0.316441000	-2.686683000	-1.138639000
C	-0.451309000	-2.134790000	0.141462000
C	0.300744000	-2.651949000	1.201482000
C	1.172977000	-3.714094000	0.979006000
C	1.304747000	-4.263221000	-0.296207000
H	0.660559000	-4.165503000	-2.351921000
H	-0.866331000	-2.255094000	-1.971609000
H	0.209531000	-2.212645000	2.188825000
H	1.756020000	-4.109849000	1.804642000
H	1.990635000	-5.087319000	-0.466053000
C	-1.404391000	-0.998798000	0.349716000

C	-2.868904000	-1.367724000	0.169508000
H	-1.143638000	-0.198237000	-0.601020000
H	-3.188727000	-2.040961000	0.972491000
H	-2.982183000	-1.893400000	-0.781429000
C	-3.813113000	-0.184881000	0.145602000
F	-5.041333000	-0.582168000	-0.240607000
F	-3.949556000	0.398940000	1.343777000
F	-3.407982000	0.758290000	-0.719655000
O	0.046028000	0.138031000	1.709758000
O	-1.291660000	-0.324555000	1.557099000
C	4.513707000	1.120112000	0.676221000
C	3.353091000	1.580806000	0.075518000
C	2.434751000	0.674257000	-0.514572000
C	2.745309000	-0.710823000	-0.474666000
C	3.907837000	-1.153027000	0.133708000
C	4.801978000	-0.247250000	0.712858000
H	5.200533000	1.831665000	1.123624000
H	3.146529000	2.645553000	0.072440000
H	2.058138000	-1.423074000	-0.917665000
H	4.117633000	-2.218213000	0.159731000
H	5.710908000	-0.601133000	1.187929000
C	1.239946000	1.129667000	-1.131195000
C	0.789122000	2.548924000	-1.267246000
H	-0.095993000	1.099336000	1.726355000
H	0.095402000	2.635406000	-2.106635000
H	1.637064000	3.218366000	-1.449333000
C	0.072789000	3.097368000	-0.048420000
F	0.846648000	3.031138000	1.061357000
F	-0.257952000	4.384606000	-0.220816000
F	-1.053461000	2.429250000	0.254127000
O	-0.844723000	0.413501000	-1.694952000
O	0.520243000	0.180889000	-1.827760000

D

C	2.769160000	-1.589813000	0.228012000
C	1.481755000	-1.119470000	0.436954000
C	1.166541000	0.243845000	0.215168000
C	2.204465000	1.105755000	-0.222347000
C	3.485444000	0.618393000	-0.427602000
C	3.781030000	-0.729247000	-0.204367000
H	2.986098000	-2.639235000	0.400555000
H	0.711053000	-1.812532000	0.755377000

H	1.985637000	2.153264000	-0.394526000
H	4.264535000	1.295159000	-0.764341000
H	4.785844000	-1.104302000	-0.367109000
C	-0.150059000	0.744698000	0.437565000
C	-1.316146000	-0.030536000	0.961369000
H	-1.564173000	2.375117000	-0.984792000
H	-2.018747000	0.649387000	1.447652000
H	-0.996491000	-0.781030000	1.691922000
C	-2.087511000	-0.775237000	-0.111712000
F	-3.173778000	-1.372474000	0.406459000
F	-2.512010000	0.033812000	-1.100015000
F	-1.344727000	-1.734807000	-0.690411000
O	-1.590447000	2.484385000	-0.019136000
O	-0.270452000	2.104999000	0.368227000

TS5, IF = -600.29 cm^{-1}

C	-2.708115000	-1.583356000	-0.273218000
C	-1.439389000	-1.099708000	-0.562101000
C	-1.111496000	0.247103000	-0.299452000
C	-2.099925000	1.088076000	0.258456000
C	-3.360842000	0.591400000	0.550411000
C	-3.674173000	-0.744397000	0.284669000
H	-2.944724000	-2.621847000	-0.481205000
H	-0.699667000	-1.769309000	-0.986802000
H	-1.849588000	2.122648000	0.464574000
H	-4.106379000	1.246433000	0.989780000
H	-4.662943000	-1.128756000	0.512832000
C	0.185485000	0.789309000	-0.622616000
C	1.397408000	-0.018473000	-0.989536000
H	1.684299000	3.335121000	-0.060947000
H	2.164495000	0.662599000	-1.363754000
H	1.169331000	-0.746505000	-1.776148000
C	2.024123000	-0.801343000	0.150511000
F	3.158912000	-1.395429000	-0.269879000
F	2.336794000	-0.036592000	1.199080000
F	1.215786000	-1.780250000	0.598616000
O	1.390637000	2.526266000	0.387300000
O	0.304776000	2.098533000	-0.641229000

8

C	4.044582000	-0.403959000	0.000028000
C	3.129779000	-1.455109000	-0.000032000

C	1.762685000	-1.187370000	-0.000050000
C	1.306943000	0.134926000	-0.000024000
C	2.230570000	1.186352000	0.000035000
C	3.593851000	0.917381000	0.000064000
H	5.109575000	-0.613907000	0.000041000
H	3.479272000	-2.482294000	-0.000066000
H	1.062761000	-2.017325000	-0.000084000
H	1.855061000	2.204501000	0.000052000
H	4.307169000	1.735095000	0.000119000
C	-0.148176000	0.485782000	-0.000065000
O	-0.522907000	1.637232000	-0.000081000
C	-1.149144000	-0.665346000	-0.000007000
H	-1.000776000	-1.294559000	-0.883290000
H	-1.000681000	-1.294416000	0.883373000
C	-2.587522000	-0.204825000	0.000011000
F	-2.892170000	0.517954000	1.084395000
F	-2.892152000	0.518161000	-1.084247000
F	-3.407959000	-1.278553000	-0.000066000

$HNEt_2$

N	0.048686000	0.605513000	0.313958000
H	0.448264000	1.536393000	0.230751000
C	-1.309356000	0.613649000	-0.220803000
C	-2.084144000	-0.638212000	0.176704000
H	-1.317546000	0.712436000	-1.322317000
H	-1.817951000	1.493365000	0.186471000
H	-3.127432000	-0.559019000	-0.141871000
H	-1.666458000	-1.536817000	-0.286049000
H	-2.055831000	-0.766254000	1.262312000
C	0.938716000	-0.349254000	-0.335028000
C	2.370270000	-0.156021000	0.144500000
H	0.896770000	-0.266948000	-1.437585000
H	0.605742000	-1.361338000	-0.081042000
H	3.038106000	-0.891593000	-0.311252000
H	2.740317000	0.840556000	-0.120753000
H	2.422297000	-0.260349000	1.231394000

HF

F	0.000000000	0.000000000	0.092312000
H	0.000000000	0.000000000	-0.830805000

H_2O

O	0.000000000	0.000000000	0.115587000
H	0.000000000	-0.768653000	-0.462347000
H	0.000000000	0.768653000	-0.462347000

TS6, IF = -493.16 cm^{-1}

C	-4.514912000	-0.038369000	-0.523077000
C	-3.662464000	-0.614796000	-1.463367000
C	-2.334827000	-0.882820000	-1.133696000
C	-1.846249000	-0.578212000	0.140746000
C	-2.714848000	-0.019603000	1.084591000
C	-4.039089000	0.254321000	0.755572000
H	-5.548125000	0.171765000	-0.782036000
H	-4.032384000	-0.861912000	-2.453617000
H	-1.689539000	-1.347408000	-1.871778000
H	-2.326878000	0.180978000	2.078964000
H	-4.703020000	0.689854000	1.496127000
C	-0.408645000	-0.800510000	0.559239000
O	-0.123846000	-0.701005000	1.761177000
C	0.599373000	-0.917390000	-0.461503000
H	0.300959000	-1.134908000	-1.480467000
H	1.038519000	0.572541000	-0.164790000
C	1.848838000	-1.621520000	-0.090815000
F	2.590240000	-0.960817000	0.848264000
F	1.695189000	-2.869801000	0.401521000
F	2.667057000	-1.748617000	-1.169414000
N	1.375639000	1.586091000	0.362745000
H	1.833471000	1.248184000	1.213412000
C	0.161036000	2.362766000	0.728645000
C	-0.691911000	2.684760000	-0.490818000
H	0.478127000	3.279378000	1.239884000
H	-0.393695000	1.742620000	1.435640000
H	-1.648724000	3.095793000	-0.160508000
H	-0.216490000	3.421199000	-1.144000000
H	-0.905471000	1.780231000	-1.068328000
C	2.340597000	2.310029000	-0.495327000
C	3.645064000	1.541359000	-0.633207000
H	2.506573000	3.305912000	-0.067342000
H	1.867276000	2.437676000	-1.472689000
H	4.337346000	2.109967000	-1.258256000
H	4.116717000	1.381404000	0.340720000
H	3.482475000	0.565143000	-1.094800000

E

C	−4.526265000	−0.140542000	−0.430727000
C	−3.679203000	−0.651973000	−1.413693000
C	−2.335367000	−0.885503000	−1.129845000
C	−1.815655000	−0.605440000	0.139456000
C	−2.676906000	−0.104566000	1.121331000
C	−4.021607000	0.127230000	0.841104000
H	−5.573691000	0.038882000	−0.653161000
H	−4.066468000	−0.873935000	−2.403459000
H	−1.697677000	−1.289448000	−1.908888000
H	−2.264643000	0.084369000	2.107901000
H	−4.677614000	0.511179000	1.616688000
C	−0.354708000	−0.779444000	0.515766000
O	−0.018398000	−0.442363000	1.678580000
C	0.568322000	−1.147538000	−0.483123000
H	0.243352000	−1.517474000	−1.445673000
H	1.010938000	0.761760000	−0.255150000
C	1.893674000	−1.656566000	−0.090922000
F	2.592156000	−0.822512000	0.743047000
F	1.897443000	−2.850575000	0.547729000
F	2.695331000	−1.826400000	−1.177017000
N	1.259192000	1.622361000	0.327594000
H	1.576009000	1.178752000	1.200026000
C	0.009447000	2.400881000	0.603341000
C	−0.780599000	2.666814000	−0.668349000
H	0.311214000	3.330084000	1.096777000
H	−0.566944000	1.793112000	1.301922000
H	−1.740828000	3.113334000	−0.400063000
H	−0.268750000	3.354337000	−1.346704000
H	−0.993006000	1.730740000	−1.193782000
C	2.336010000	2.408617000	−0.333127000
C	3.583323000	1.580706000	−0.590969000
H	2.548341000	3.267569000	0.310487000
H	1.918957000	2.782355000	−1.270964000
H	4.318930000	2.203747000	−1.104901000
H	4.025042000	1.218794000	0.339756000
H	3.362522000	0.713535000	−1.217899000

Et_2NCOO^- $H_2NEt_2^+$

N	−2.108433000	0.082643000	−0.011335000
C	−2.598966000	0.853527000	1.124372000
C	−2.752348000	2.336898000	0.798783000

H	-1.911946000	0.719276000	1.961548000
H	-3.563017000	0.421981000	1.416382000
H	-3.159305000	2.882115000	1.655661000
H	-1.778011000	2.762488000	0.545627000
H	-3.426104000	2.481541000	-0.051557000
C	-3.070927000	-0.519057000	-0.924163000
C	-3.456754000	-1.935170000	-0.505973000
H	-3.952346000	0.131744000	-0.950590000
H	-2.628926000	-0.529096000	-1.922366000
H	-4.200696000	-2.353097000	-1.190701000
H	-2.571527000	-2.576079000	-0.520273000
H	-3.877715000	-1.944368000	0.504566000
C	-0.782270000	-0.082017000	-0.260617000
O	-0.350447000	-0.747763000	-1.202402000
O	0.006245000	0.547629000	0.613983000
H	0.973493000	0.352424000	0.334550000
N	2.363180000	-0.193650000	-0.315398000
H	1.967547000	-0.297256000	-1.251075000
C	2.571271000	-1.539045000	0.236330000
C	3.561913000	0.644210000	-0.364510000
C	2.839499000	-1.503203000	1.736090000
H	3.398095000	-2.049976000	-0.282253000
H	1.653881000	-2.099776000	0.032518000
C	3.269533000	1.942235000	-1.104035000
H	4.396259000	0.107920000	-0.845800000
H	3.870514000	0.865241000	0.662176000
H	2.882663000	-2.520072000	2.135134000
H	3.790807000	-1.016940000	1.969971000
H	2.039229000	-0.964261000	2.252480000
H	4.153064000	2.585030000	-1.123252000
H	2.973769000	1.743629000	-2.139271000
H	2.454950000	2.485393000	-0.616659000

TS6′, IF = -199.13 cm^{-1}

C	-3.990840000	2.188167000	-1.753582000
C	-4.151965000	1.571318000	-0.515376000
C	-3.032538000	1.194304000	0.227679000
C	-1.747239000	1.420662000	-0.265054000
C	-1.590151000	2.055737000	-1.500681000
C	-2.706083000	2.434459000	-2.241675000
H	-4.859503000	2.481247000	-2.335021000
H	-5.148181000	1.387965000	-0.123916000

H	-3.140687000	0.722471000	1.200190000
H	-0.592078000	2.217672000	-1.895126000
H	-2.575064000	2.915374000	-3.206208000
C	-0.567500000	0.976176000	0.595558000
O	-0.817700000	0.142100000	1.525187000
C	0.339621000	2.148546000	0.989915000
H	-0.275879000	2.905959000	1.485883000
N	2.402684000	-0.536679000	-1.247228000
C	3.340432000	-1.651975000	-1.285336000
C	3.020080000	-2.641682000	-2.403003000
H	3.316362000	-2.153359000	-0.316204000
H	4.342438000	-1.230928000	-1.420278000
H	3.755581000	-3.451324000	-2.427776000
H	2.030412000	-3.074987000	-2.237132000
H	3.025196000	-2.145095000	-3.378643000
C	2.741794000	0.665146000	-1.996490000
C	3.662503000	1.607352000	-1.224812000
H	3.225313000	0.348104000	-2.929408000
H	1.814376000	1.171855000	-2.266683000
H	3.937410000	2.466727000	-1.843978000
H	3.172942000	1.970715000	-0.318760000
H	4.582371000	1.097745000	-0.921925000
C	1.210477000	-0.700729000	-0.602924000
O	0.393940000	0.319022000	-0.686288000
O	0.963837000	-1.792308000	-0.047982000
H	-0.545057000	-2.219391000	0.339855000
N	-1.511117000	-2.161001000	0.769326000
H	-1.440000000	-1.100453000	1.056141000
C	-1.543418000	-2.953988000	2.018678000
C	-2.576955000	-2.444678000	-0.213633000
C	-0.995888000	-4.359846000	1.818411000
H	-2.576114000	-2.968788000	2.382990000
H	-0.937081000	-2.403646000	2.743049000
C	-2.191048000	-1.919025000	-1.588797000
H	-3.497965000	-1.972941000	0.145971000
H	-2.743530000	-3.526117000	-0.247232000
H	-1.005858000	-4.904047000	2.765829000
H	-1.589228000	-4.932046000	1.099564000
H	0.036165000	-4.313683000	1.459492000
H	-3.004329000	-2.095309000	-2.296789000
H	-1.984926000	-0.845678000	-1.557129000
H	-1.292909000	-2.425542000	-1.955069000

H	0.804626000	2.599742000	0.111364000
C	1.426935000	1.764009000	1.965768000
F	2.339416000	2.764276000	2.056796000
F	2.105404000	0.664847000	1.598305000
F	0.967882000	1.558353000	3.206794000

E′

C	-1.405881000	4.149534000	0.726322000
C	-2.165440000	3.619126000	-0.314569000
C	-2.014484000	2.283205000	-0.681906000
C	-1.097375000	1.472199000	-0.013527000
C	-0.343728000	2.002287000	1.034534000
C	-0.494653000	3.337922000	1.400036000
H	-1.521530000	5.190677000	1.010253000
H	-2.875755000	4.245745000	-0.844620000
H	-2.600397000	1.865490000	-1.495068000
H	0.373752000	1.374749000	1.555477000
H	0.102751000	3.745289000	2.209627000
C	-0.995739000	-0.005182000	-0.389838000
O	-1.300076000	-0.246605000	-1.717413000
C	-1.967673000	-0.809063000	0.475643000
H	-2.972536000	-0.403368000	0.335480000
H	-0.655768000	0.257228000	-2.244258000
N	2.521582000	-0.581499000	-0.369484000
C	2.586381000	-1.569270000	0.710385000
C	2.447739000	-0.968658000	2.106720000
H	3.555959000	-2.066433000	0.608544000
H	1.810659000	-2.322312000	0.548039000
H	2.599080000	-1.742997000	2.864319000
H	3.182088000	-0.174939000	2.269329000
H	1.446501000	-0.553523000	2.243569000
C	3.752231000	-0.208474000	-1.060316000
C	4.700591000	0.588327000	-0.170102000
H	4.239074000	-1.126858000	-1.410777000
H	3.464460000	0.375642000	-1.934512000
H	5.596717000	0.867460000	-0.731056000
H	4.213204000	1.501576000	0.182849000
H	5.019046000	0.005897000	0.700227000
C	1.350935000	-0.052044000	-0.788054000
O	1.211885000	0.735280000	-1.715518000
O	0.309332000	-0.509811000	-0.046657000
H	-1.689944000	-0.686440000	1.525503000

C	−2.047939000	−2.296138000	0.197655000
F	−2.562518000	−2.583889000	−1.002356000
F	−0.862058000	−2.921183000	0.288873000
F	−2.857352000	−2.870032000	1.117068000

TS6′′, IF = -1663.39 cm^{-1}

C	4.009322000	−0.504057000	−0.050807000
C	3.037430000	−1.501385000	0.004361000
C	1.687551000	−1.157885000	0.023345000
C	1.306104000	0.186894000	−0.004525000
C	2.285739000	1.184333000	−0.046871000
C	3.632205000	0.839544000	−0.076009000
H	5.060771000	−0.773166000	−0.070166000
H	3.329301000	−2.546012000	0.036352000
H	0.940251000	−1.942845000	0.085069000
H	1.967381000	2.221715000	−0.055313000
H	4.389187000	1.616089000	−0.115928000
C	−0.127623000	0.624395000	0.028580000
O	−0.425247000	1.776524000	0.281767000
C	−1.148999000	−0.421648000	−0.250640000
H	−0.900304000	−1.227351000	−0.933763000
H	−1.686701000	−0.982196000	0.892305000
C	−2.527671000	−0.070957000	−0.301697000
F	−2.833703000	−0.979085000	1.261016000
F	−3.001391000	1.076606000	0.026604000
F	−3.345158000	−0.725725000	−1.070634000

TS7, IF = -429.64 cm^{-1}

C	5.029629000	−0.744703000	−0.055435000
C	4.618532000	0.530571000	−0.439979000
C	3.285103000	0.907665000	−0.297647000
C	2.352057000	0.012889000	0.235975000
C	2.775718000	−1.258540000	0.636261000
C	4.105363000	−1.639046000	0.485090000
H	6.068517000	−1.038277000	−0.170167000
H	5.337702000	1.235066000	−0.845634000
H	2.980892000	1.910873000	−0.577891000
H	2.043813000	−1.931774000	1.070725000
H	4.423620000	−2.630520000	0.791883000
C	0.899569000	0.361844000	0.421271000
O	0.237266000	−0.323978000	1.225026000
C	0.374461000	1.440127000	−0.356624000

H	0.928910000	1.853251000	-1.185906000
H	-2.235827000	-0.096927000	-0.500833000
C	-0.875735000	1.977652000	-0.158091000
F	-2.169492000	1.073052000	-1.169704000
F	-1.539698000	1.799104000	0.967121000
F	-1.183158000	3.134077000	-0.697969000
N	-2.139353000	-1.047354000	0.079238000
H	-1.420050000	-0.812832000	0.791253000
C	-1.552629000	-2.063856000	-0.827919000
C	-2.402820000	-2.269035000	-2.072470000
H	-1.418511000	-2.994954000	-0.266747000
H	-0.562629000	-1.685712000	-1.097988000
H	-1.872865000	-2.915036000	-2.776002000
H	-3.359647000	-2.744869000	-1.842680000
H	-2.592392000	-1.309003000	-2.561499000
C	-3.422435000	-1.411051000	0.717488000
C	-3.838586000	-0.327852000	1.700986000
H	-3.298275000	-2.379822000	1.214306000
H	-4.170750000	-1.524013000	-0.070791000
H	-4.784349000	-0.597891000	2.175861000
H	-3.083949000	-0.198332000	2.482196000
H	-3.965094000	0.627976000	1.186571000

$Et_2NH{\cdot}HF$

H	-0.049936000	1.328631000	0.277332000
F	-0.055359000	2.262887000	-0.029416000
N	-0.043121000	-0.196839000	0.621847000
H	-0.447446000	-0.334026000	1.546677000
C	1.341871000	-0.697400000	0.628643000
C	2.079841000	-0.336826000	-0.654851000
H	1.357632000	-1.787536000	0.781651000
H	1.844752000	-0.234080000	1.482593000
H	3.136577000	-0.599504000	-0.561543000
H	1.680989000	-0.877469000	-1.517247000
H	2.001959000	0.736264000	-0.850762000
C	-0.916036000	-0.843130000	-0.369550000
C	-2.361928000	-0.423259000	-0.150252000
H	-0.814030000	-1.938652000	-0.320714000
H	-0.586845000	-0.523912000	-1.362774000
H	-3.009613000	-0.869025000	-0.908718000
H	-2.722286000	-0.749613000	0.831306000
H	-2.454151000	0.664496000	-0.209938000

F

C	3.708966000	−0.464745000	−0.025182000
C	2.764256000	−1.472595000	−0.207147000
C	1.405184000	−1.166291000	−0.183401000
C	0.986135000	0.153177000	0.012551000
C	1.940165000	1.163125000	0.180346000
C	3.295215000	0.854437000	0.168379000
H	4.767340000	−0.705729000	−0.037637000
H	3.084105000	−2.496646000	−0.370064000
H	0.682068000	−1.959166000	−0.345477000
H	1.593966000	2.182282000	0.318311000
H	4.030841000	1.640061000	0.307556000
C	−0.458195000	0.556347000	0.024768000
O	−0.779107000	1.723753000	−0.105062000
C	−1.466428000	−0.511899000	0.222856000
H	−1.187341000	−1.503636000	0.549845000
C	−2.768660000	−0.299855000	0.043943000
F	−3.683305000	−1.229295000	0.239119000
F	−3.336466000	0.805139000	−0.350753000

TS8′, IF = -177.36 cm^{-1}

C	5.187486000	0.479527000	−0.937856000
C	4.381836000	1.432905000	−1.555336000
C	3.044850000	1.568194000	−1.180907000
C	2.507556000	0.753511000	−0.186357000
C	3.318166000	−0.202916000	0.430751000
C	4.651044000	−0.341199000	0.056004000
H	6.228241000	0.372996000	−1.228352000
H	4.793659000	2.074280000	−2.328680000
H	2.398615000	2.303029000	−1.648962000
H	2.893457000	−0.860713000	1.183260000
H	5.271568000	−1.092869000	0.534405000
C	1.055608000	0.970339000	0.208045000
O	0.372083000	1.698346000	−0.574954000
C	0.850948000	1.061493000	1.692302000
H	1.589624000	0.636933000	2.359406000
C	−0.197992000	1.623499000	2.263864000
N	−0.771625000	−2.567271000	0.182333000
C	−2.032075000	−3.167068000	0.596071000
C	−3.089701000	−3.131316000	−0.504812000
H	−2.396118000	−2.635758000	1.478216000

H	-1.822951000	-4.201893000	0.889551000
H	-4.002052000	-3.645857000	-0.187842000
H	-3.343787000	-2.092481000	-0.736878000
H	-2.720961000	-3.613207000	-1.416412000
C	0.296983000	-3.428957000	-0.303342000
C	1.195090000	-3.937823000	0.821494000
H	-0.171010000	-4.268824000	-0.830679000
H	0.887944000	-2.866041000	-1.028514000
H	1.975423000	-4.597476000	0.430155000
H	1.673005000	-3.089923000	1.319209000
H	0.615580000	-4.493641000	1.565621000
C	-0.589950000	-1.215232000	0.326339000
O	0.591091000	-0.789295000	0.010229000
O	-1.549224000	-0.508147000	0.719759000
H	-2.210958000	0.648716000	-0.351742000
N	-2.123843000	1.455216000	-1.012509000
H	-1.083273000	1.711405000	-0.786269000
C	-3.087712000	2.530107000	-0.674570000
C	-2.204273000	0.985911000	-2.418600000
C	-4.443933000	1.957955000	-0.287304000
H	-3.162542000	3.191495000	-1.543126000
H	-2.663850000	3.105137000	0.149070000
C	-1.291219000	-0.206597000	-2.662564000
H	-1.913335000	1.831726000	-3.049202000
H	-3.247737000	0.739643000	-2.641664000
H	-5.138580000	2.765648000	-0.045499000
H	-4.882531000	1.369721000	-1.098615000
H	-4.345194000	1.315476000	0.592594000
H	-1.305911000	-0.461244000	-3.725247000
H	-0.265563000	0.025839000	-2.363965000
H	-1.622963000	-1.083404000	-2.098054000
F	-1.222982000	2.192794000	1.656311000
F	-0.375619000	1.706588000	3.574782000

F′

C	3.031450000	-2.972134000	0.844937000
C	3.483906000	-2.289444000	-0.282116000
C	2.810261000	-1.154829000	-0.731576000
C	1.676498000	-0.701946000	-0.058117000
C	1.230500000	-1.378637000	1.077421000
C	1.903348000	-2.513616000	1.523888000
H	3.553998000	-3.857511000	1.192956000

H	4.361446000	-2.640732000	-0.815771000
H	3.156187000	-0.619515000	-1.610262000
H	0.350506000	-1.023495000	1.605488000
H	1.544695000	-3.041235000	2.402157000
C	0.994695000	0.582064000	-0.529671000
O	1.132593000	0.792392000	-1.895343000
C	1.589800000	1.769632000	0.188559000
H	2.553848000	1.668097000	0.667765000
C	1.008376000	2.956284000	0.223685000
H	0.728929000	0.021705000	-2.332711000
N	-2.466302000	-0.273449000	-0.346577000
C	-2.894390000	0.707015000	0.653338000
C	-2.483240000	0.356444000	2.080884000
H	-3.984853000	0.760552000	0.577351000
H	-2.497398000	1.688444000	0.379521000
H	-2.917869000	1.074307000	2.782675000
H	-2.825466000	-0.645752000	2.353408000
H	-1.396563000	0.397539000	2.183854000
C	-3.461739000	-1.168329000	-0.928390000
C	-3.989276000	-2.185502000	0.078590000
H	-4.284323000	-0.556920000	-1.319606000
H	-2.986207000	-1.672386000	-1.769826000
H	-4.713799000	-2.848973000	-0.401609000
H	-3.168411000	-2.792746000	0.470462000
H	-4.490576000	-1.695356000	0.919224000
C	-1.190388000	-0.337824000	-0.790229000
O	-0.774361000	-1.096799000	-1.656512000
O	-0.401274000	0.563595000	-0.152932000
F	-0.150071000	3.277399000	-0.311785000
F	1.524016000	4.012552000	0.830901000

TS8′′, IF = -1601.28 cm^{-1}

C	5.090819000	0.403349000	0.319445000
C	4.220732000	1.424380000	-0.060234000
C	2.859488000	1.164728000	-0.203469000
C	2.356354000	-0.116877000	0.040500000
C	3.232239000	-1.132622000	0.433931000
C	4.593648000	-0.876454000	0.566441000
H	6.152253000	0.605551000	0.425603000
H	4.601787000	2.424329000	-0.243022000
H	2.189577000	1.970895000	-0.485075000
H	2.819342000	-2.116704000	0.630800000

H	5.268201000	-1.673364000	0.863893000
C	0.895563000	-0.466884000	-0.089156000
O	0.479868000	-1.507128000	0.431454000
C	0.019750000	0.480270000	-0.750621000
H	0.437952000	1.185780000	-1.459698000
C	-1.363267000	0.003753000	-1.062782000
F	-1.543829000	-1.274585000	-1.451552000
F	-1.968876000	0.763762000	-2.011020000
N	-2.029711000	0.242056000	0.289369000
H	-0.835387000	0.718956000	0.433016000
C	-2.531220000	-0.973894000	0.985095000
C	-3.891027000	-1.444285000	0.482298000
H	-2.564690000	-0.726164000	2.048729000
H	-1.762764000	-1.734614000	0.850434000
H	-4.144887000	-2.388741000	0.970254000
H	-4.688544000	-0.730064000	0.707459000
H	-3.870633000	-1.618232000	-0.596481000
C	-2.956940000	1.399388000	0.286346000
C	-3.356918000	1.790638000	1.700948000
H	-3.830953000	1.174674000	-0.332400000
H	-2.421974000	2.225330000	-0.190781000
H	-3.997917000	1.041975000	2.172746000
H	-2.472362000	1.935932000	2.328236000
H	-3.910950000	2.731567000	1.669774000

F″

C	-5.073385000	0.360165000	0.265171000
C	-4.267119000	-0.121860000	1.294223000
C	-2.910231000	-0.346000000	1.069381000
C	-2.354655000	-0.092384000	-0.188855000
C	-3.171440000	0.387134000	-1.219054000
C	-4.523594000	0.614909000	-0.992637000
H	-6.129881000	0.536268000	0.442022000
H	-4.693193000	-0.324148000	2.271558000
H	-2.296629000	-0.725877000	1.880243000
H	-2.721550000	0.573114000	-2.188951000
H	-5.151709000	0.989384000	-1.794572000
C	-0.902277000	-0.322677000	-0.496735000
O	-0.474205000	-0.162163000	-1.618436000
C	-0.008516000	-0.779110000	0.649658000
H	-0.315811000	-1.782502000	0.966183000
C	1.465340000	-0.850425000	0.282541000

F	1.621690000	-1.773746000	-0.700661000
F	2.110131000	-1.415470000	1.391044000
N	2.062069000	0.374178000	-0.096141000
H	-0.142504000	-0.123535000	1.513658000
C	3.163868000	0.282629000	-1.061311000
C	4.470001000	-0.290481000	-0.509943000
H	3.324339000	1.292793000	-1.446576000
H	2.808687000	-0.311643000	-1.903526000
H	5.227067000	-0.319710000	-1.299039000
H	4.865497000	0.319465000	0.308560000
H	4.322675000	-1.306971000	-0.135680000
C	2.283098000	1.289699000	1.027134000
C	2.552240000	2.716641000	0.564673000
H	3.100605000	0.941641000	1.675373000
H	1.379690000	1.288313000	1.643604000
H	3.535846000	2.818170000	0.098678000
H	1.792431000	3.035509000	-0.154418000
H	2.527226000	3.391271000	1.424436000

TS8, IF = -165.30 cm^{-1}

C	5.094031000	-0.339892000	0.392079000
C	4.399235000	0.704716000	0.999703000
C	3.047886000	0.897916000	0.720770000
C	2.385641000	0.048899000	-0.170689000
C	3.091007000	-0.989041000	-0.787302000
C	4.438346000	-1.186004000	-0.503659000
H	6.146491000	-0.491313000	0.611504000
H	4.910682000	1.372550000	1.685675000
H	2.516432000	1.726990000	1.177841000
H	2.561066000	-1.625280000	-1.488871000
H	4.980263000	-1.996355000	-0.981105000
C	0.933826000	0.221385000	-0.513259000
O	0.469747000	-0.348574000	-1.505820000
C	0.107934000	1.010564000	0.376485000
H	0.366392000	1.167020000	1.414431000
C	-1.158022000	1.346125000	-0.004452000
F	-1.488123000	1.659526000	-1.247111000
F	-1.965084000	1.971891000	0.841831000
N	-2.250255000	-0.449685000	-0.202168000
H	-1.612213000	-0.786441000	-0.928387000
C	-3.609710000	-0.342822000	-0.748599000
C	-4.621383000	0.154391000	0.276155000

H	-3.940143000	-1.309489000	-1.156664000
H	-3.553479000	0.355998000	-1.588103000
H	-5.580028000	0.334909000	-0.216278000
H	-4.792149000	-0.579104000	1.069685000
H	-4.288000000	1.088616000	0.734265000
C	-2.090045000	-1.264104000	1.000832000
C	-2.529200000	-2.717574000	0.842169000
H	-2.640849000	-0.781235000	1.815494000
H	-1.027477000	-1.219716000	1.263907000
H	-3.603379000	-2.795980000	0.648187000
H	-1.996230000	-3.193628000	0.012842000
H	-2.311995000	-3.281259000	1.753428000

G

C	5.036898000	0.116166000	-0.094353000
C	4.236677000	1.251380000	0.035591000
C	2.850688000	1.134082000	0.034276000
C	2.246480000	-0.121211000	-0.102944000
C	3.054007000	-1.258287000	-0.215189000
C	4.441471000	-1.137546000	-0.216630000
H	6.118352000	0.209255000	-0.091616000
H	4.693154000	2.229552000	0.148890000
H	2.237989000	2.020513000	0.164125000
H	2.583758000	-2.231200000	-0.304306000
H	5.057977000	-2.025805000	-0.311991000
C	0.771619000	-0.275606000	-0.124515000
O	0.368335000	-1.517671000	0.207753000
C	-0.072880000	0.724748000	-0.450192000
H	0.310517000	1.684633000	-0.769580000
C	-1.549095000	0.562702000	-0.567326000
F	-2.161529000	1.772460000	-0.291654000
F	-1.870569000	0.322467000	-1.882782000
N	-2.124573000	-0.495416000	0.233512000
H	-0.621735000	-1.493955000	0.231149000
C	-3.295327000	-1.167579000	-0.375016000
C	-4.534218000	-0.297059000	-0.580873000
H	-3.528824000	-2.004667000	0.290598000
H	-2.976289000	-1.594429000	-1.326864000
H	-4.920106000	0.095916000	0.363282000
H	-4.316262000	0.544064000	-1.242330000
H	-5.325593000	-0.897385000	-1.038532000
C	-2.395989000	-0.101576000	1.636900000

C	-1.193693000	0.400238000	2.428158000
H	-2.787974000	-1.004190000	2.115891000
H	-3.186123000	0.658133000	1.666942000
H	-1.501371000	0.527716000	3.469706000
H	-0.363839000	-0.310643000	2.400078000
H	-0.839243000	1.364734000	2.060559000

TS9, IF = -422.13 cm^{-1}

C	-5.059763000	0.621425000	0.005419000
C	-4.120396000	1.380223000	-0.692880000
C	-2.787424000	0.982226000	-0.724531000
C	-2.381167000	-0.176079000	-0.052779000
C	-3.329841000	-0.942732000	0.631950000
C	-4.662345000	-0.541476000	0.664166000
H	-6.099925000	0.931304000	0.027654000
H	-4.429206000	2.275450000	-1.223226000
H	-2.065472000	1.555695000	-1.297821000
H	-3.004718000	-1.847535000	1.133882000
H	-5.392197000	-1.137696000	1.202576000
C	-0.964898000	-0.620797000	-0.053761000
O	-0.776706000	-1.890235000	0.196987000
C	0.069380000	0.259482000	-0.247130000
H	-0.103092000	1.326690000	-0.244501000
C	1.428984000	-0.186400000	-0.452028000
F	1.490218000	-1.676290000	0.785862000
F	1.649664000	-1.015094000	-1.472498000
N	2.486005000	0.534862000	-0.123782000
H	0.246440000	-1.986400000	0.484523000
C	3.822109000	0.159772000	-0.608136000
C	4.397312000	-1.038913000	0.140536000
H	4.450374000	1.046425000	-0.481772000
H	3.753132000	-0.044071000	-1.677729000
H	4.454269000	-0.840064000	1.214288000
H	3.760487000	-1.913481000	0.000876000
H	5.404948000	-1.250883000	-0.227221000
C	2.420446000	1.426653000	1.038089000
C	2.418472000	2.895421000	0.631824000
H	3.287929000	1.197971000	1.666242000
H	1.530402000	1.166047000	1.613569000
H	2.417040000	3.531686000	1.520556000
H	3.303489000	3.142345000	0.038196000
H	1.533572000	3.133998000	0.035776000

H

C	−4.879510000	0.739349000	0.137390000
C	−3.816299000	1.570322000	−0.210208000
C	−2.522617000	1.055996000	−0.280469000
C	−2.283752000	−0.295211000	−0.013417000
C	−3.358583000	−1.126465000	0.316977000
C	−4.648065000	−0.611542000	0.400462000
H	−5.886255000	1.141384000	0.197429000
H	−3.994140000	2.618119000	−0.431669000
H	−1.706108000	1.708711000	−0.574417000
H	−3.155678000	−2.176663000	0.500888000
H	−5.475013000	−1.262467000	0.666879000
C	−0.912897000	−0.924959000	−0.095478000
O	−0.824625000	−2.136828000	−0.247531000
C	0.229378000	−0.028618000	0.042034000
H	0.060147000	0.990757000	0.354780000
C	1.518038000	−0.421319000	−0.165426000
F	1.778091000	−1.635409000	−0.644986000
N	2.647864000	0.284649000	0.048992000
C	3.953857000	−0.209590000	−0.390848000
C	4.661673000	−1.019131000	0.691477000
H	4.547567000	0.667555000	−0.669095000
H	3.821053000	−0.808447000	−1.293064000
H	4.784495000	−0.427751000	1.603836000
H	4.082132000	−1.912722000	0.934900000
H	5.652716000	−1.329208000	0.348692000
C	2.587187000	1.593648000	0.685048000
C	2.331881000	2.723109000	−0.311287000
H	3.542820000	1.746135000	1.197012000
H	1.814908000	1.567766000	1.459684000
H	2.294015000	3.686760000	0.203752000
H	3.129714000	2.765448000	−1.058434000
H	1.385012000	2.571848000	−0.836532000

TS10, IF = -699.17 cm^{-1}

C	5.021997000	0.838855000	0.136457000
C	4.016667000	1.735649000	−0.224266000
C	2.704881000	1.292020000	−0.369697000
C	2.385753000	−0.052488000	−0.153211000
C	3.401204000	−0.950460000	0.189667000
C	4.711560000	−0.505446000	0.340179000

H	6.044758000	1.185332000	0.249034000
H	4.256715000	2.779137000	-0.403215000
H	1.931663000	1.987477000	-0.681718000
H	3.140040000	-1.993590000	0.332663000
H	5.492654000	-1.208004000	0.613786000
C	0.992145000	-0.573190000	-0.291498000
O	0.871318000	-1.837114000	-0.497696000
C	-0.087854000	0.279979000	-0.129960000
H	0.055885000	1.281851000	0.246886000
C	-1.439373000	-0.114497000	-0.429589000
F	-1.711595000	-0.471828000	-1.711470000
N	-2.496545000	0.454789000	0.156712000
C	-3.851342000	0.179103000	-0.333369000
C	-4.406615000	1.347180000	-1.139985000
H	-4.477358000	-0.024269000	0.541545000
H	-3.835191000	-0.730339000	-0.935860000
H	-4.412247000	2.263862000	-0.542849000
H	-3.792774000	1.518493000	-2.027377000
H	-5.431846000	1.138703000	-1.457724000
C	-2.390122000	0.968910000	1.525980000
C	-2.335560000	-0.142902000	2.569177000
H	-3.262676000	1.611615000	1.678526000
H	-1.509245000	1.607909000	1.600157000
H	-2.307013000	0.291046000	3.572335000
H	-3.212888000	-0.792287000	2.496197000
H	-1.449420000	-0.762042000	2.416877000
O	-1.421758000	-1.957467000	0.138398000
H	-1.951811000	-2.472261000	-0.483793000
H	-0.335621000	-2.079328000	-0.174141000

I

C	-4.952495000	-0.665132000	0.627614000
C	-4.023139000	-1.670094000	0.360172000
C	-2.732368000	-1.341240000	-0.041768000
C	-2.351944000	-0.000837000	-0.175148000
C	-3.294511000	1.002737000	0.074529000
C	-4.584865000	0.670793000	0.479842000
H	-5.959862000	-0.923303000	0.938738000
H	-4.307555000	-2.713576000	0.452049000
H	-2.026675000	-2.130654000	-0.280207000
H	-3.005169000	2.040290000	-0.050224000
H	-5.305040000	1.458468000	0.677883000

C	−0.974525000	0.380753000	−0.580608000
O	−0.939098000	1.598084000	−1.164478000
C	0.091801000	−0.405049000	−0.336189000
H	−0.062164000	−1.342665000	0.182061000
C	1.516013000	−0.159087000	−0.716007000
F	1.880342000	−1.057344000	−1.727787000
N	2.415053000	−0.396932000	0.366106000
C	3.832675000	−0.229546000	0.034750000
C	4.703382000	−1.256973000	0.751107000
H	4.177990000	0.790374000	0.268026000
H	3.952446000	−0.376906000	−1.042396000
H	4.627466000	−1.164837000	1.837908000
H	4.391099000	−2.265767000	0.471423000
H	5.753981000	−1.121902000	0.478163000
C	2.030751000	0.196511000	1.651874000
C	1.837509000	1.715862000	1.664230000
H	2.814553000	−0.081954000	2.362405000
H	1.113849000	−0.288997000	1.996849000
H	1.690029000	2.058730000	2.692541000
H	2.706457000	2.238941000	1.253739000
H	0.961350000	2.007389000	1.079347000
O	1.641708000	1.119429000	−1.316398000
H	2.460240000	1.146011000	−1.828144000
H	−0.022031000	1.792681000	−1.422186000

TS10′, IF = -438.19 cm^{-1}

C	−5.244396000	1.370631000	−1.182919000
C	−4.414830000	2.488991000	−1.171977000
C	−3.045803000	2.346119000	−0.944199000
C	−2.495145000	1.083706000	−0.730075000
C	−3.331900000	−0.035361000	−0.738767000
C	−4.697969000	0.105172000	−0.962301000
H	−6.310242000	1.481302000	−1.358034000
H	−4.832613000	3.477087000	−1.340363000
H	−2.385639000	3.206186000	−0.927248000
H	−2.912995000	−1.016562000	−0.538557000
H	−5.339063000	−0.771445000	−0.957294000
C	−0.990003000	0.976354000	−0.535874000
O	−0.422528000	2.104840000	−0.267217000
C	−0.352251000	−0.021455000	−1.436290000
H	−0.981236000	−0.835164000	−1.769661000
C	0.961402000	−0.088394000	−1.714361000

N	1.653141000	-1.022525000	-2.438736000
C	0.944030000	-2.238089000	-2.821960000
C	0.764375000	-3.220822000	-1.662255000
H	1.515398000	-2.700388000	-3.633089000
H	-0.020331000	-1.950984000	-3.249766000
H	1.735083000	-3.590477000	-1.316621000
H	0.268574000	-2.738286000	-0.813749000
H	0.164891000	-4.081462000	-1.973967000
C	3.096976000	-1.148616000	-2.192643000
C	3.927906000	-0.214111000	-3.065276000
H	3.359920000	-2.187076000	-2.414861000
H	3.310541000	-0.986423000	-1.129736000
H	4.995099000	-0.376761000	-2.885224000
H	3.721405000	-0.397800000	-4.123354000
H	3.694541000	0.830144000	-2.846908000
N	-0.383506000	-2.020438000	1.724909000
C	0.676864000	-2.893406000	2.208067000
C	1.102470000	-2.559185000	3.636269000
H	1.531029000	-2.804803000	1.532349000
H	0.308021000	-3.923490000	2.149586000
H	1.872083000	-3.253523000	3.987055000
H	1.508349000	-1.544823000	3.668681000
H	0.250220000	-2.617058000	4.320787000
C	-1.762018000	-2.452006000	1.902680000
C	-2.195687000	-3.456857000	0.836203000
H	-1.859666000	-2.900792000	2.900338000
H	-2.397940000	-1.566499000	1.873514000
H	-3.231629000	-3.770486000	0.997363000
H	-2.118920000	-3.010458000	-0.160311000
H	-1.563845000	-4.351175000	0.848234000
C	-0.050622000	-0.767829000	1.262739000
O	-1.059779000	0.000720000	0.963349000
O	1.154226000	-0.462631000	1.155293000
H	1.820243000	1.284580000	1.209377000
N	1.632765000	2.293586000	1.093249000
H	0.652383000	2.198636000	0.389097000
C	2.744675000	2.978691000	0.398941000
C	1.286059000	2.895796000	2.397553000
C	4.090517000	2.338778000	0.711281000
H	2.728343000	4.029285000	0.705759000
H	2.543550000	2.948138000	-0.673915000
C	0.272122000	2.045185000	3.145920000

H	0.875087000	3.889535000	2.190447000
H	2.201646000	3.028933000	2.988452000
H	4.900114000	2.878194000	0.212791000
H	4.291877000	2.341806000	1.787219000
H	4.103373000	1.301399000	0.362345000
H	-0.021035000	2.548232000	4.070963000
H	-0.615320000	1.875570000	2.530945000
H	0.695714000	1.069058000	3.400311000
F	1.792246000	0.876701000	-1.280540000

I′

C	2.257017000	4.122219000	0.564370000
C	1.535069000	4.135315000	-0.627287000
C	0.834804000	3.001041000	-1.035726000
C	0.857515000	1.844427000	-0.257364000
C	1.571060000	1.836517000	0.941673000
C	2.272387000	2.969424000	1.348548000
H	2.805807000	5.003957000	0.880291000
H	1.518166000	5.029101000	-1.243435000
H	0.270316000	3.002076000	-1.962790000
H	1.585488000	0.937842000	1.551239000
H	2.833928000	2.950590000	2.277633000
C	0.027125000	0.636094000	-0.690868000
O	-0.106548000	0.554861000	-2.073587000
C	-1.330303000	0.697900000	-0.054884000
H	-1.569481000	1.561110000	0.548196000
C	-2.258212000	-0.256180000	-0.258959000
N	-3.568913000	-0.271274000	0.105518000
C	-4.162766000	0.912013000	0.703938000
C	-3.938156000	1.005801000	2.213638000
H	-5.235573000	0.884069000	0.482962000
H	-3.756496000	1.791013000	0.193562000
H	-4.379467000	0.144612000	2.724519000
H	-2.870975000	1.028216000	2.448932000
H	-4.400780000	1.911983000	2.614630000
C	-4.335649000	-1.514776000	0.125634000
C	-5.163715000	-1.705157000	-1.141916000
H	-4.986504000	-1.484581000	1.007190000
H	-3.652119000	-2.355203000	0.262839000
H	-5.764229000	-2.617294000	-1.076339000
H	-5.840874000	-0.859055000	-1.293352000
H	-4.507340000	-1.778714000	-2.012199000

H	0.795092000	0.477375000	-2.431756000
N	2.348606000	-2.043647000	-0.131979000
C	1.597811000	-2.786205000	0.880101000
C	1.608717000	-2.138277000	2.262495000
H	2.052272000	-3.781130000	0.926891000
H	0.566854000	-2.909717000	0.535729000
H	1.122672000	-2.796237000	2.989349000
H	2.631875000	-1.946760000	2.598068000
H	1.061475000	-1.193354000	2.239503000
C	3.636821000	-2.561339000	-0.576591000
C	4.709634000	-2.460567000	0.503719000
H	3.501390000	-3.606662000	-0.881943000
H	3.925268000	-1.987279000	-1.457307000
H	5.664215000	-2.836576000	0.124817000
H	4.842279000	-1.418683000	0.808851000
H	4.444771000	-3.049678000	1.387687000
C	1.856337000	-0.918698000	-0.708927000
O	2.414225000	-0.282701000	-1.596376000
O	0.659218000	-0.581469000	-0.185113000
F	-1.922667000	-1.371044000	-0.929722000

TS10′′, IF = -1227.07 cm^{-1}

C	-5.018792000	-1.121586000	-0.086911000
C	-3.924199000	-1.933910000	-0.380516000
C	-2.643074000	-1.389980000	-0.425760000
C	-2.442475000	-0.028127000	-0.175875000
C	-3.547590000	0.784500000	0.097218000
C	-4.827318000	0.239497000	0.149016000
H	-6.017469000	-1.546063000	-0.052225000
H	-4.069791000	-2.989836000	-0.586440000
H	-1.799511000	-2.020758000	-0.689100000
H	-3.380495000	1.842855000	0.266153000
H	-5.677193000	0.877426000	0.371074000
C	-1.084547000	0.605845000	-0.210388000
O	-1.085328000	1.860631000	-0.494826000
C	0.015689000	-0.186603000	0.074017000
H	-0.164897000	-1.165211000	0.488731000
C	1.382464000	0.181947000	-0.149280000
F	1.584085000	1.134209000	-1.087570000
N	2.368619000	-0.753321000	-0.174449000
C	3.735778000	-0.336631000	-0.494524000
C	4.247354000	-1.010481000	-1.762955000

H	4.382303000	-0.578932000	0.360187000
H	3.754249000	0.747202000	-0.623188000
H	4.213843000	-2.100014000	-1.672018000
H	3.628449000	-0.719480000	-2.614846000
H	5.282187000	-0.717844000	-1.960910000
C	2.244973000	-1.971602000	0.625515000
C	2.267602000	-1.721347000	2.132383000
H	3.081149000	-2.613077000	0.331986000
H	1.336715000	-2.501758000	0.328164000
H	2.195450000	-2.670676000	2.670136000
H	3.199203000	-1.230499000	2.431726000
H	1.440653000	-1.073655000	2.432344000
O	1.811629000	1.283783000	1.281274000
H	2.767163000	1.404897000	1.362016000
H	1.274580000	2.317055000	0.989737000
O	0.580021000	3.204752000	0.573421000
H	1.050374000	3.767191000	-0.050891000
H	-0.219832000	2.574067000	-0.003965000

TS11, IF = -358.10 cm^{-1}

C	-5.062198000	-0.629248000	0.007200000
C	-4.122391000	-1.370752000	0.723746000
C	-2.790011000	-0.971592000	0.748236000
C	-2.380900000	0.169792000	0.048574000
C	-3.330275000	0.919015000	-0.654472000
C	-4.663308000	0.517219000	-0.677829000
H	-6.102240000	-0.939716000	-0.008454000
H	-4.430715000	-2.253947000	1.274232000
H	-2.070298000	-1.534232000	1.334923000
H	-3.006467000	1.811249000	-1.178952000
H	-5.392064000	1.101263000	-1.230971000
C	-0.965427000	0.611579000	0.036522000
O	-0.784963000	1.898534000	-0.254874000
C	0.075293000	-0.226344000	0.274962000
H	-0.083850000	-1.289907000	0.392348000
C	1.459169000	0.257979000	0.464418000
F	1.498064000	1.556563000	-0.854563000
N	2.485892000	-0.542161000	0.161569000
C	3.838175000	-0.187732000	0.607796000
C	4.420149000	1.006222000	-0.144669000
H	4.451411000	-1.081830000	0.459457000
H	3.803044000	0.010704000	1.680433000

H	4.430687000	0.824413000	-1.222942000
H	3.816275000	1.896871000	0.034165000
H	5.446386000	1.187038000	0.187558000
C	2.390752000	-1.407639000	-1.015994000
C	2.423110000	-2.885454000	-0.644350000
H	3.227138000	-1.156062000	-1.678143000
H	1.477518000	-1.152399000	-1.556326000
H	2.404035000	-3.504288000	-1.545465000
H	3.328571000	-3.132114000	-0.082050000
H	1.560383000	-3.148766000	-0.026155000
O	1.710089000	1.073525000	1.502955000
H	0.912575000	1.587086000	1.692637000
H	0.189960000	1.965951000	-0.595696000

J

C	-4.864904000	0.798154000	-0.013218000
C	-3.784572000	1.537224000	-0.491412000
C	-2.503499000	0.987278000	-0.481367000
C	-2.294316000	-0.309264000	-0.002435000
C	-3.386330000	-1.050731000	0.458960000
C	-4.663176000	-0.498686000	0.461715000
H	-5.861788000	1.228455000	-0.016118000
H	-3.939397000	2.540189000	-0.877205000
H	-1.671671000	1.562851000	-0.876592000
H	-3.206686000	-2.062931000	0.807118000
H	-5.503618000	-1.078828000	0.830289000
C	-0.935887000	-0.974546000	0.011975000
O	-0.880377000	-2.197107000	0.053480000
C	0.222543000	-0.086406000	0.023466000
H	0.057260000	0.956034000	0.252348000
C	1.508227000	-0.511562000	-0.165050000
N	2.625429000	0.224583000	0.123233000
C	3.902668000	-0.035052000	-0.539984000
C	4.893155000	-0.784983000	0.349812000
H	4.330005000	0.931088000	-0.830740000
H	3.715376000	-0.584598000	-1.465798000
H	5.061252000	-0.245222000	1.286074000
H	4.526936000	-1.784001000	0.608290000
H	5.855027000	-0.898882000	-0.157664000
C	2.518710000	1.473976000	0.865763000
C	2.246110000	2.691650000	-0.018325000
H	3.461138000	1.611168000	1.408059000

H	1.733695000	1.352759000	1.616760000
H	2.169543000	3.594294000	0.594046000
H	3.053966000	2.843338000	-0.740224000
H	1.314854000	2.572998000	-0.577824000
O	1.738830000	-1.726658000	-0.702623000
H	2.506110000	-2.142986000	-0.289709000

TS12, IF = -327.35 cm^{-1}

C	-3.330236000	-4.039917000	-0.168812000
C	-3.381682000	-3.221970000	-1.294206000
C	-2.504670000	-2.143244000	-1.419629000
C	-1.571062000	-1.872441000	-0.420378000
C	-1.520698000	-2.699168000	0.705699000
C	-2.393406000	-3.775014000	0.832281000
H	-4.011957000	-4.879096000	-0.069788000
H	-4.103445000	-3.423723000	-2.080236000
H	-2.527204000	-1.501331000	-2.294064000
H	-0.801604000	-2.487419000	1.491332000
H	-2.347459000	-4.406870000	1.714382000
C	-0.602859000	-0.716118000	-0.611315000
O	-0.948997000	0.112303000	-1.605105000
C	0.819569000	-1.083041000	-0.554293000
H	1.110283000	-1.847584000	0.150374000
C	1.759904000	-0.444711000	-1.330918000
N	3.103597000	-0.679387000	-1.279013000
C	3.665547000	-1.555416000	-0.267978000
C	3.830130000	-0.850696000	1.079775000
H	4.635144000	-1.904206000	-0.638876000
H	3.038274000	-2.447064000	-0.168860000
H	4.531687000	-0.015332000	0.988768000
H	2.866011000	-0.452953000	1.412683000
H	4.208897000	-1.540005000	1.841469000
C	4.021012000	0.046216000	-2.149707000
C	4.268003000	-0.682925000	-3.468248000
H	4.960368000	0.172169000	-1.598996000
H	3.616844000	1.041843000	-2.338220000
H	4.984894000	-0.134546000	-4.087401000
H	4.664861000	-1.687397000	-3.289330000
H	3.328693000	-0.776133000	-4.019028000
O	1.413832000	0.459118000	-2.249112000
H	0.398593000	0.487927000	-2.177965000
N	0.582125000	0.644216000	2.448170000

C	1.551068000	1.590932000	2.987039000
C	0.886101000	2.780636000	3.675871000
H	2.180087000	1.936281000	2.163658000
H	2.188229000	1.044146000	3.691059000
H	1.638026000	3.453112000	4.099134000
H	0.291279000	3.339266000	2.948870000
H	0.230054000	2.449326000	4.487182000
C	0.108710000	-0.419439000	3.324204000
C	1.080774000	-1.593967000	3.412887000
H	-0.048250000	0.007190000	4.324167000
H	-0.861534000	-0.751102000	2.953226000
H	0.690356000	-2.361977000	4.087742000
H	1.234087000	-2.040882000	2.425963000
H	2.058339000	-1.277084000	3.790076000
C	0.004991000	0.927972000	1.241472000
O	-0.935465000	0.082568000	0.845604000
O	0.342951000	1.929104000	0.595244000
H	-1.563229000	2.381307000	0.024617000
N	-1.950810000	2.279921000	-0.919019000
H	-1.557276000	1.221256000	-1.212521000
C	-1.249955000	3.243952000	-1.795256000
C	-3.424467000	2.319466000	-0.924317000
C	-1.403448000	4.687137000	-1.338567000
H	-1.631042000	3.098499000	-2.811254000
H	-0.198175000	2.945235000	-1.772550000
C	-3.976495000	1.241011000	-0.002773000
H	-3.745595000	2.152696000	-1.957900000
H	-3.770444000	3.312762000	-0.619701000
H	-0.806689000	5.343202000	-1.976796000
H	-2.440625000	5.030089000	-1.386321000
H	-1.040857000	4.798463000	-0.311790000
H	-5.068836000	1.253759000	-0.024125000
H	-3.627538000	0.250364000	-0.307724000
H	-3.647175000	1.402289000	1.027737000

K

C	1.884672000	4.099515000	0.858458000
C	1.027941000	4.156745000	-0.240033000
C	0.411824000	2.999088000	-0.709367000
C	0.654847000	1.773436000	-0.088859000
C	1.505189000	1.718569000	1.015158000
C	2.120443000	2.877774000	1.485253000

H	2.366161000	5.001525000	1.222935000
H	0.837969000	5.105185000	-0.732939000
H	-0.261268000	3.035448000	-1.560006000
H	1.696528000	0.767247000	1.502233000
H	2.787212000	2.824019000	2.340416000
C	-0.087726000	0.536854000	-0.584501000
O	-0.274412000	0.574336000	-1.979800000
C	-1.394014000	0.387119000	0.114647000
H	-1.471010000	0.850866000	1.085693000
C	-2.401394000	-0.398580000	-0.365785000
N	-3.562699000	-0.685248000	0.299212000
C	-3.819878000	-0.066372000	1.590909000
C	-3.164599000	-0.825323000	2.743638000
H	-4.905000000	-0.046866000	1.730782000
H	-3.492386000	0.980731000	1.575138000
H	-3.566813000	-1.840638000	2.802964000
H	-2.084140000	-0.896470000	2.594137000
H	-3.352472000	-0.319933000	3.695586000
C	-4.699016000	-1.253741000	-0.422688000
C	-5.491358000	-0.203573000	-1.198613000
H	-5.333132000	-1.745412000	0.322342000
H	-4.332642000	-2.027603000	-1.097337000
H	-6.350820000	-0.658626000	-1.700010000
H	-5.861167000	0.581530000	-0.531203000
H	-4.853086000	0.259798000	-1.955630000
O	-2.349286000	-0.998498000	-1.573541000
H	0.620290000	0.574036000	-2.371843000
N	2.608699000	-1.836270000	-0.361734000
C	2.054244000	-2.720996000	0.664723000
C	2.012633000	-2.114122000	2.064814000
H	2.684695000	-3.615596000	0.662316000
H	1.047894000	-3.026584000	0.364096000
H	1.727129000	-2.878414000	2.793794000
H	2.990156000	-1.713129000	2.348294000
H	1.272997000	-1.311773000	2.108096000
C	3.938118000	-2.118217000	-0.892207000
C	5.038819000	-1.827166000	0.123487000
H	3.969044000	-3.170876000	-1.199118000
H	4.066143000	-1.502253000	-1.782461000
H	6.020762000	-2.029468000	-0.313369000
H	5.002664000	-0.777127000	0.427671000
H	4.933830000	-2.451170000	1.016875000

C	1.910562000	-0.789797000	-0.862749000
O	2.304465000	-0.046920000	-1.758807000
O	0.705465000	-0.662863000	-0.267704000
H	-1.579226000	-0.633552000	-2.050696000

TS13, IF = -588.14 cm^{-1}

C	2.564154000	3.926004000	0.691292000
C	1.424682000	4.140521000	-0.083951000
C	0.594657000	3.073528000	-0.415438000
C	0.900989000	1.785089000	0.027399000
C	2.043744000	1.570598000	0.798984000
C	2.872045000	2.640293000	1.131311000
H	3.212338000	4.758040000	0.948098000
H	1.185832000	5.139056000	-0.436007000
H	-0.285548000	3.217329000	-1.034073000
H	2.286195000	0.571175000	1.149389000
H	3.757876000	2.468274000	1.734515000
C	-0.050789000	0.675053000	-0.287648000
O	-0.273673000	0.790615000	-2.062661000
C	-1.352908000	0.739666000	0.241087000
H	-1.604653000	1.575756000	0.875095000
C	-2.335972000	-0.119846000	-0.342273000
N	-3.548572000	-0.310093000	0.241744000
C	-3.869215000	0.216047000	1.561271000
C	-3.338724000	-0.671132000	2.685362000
H	-4.959697000	0.296362000	1.619398000
H	-3.482784000	1.233492000	1.660148000
H	-3.756843000	-1.679326000	2.606396000
H	-2.249529000	-0.741017000	2.619404000
H	-3.606404000	-0.261582000	3.663867000
C	-4.563037000	-1.104675000	-0.443150000
C	-5.478074000	-0.241799000	-1.308025000
H	-5.139535000	-1.634593000	0.323813000
H	-4.053512000	-1.848027000	-1.056969000
H	-6.246476000	-0.853707000	-1.789799000
H	-5.977675000	0.525666000	-0.707951000
H	-4.889722000	0.253928000	-2.084305000
O	-2.107706000	-0.694131000	-1.461381000
H	0.547376000	0.442215000	-2.459963000
N	2.198078000	-2.068547000	-0.324564000
C	1.568075000	-2.777174000	0.794471000
C	1.693170000	-2.065490000	2.139080000

H	2.056354000	-3.755190000	0.840237000
H	0.513498000	-2.944842000	0.558345000
H	1.318946000	-2.713731000	2.936950000
H	2.736764000	-1.819136000	2.357663000
H	1.101449000	-1.146949000	2.144121000
C	3.434730000	-2.598666000	-0.890881000
C	4.628663000	-2.382637000	0.033847000
H	3.287986000	-3.667133000	-1.087366000
H	3.593998000	-2.097396000	-1.845761000
H	5.540496000	-2.773362000	-0.426133000
H	4.767220000	-1.314656000	0.226485000
H	4.489201000	-2.893682000	0.991797000
C	1.661299000	-0.953789000	-0.866770000
O	2.121742000	-0.332741000	-1.815688000
O	0.508042000	-0.620973000	-0.225610000
H	-1.061867000	0.061807000	-2.020762000

TS13′, IF = -516.30 cm^{-1}

C	2.198223000	4.270452000	0.536607000
C	1.395447000	4.272873000	-0.602536000
C	0.737176000	3.110136000	-0.998540000
C	0.879967000	1.939380000	-0.253133000
C	1.678854000	1.938327000	0.890629000
C	2.338186000	3.100359000	1.282036000
H	2.714042000	5.175381000	0.841926000
H	1.284061000	5.179992000	-1.188305000
H	0.117424000	3.098401000	-1.889605000
H	1.781035000	1.028692000	1.476605000
H	2.961930000	3.091972000	2.170328000
C	0.091058000	0.707065000	-0.622780000
O	0.353465000	0.613550000	-2.289555000
C	-1.298959000	0.789619000	-0.317433000
H	-1.650027000	1.782281000	-0.086537000
C	-2.162659000	-0.324624000	-0.176576000
N	-3.400187000	-0.152360000	0.388039000
C	-3.887320000	1.131275000	0.869889000
C	-3.385079000	1.466811000	2.273602000
H	-4.981299000	1.080215000	0.865996000
H	-3.621438000	1.920237000	0.160475000
H	-3.702750000	0.697390000	2.983998000
H	-2.292880000	1.513686000	2.285692000
H	-3.781173000	2.430181000	2.608492000

C	-4.289108000	-1.300005000	0.531355000
C	-5.195873000	-1.483875000	-0.683274000
H	-4.886363000	-1.141287000	1.436716000
H	-3.679400000	-2.190803000	0.683130000
H	-5.875355000	-2.329308000	-0.537961000
H	-5.798035000	-0.587331000	-0.863345000
H	-4.586163000	-1.674465000	-1.570189000
O	-1.874111000	-1.523189000	-0.533734000
H	1.329024000	0.549076000	-2.375399000
N	2.251331000	-2.014959000	0.113256000
C	1.279536000	-2.740282000	0.942262000
C	1.079635000	-2.126449000	2.325095000
H	1.662394000	-3.761780000	1.029765000
H	0.324077000	-2.780043000	0.411703000
H	0.419366000	-2.762225000	2.922047000
H	2.031914000	-2.022102000	2.853497000
H	0.611608000	-1.142805000	2.237345000
C	3.565188000	-2.603841000	-0.120314000
C	4.417488000	-2.636905000	1.144342000
H	3.420471000	-3.619055000	-0.509864000
H	4.050204000	-2.011125000	-0.896201000
H	5.397773000	-3.069282000	0.925659000
H	4.562694000	-1.624573000	1.532019000
H	3.950505000	-3.243433000	1.926614000
C	1.924728000	-0.869433000	-0.516315000
O	2.639072000	-0.238063000	-1.286869000
O	0.659084000	-0.498374000	-0.180454000
H	-0.047489000	-0.373203000	-2.533212000
O	-0.493627000	-1.645554000	-2.527354000
H	-1.100093000	-1.646615000	-1.624584000
H	-1.044049000	-1.909081000	-3.271639000

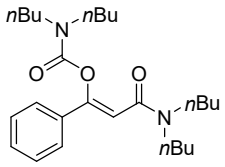
4ab

C	-5.105232000	-1.134441000	0.294833000
C	-4.457192000	-1.912613000	-0.664717000
C	-3.087310000	-1.780481000	-0.863590000
C	-2.346627000	-0.872747000	-0.097969000
C	-3.003253000	-0.083984000	0.851944000
C	-4.374887000	-0.217641000	1.048422000
H	-6.175638000	-1.233852000	0.444397000
H	-5.023595000	-2.612438000	-1.270938000
H	-2.595030000	-2.359738000	-1.638735000

H	-2.433421000	0.634412000	1.432743000
H	-4.874717000	0.399163000	1.788588000
C	-0.887329000	-0.754521000	-0.268907000
C	-0.047966000	-1.683221000	-0.730485000
H	-0.403717000	-2.663051000	-1.030765000
C	1.408532000	-1.340614000	-0.893873000
N	2.264838000	-1.832036000	0.043216000
C	1.827184000	-2.543453000	1.239429000
C	1.539580000	-1.594791000	2.400965000
H	2.615133000	-3.257566000	1.503321000
H	0.935304000	-3.127418000	1.001917000
H	2.420899000	-0.988135000	2.634533000
H	0.721320000	-0.918206000	2.136410000
H	1.259940000	-2.152668000	3.299273000
C	3.680291000	-1.489073000	-0.074289000
C	4.427835000	-2.471457000	-0.970808000
H	4.104200000	-1.480991000	0.935383000
H	3.753319000	-0.478326000	-0.484135000
H	5.487640000	-2.208271000	-1.032349000
H	4.348243000	-3.491494000	-0.582067000
H	4.004082000	-2.445435000	-1.977573000
O	1.788563000	-0.639355000	-1.824884000
N	0.565168000	2.421393000	-0.268355000
C	1.631691000	2.104980000	0.681779000
C	1.212075000	2.267405000	2.140084000
H	2.463370000	2.778056000	0.449002000
H	1.979261000	1.083268000	0.496277000
H	2.050431000	2.036598000	2.804905000
H	0.881686000	3.290427000	2.340419000
H	0.389703000	1.586849000	2.375003000
C	0.649530000	3.662882000	-1.030039000
C	0.512755000	4.897842000	-0.145625000
H	1.609483000	3.678625000	-1.562176000
H	-0.144163000	3.632056000	-1.776711000
H	0.563012000	5.803483000	-0.756432000
H	-0.445282000	4.886909000	0.381712000
H	1.315081000	4.952593000	0.597250000
C	-0.382300000	1.515544000	-0.612089000
O	-1.216304000	1.618219000	-1.482325000
O	-0.297366000	0.410129000	0.21175100

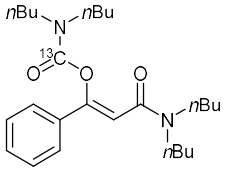
E. Analytical data

(*Z*)-3-(Dibutylamino)-3-oxo-1-phenylprop-1-en-1-yl dibutylcarbamate (4aa)



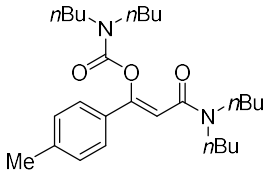
Yellow oil (30.1 mg, 70%). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.51 – 7.46 (m, 2 H), 7.38 – 7.31 (m, 3 H), 6.26 (s, 1 H), 3.39 – 3.30 (m, 6 H), 3.23 (t, J = 7.8 Hz, 2 H), 1.70 – 1.61 (m, 2 H), 1.60 – 1.50 (m, 6 H), 1.38 – 1.27 (m, 8 H), 0.96 – 0.88 (m, 12 H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 164.9, 153.1, 152.2, 135.2, 129.3, 128.4, 125.4, 109.2, 48.0, 47.6, 47.5, 44.8, 31.0, 30.9, 30.0, 29.7, 20.2, 20.1, 20.0, 19.9, 13.9, 13.8, 13.8. IR (KBr): 2958, 2929, 2876, 1724, 1626, 1463, 1425, 1213, 1147, 1075, 755 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{26}H_{43}N_2O_3$ $[M + H]^+$: 431.3268, found: 431.3267.

(*Z*)-3-(Dibutylamino)-3-oxo-1-phenylprop-1-en-1-yl dibutylcarbamate-^{13}C (4aa-^{13}C)



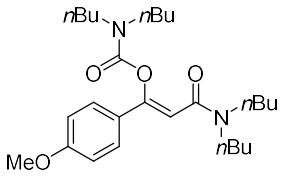
Yellow oil (11.2 mg, 26%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.51 – 7.46 (m, 2 H), 7.39 – 7.32 (m, 3 H), 6.26 (d, J = 1.2 Hz , 1 H), 3.40 – 3.31 (m, 6 H), 3.27 – 3.21 (m, 2 H), 1.70 – 1.62 (m, 2 H), 1.60 – 1.50 (m, 6 H), 1.36 – 1.26 (m, 8 H), 0.96 – 0.89 (m, 12 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 164.9, 153.1, 152.9, 135.3, 129.3, 128.5, 125.4, 109.2, 48.0, 47.7, 47.6, 44.9, 31.0, 30.9, 30.1, 29.8, 20.2, 20.1, 20.0, 20.0, 14.0, 13.9, 13.9. HRMS-ESI (*m/z*): calcd for $C_{25}{}^{13}CH_{43}N_2O_3$ $[M + H]^+$: 432.3302, found: 432.3300.

(*Z*)-3-(Dibutylamino)-3-oxo-1-(*p*-tolyl)prop-1-en-1-yl dibutylcarbamate (4ba)



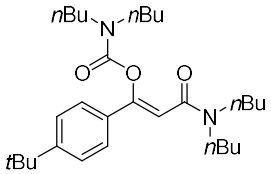
Pale yellow oil (28.4 mg, 64%). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.37 (d, J = 7.5 Hz, 2 H), 7.16 (d, J = 8.0 Hz, 2 H), 6.22 (s, 1 H), 3.39 – 3.30 (m, 6 H), 3.23 (t, J = 7.6 Hz, 2 H), 2.35 (s, 3 H), 1.65 (p, J = 7.8 Hz, 2 H), 1.60 – 1.49 (m, 6 H), 1.36 – 1.27 (m, 8 H), 0.96 – 0.89 (m, 12 H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.1, 153.2, 152.4, 139.4, 132.5, 129.2, 125.4, 108.3, 48.0, 47.6, 47.6, 44.9, 31.0, 30.9, 30.1, 29.8, 21.2, 20.2, 20.1, 20.0, 20.0, 13.9, 13.9, 13.8. IR (KBr): 3011, 2954, 2866, 1783, 1723, 1630, 1517, 1465, 1424, 1376, 1266, 1211, 1150, 934, 885, 808, 716, 661 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{27}H_{45}N_2O_3$ $[M + H]^+$: 445.3425; found: 445.3420.

(*Z*)-3-(Dibutylamino)-1-(4-methoxyphenyl)-3-oxoprop-1-en-1-yl dibutylcarbamate (4ca)



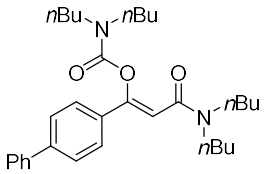
Pale yellow oil (23.0 mg, 50%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.42 (d, J = 8.4 Hz, 2 H), 6.87 (d, J = 8.4 Hz, 2 H), 6.16 (s, 1 H), 3.80 (s, 3 H), 3.34 (p, J = 7.6 Hz, 6 H), 3.23 (t, J = 7.6 Hz, 2 H), 1.71 – 1.61 (m, 2 H), 1.59 – 1.47 (m, 6 H), 1.38 – 1.27 (m, 8 H), 0.96 – 0.88 (m, 12 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.0, 160.5, 153.2, 152.3, 127.9, 126.9, 113.9, 107.2, 55.3, 48.0, 47.6, 47.5, 44.9, 31.0, 30.9, 30.0, 29.8, 20.2, 20.1, 20.0, 20.0, 13.9, 13.8, 13.8. IR (KBr): 2951, 2868, 1722, 1616, 1513, 1458, 1373, 1253, 1149, 1077, 1030, 933, 821, 747 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{27}H_{45}N_2O_4$ $[M + H]^+$: 461.3374; found: 461.3371.

(*Z*)-1-(4-(*tert*-Butyl)phenyl)-3-(dibutylamino)-3-oxoprop-1-en-1-yl dibutylcarbamate (4da)



Pale yellow oil (34.5 mg, 71%). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.42 (d, J = 8.5 Hz, 2 H), 7.36 (d, J = 8.5 Hz, 2 H), 6.24 (s, 1 H), 3.39 – 3.30 (m, 6 H), 3.23 (t, J = 7.5 Hz, 2 H), 1.65 (p, J = 7.8 Hz, 2 H), 1.58 – 1.49 (m, 6 H), 1.36 – 1.27 (m, 17 H), 0.96 – 0.88 (m, 12 H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.0, 153.2, 152.4, 152.3, 132.3, 125.4, 125.1, 108.3, 48.0, 47.6, 47.5, 44.8, 34.6, 31.1, 31.0, 30.9, 30.0, 29.8, 20.2, 20.0, 20.0, 19.9, 13.9, 13.8, 13.8, 13.8. IR (KBr): 3044, 2953, 2872, 1724, 1634, 1459, 1373, 1271, 1210, 1144, 1080, 1011, 938, 823, 743 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{30}H_{51}N_2O_3$ $[M + H]^+$: 487.3894; found: 487.3890.

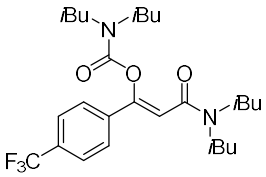
(*Z*)-1-([1,1'-Biphenyl]-4-yl)-3-(dibutylamino)-3-oxoprop-1-en-1-yl dibutylcarbamate (4ea)



Pale yellow oil (28.8 mg, 57%). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.64 – 7.55 (m, 6 H), 7.44 (t, J = 7.5 Hz, 2 H), 7.35 (t, J = 7.5 Hz, 1 H), 6.32 (s, 1 H), 3.43 – 3.33 (m, 6 H), 3.26 (t, J = 7.8 Hz, 2 H), 1.69 (p, J = 7.9 Hz, 2 H), 1.57 (hept, J = 7.8 Hz, 6 H), 1.41 – 1.30 (m, 8 H), 0.99 – 0.90 (m, 12 H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 164.9, 153.2, 152.0, 142.1, 140.3, 134.2, 128.8, 127.6, 127.2, 127.0, 125.8, 109.1, 48.0, 47.7, 47.6, 44.9, 31.0, 30.9, 30.0, 29.8, 20.2, 20.1, 20.0, 20.0, 13.9, 13.9, 13.8. IR

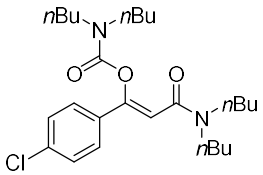
(KBr): 3035, 2949, 2868, 1722, 1631, 1531, 1464, 1428, 1268, 1209, 1146, 1071, 999, 825, 758, 659 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{32}H_{47}N_2O_3$ $[M + H]^+$: 507.3581; found: 507.3575.

(*Z*)-3-(Diisobutylamino)-3-oxo-1-(4-(trifluoromethyl)phenyl)prop-1-en-1-yl diisobutylcarbamate (4fa)



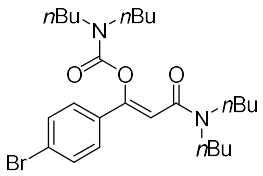
Brown solid (35.4 mg, 71%). mp: 138 – 140 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.59 (q, *J* = 8.0 Hz, 4 H), 6.35 (s, 1 H), 3.24-3.19 (m, 6 H), 3.09 (d, *J* = 4.0 Hz, 2 H), 2.13-1.95 (m, 4 H), 0.96-0.88 (m, 24 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 164.94, 153.55, 150.90, 139.05, 131.05 (q, *J* = 32.0 Hz), 125.90, 125.72, 125.58 (q, *J* = 4.0 Hz), 123.88 (q, *J* = = 270.0 Hz), 111.98, 56.08, 55.64, 55.50, 52.52, 27.71, 27.43, 26.70, 26.54, 20.28, 20.20, 20.12, 20.05. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -62.81 (s). IR (KBr): 2952, 1722, 1633, 1448, 1322, 1238, 1138, 938, 830, 744 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{27}H_{42}F_3N_2O_3$ $(M + H)^+$: 499.3142, found: 499.3144.

(*Z*)-1-(4-Chlorophenyl)-3-(dibutylamino)-3-oxoprop-1-en-1-yl dibutylcarbamate (4ga)



Pale yellow oil (33.4 mg, 72%). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.40 (d, *J* = 8.0 Hz, 2 H), 7.32 (d, *J* = 8.5 Hz, 2 H), 6.23 (s, 1 H), 3.37 – 3.29 (m, 6 H), 3.23 (t, *J* = 7.5 Hz, 2 H), 1.64 (p, *J* = 7.6 Hz, 2 H), 1.59 – 1.49 (m, 6 H), 1.38 – 1.28 (m, 8 H), 0.97 – 0.89 (m, 12 H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 164.6, 153.0, 151.2, 135.2, 133.9, 128.8, 126.7, 109.7, 48.0, 47.7, 47.6, 44.9, 31.0, 30.9, 30.0, 29.8, 20.2, 20.1, 20.0, 20.0, 13.9, 13.9, 13.8. IR (KBr): 2949, 2868, 1722, 1631, 1461, 1376, 1214, 1148, 1081, 1007, 934, 811, 739, 657 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{26}H_{42}ClN_2O_3$ $[M + H]^+$: 465.2878; found: 465.2877.

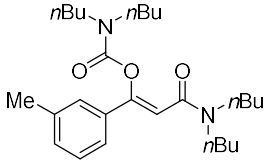
(*Z*)-1-(4-Bromophenyl)-3-(dibutylamino)-3-oxoprop-1-en-1-yl dibutylcarbamate (4ha)



Pale yellow oil (35.1 mg, 69%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.48 (d, *J* = 8.4 Hz, 2 H), 7.33 (d, *J* = 8.0 Hz, 2 H), 6.24 (s, 1 H), 3.38 – 3.29 (m, 6 H), 3.22 (t, *J* = 7.8 Hz, 2 H), 1.68 – 1.60 (m, 2 H), 1.58 – 1.48 (m,

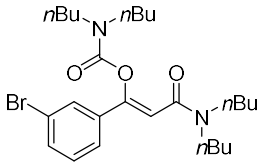
6 H), 1.36 – 1.27 (m, 8 H), 0.95 – 0.88 (m, 12 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 164.6, 153.0, 151.2, 134.3, 131.7, 126.9, 123.5, 109.8, 48.0, 47.7, 47.6, 44.9, 31.0, 30.9, 30.0, 29.8, 20.2, 20.1, 20.0, 19.9, 13.9, 13.8, 13.8. IR (KBr): 3031, 2950, 2867, 1724, 1634, 1551, 1468, 1376, 1214, 1148, 1072, 1002, 922, 811, 736, 655 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{26}H_{42}BrN_2O_3$ $[M + H]^+$: 509.2373; found: 509.2368.

(*Z*)-3-(Dibutylamino)-3-oxo-1-(*m*-tolyl)prop-1-en-1-yl dibutylcarbamate (4ia)



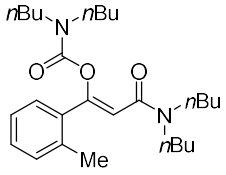
Pale yellow oil (32.9 mg, 74%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.33 – 7.23 (m, 3 H), 7.17 (d, *J* = 7.2 Hz, 1 H), 6.26 (s, 1 H), 3.43 – 3.33 (m, 6 H), 3.26 (t, *J* = 7.6 Hz, 2 H), 2.37 (s, 3 H), 1.68 (p, *J* = 8.0 Hz, 2 H), 1.61 – 1.51 (m, 6 H), 1.41 – 1.29 (m, 8 H), 0.99 – 0.91 (m, 12 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.0, 153.2, 152.4, 138.0, 135.3, 130.1, 128.4, 126.1, 122.6, 109.1, 48.0, 47.6, 47.5, 44.9, 31.0, 30.9, 30.0, 29.8, 21.4, 20.2, 20.1, 20.0, 20.0, 13.9, 13.9, 13.8. IR (KBr): 3047, 2953, 2866, 1723, 1629, 1466, 1424, 1372, 1264, 1211, 1148, 1079, 995, 937, 748 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{27}H_{45}N_2O_3$ $[M + H]^+$: 445.3425; found: 445.3422.

(*Z*)-1-(3-Bromophenyl)-3-(dibutylamino)-3-oxoprop-1-en-1-yl dibutylcarbamate (4ja)



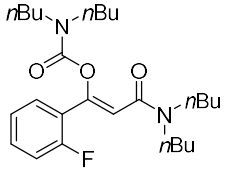
Pale yellow oil (34.5 mg, 68%). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.61 (t, *J* = 2.0 Hz, 1 H), 7.47 (dd, *J* = 8.0, 2.0 Hz, 1 H), 7.41 (dt, *J* = 8.0, 1.3 Hz, 1 H), 7.23 (t, *J* = 7.8 Hz, 1 H), 6.25 (s, 1 H), 3.42 – 3.30 (m, 6 H), 3.24 (t, *J* = 7.5 Hz, 2 H), 1.67 – 1.62 (m, 2 H), 1.59 – 1.49 (m, 6 H), 1.40 – 1.29 (m, 8 H), 0.94 (dq, *J* = 15.0, 7.5 Hz, 12 H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 164.5, 153.0, 150.6, 137.4, 132.2, 130.1, 128.5, 124.0, 122.7, 110.5, 48.0, 47.7, 47.6, 44.9, 31.0, 30.9, 30.0, 29.8, 20.2, 20.1, 20.0, 20.0, 13.9, 13.9, 13.8. IR (KBr): 3119, 3026, 2939, 2851, 1784, 1724, 1635, 1542, 1468, 1386, 1222, 1150, 1058, 979, 789, 658 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{26}H_{42}BrN_2O_3$ $[M + H]^+$: 509.2373; found: 509.2371.

(*Z*)-3-(Dibutylamino)-3-oxo-1-(*o*-tolyl)prop-1-en-1-yl dibutylcarbamate (4ka)



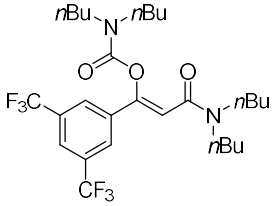
Pale yellow oil (22.6 mg, 51%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.38 (d, *J* = 7.2 Hz, 1 H), 7.28 – 7.15 (m, 3 H), 5.83 (s, 1 H), 3.42 – 3.26 (m, 6 H), 3.17 (t, *J* = 7.6 Hz, 2 H), 2.46 (s, 3 H), 1.61 – 1.47 (m, 8 H), 1.36 – 1.24 (m, 8 H), 0.96 – 0.86 (m, 12 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.0, 152.9, 152.4, 136.1, 135.8, 130.6, 128.9, 128.8, 125.6, 113.0, 48.1, 47.4, 44.8, 31.1, 30.8, 30.0, 29.8, 20.3, 20.1, 20.0, 13.9, 13.8. IR (KBr): 2951, 2866, 1726, 1633, 1548, 1465, 1376, 1243, 1151, 1055, 984, 918, 743, 655 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{27}H_{45}N_2O_3$ $[M + H]^+$: 445.3425; found: 445.3421.

(*Z*)-3-(Dibutylamino)-1-(2-fluorophenyl)-3-oxoprop-1-en-1-yl dibutylcarbamate (4la)



Pale yellow oil (32.3 mg, 72%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.46 – 7.37 (m, 1 H), 7.34 – 7.27 (m, 1 H), 7.18 – 7.03 (m, 2 H), 6.38 (s, 1 H), 3.46 – 3.30 (m, 6 H), 3.21 (t, *J* = 7.6 Hz, 2 H), 1.67 – 1.51 (m, 8 H), 1.35 – 1.25 (m, 8 H), 1.00 – 0.88 (m, 12 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 164.9, 159.9 (d, J = 250.1 Hz), 153.0, 146.2, 130.4 (d, *J* = 8.5 Hz), 128.4 (d, *J* = 1.9 Hz), 124.1 (d, *J* = 3.6 Hz), 123.2 (d, *J* = 10.7 Hz), 116.2 (d, *J* = 22.6 Hz), 114.7 (d, *J* = 10.1 Hz), 48.1, 47.6, 47.5, 44.8, 30.9, 30.8, 30.0, 29.8, 20.2, 20.1, 20.0, 19.9, 13.9, 13.9, 13.8. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -113.49 – -113.61 (m). IR (KBr): 2948, 2869, 1725, 1634, 1431, 1373, 1214, 1148, 1067, 825, 756, 662 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{26}H_{42}FN_2O_3$ $[M + H]^+$: 449.3174; found: 449.3170.

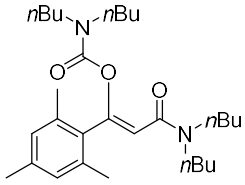
(*Z*)-1-(3,5-Bis(trifluoromethyl)phenyl)-3-(dibutylamino)-3-oxoprop-1-en-1-yl dibutylcarbamate (4ma)



Pale yellow oil (32.3 mg, 57%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.89 (s, 2 H), 7.84 (s, 1 H), 6.38 (s, 1 H), 3.42 – 3.30 (m, 6 H), 3.27 – 3.21 (m, 2 H), 1.68 – 1.50 (m, 8 H), 1.38 – 1.26 (m, 8 H), 0.97 – 0.88 (m, 12 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 163.9, 152.7, 149.1, 137.6, 132.1 (q, *J* = 33.4 Hz), 125.4, 123.0 (q, *J* = 271.2 Hz), 122.8 (p, J = 3.6 Hz), 112.4, 48.0, 47.7, 47.5, 44.9, 30.9, 30.9, 29.9, 29.7, 20.2, 20.1, 20.0, 19.9, 13.9, 13.8, 13.7, 13.7. ^{19}F NMR (376 MHz, $CDCl_3$): δ =

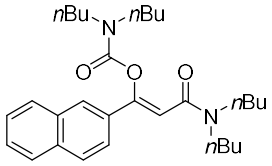
-63.11 (s). IR (KBr): 2948, 2870, 1727, 1633, 1454, 1378, 1280, 1145, 905, 836, 697 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{28}H_{41}F_6N_2O_3$ $[M + H]^+$: 567.3016; found: 567.3008.

(*Z*)-3-(Dibutylamino)-1-mesityl-3-oxoprop-1-en-1-yl dibutylcarbamate (4na)



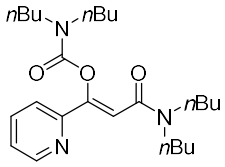
Pale yellow oil (30.7 mg, 65%). ^1H NMR (400 MHz, $CDCl_3$): δ = 6.87 (s, 2 H), 5.69 (s, 1 H), 3.44 – 3.28 (m, 4 H), 3.24 (t, *J* = 7.8 Hz, 2 H), 3.16 (t, *J* = 7.6 Hz, 2 H), 2.41 (s, 6 H), 2.27 (s, 3 H), 1.64 – 1.43 (m, 8 H), 1.39 – 1.21 (m, 8 H), 1.02 – 0.81 (m, 12 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.0, 152.6, 151.0, 138.3, 137.0, 132.6, 128.3, 113.5, 48.2, 47.6, 47.6, 44.9, 31.1, 30.7, 30.0, 29.8, 21.0, 20.3, 20.2, 20.1, 20.1, 20.0, 13.9, 13.9, 13.8. IR (KBr): 2943, 1723, 1632, 1447, 1226, 1143, 1062, 930, 844, 746, 663 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{29}H_{49}N_2O_3$ $[M + H]^+$: 473.3738; found: 473.3732.

(*Z*)-3-(Dibutylamino)-1-(naphthalen-2-yl)-3-oxoprop-1-en-1-yl dibutylcarbamate (4oa)



Pale yellow oil (24.5 mg, 51%). ^1H NMR (400 MHz, $CDCl_3$): δ = 7.95 (s, 1 H), 7.86 – 7.76 (m, 3 H), 7.59 (d, *J* = 8.4 Hz, 1 H), 7.52 – 7.42 (m, 2 H), 6.41 (s, 1 H), 3.48 – 3.33 (m, 6 H), 3.27 (t, *J* = 7.6 Hz, 2 H), 1.76 – 1.67 (m, 2 H), 1.63 – 1.52 (m, 6 H), 1.44 – 1.31 (m, 8 H), 1.00 – 0.90 (m, 12 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.0, 153.2, 152.3, 133.7, 133.0, 132.6, 128.5, 128.3, 127.6, 126.7, 126.5, 125.2, 122.8, 109.7, 48.1, 47.7, 47.6, 45.0, 31.1, 31.0, 30.1, 29.8, 20.3, 20.2, 20.0, 20.0, 13.9, 13.8. IR (KBr): 2946, 2866, 1780, 1722, 1633, 1530, 1460, 1371, 1211, 1146, 1061, 978, 808, 746, 658 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{30}H_{45}N_2O_3$ $[M + H]^+$: 481.3425; found: 481.3422.

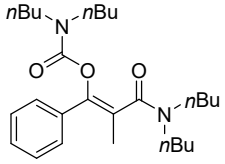
(*Z*)-3-(Dibutylamino)-3-oxo-1-(pyridin-2-yl)prop-1-en-1-yl dibutylcarbamate (4pa)



Yellow oil (18.1 mg, 42%). ^1H NMR (400 MHz, $CDCl_3$): δ = 8.56 (ddd, *J* = 4.7, 1.8, 0.9 Hz, 1 H), 7.68 (td, *J* = 7.8, 1.8 Hz, 1 H), 7.41 (dt, *J* = 7.9, 1.1 Hz, 1 H), 7.21 (ddd, *J* = 7.5, 4.7, 1.2 Hz, 1 H), 7.14 (s, 1 H), 3.43 – 3.31 (m, 6 H), 3.29 – 3.21 (m, 2 H), 1.73 – 1.62 (m, 2 H), 1.61 – 1.48 (m, 6 H), 1.42 – 1.27 (m, 8 H), 0.98 – 0.87 (m, 12 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.0, 153.2, 152.1, 150.3, 149.3, 136.6, 123.6, 119.5,

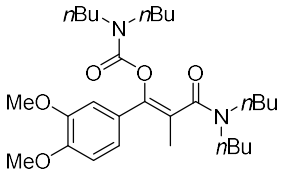
111.3, 48.0, 47.7, 47.6, 44.7, 31.0, 31.0, 30.0, 29.8, 20.2, 20.1, 20.0, 20.0, 13.9, 13.9, 13.8, 13.8. IR (KBr): 2946, 2863, 1734, 1627, 1449, 1240, 1139, 1069, 916, 745, 639 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{25}H_{42}N_3O_3$ $[M + H]^+$: 432.3221; found: 432.3218.

(*Z*)-3-(Dibutylamino)-2-methyl-3-oxo-1-phenylprop-1-en-1-yl dibutylcarbamate (4qa)



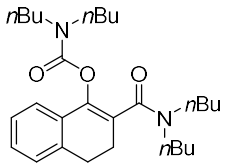
Pale yellow oil (25.3 mg, 57%). ^1H NMR (400 MHz, $CDCl_3$): δ = 7.42 – 7.19 (m, 5 H), 3.74 – 3.44 (m, 2 H), 3.25 – 2.95 (m, 6 H), 1.87 (s, 3 H), 1.55 – 1.41 (m, 6 H), 1.35 (t, *J* = 7.8 Hz, 2 H), 1.31 – 1.21 (m, 6 H), 1.19 – 1.11 (m, 2 H), 0.91 – 0.86 (m, 8 H), 0.82 – 0.75 (m, 3 H).^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.0, 153.2, 152.3, 133.7, 133.0, 132.6, 128.5, 128.3, 127.6, 126.7, 126.5, 125.2, 122.8, 109.7, 48.1, 47.7, 47.6, 45.0, 31.1, 31.0, 30.1, 29.8, 20.3, 20.2, 20.0, 20.0, 13.9, 13.8. IR (KBr): 2948, 2866, 1777, 1716, 1630, 1529, 1460, 1426, 1374, 1305, 1220, 1154, 1100, 1005, 756, 700 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{27}H_{45}N_2O_3$ $[M + H]^+$: 445.3425; found: 445.3420.

(*Z*)-3-(Dibutylamino)-1-(3,4-dimethoxyphenyl)-2-methyl-3-oxoprop-1-en-1-yl dibutylcarbamate (4ra)



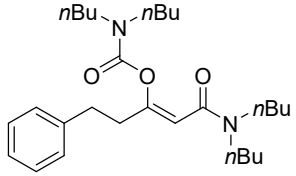
Pale yellow oil (29.2 mg, 58%). ^1H NMR (400 MHz, $CDCl_3$): δ = 6.96 (d, *J* = 8.4 Hz, 1 H), 6.89 (s, 1 H), 6.83 (d, *J* = 8.4 Hz, 1 H), 3.86 (s, 3 H), 3.83 (s, 3 H), 3.75 – 3.56 (m, 2 H), 3.36 – 3.24 (m, 1 H), 3.22 – 3.00 (m, 5 H), 1.93 (s, 3 H), 1.60 – 1.46 (m, 6 H), 1.45 – 1.38 (m, 2 H), 1.37 – 1.27 (m, 6 H), 1.24 – 1.17 (m, 2 H), 0.96 – 0.90 (m, 9 H), 0.85 (t, *J* = 7.2 Hz, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 169.8, 153.5, 148.9, 148.4, 143.1, 127.3, 121.6, 120.2, 111.2, 110.5, 55.7, 55.7, 47.7, 47.1, 43.5, 31.0, 30.9, 29.9, 29.5, 20.2, 20.1, 20.0, 19.9, 16.1, 13.9, 13.9, 13.8, 13.7. IR (KBr): 2949, 2868, 1782, 1717, 1629, 1516, 1459, 1259, 1221, 1151, 1100, 1025, 878, 812, 755, 668 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{29}H_{49}N_2O_5$ $[M + H]^+$: 505.3636; found: 505.3632.

2-(Dibutylcarbamoyl)-3,4-dihydronaphthalen-1-yl dibutylcarbamate (4sa)



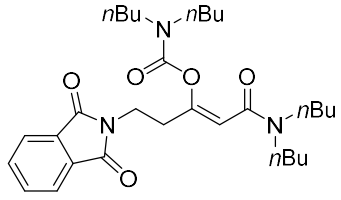
Pale yellow oil (28.7 mg, 63%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.21 – 7.10 (m, 3 H), 7.08 – 7.02 (m, 1 H), 3.66 (br, 2 H), 3.33 (t, J = 7.8 Hz, 2 H), 3.25 (t, J = 7.6 Hz, 2 H), 3.11 (br, 2 H), 2.96 – 2.87 (m, 2 H), 2.74 (br, 1 H), 2.42 (br, 1 H), 1.70 – 1.60 (m, 2 H), 1.59 – 1.44 (m, 6 H), 1.39 – 1.25 (m, 8 H), 0.99 – 0.86 (m, 12 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 168.6, 153.3, 141.9, 135.8, 130.8, 128.0, 127.4, 126.5, 122.5, 121.5, 47.9, 47.5, 47.4, 43.6, 31.0, 30.9, 30.0, 29.6, 27.4, 25.6, 20.2, 20.1, 20.0, 19.9, 13.9, 13.9, 13.9, 13.8. IR (KBr): 2947, 2867, 1784, 1719, 1627, 1540, 1457, 1291, 1223, 1149, 978, 757, 659 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{28}H_{45}N_2O_3$ $[M + H]^+$: 457.3425; found: 457.3421.

(*Z*)-1-(Dibutylamino)-1-oxo-5-phenylpent-2-en-3-yl dibutylcarbamate (4ta)



Yellow oil (22.0 mg, 48%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.33 – 7.18 (m, 5 H), 5.56 (s, 1 H), 3.30 – 3.16 (m, 8 H), 2.86 (t, J = 7.6 Hz, 2 H), 2.65 (t, J = 7.6 Hz, 2 H), 1.61 – 1.48 (m, 6 H), 1.48 – 1.40 (m, 2 H), 1.36 – 1.28 (m, 6 H), 1.26 – 1.19 (m, 2 H), 0.97 – 0.89 (m, 12 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.1, 154.5, 153.0, 140.7, 128.4, 128.4, 126.1, 109.8, 47.8, 47.5, 47.4, 44.6, 36.0, 32.4, 30.8, 30.8, 30.1, 29.7, 20.2, 20.0, 20.0, 19.9, 13.9, 13.9, 13.8. IR (KBr): 2943, 2873, 1735, 1630, 1450, 1379, 1240, 1144, 1057, 914, 831, 744, 663 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{28}H_{47}N_2O_3$ $[M + H]^+$: 459.3581; found: 459.3578.

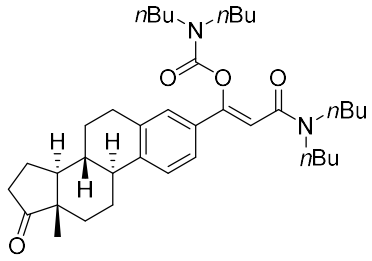
(*Z*)-1-(Dibutylamino)-5-(1,3-dioxoisoindolin-2-yl)-1-oxopent-2-en-3-yl dibutylcarbamate (4ua)



Yellow oil (30.6 mg, 57%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.86 – 7.80 (m, 2 H), 7.74 – 7.68 (m, 2 H), 5.74 (s, 1 H), 3.90 (t, J = 7.2 Hz, 2 H), 3.30 – 3.15 (m, 8 H), 2.75 (t, J = 7.2 Hz, 2 H), 1.63 – 1.42 (m, 8 H), 1.37 – 1.20 (m, 8 H), 0.98 – 0.86 (m, 12 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 167.9, 164.5, 152.7, 151.6, 133.9, 132.0, 123.2, 111.2, 47.8, 47.5, 47.4, 44.6, 35.1, 33.4, 30.8, 30.6, 30.0, 29.6, 20.1, 20.0, 19.9, 19.9, 13.8, 13.8, 13.7. IR (KBr): 2947, 2870, 1718,

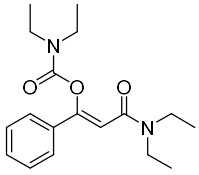
1629, 1448, 1387, 1239, 1147, 1052, 917, 816, 731 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{30}H_{46}N_3O_5$ $[M + H]^+$: 528.3432; found: 528.3428.

(*Z*)-3-(Dibutylamino)-1-((8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[a]phenanthren-3-yl)-3-oxoprop-1-en-1-yl dibutylcarbamate (4va)



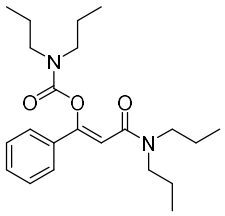
Yellow oil (35.6 mg, 62%). ^1H NMR (400 MHz, $CDCl_3$): δ = 7.22 – 7.18 (m, 2 H), 7.14 (s, 1 H), 6.14 (s, 1 H), 3.33 – 3.24 (m, 6 H), 3.19 – 3.12 (m, 2 H), 2.88 – 2.81 (m, 2 H), 2.44 (dd, *J* = 18.9, 8.7 Hz, 2 H), 2.37 – 2.31 (m, 1 H), 2.26 – 2.21 (m, 1 H), 2.12 – 2.04 (m, 2 H), 2.02 – 1.83 (m, 6 H), 1.60 – 1.56 (m, 3 H), 1.49 – 1.43 (m, 8 H), 1.30 – 1.21 (m, 8 H), 0.90 – 0.83 (m, 15 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 220.7, 165.0, 153.2, 152.3, 141.2, 136.6, 132.8, 126.0, 125.6, 122.8, 108.6, 50.5, 48.0, 47.9, 47.6, 47.5, 44.9, 44.4, 37.9, 35.8, 31.5, 31.0, 30.9, 30.0, 29.8, 29.4, 26.3, 25.6, 21.5, 20.2, 20.1, 20.0, 13.9, 13.8, 13.8. IR (KBr): 2943, 2863, 1733, 1631, 1450, 1245, 1087, 914, 810, 740, 649 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{38}H_{59}N_2O_4$ $[M + H]^+$: 607.4469; found: 607.4464.

(*Z*)-3-(Diethylamino)-3-oxo-1-phenylprop-1-en-1-yl diethylcarbamate (4ab)



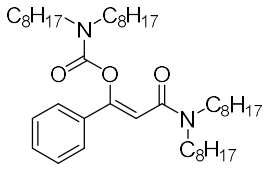
Yellow oil (22.9 mg, 72%). ^1H NMR (400 MHz, $CDCl_3$): δ = 7.51 – 7.49 (m, 2 H), 7.37 – 7.34 (m, 3 H), 6.28 (s, 1 H), 3.47 – 3.36 (m, 4 H), 3.30 (q, *J* = 6.0 Hz, 4 H), 1.25 (t, *J* = 8.0 Hz, 3 H), 1.30 – 1.21 (m, 9 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 164.6, 152.7, 152.4, 135.1, 135.1, 129.4, 128.3, 125.4, 108.7, 42.4, 42.2, 42.1, 39.4, 14.2, 14.2, 13.3, 12.9. IR (KBr): 3061, 2976, 2933, 2877, 1729, 1622, 1458, 1425, 1378, 1317, 1253, 1070, 963, 789, 759, 696, 605 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{18}H_{27}N_2O_3$ $[M + H]^+$: 319.2016, found: 319.2020.

(*Z*)-3-(Dipropylamino)-3-oxo-1-phenylprop-1-en-1-yl dipropylcarbamate (4ac)



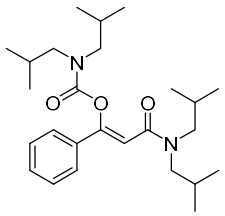
Yellow oil (24.3 mg, 65%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.51-7.49 (m, 2 H), 7.35 (d, J = 4.0 Hz, 3 H), 6.29 (s, 1H), 3.33 (q, J = 8.0 Hz, 6 H), 3.22 (t, J = 8.0 Hz, 2 H), 1.76-1.60 (m, 8 H), 0.95-0.87 (m, 12 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.06, 153.24, 152.32, 135.32, 129.34, 128.52, 125.48, 109.26, 50.03, 49.63, 46.80, 22.12, 22.03, 21.17, 20.83, 11.42, 11.35, 11.30, 11.16. IR (KBr): 2963, 2876, 1724, 1630, 1426, 1229, 1149, 1080, 755 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{22}H_{35}N_2O_3$ [M + H]$^+$: 375.2642, found: 375.2643.

(*Z*)-3-(Dioctylamino)-3-oxo-1-phenylprop-1-en-1-yl dioctylcarbamate (4ad)



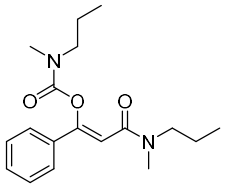
Faint yellow oil (39.2 mg, 60%). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.51 – 7.46 (m, 2 H), 7.37 – 7.30 (m, 3 H), 6.26 (s, 1 H), 3.39 – 3.28 (m, 6 H), 3.22 (t, J = 7.8 Hz, 2 H), 1.66 (p, J = 7.4 Hz, 2 H), 1.56 (hept, J = 7.3 Hz, 6 H), 1.34 – 1.21 (m, 40 H), 0.91 – 0.83 (m, 12 H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 164.8, 153.0, 152.2, 135.2, 129.2, 128.4, 125.4, 109.1, 48.2, 47.9, 47.8, 45.2, 31.8, 31.7, 31.7, 29.4, 29.3, 29.2, 29.2, 29.1, 28.8, 28.8, 27.9, 27.6, 27.1, 26.9, 26.8, 26.7, 22.6, 22.6, 22.5, 14.0, 14.0. IR (KBr): 3063, 2926, 2857, 1727, 1649, 1627, 1463, 1424, 1375, 1236, 1179, 1141, 1084, 916, 847, 757, 693 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{42}H_{75}N_2O_3$ [M + H]$^+$: 655.5772; found: 655.5766.

(*Z*)-3-(Diisobutylamino)-3-oxo-1-phenylprop-1-en-1-yl diisobutylcarbamate (4ae)



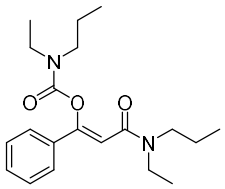
Brown oil (31.4 mg, 73%). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.53 – 7.44 (m, 2 H), 7.39 – 7.30 (m, 3 H), 6.29 (s, 1 H), 3.29 – 3.17 (m, 6 H), 3.08 (d, J = 7.5 Hz, 2 H), 2.15 – 2.08 (m, 1 H), 2.06 – 1.95 (m, 3 H), 1.02 – 0.86 (m, 24 H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.4, 153.7, 152.3, 135.4, 129.2, 128.4, 125.4, 109.8, 56.0, 55.6, 55.4, 52.5, 27.7, 27.4, 26.7, 26.5, 20.2, 20.2, 20.1, 20.0. IR (KBr): 2954, 1722, 1632, 1453, 1231, 1149, 1078, 941, 754, 694 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{26}H_{42}N_2NaO_3$ [M + Na]$^+$: 453.3084, found: 453.3096.

(*Z*)-3-(Methyl(propyl)amino)-3-oxo-1-phenylprop-1-en-1-yl methyl(propyl)carbamate (4af)



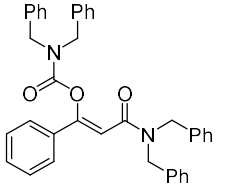
Faint yellow oil (22.6 mg, 71%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.54 – 7.45 (m, 2 H), 7.39 – 7.30 (m, 3 H), 6.27 (s, 1 H), 3.41 – 3.31 (m, 3 H), 3.27 – 3.20 (m, 1 H), 3.05 (d, *J* = 11.6 Hz, 3 H), 2.92 (s, 3 H), 1.73 – 1.52 (m, 4 H), 0.96 – 0.85 (m, 6 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.1, 153.2, 152.3, 152.2, 135.1, 135.0, 129.4, 129.3, 128.4, 125.4, 125.4, 109.2, 108.8, 108.2, 107.8, 51.9, 51.1, 50.9, 48.6, 35.7, 34.8, 34.5, 32.8, 21.5, 21.1, 20.5, 20.2, 11.1, 11.0, 10.9. IR (KBr): 3060, 2960, 2927, 2873, 1767, 1721, 1622, 1458, 1398, 1233, 1151, 1070, 911, 841, 750, 692 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{18}H_{27}N_2O_3$ $[M + H]^+$: 319.2016; found: 319.2014.

(*Z*)-3-(Methyl(propyl)amino)-3-oxo-1-phenylprop-1-en-1-yl ethyl(propyl)carbamate (4ag)



Faint yellow oil (21.5 mg, 62%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.54 – 7.45 (m, 2 H), 7.40 – 7.30 (m, 3 H), 6.28 (s, 1 H), 3.51 – 3.37 (m, 3 H), 3.37 – 3.25 (m, 4 H), 3.22 (t, J = 7.6 Hz, 1 H), 1.69 (q, *J* = 7.7 Hz, 1 H), 1.64 – 1.48 (m, 3 H), 1.26 (t, *J* = 7.0 Hz, 2 H), 1.20 – 1.10 (m, 4 H), 0.90 (p, *J* = 8.8 Hz, 6 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 164.8, 153.0, 152.9, 152.3, 135.1, 129.3, 128.4, 125.4, 109.0, 108.8, 49.6, 49.1, 46.2, 42.7, 42.5, 39.9, 22.0, 21.3, 20.9, 14.1, 13.1, 12.8, 11.3, 11.1. IR (KBr): 3061, 2967, 2931, 2875, 1723, 1623, 1462, 1424, 1378, 1243, 1151, 1072, 1031, 958, 912, 835, 795, 756 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{20}H_{31}N_2O_3$ $[M + H]^+$: 347.2329; found: 347.2326.

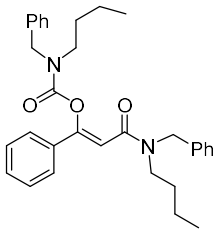
(*Z*)-3-(Dibenzylamino)-3-oxo-1-phenylprop-1-en-1-yl dibenzylcarbamate (4ah)



Faint yellow solid (32.3 mg, 57%). mp: 118 – 120 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.41 – 7.32 (m, 11 H), 7.32 – 7.25 (m, 9 H), 7.23 – 7.18 (m, 5 H), 6.45 (s, 1 H), 4.68 (s, 2 H), 4.62 (s, 2 H), 4.59 (s, 2 H), 4.57 (s, 2 H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.7, 154.4, 153.8, 137.1, 137.1, 137.1, 136.7, 136.5, 134.6, 129.8, 128.9, 128.6, 128.5, 128.5, 128.4, 128.3, 128.1, 127.7, 127.5, 127.4, 127.2, 126.7, 125.6, 107.6, 50.4, 50.0, 49.7, 47.5. IR (KBr): 3030, 2924, 2857, 1767, 1724, 1649,

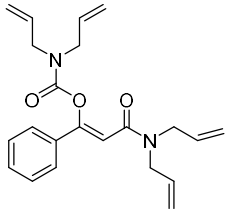
1623, 1495, 1454, 1422, 1362, 1311, 1252, 1098, 958, 816, 743, 699 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{38}H_{35}N_2O_3$ $[M + H]^+$: 567.2642; found: 567.2637.

(*Z*)-3-(Benzyl(butyl)amino)-3-oxo-1-phenylprop-1-en-1-yl benzyl(butyl)carbamate (4ai)



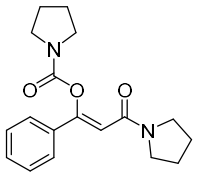
Faint yellow oil (25.9 mg, 52%). ^1H NMR (400 MHz, $CDCl_3$): δ = 7.63 – 7.27 (m, 15 H), 6.40 (dd, *J* = 47.2, 15.2 Hz, 1 H), 4.85 – 4.69 (m, 3 H), 4.67 – 4.55 (m, 1 H), 3.51 – 3.30 (m, 4 H), 1.79 – 1.55 (m, 4 H), 1.43 – 1.27 (m, 4 H), 1.03 – 0.84 (m, 6 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.5, 165.5, 165.1, 153.8, 153.6, 153.5, 153.1, 153.1, 153.0, 153.0, 137.8, 137.7, 137.7, 137.4, 137.2, 135.2, 135.1, 134.8, 134.7, 129.6, 129.5, 129.4, 128.7, 128.5, 128.5, 128.4, 128.4, 128.3, 127.9, 127.8, 127.4, 127.3, 127.2, 127.2, 127.0, 126.6, 125.5, 125.5, 108.8, 108.6, 108.0, 107.8, 51.5, 50.9, 50.7, 47.7, 47.3, 47.2, 47.1, 46.7, 45.1, 30.5, 30.3, 29.6, 29.5, 29.4, 29.4, 20.1, 20.0, 19.9, 13.7, 13.7. IR (KBr): 3113, 3000, 2894, 2822, 1774, 1684, 1539, 1391, 1339, 1161, 1104, 1046, 982, 791, 660 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{32}H_{39}N_2O_3$ $[M + H]^+$: 499.2955; found: 499.2949.

(*Z*)-3-(Diallylamino)-3-oxo-1-phenylprop-1-en-1-yl diallylcarbamate (4aj)



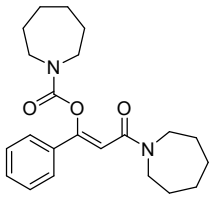
Faint yellow oil (23.1 mg, 63%). ^1H NMR (500 MHz, $CDCl_3$): δ = 7.54 – 7.47 (m, 2 H), 7.40 – 7.31 (m, 3 H), 6.32 (s, 1 H), 5.98 – 5.88 (m, 1 H), 5.87 – 5.70 (m, 3 H), 5.29 – 5.12 (m, 8 H), 4.04 (d, *J* = 6.0 Hz, 2 H), 4.02 – 3.95 (m, 4 H), 3.92 (d, *J* = 6.0 Hz, 2 H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.2, 153.4, 153.0, 134.7, 133.6, 133.1, 133.0, 132.9, 129.6, 128.4, 125.5, 117.3, 117.0, 116.8, 116.5, 107.8, 49.5, 49.3, 49.3, 47.2. IR (KBr): 3080, 2993, 2919, 1724, 1635, 1415, 1336, 1282, 1221, 1143, 1090, 995, 924, 845, 756, 696 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{22}H_{27}N_2O_3$ $[M + H]^+$: 367.2016; found: 367.2013.

(*Z*)-3-Oxo-1-phenyl-3-(pyrrolidin-1-yl)prop-1-en-1-yl pyrrolidine-1-carboxylate (4ak)



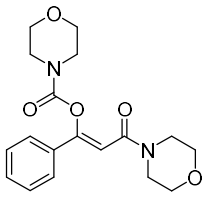
Yellow oil (22.0 mg, 70%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.58-7.59 (m, 2 H), 7.37 (s, 3 H), 6.30 (s, 1 H), 3.65 (t, J = 8.0 Hz, 2 H), 3.56 (t, J = 8.0 Hz, 2 H), 3.51 (t, J = 8.0 Hz, 2 H), 3.46 (t, J = 8.0 Hz, 2 H), 1.99-1.84 (m, 8 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 163.4, 154.1, 151.9, 135.3, 129.8, 128.5, 128.5, 125.9, 107.8, 46.9, 46.5, 46.4, 45.6, 26.0, 25.7, 25.0, 24.4. IR (KBr): 2958, 2929, 2876, 1724, 1626, 1463, 1425, 1213, 1147, 1075, 755 cm^{-1}. HRMS-ESI (m/z): calcd for $C_{18}H_{22}N_2O_3$ $[M + H]^+$: 315.1703; found: 315.1700.

(*Z*)-3-(Azepan-1-yl)-3-oxo-1-phenylprop-1-en-1-yl azepane-1-carboxylate (4al)



Brown oil (27.0 mg, 73%). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.57 – 7.47 (m, 2 H), 7.41 – 7.30 (m, 3 H), 6.31 (s, 1 H), 3.60 (t, J = 5.8 Hz, 2 H), 3.54 (dt, J = 9.5, 6.0 Hz, 4 H), 3.45 (t, J = 6.0 Hz, 2 H), 1.80 (p, J = 5.5 Hz, 2 H), 1.76 – 1.68 (m, 6 H), 1.67 – 1.52 (m, 8 H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.1, 153.1, 152.6, 135.2, 129.4, 128.5, 125.5, 108.9, 48.3, 47.4, 47.2, 45.3, 29.0, 28.5, 28.1, 27.5, 27.4, 27.3, 26.9, 26.7. IR (KBr): 2927, 2856, 1720, 1618, 1423, 1255, 1171, 1076, 694 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{22}H_{30}N_2O_3Na$ $[M + Na]^+$: 393.2149, found: 393.2151.

(*Z*)-3-Morpholino-3-oxo-1-phenylprop-1-en-1-yl morpholine-4-carboxylate (4am)



Faint yellow oil (17.6 mg, 51%). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.55 – 7.48 (m, 2 H), 7.43 – 7.33 (m, 3 H), 6.29 (s, 1 H), 3.81 – 3.63 (m, 12 H), 3.61 – 3.46 (m, 4 H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 164.1, 153.6, 152.3, 134.3, 130.0, 128.6, 125.5, 107.4, 66.9, 66.8, 66.6, 46.8, 45.3, 44.4, 41.8. IR (KBr): 2996, 2914, 2849, 1721, 1628, 1527, 1431, 1279, 1222, 1111, 974, 853, 762 cm^{-1}. HRMS-ESI (*m/z*): calcd for $C_{18}H_{23}N_2O_5$ $[M + H]^+$: 347.1601; found: 347.1598.

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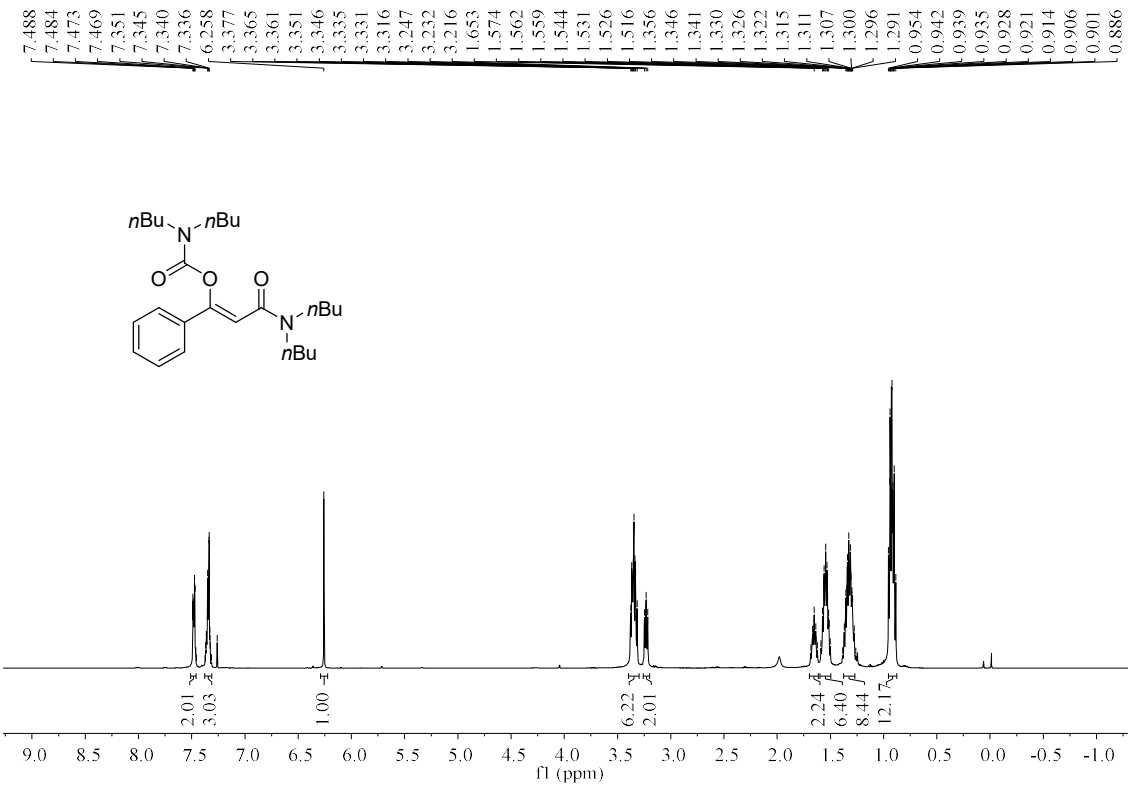
[1] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. 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 16, Revision A.03, Gaussian, Inc., Wallingford, CT, 2016.

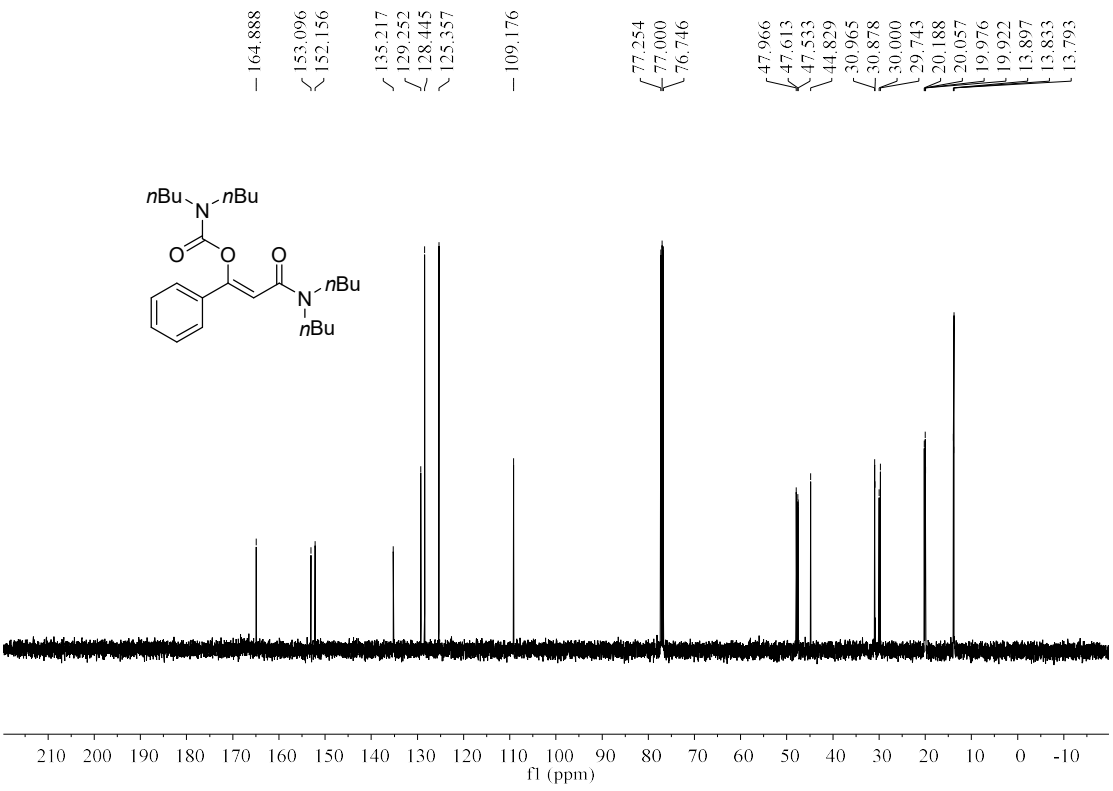
[2] Y. Zhao, D. G. Truhlar, The Mo6 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four Mo6-class functionals and 12 other functionals, *Theor. Chem. Acc*. 2008, **120**, 215−241.

[3] A. V. Marenich, C. J. Cramer, D. G. Truhlar, Universal solvation model based on solute electron density and on a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions, *J. Phys. Chem. B* 2009, **113**, 6378−6396.

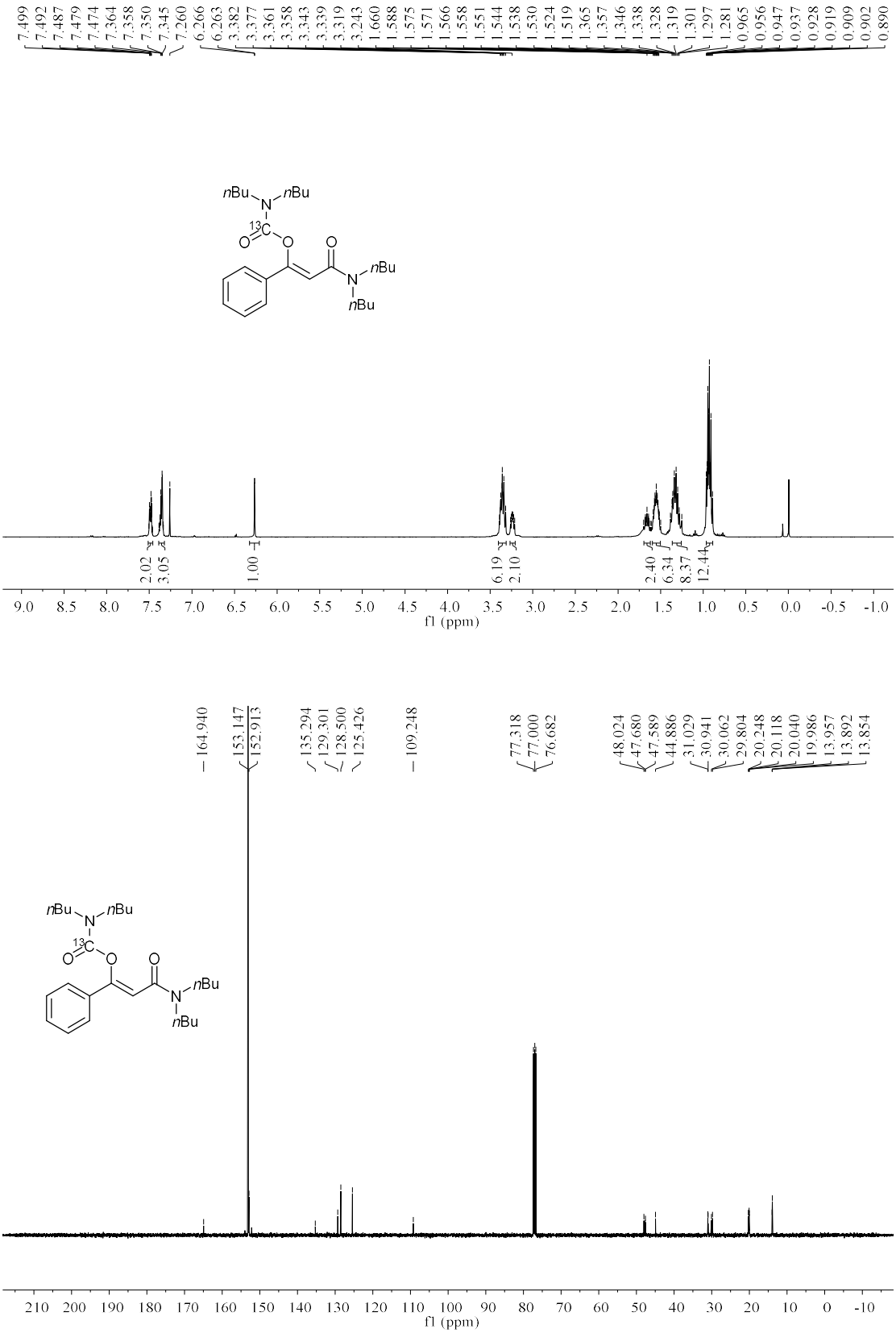
F. NMR Spectra

(*Z*)-3-(Dibutylamino)-3-oxo-1-phenylprop-1-en-1-yl dibutylcarbamate (4aa)

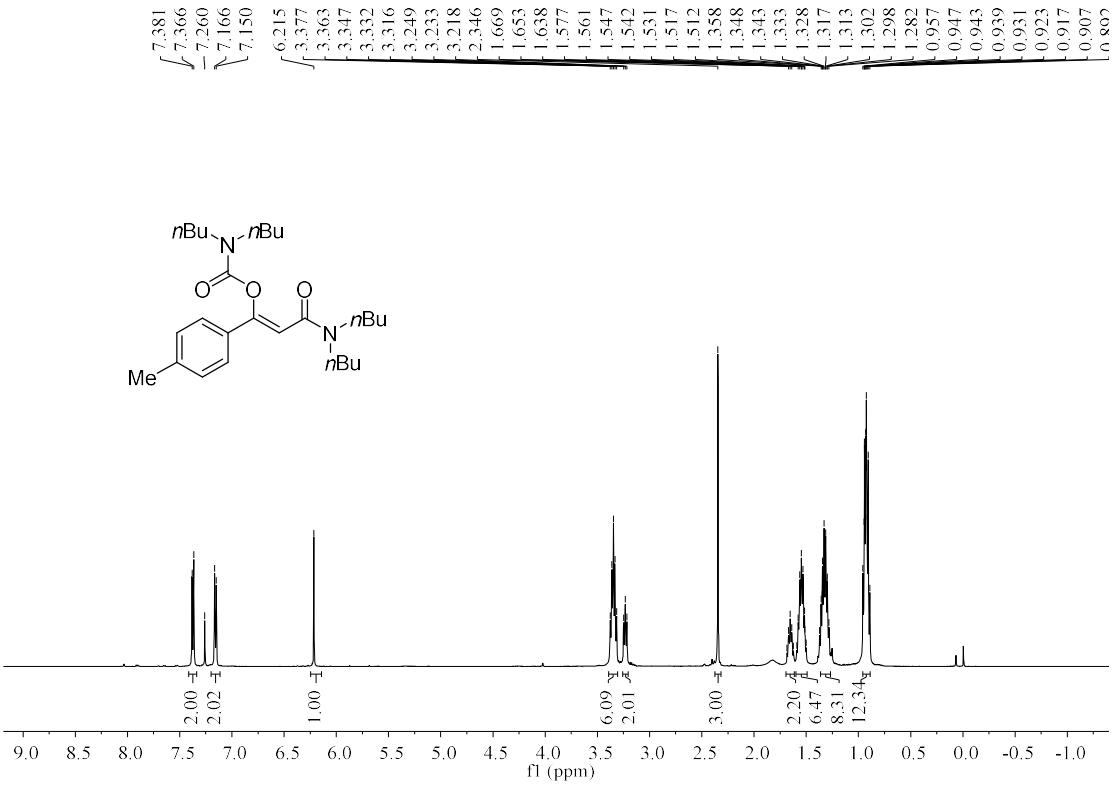


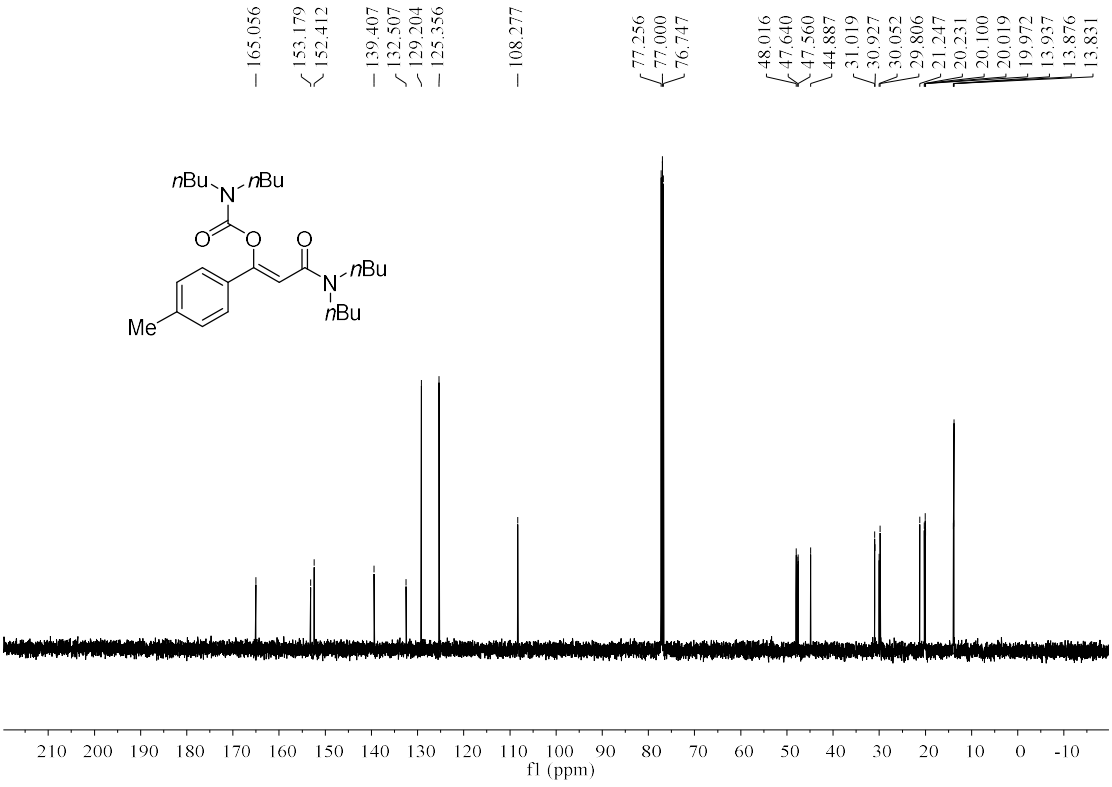


(*Z*)-3-(Dibutylamino)-3-oxo-1-phenylprop-1-en-1-yl dibutylcarbamate-^{13}C (4aa-^{13}C)

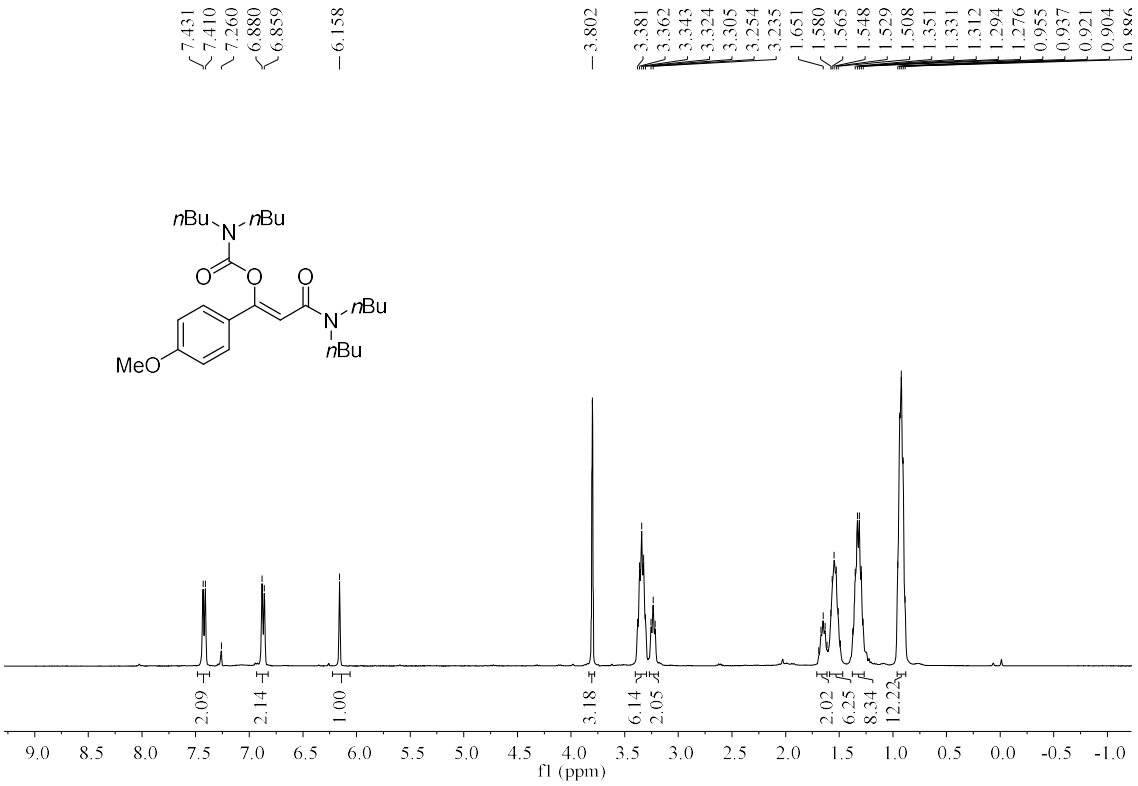


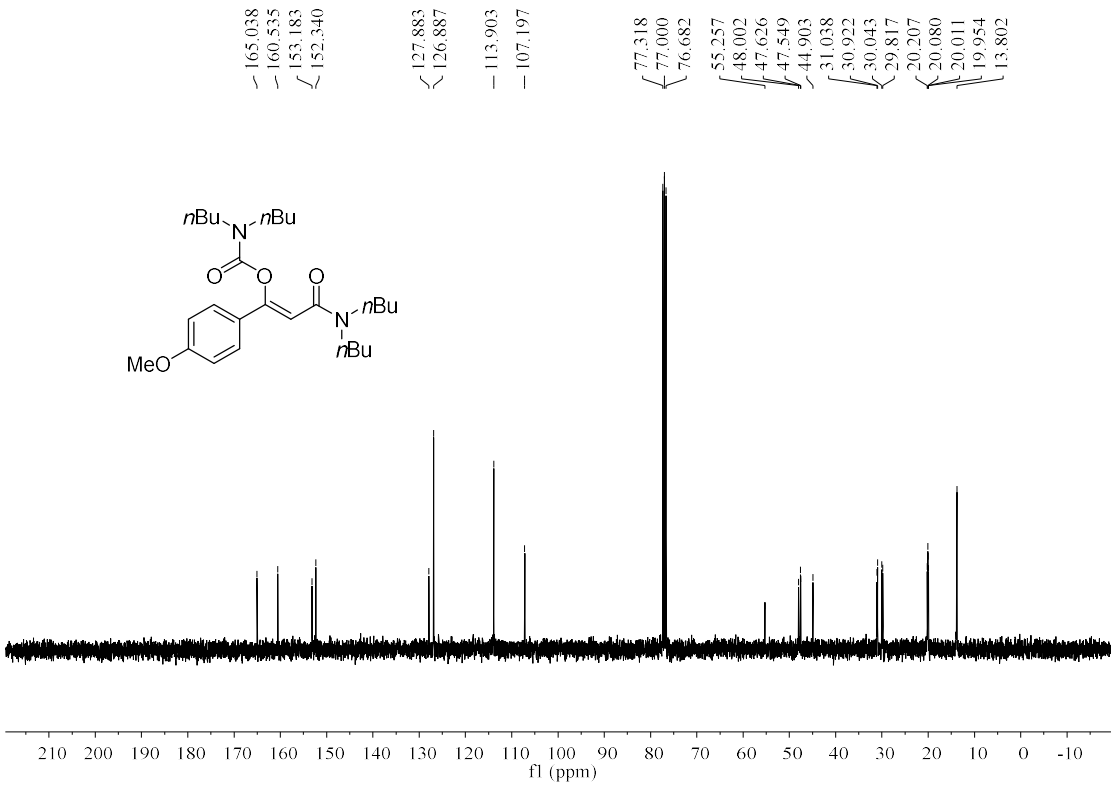
(*Z*)-3-(Dibutylamino)-3-oxo-1-(*p*-tolyl)prop-1-en-1-yl dibutylcarbamate (4ba)



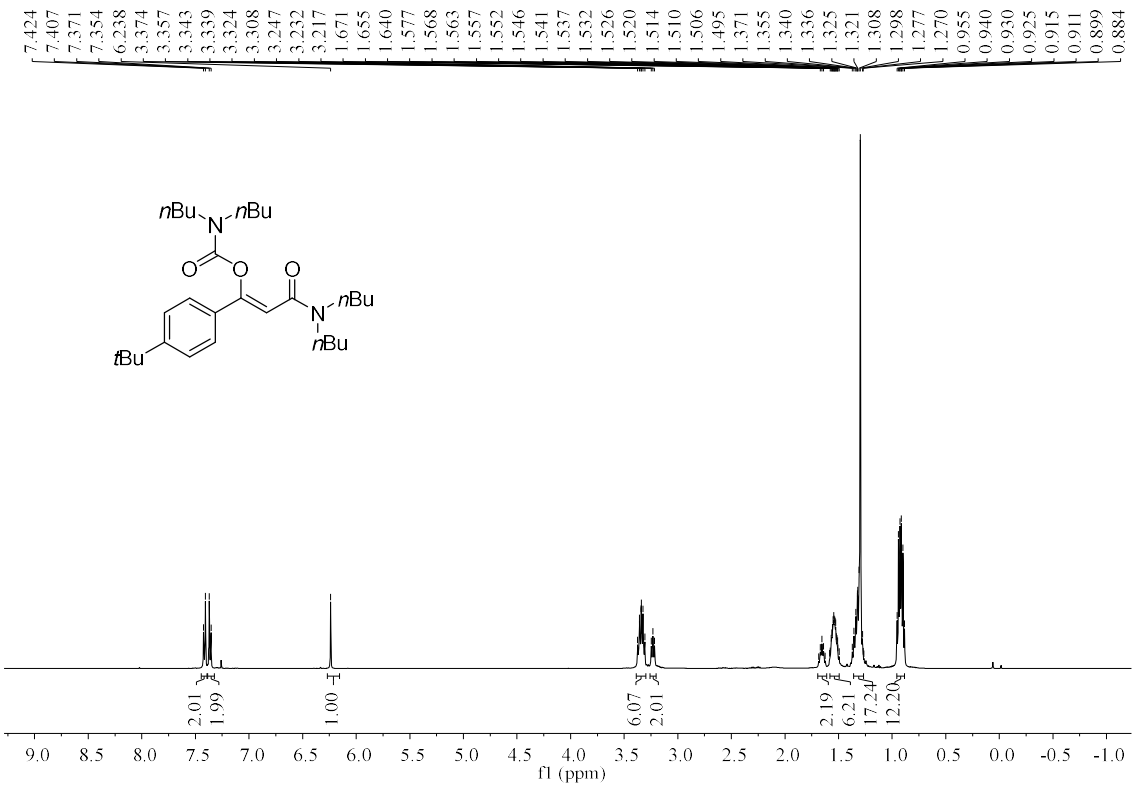


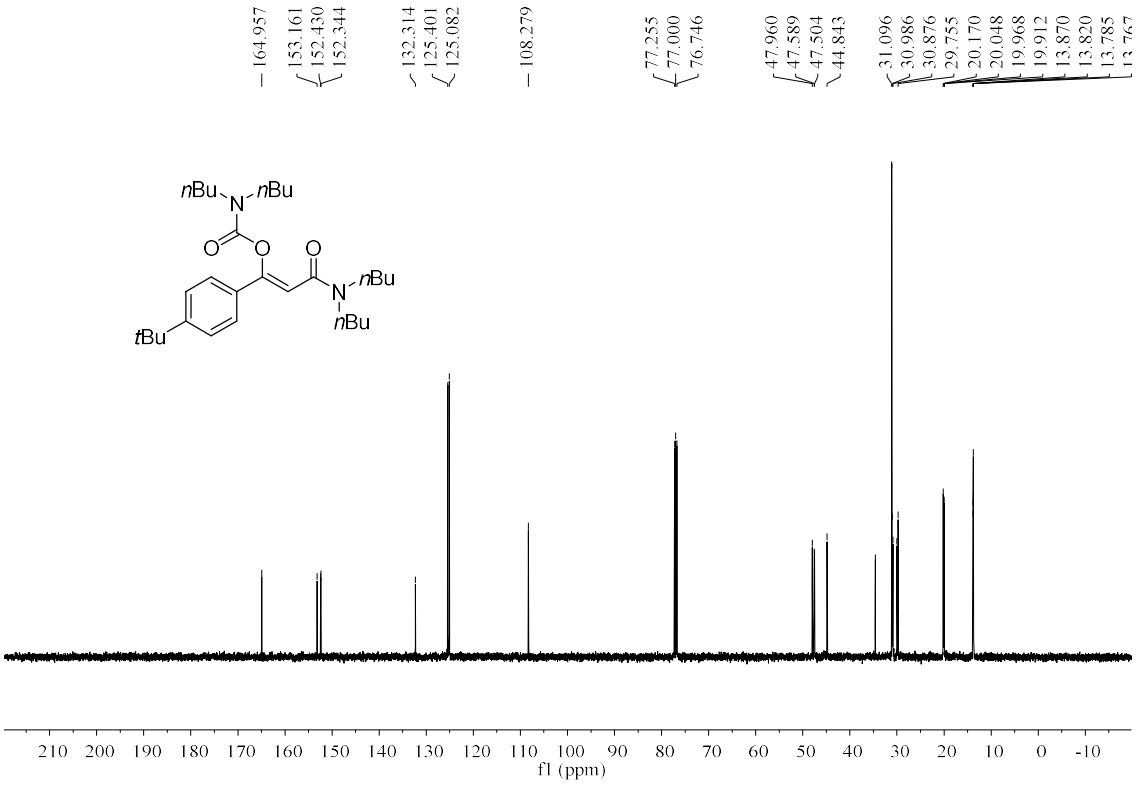
(*Z*)-3-(Dibutylamino)-1-(4-methoxyphenyl)-3-oxoprop-1-en-1-yl dibutylcarbamate (4ca)





(*Z*)-1-(4-(*tert*-butyl)phenyl)-3-(dibutylamino)-3-oxoprop-1-en-1-yl dibutylcarbamate (4da)





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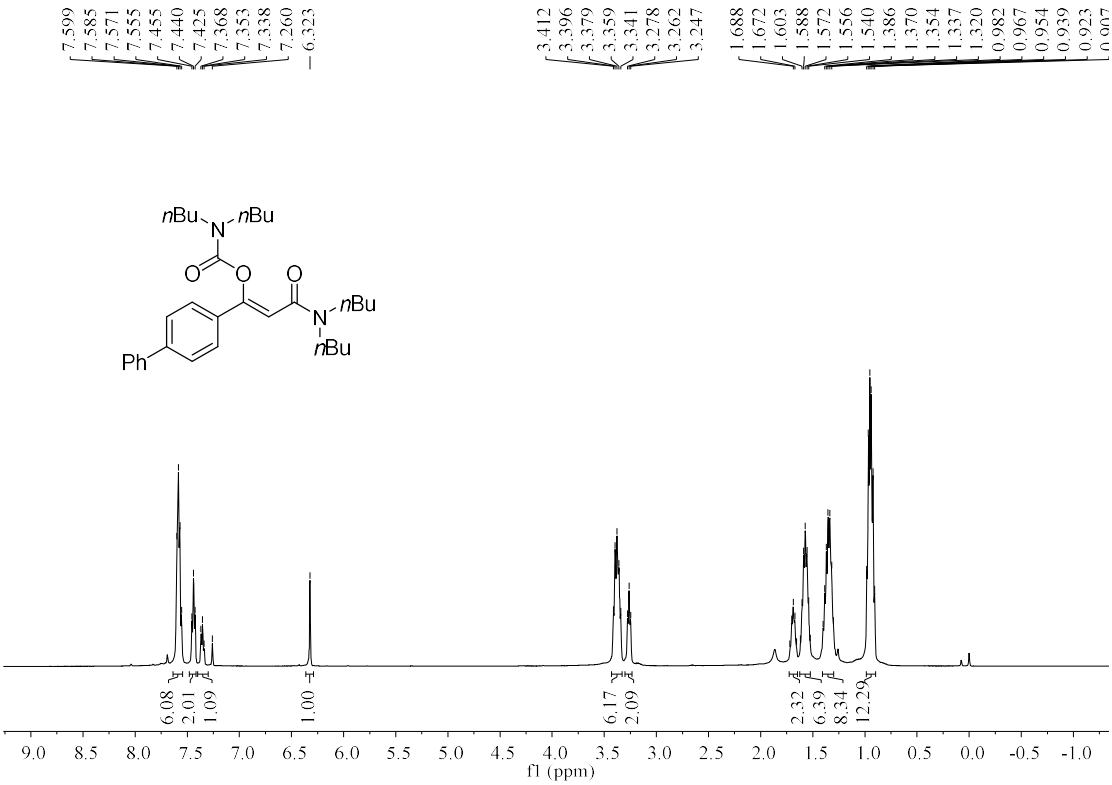
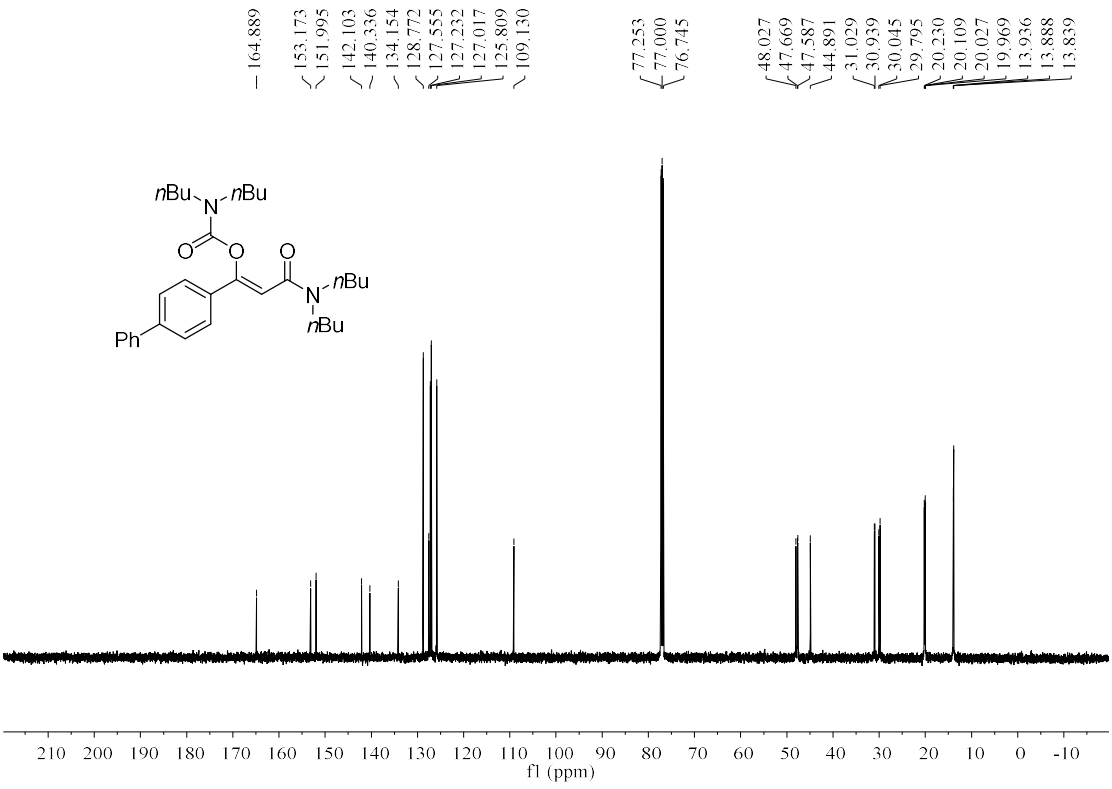
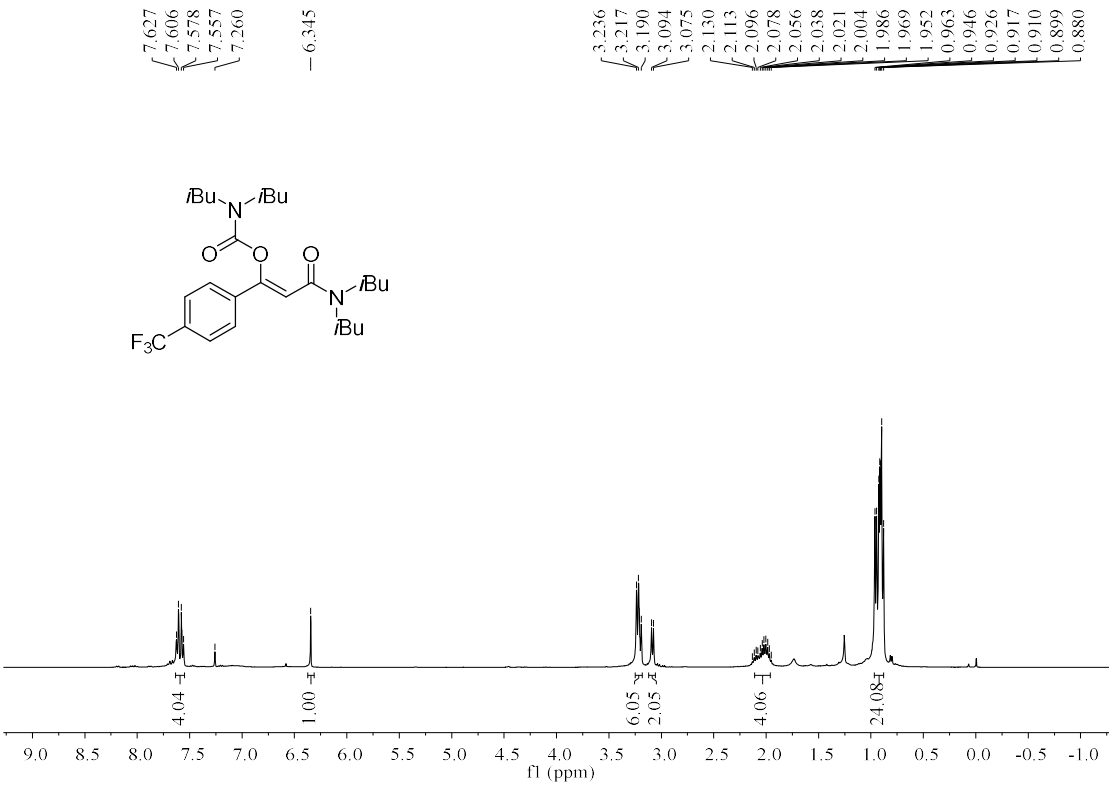
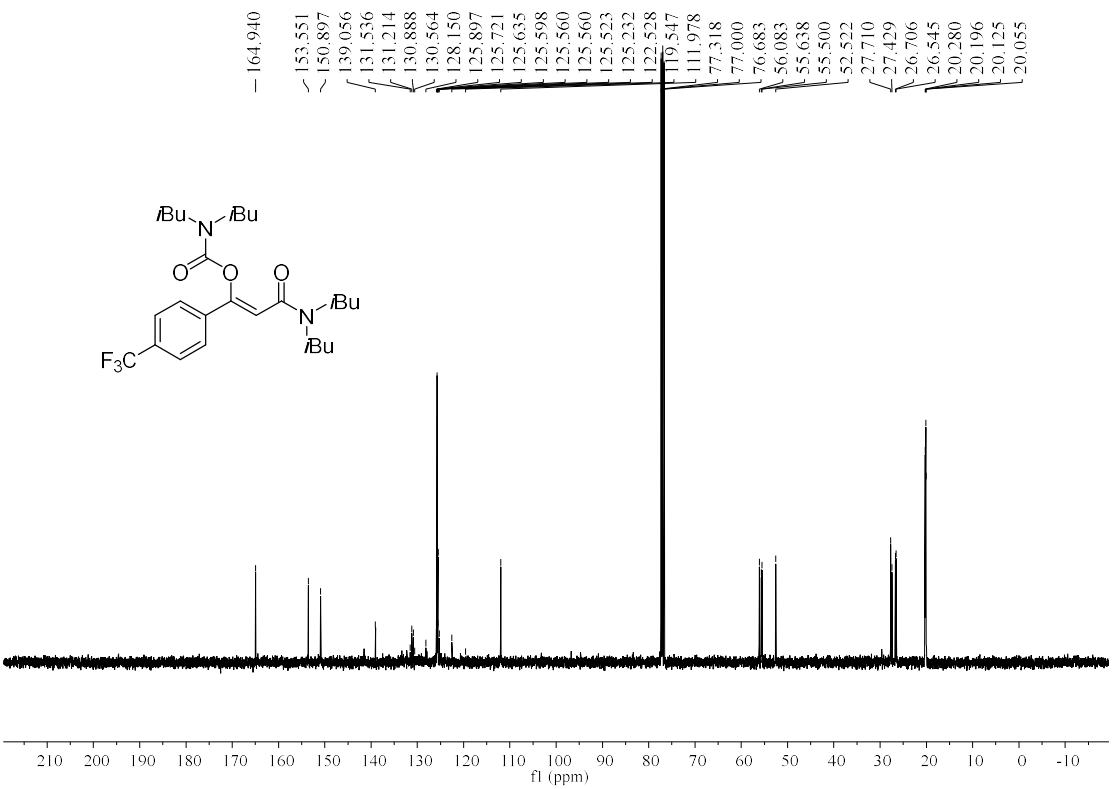
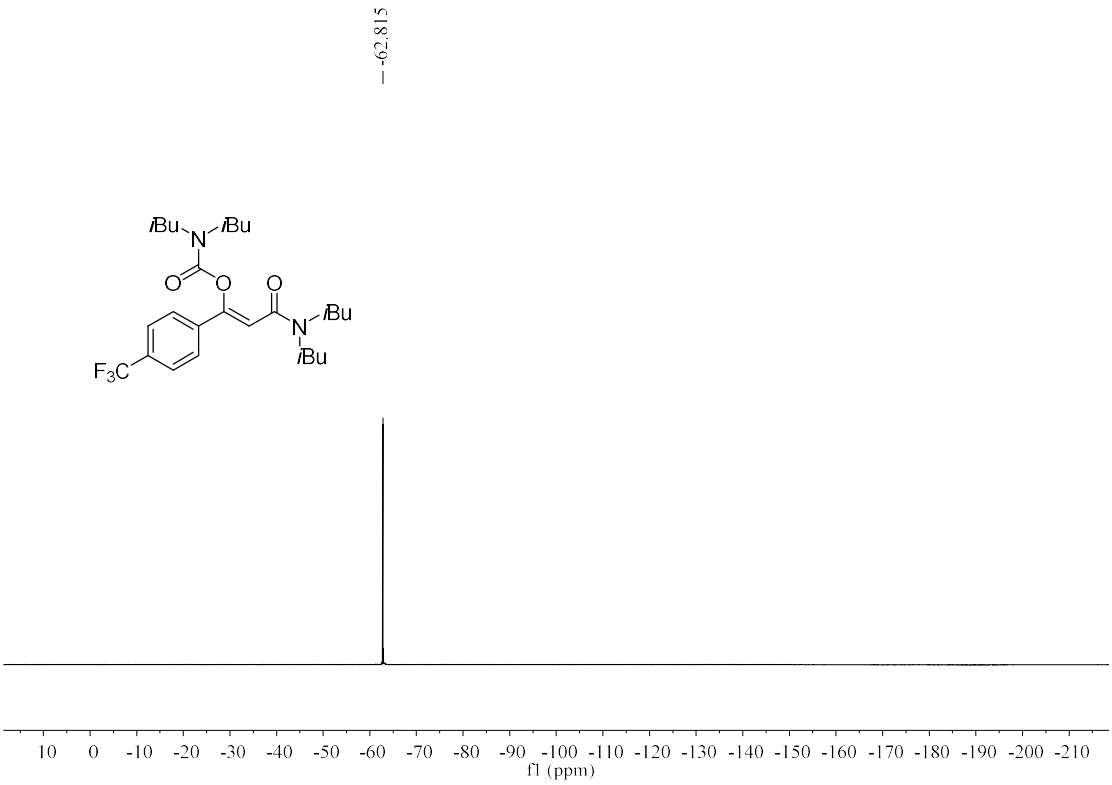




(*Z*)-3-(Diisobutylamino)-3-oxo-1-(4-(trifluoromethyl)phenyl)prop-1-en-1-yl diisobutylcarbamate (4fa)



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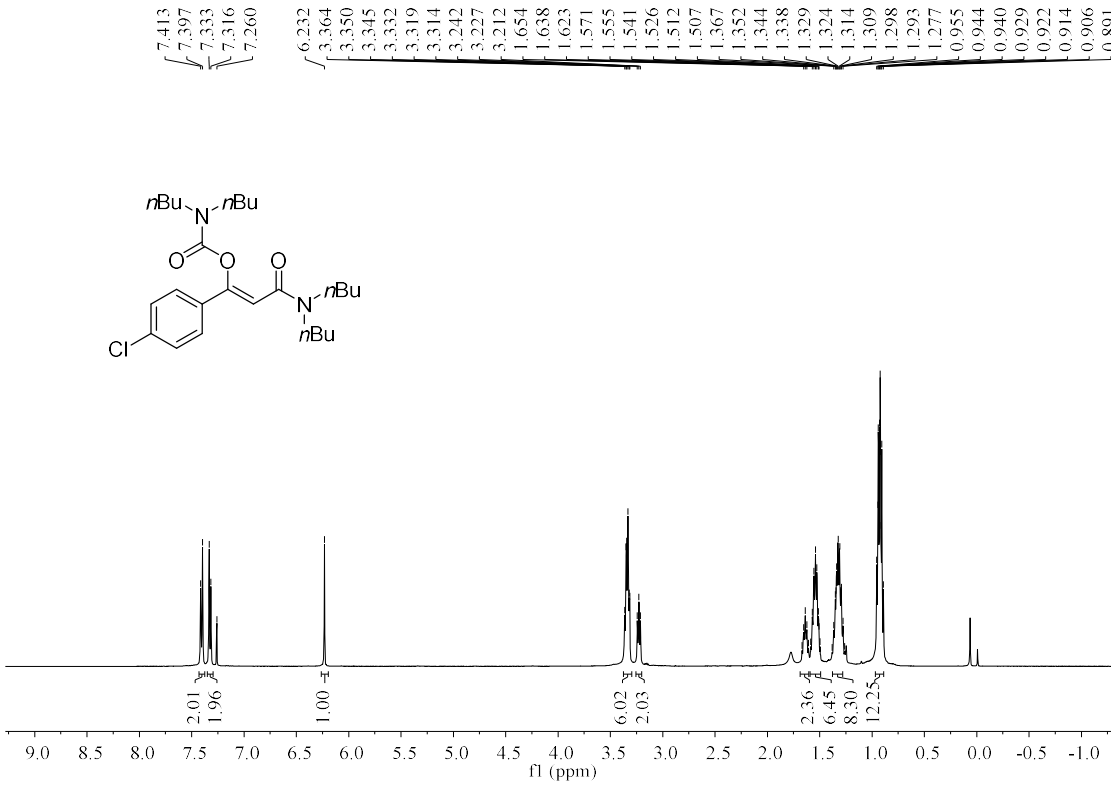
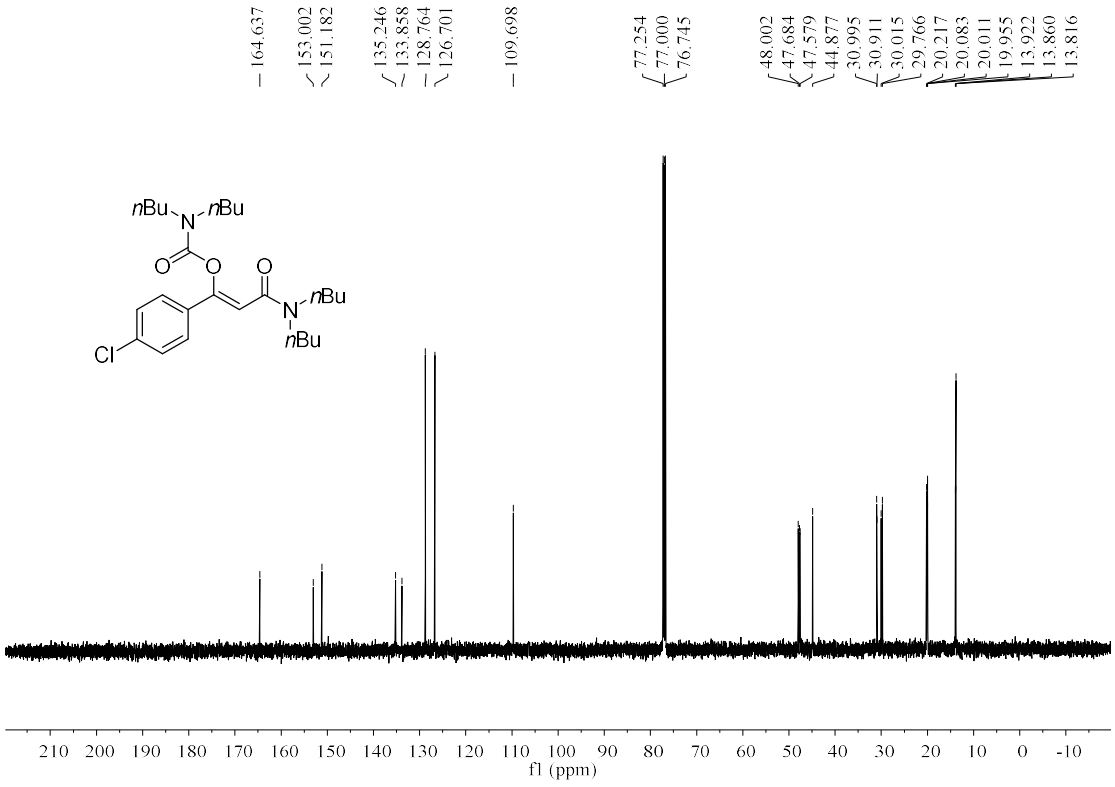
f1 (ppm)

(*Z*)-1-(4-Chlorophenyl)-3-(dibutylamino)-3-oxoprop-1-en-1-yl dibutylcarbamate (4ga)





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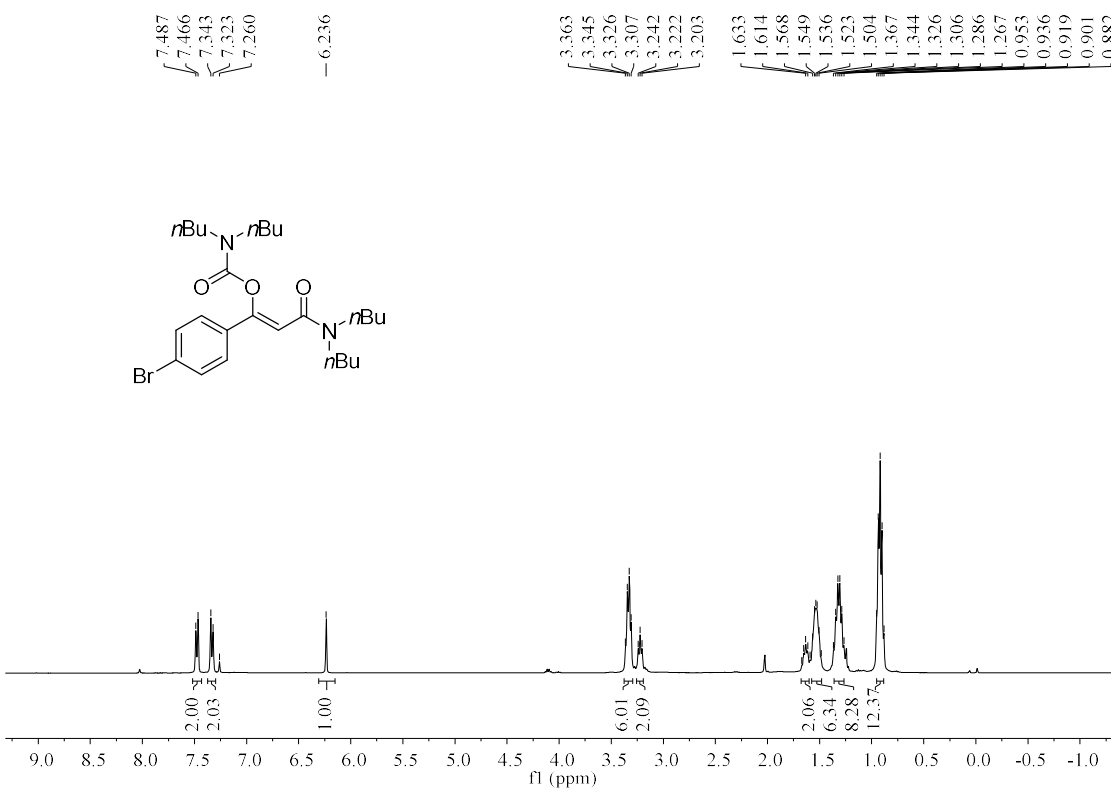

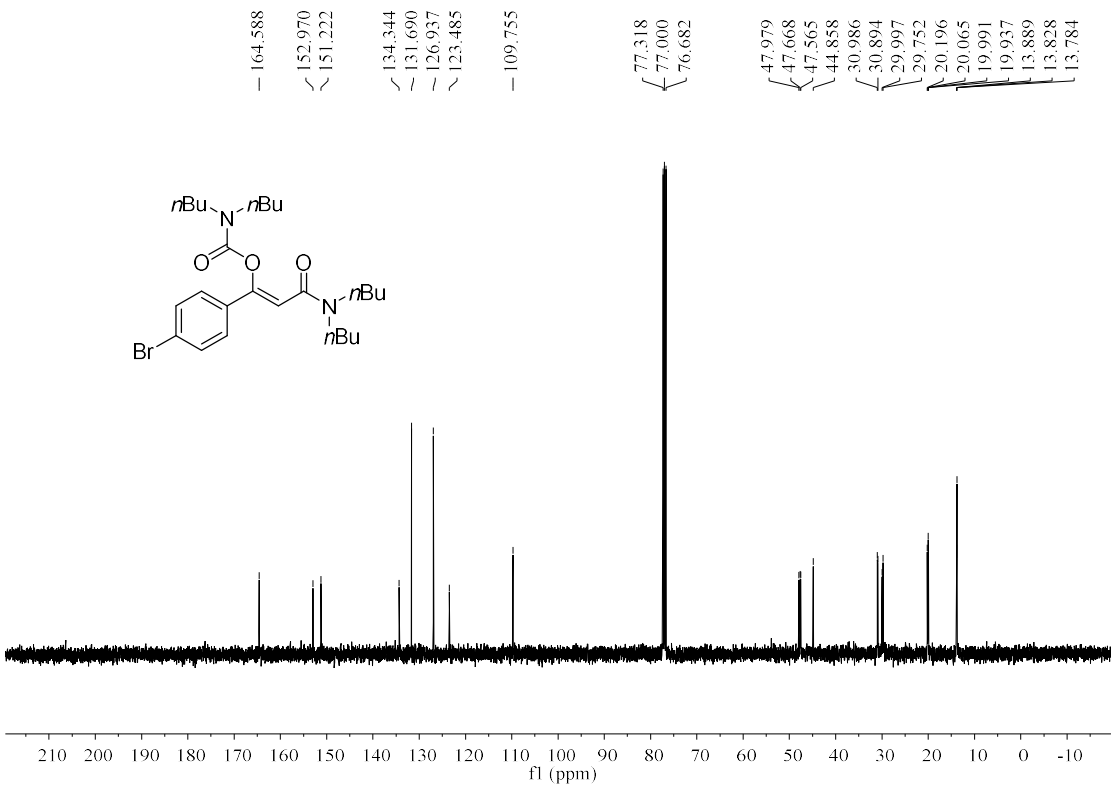

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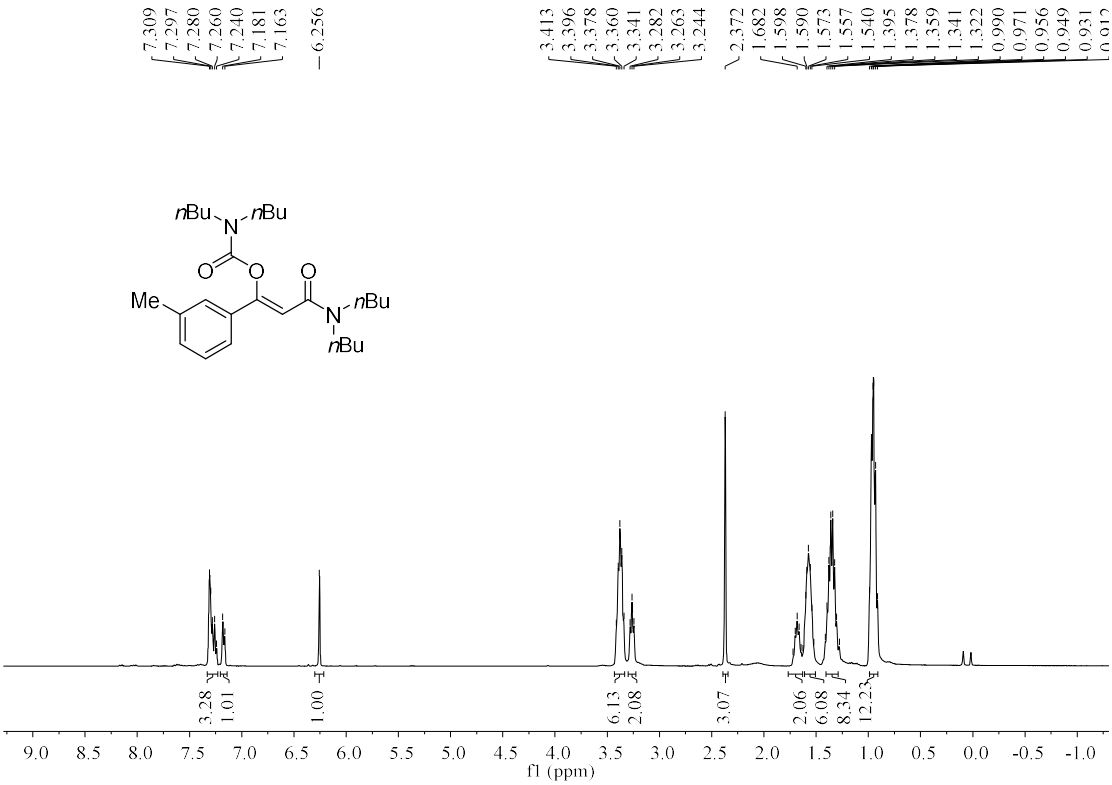

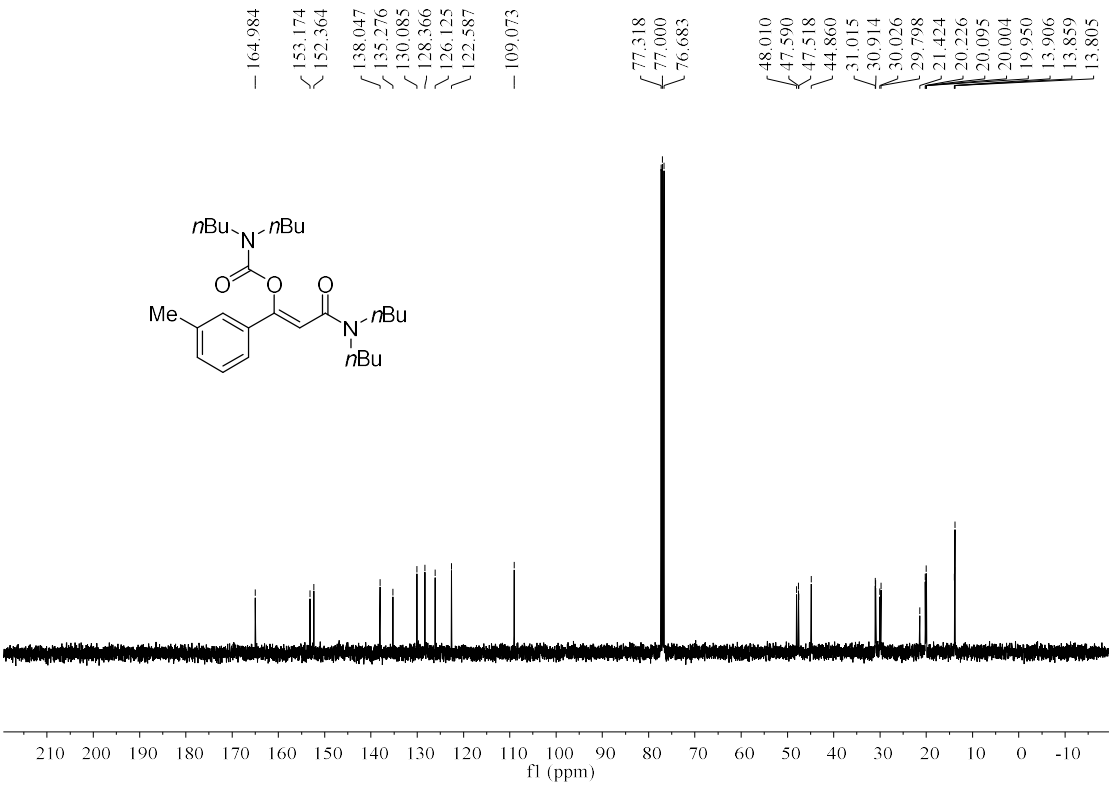

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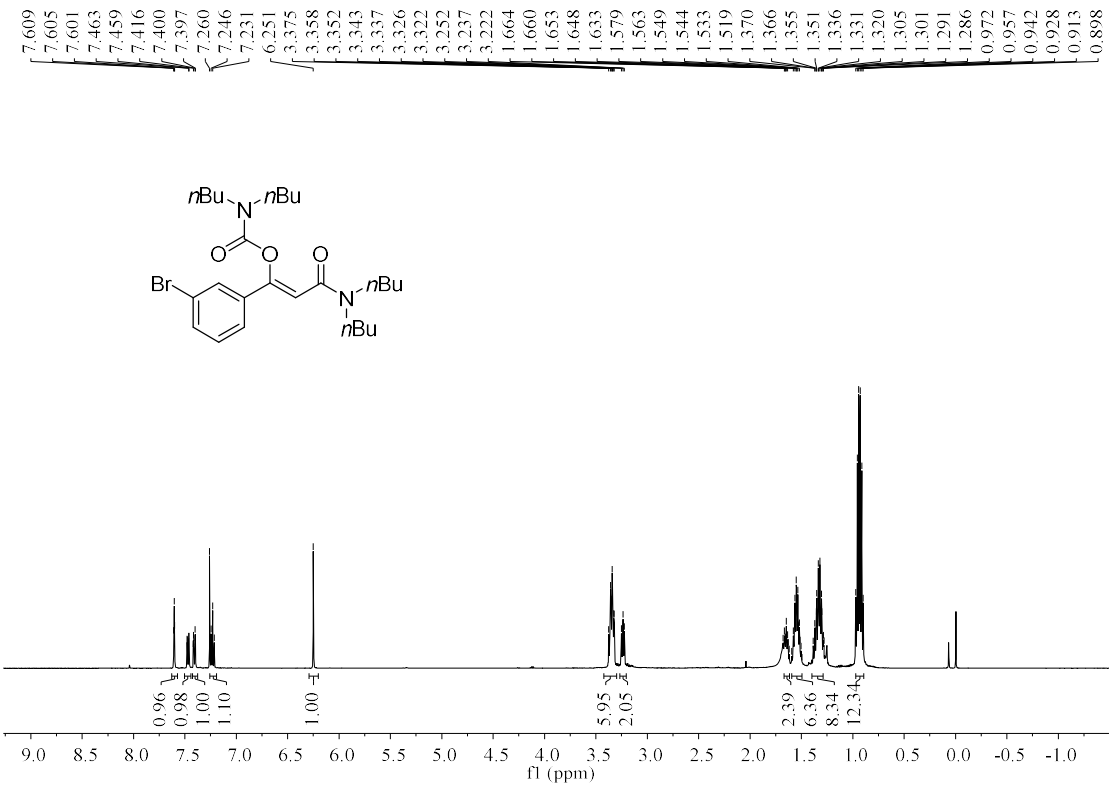
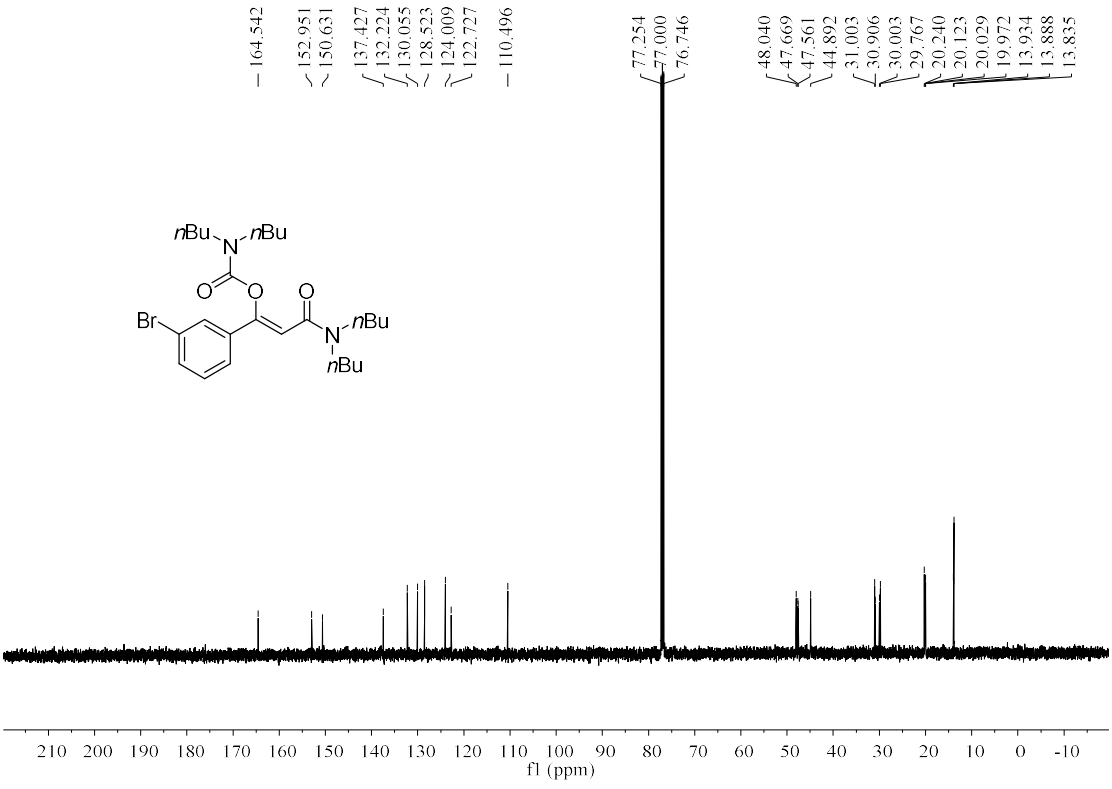
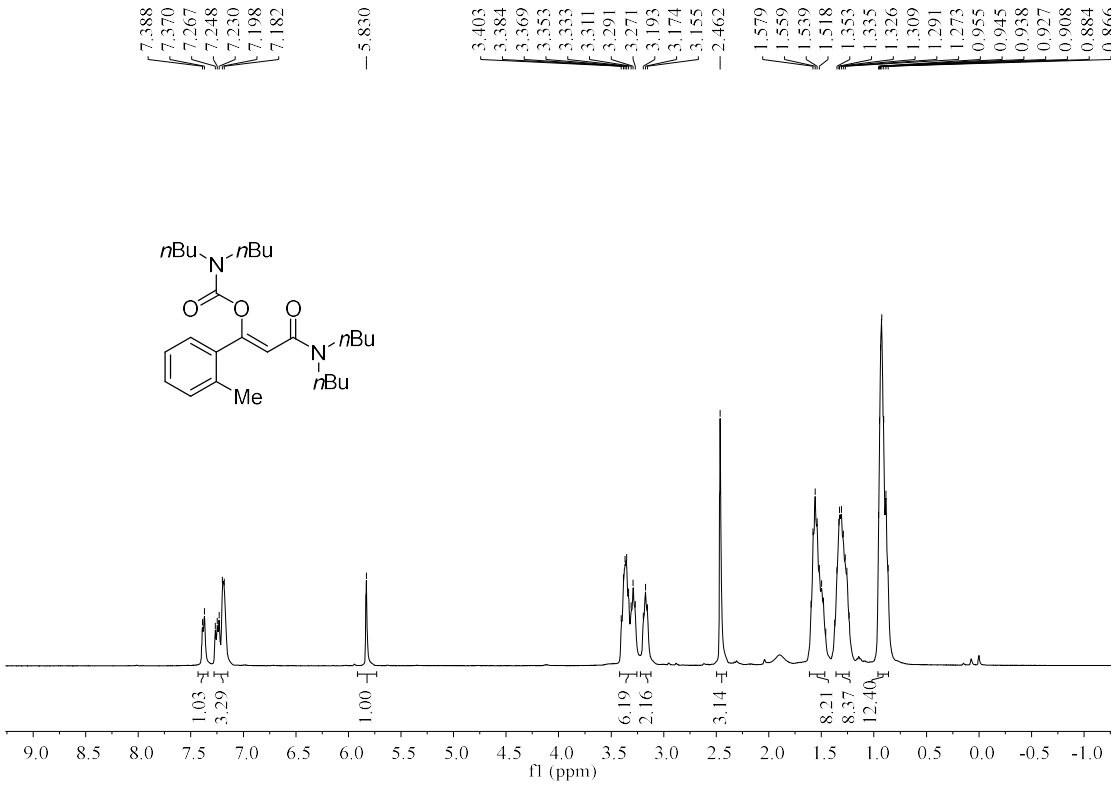
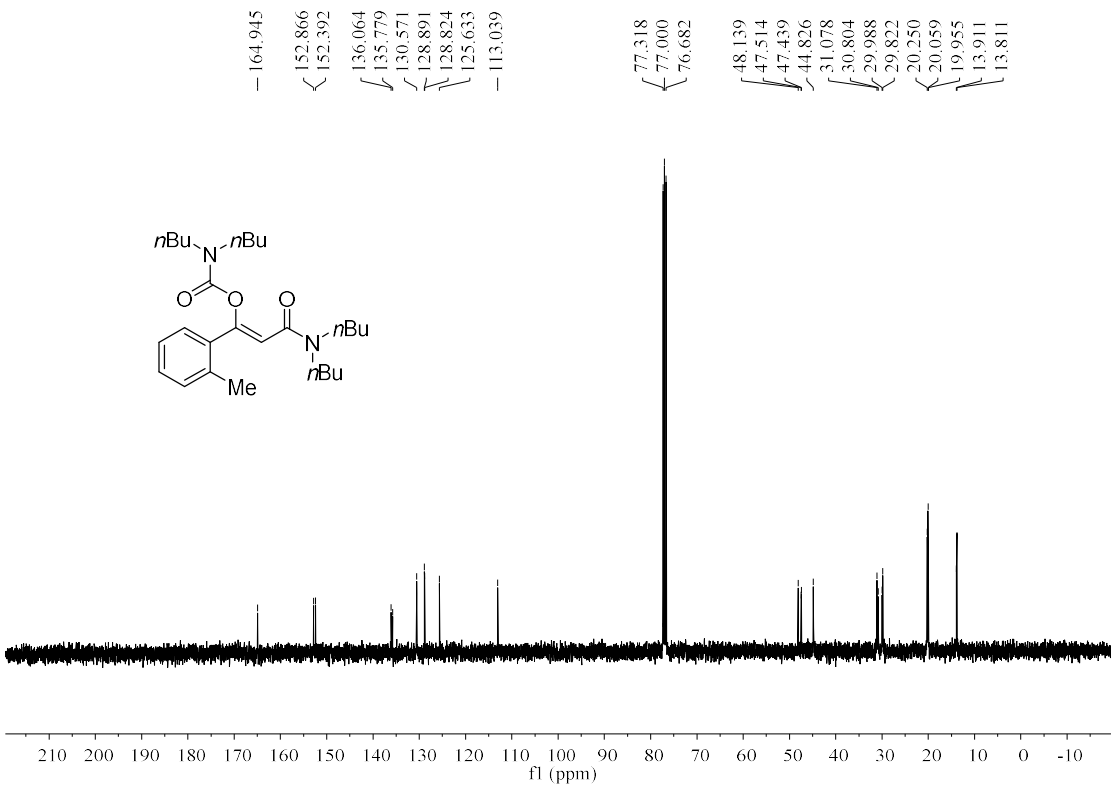




(*Z*)-3-(Dibutylamino)-3-oxo-1-(*o*-tolyl)prop-1-en-1-yl dibutylcarbamate (4ka)





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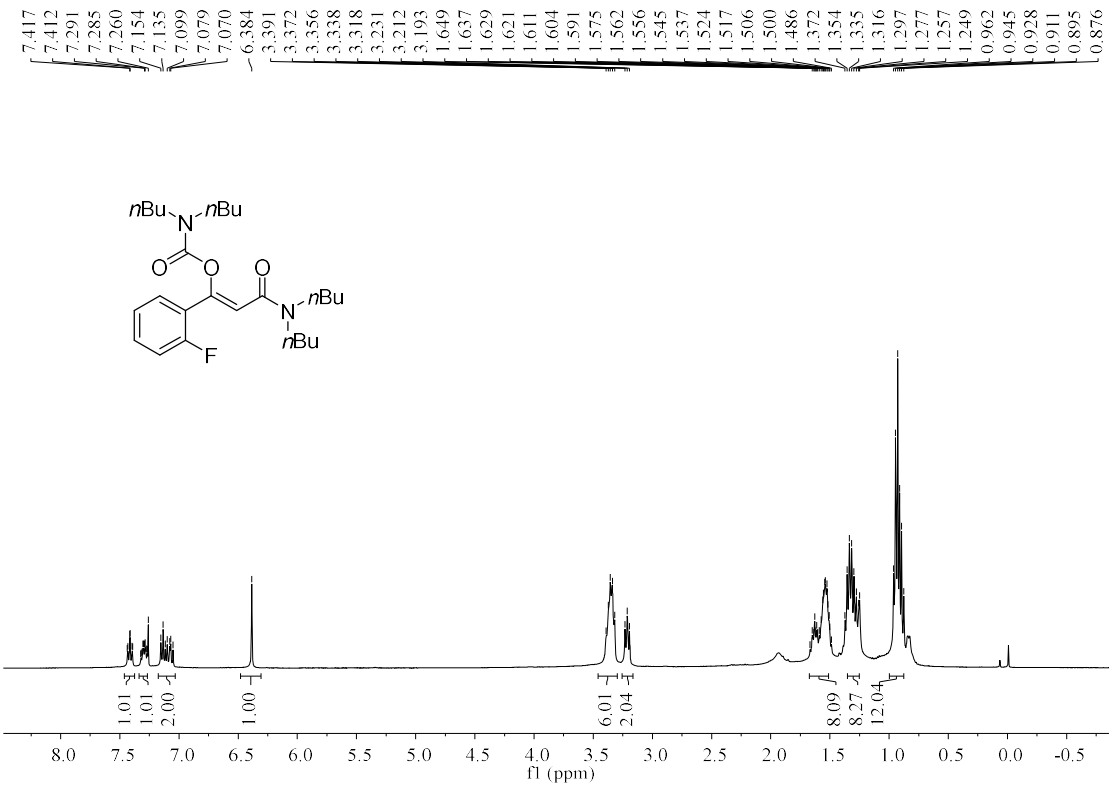

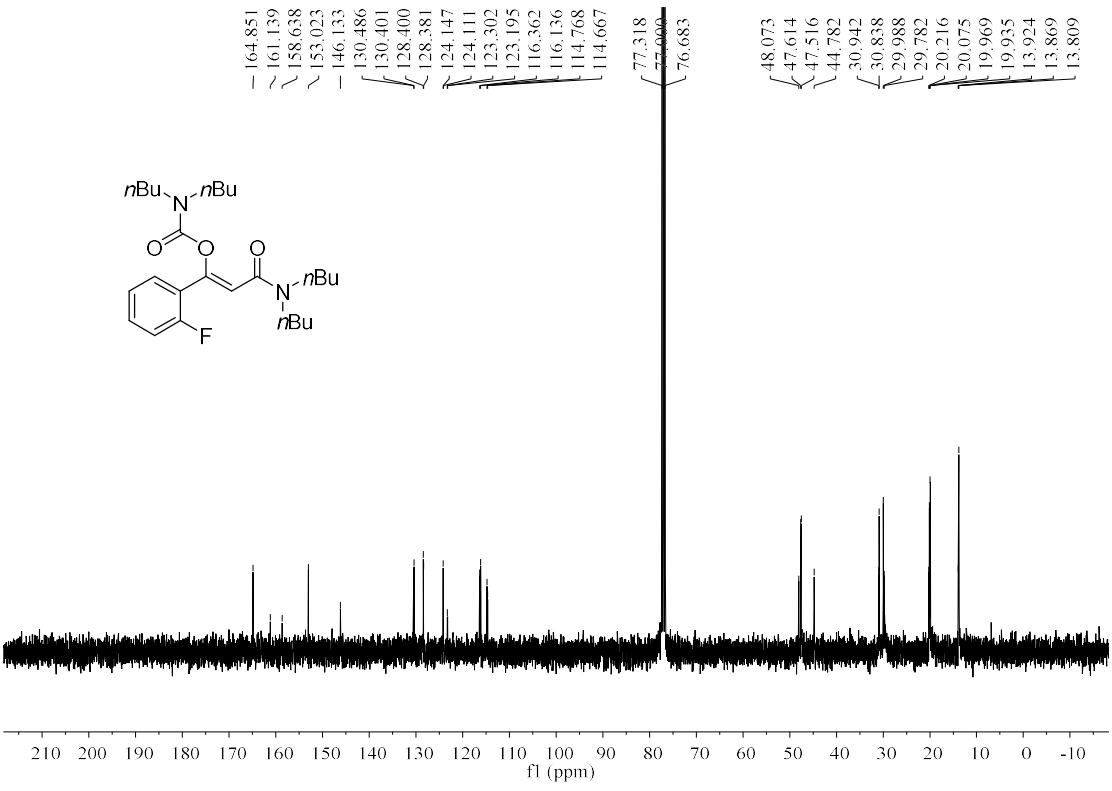

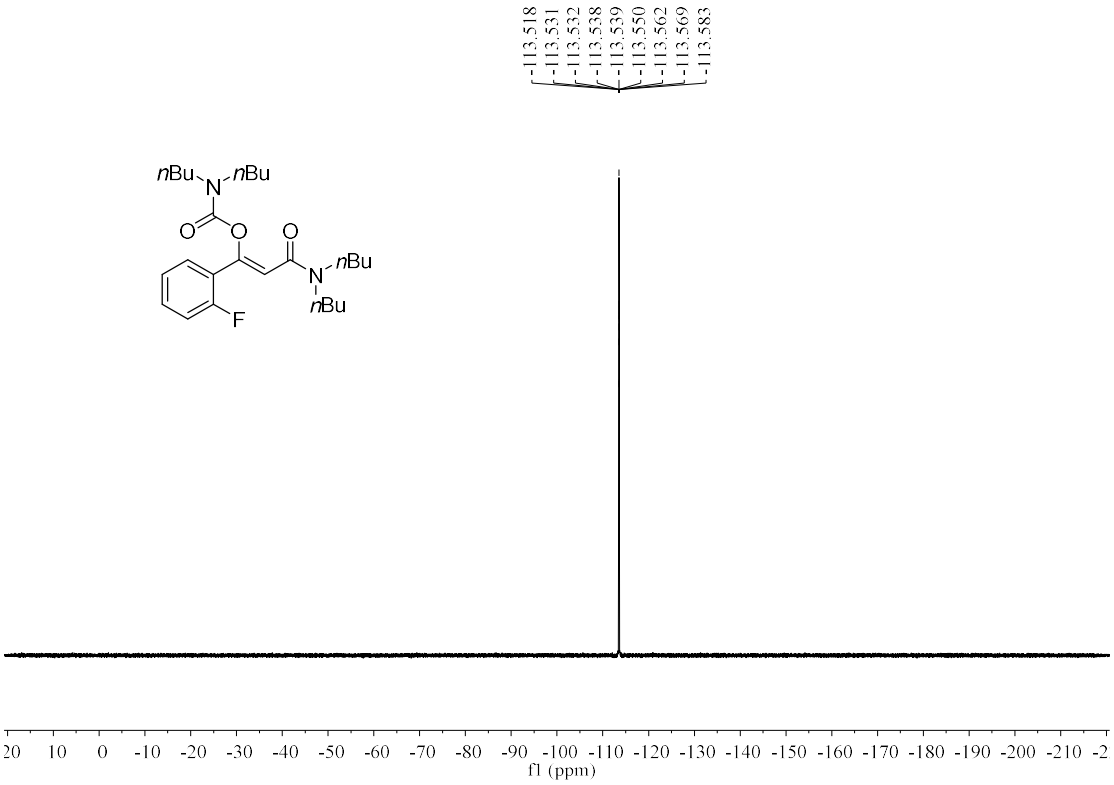
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F
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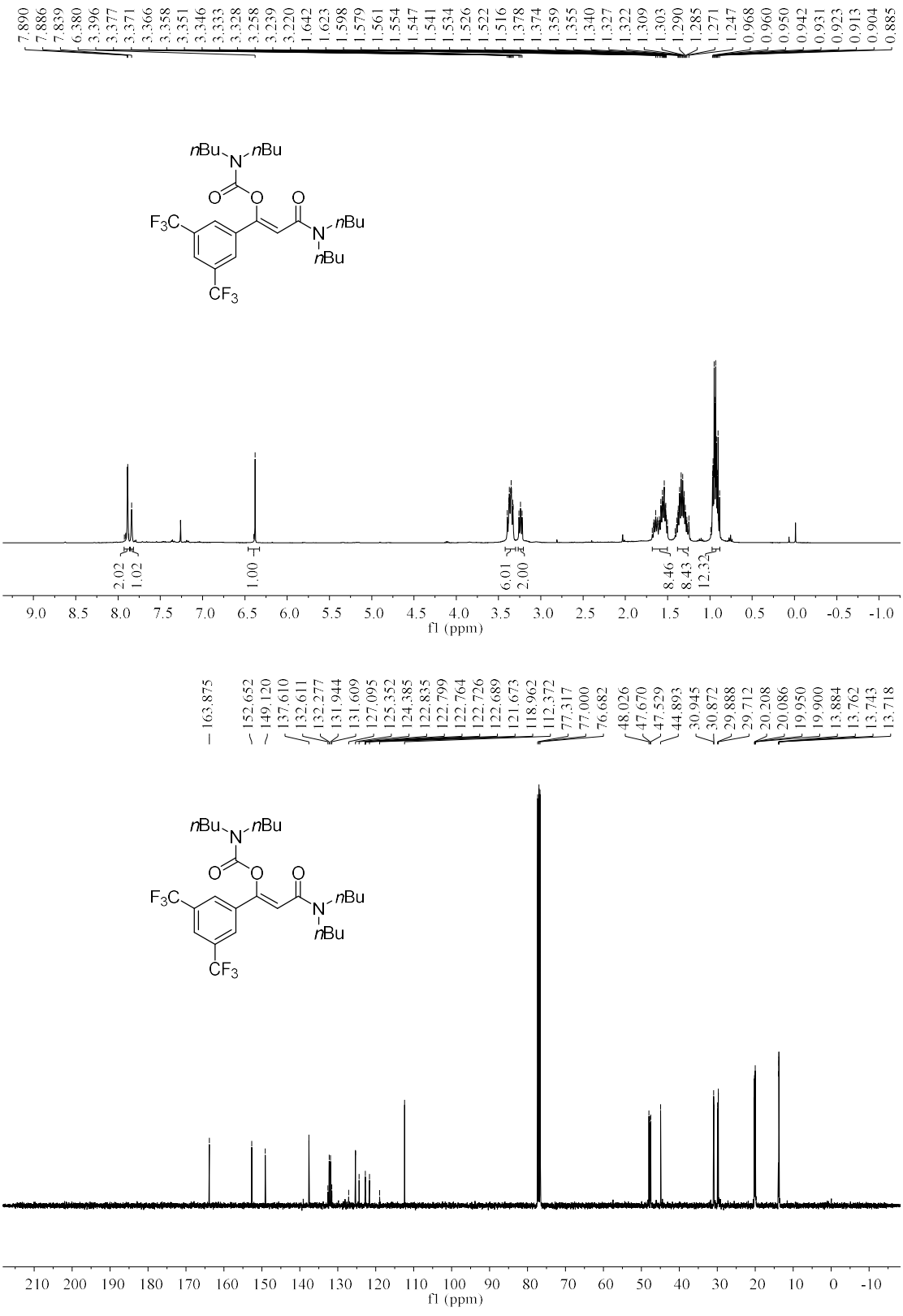
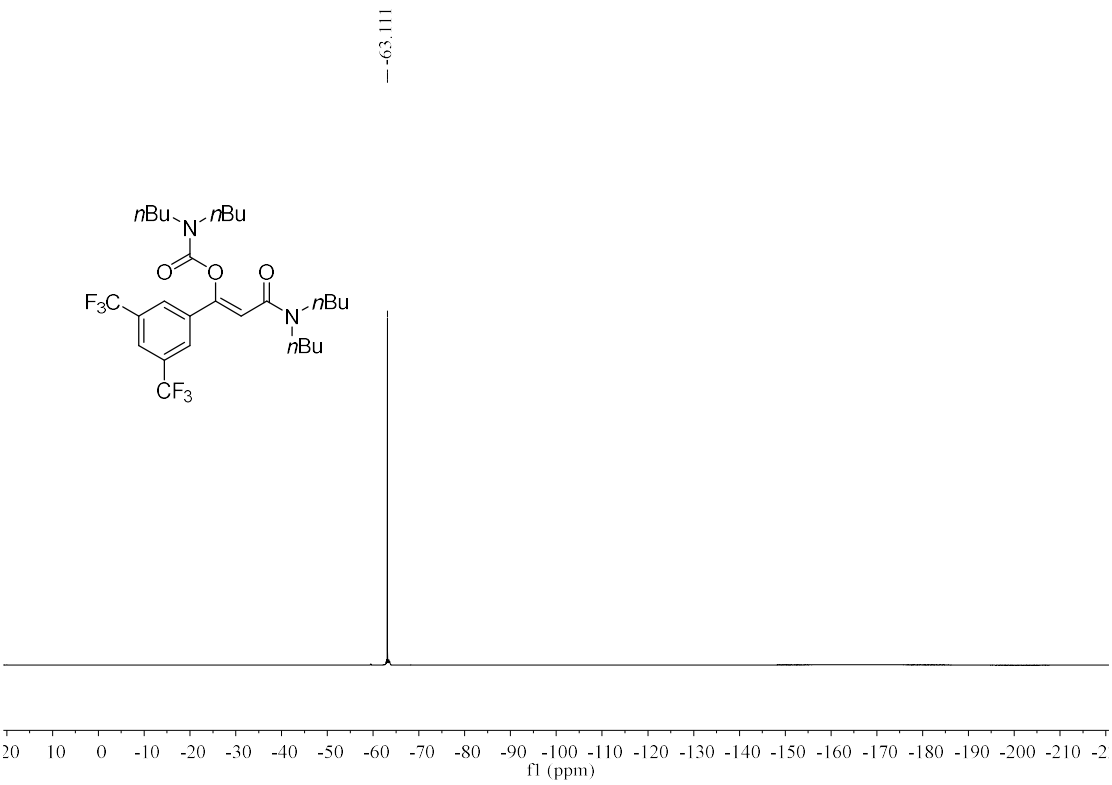
f1 (ppm)

(*Z*)-1-(3,5-Bis(trifluoromethyl)phenyl)-3-(dibutylamino)-3-oxoprop-1-en-1-yl dibutylcarbamate (4ma)

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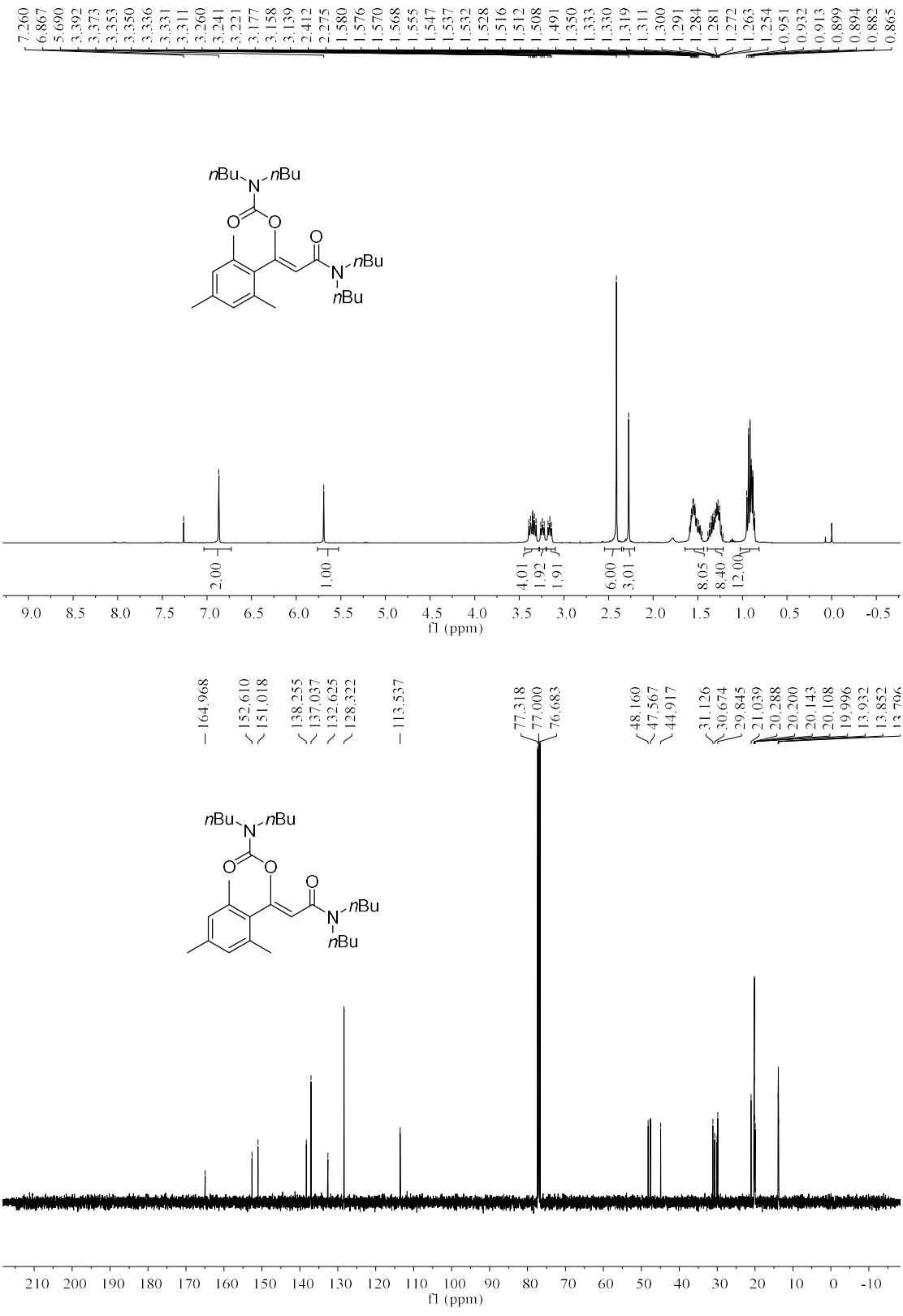
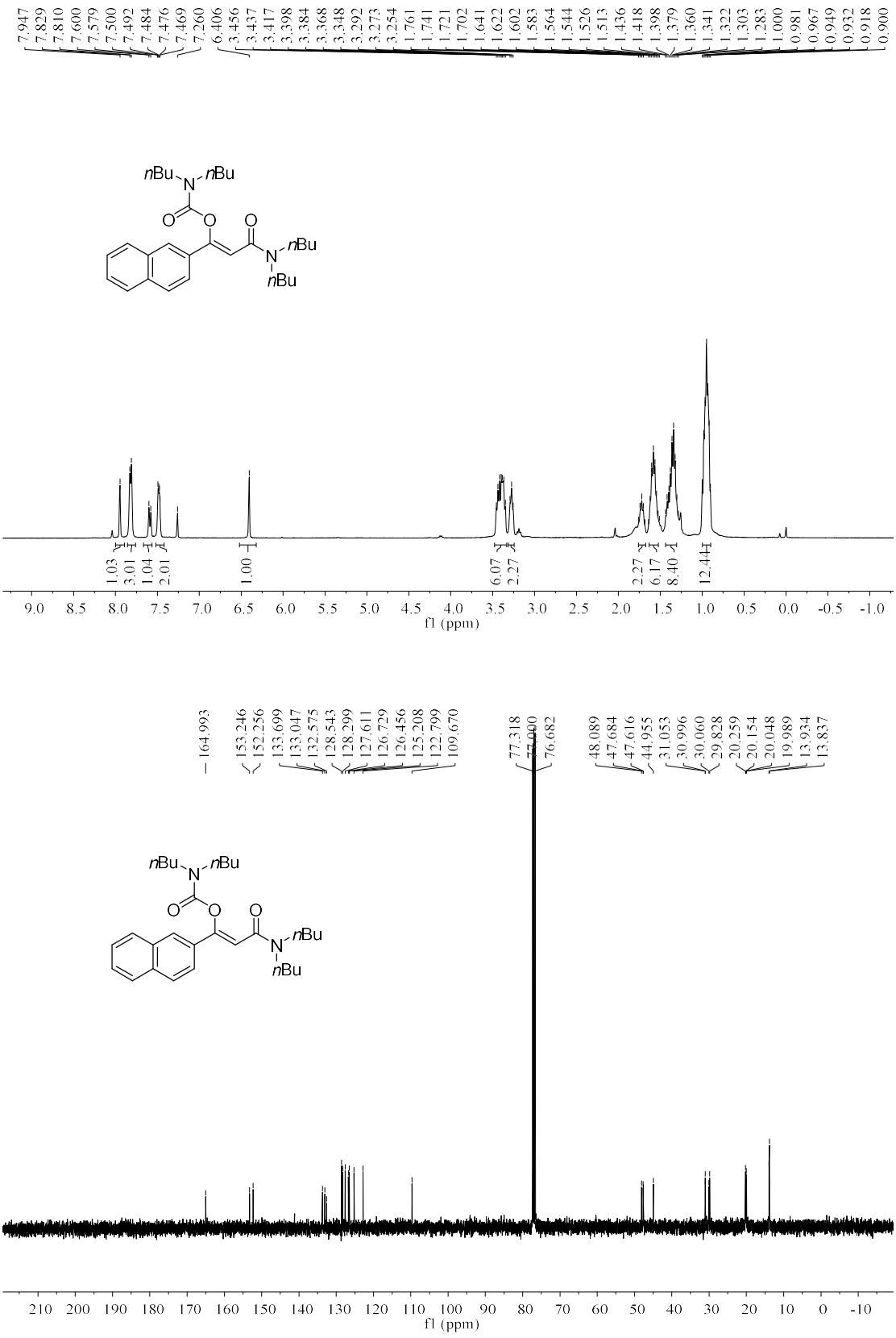
f1 (ppm)

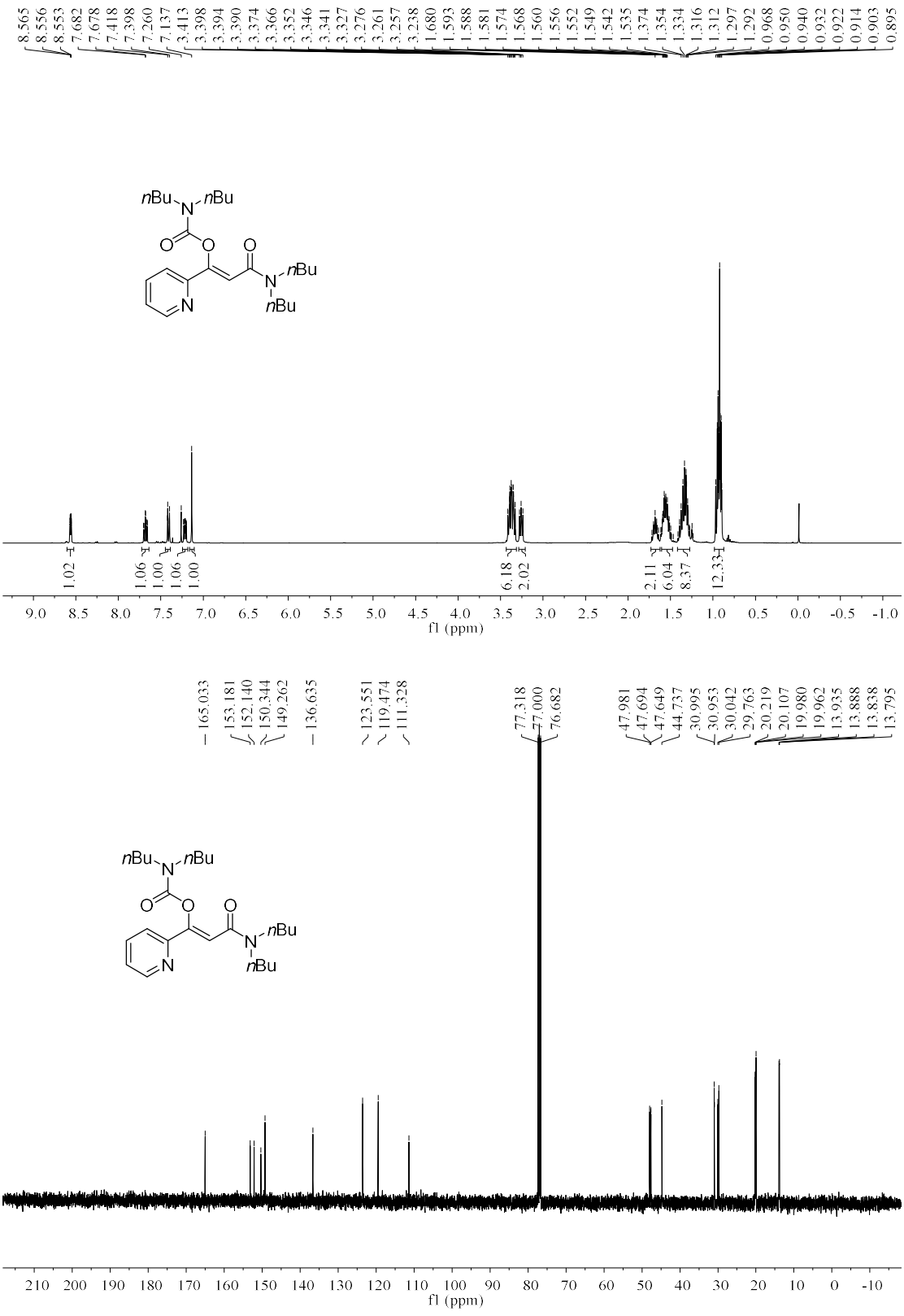
(*Z*)-3-(Dibutylamino)-1-mesityl-3-oxoprop-1-en-1-yl dibutylcarbamate (4na)



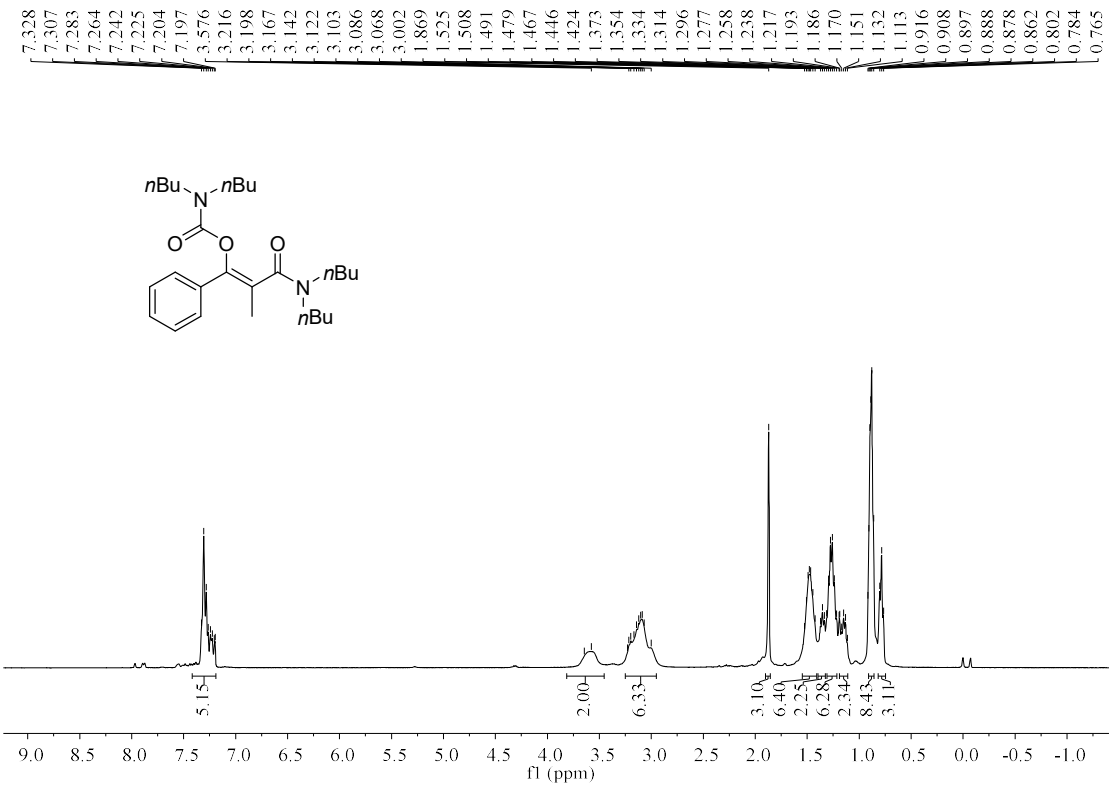
(*Z*)-3-(Dibutylamino)-1-(naphthalen-2-yl)-3-oxoprop-1-en-1-yl dibutylcarbamate (4oa)

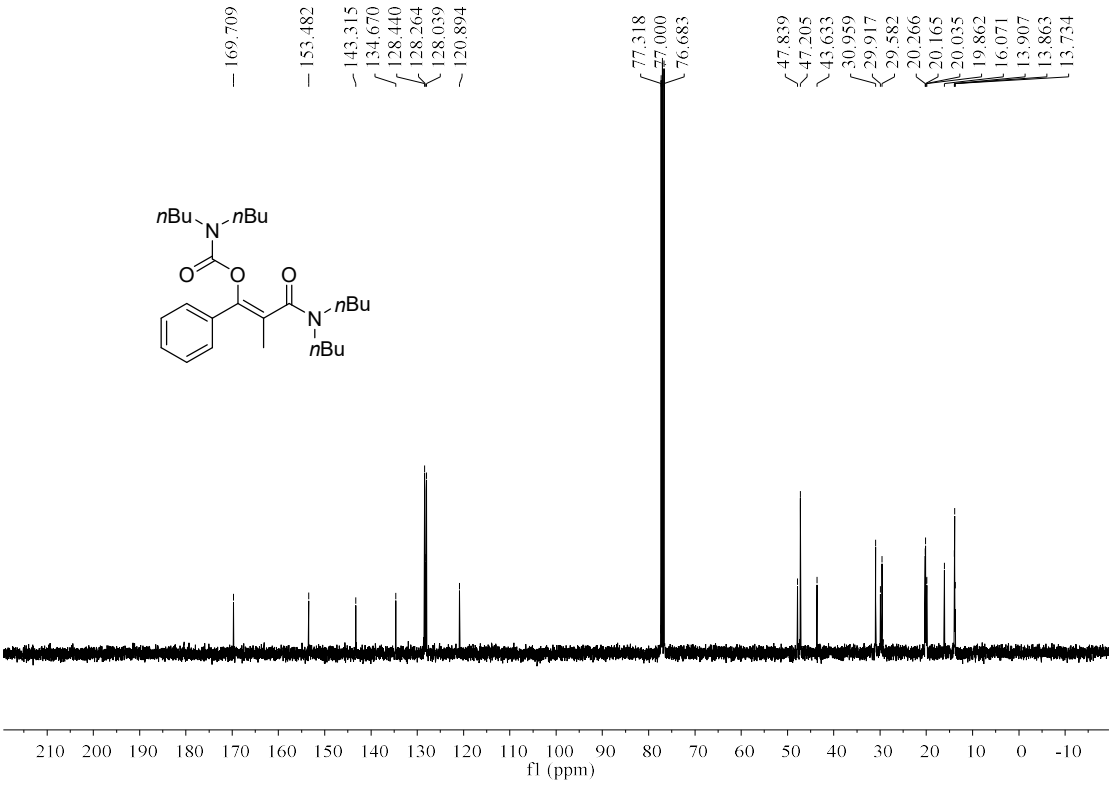


(*Z*)-3-(Dibutylamino)-3-oxo-1-(pyridin-2-yl)prop-1-en-1-yl dibutylcarbamate (4pa)

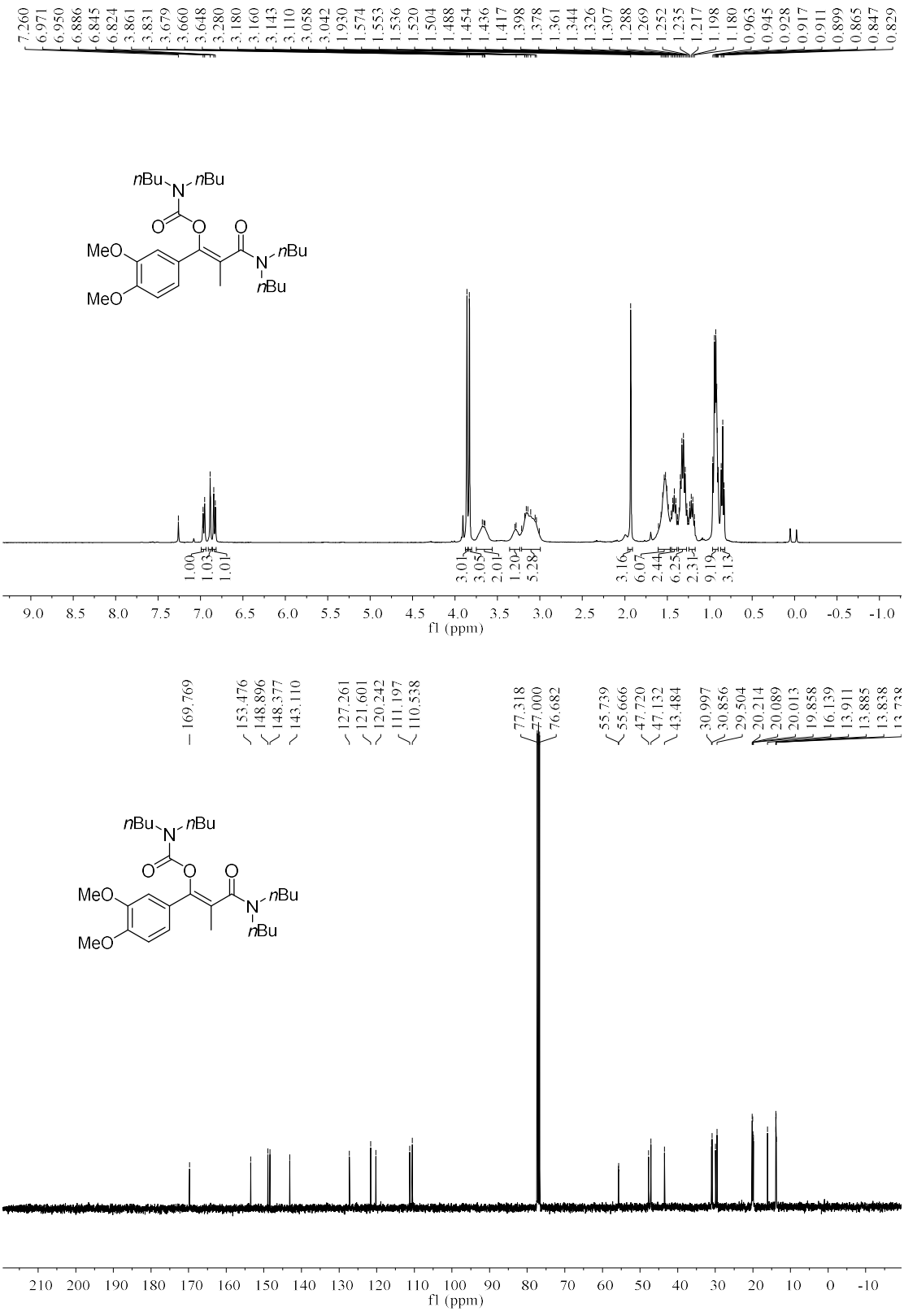


(*Z*)-3-(Dibutylamino)-2-methyl-3-oxo-1-phenylprop-1-en-1-yl dibutylcarbamate (4qa)

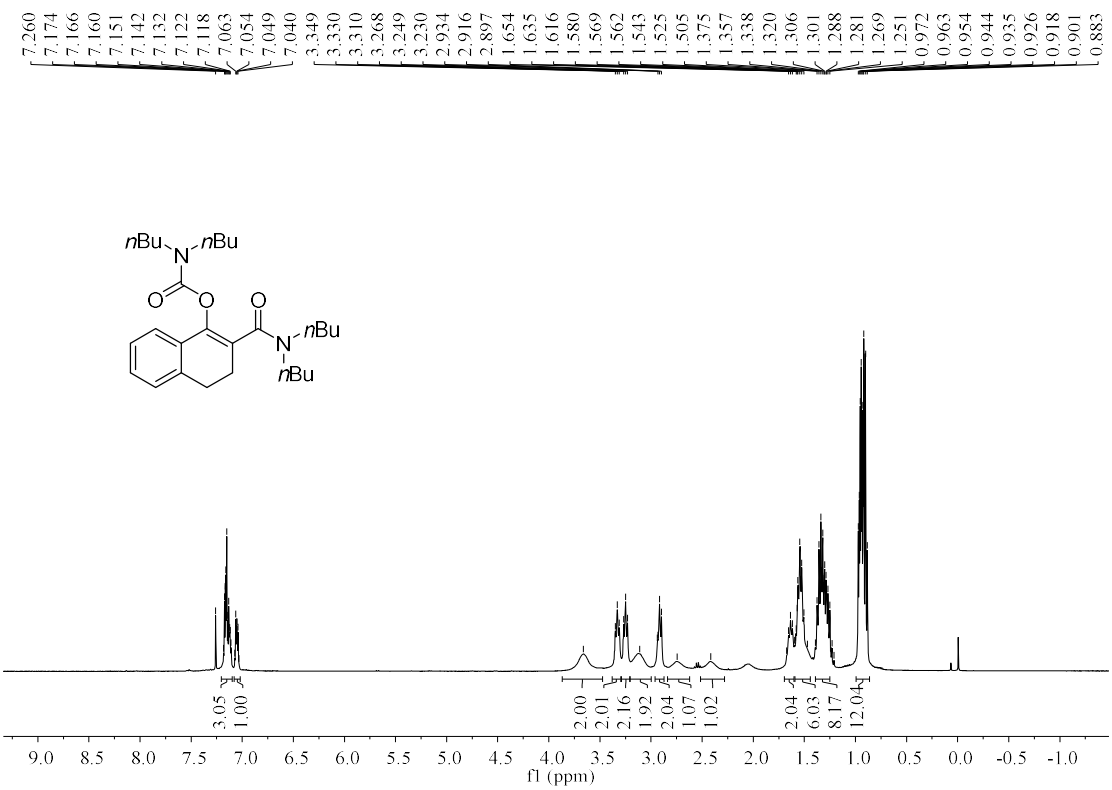


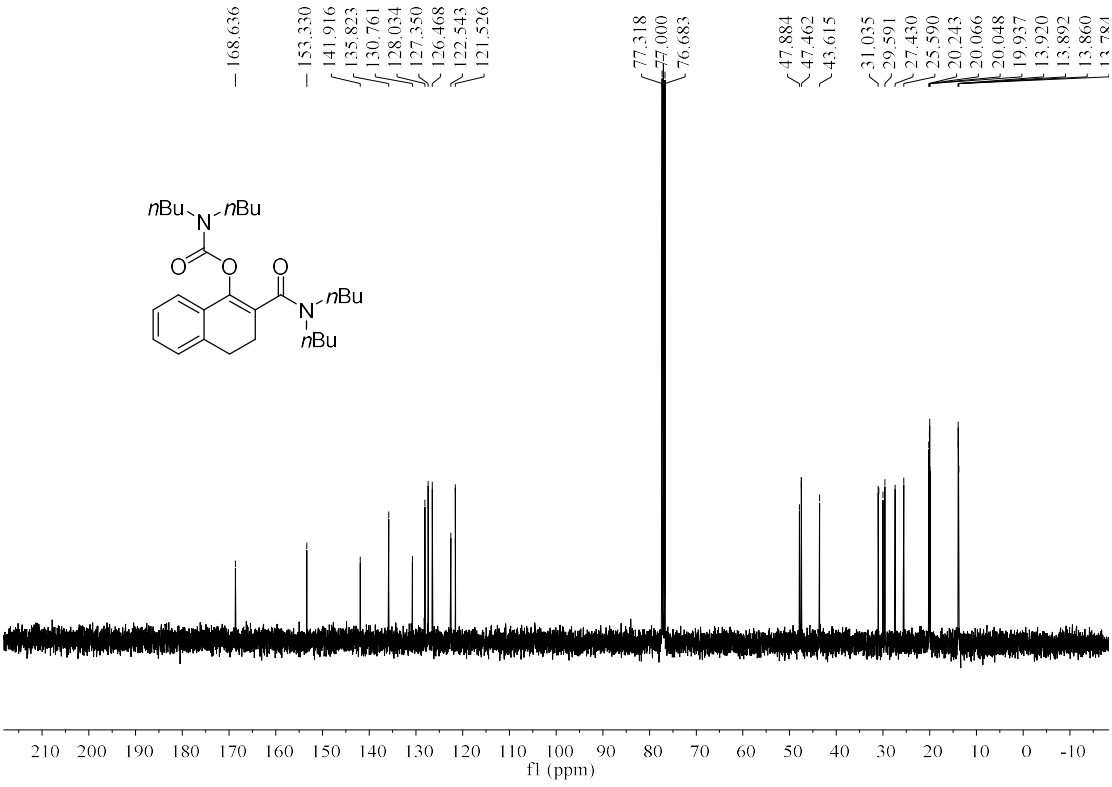


(*Z*)-3-(Dibutylamino)-1-(3,4-dimethoxyphenyl)-2-methyl-3-oxoprop-1-en-1-yl dibutylcarbamate (4ra)

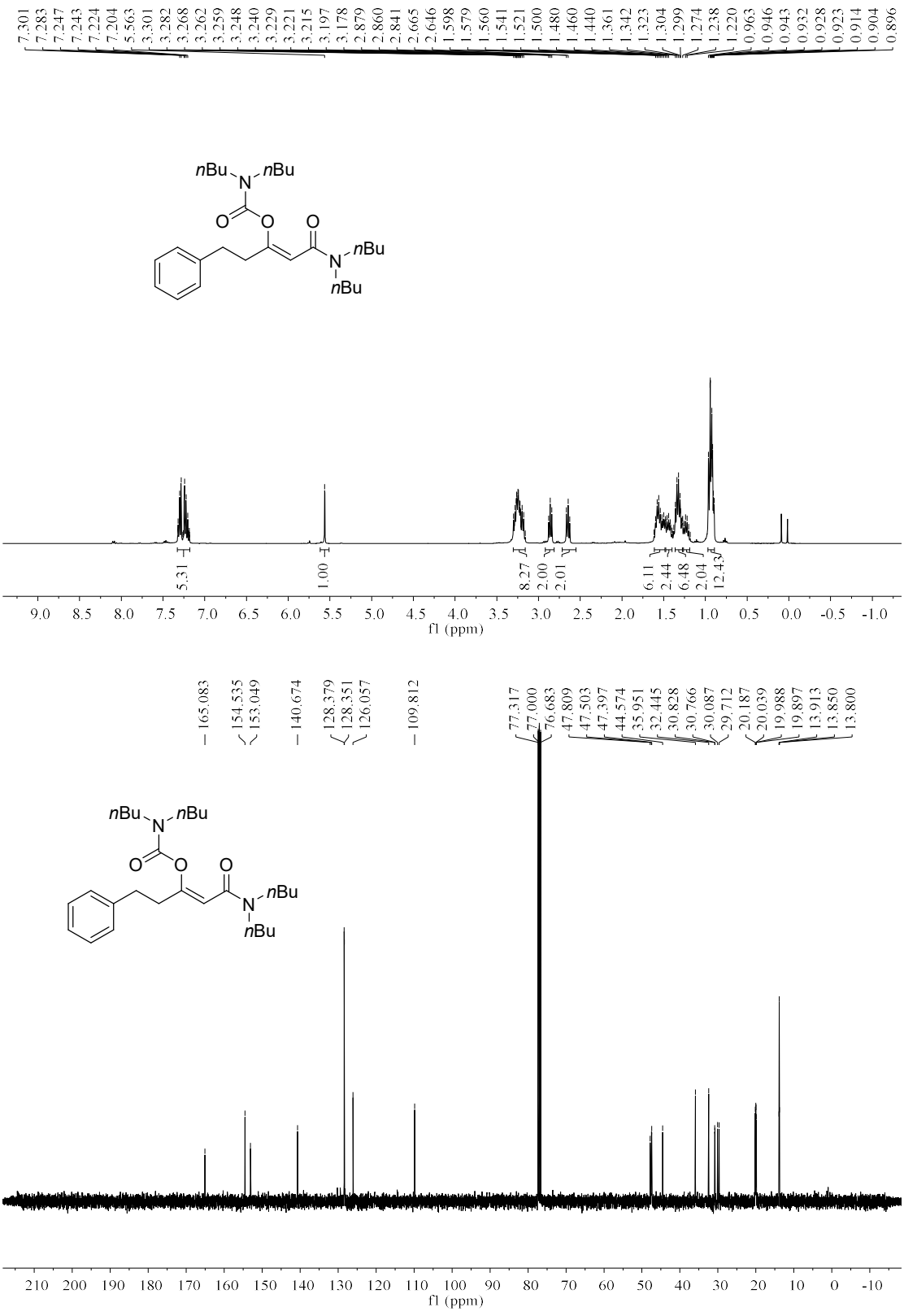


2-(Dibutylcarbamoyl)-3,4-dihydronaphthalen-1-yl dibutylcarbamate (4sa)



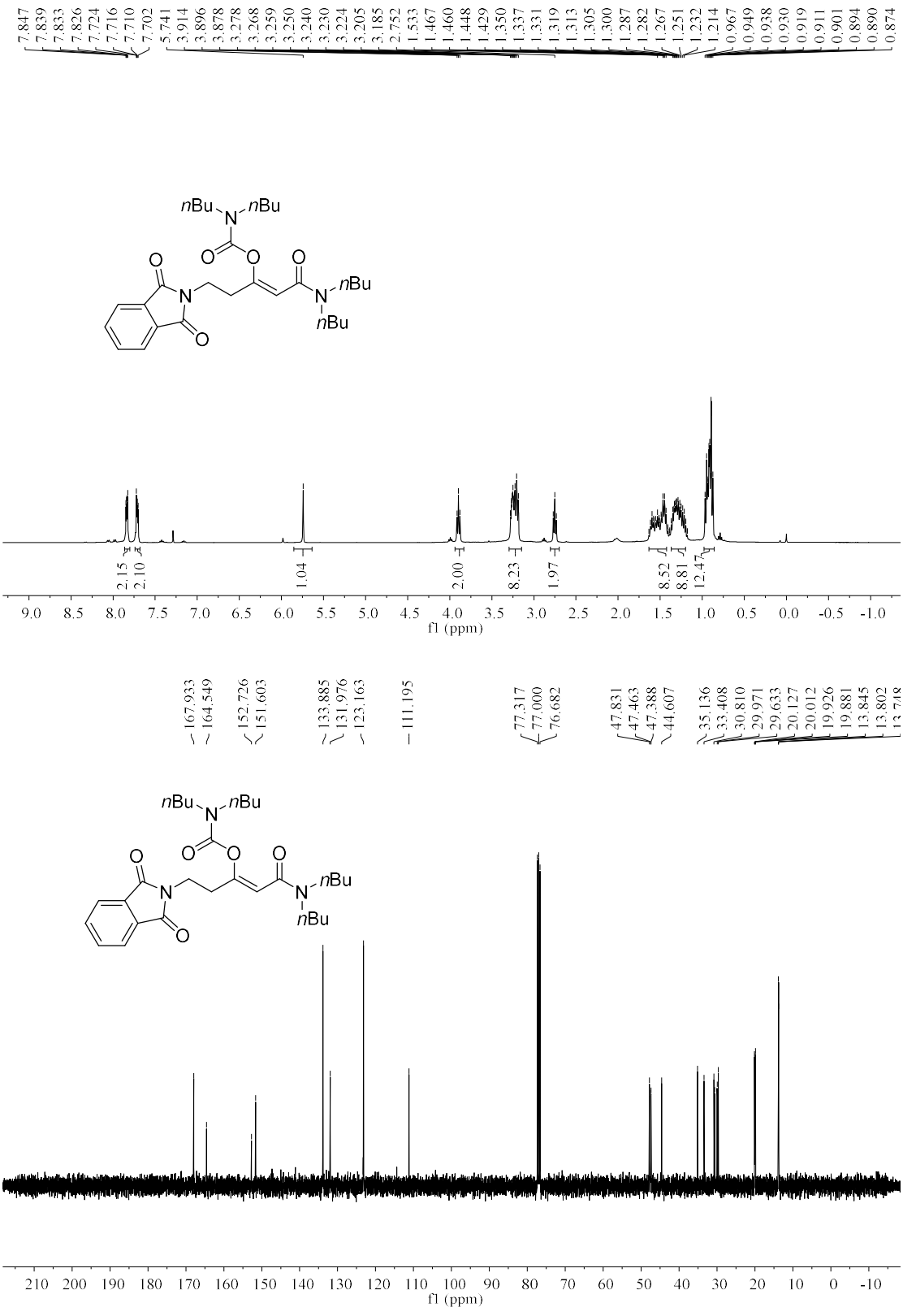


(*Z*)-1-(Dibutylamino)-1-oxo-5-phenylpent-2-en-3-yl dibutylcarbamate (4ta)

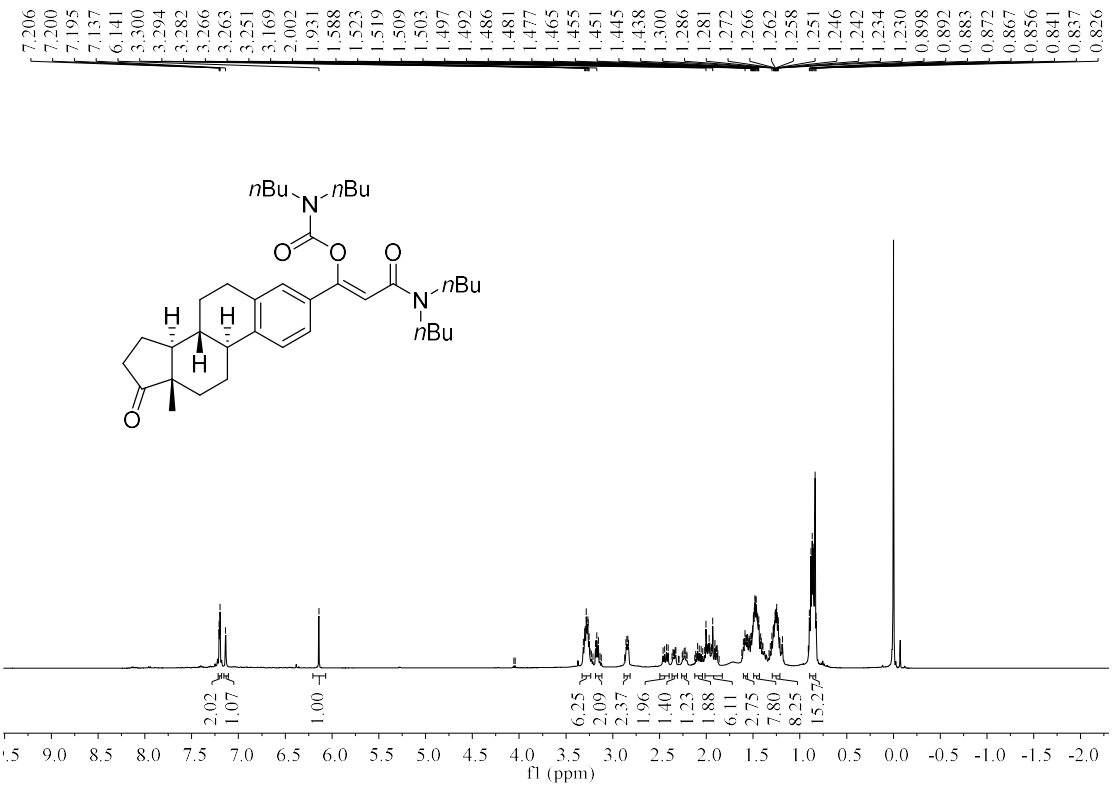


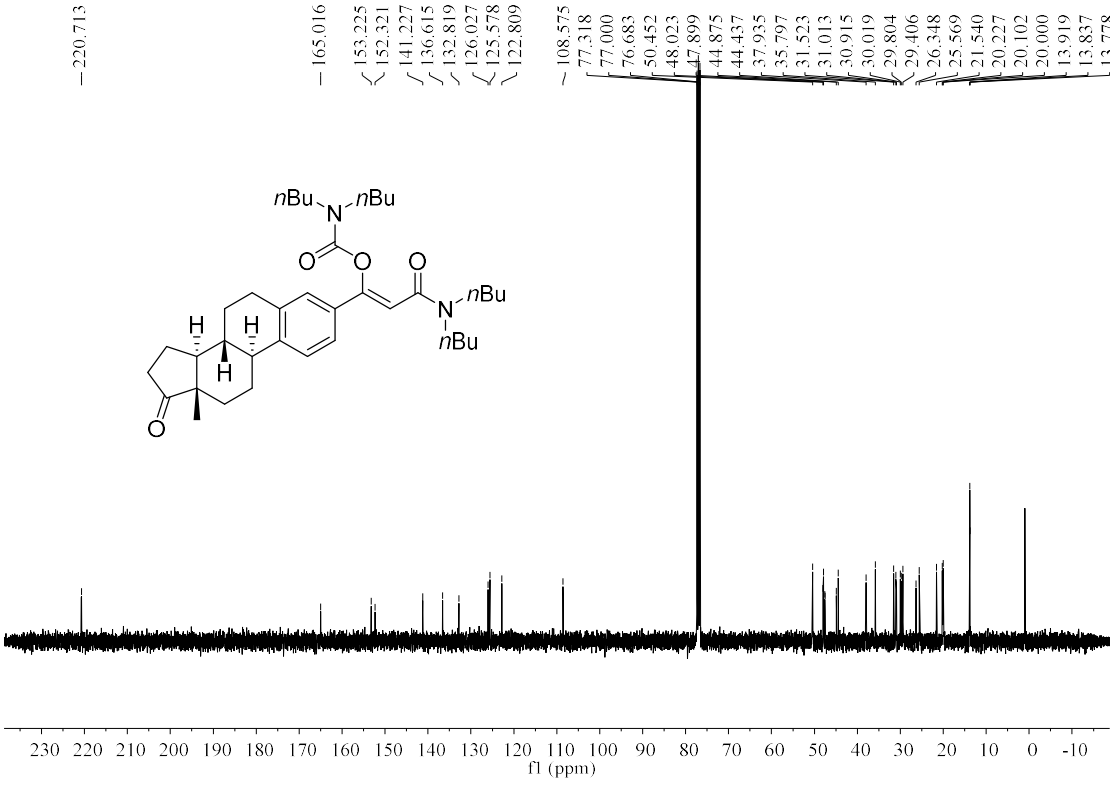
(*Z*)-1-(Dibutylamino)-5-(1,3-dioxoisoindolin-2-yl)-1-oxopent-2-en-3-yl dibutylcarbamate

(4ua)

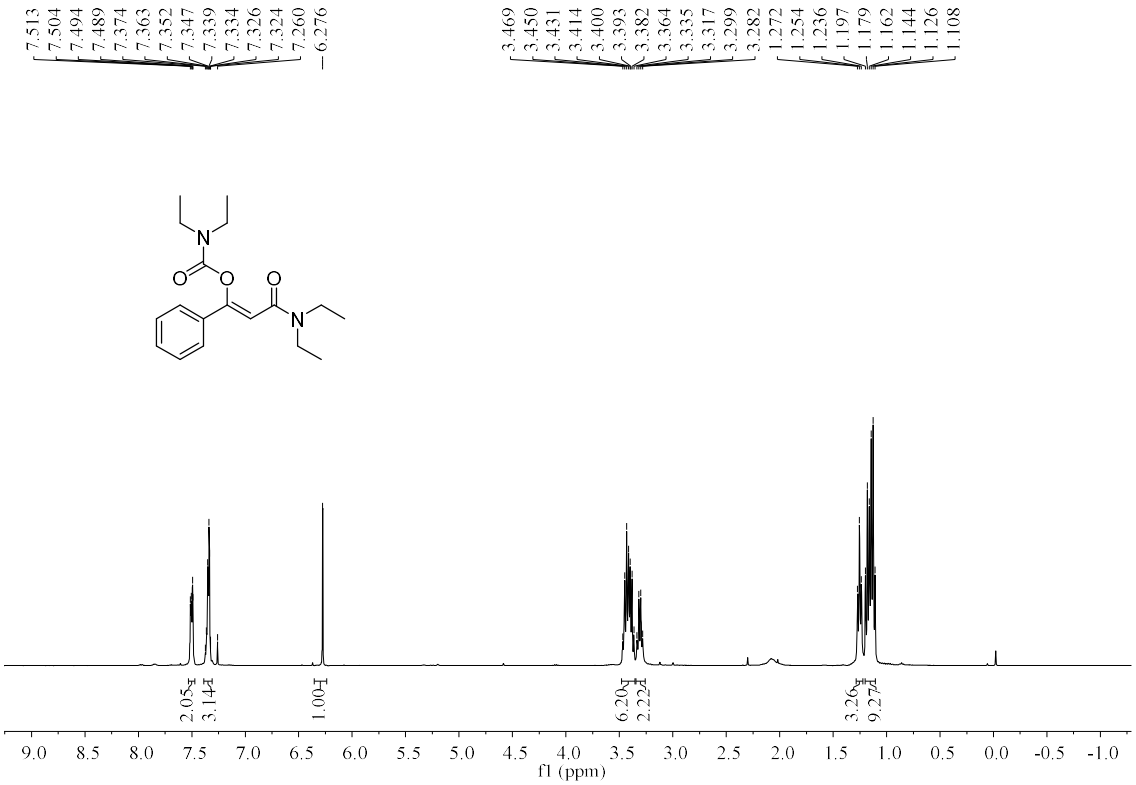


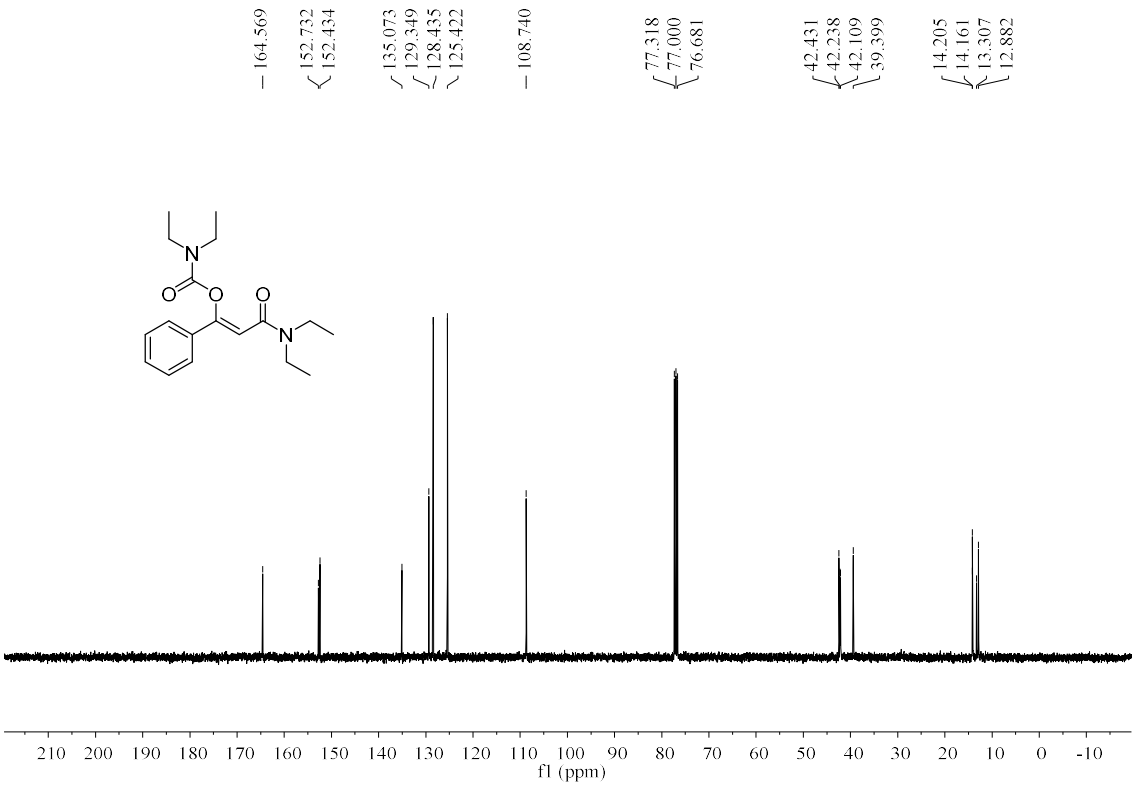
(*Z*)-3-(Dibutylamino)-1-((8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[a]phenanthren-3-yl)-3-oxoprop-1-en-1-yl dibutylcarbamate (4va)



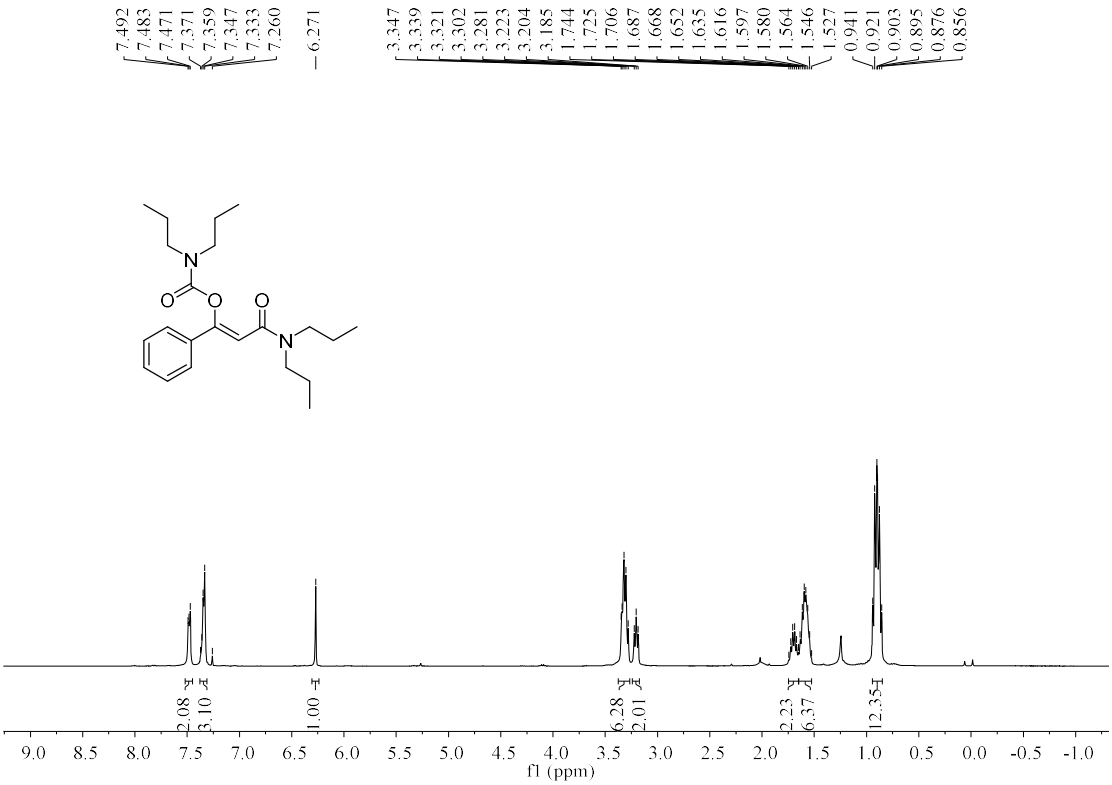


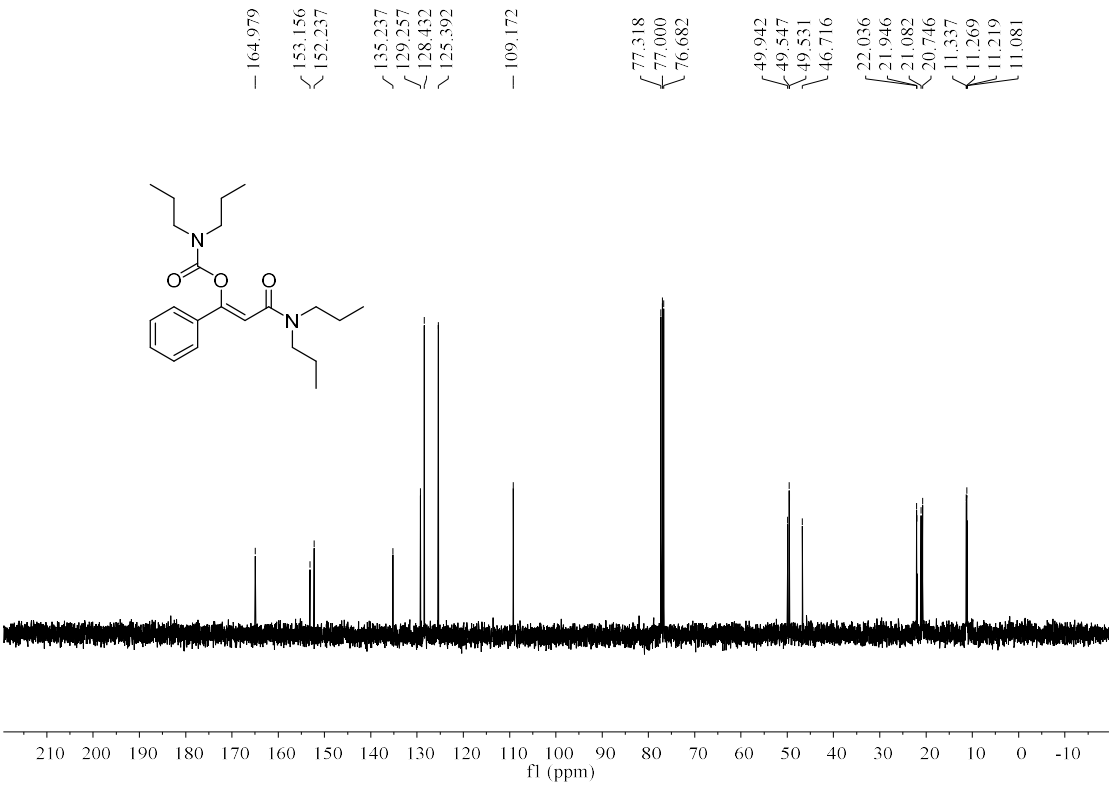
(*Z*)-3-(Diethylamino)-3-oxo-1-phenylprop-1-en-1-yl diethylcarbamate (4ab)



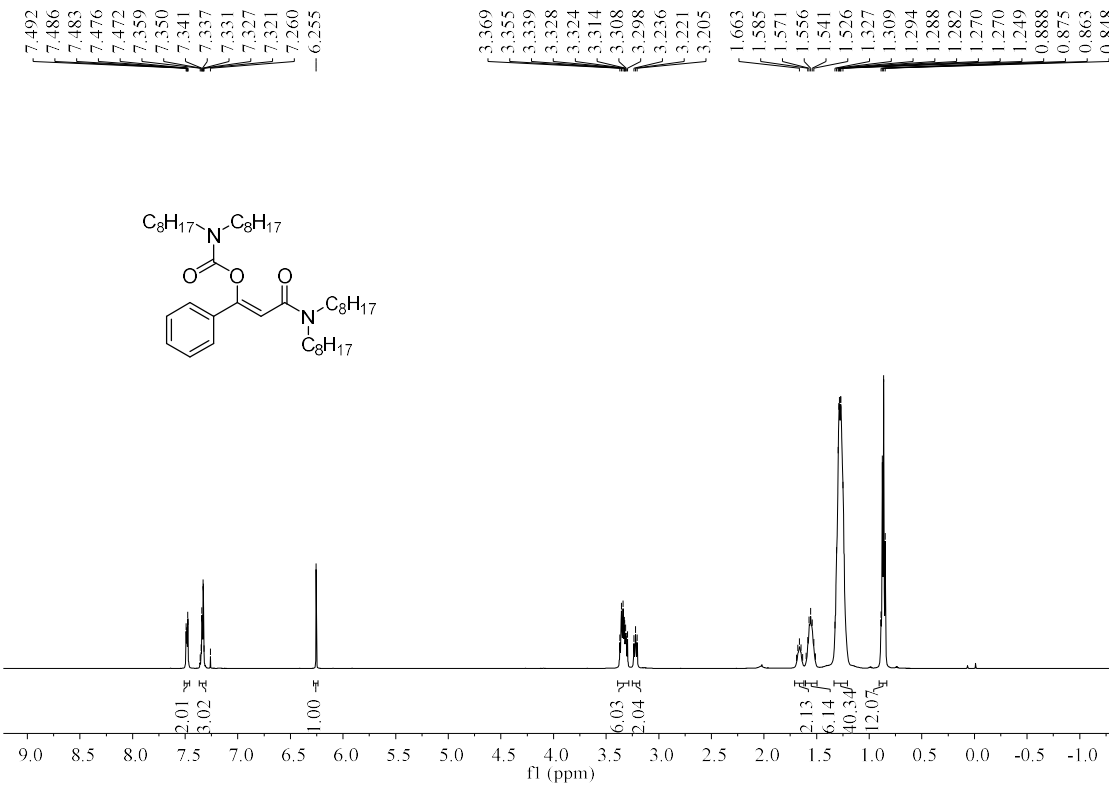


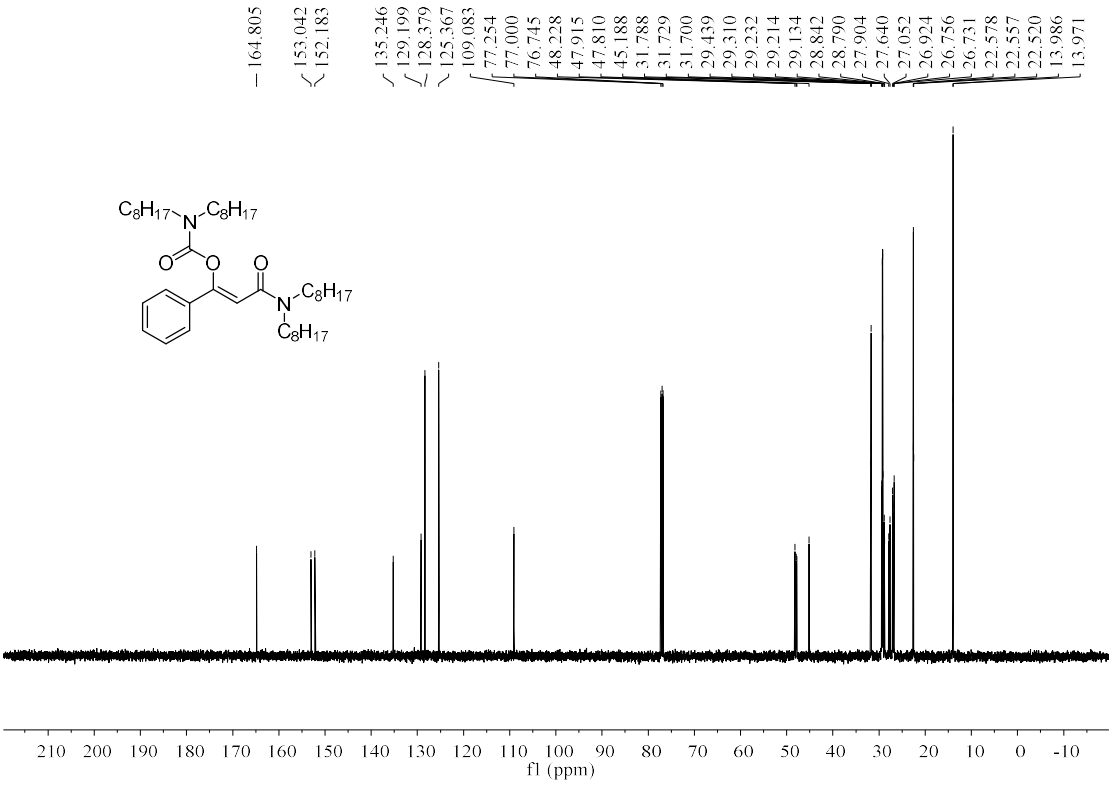
(*Z*)-3-(Dipropylamino)-3-oxo-1-phenylprop-1-en-1-yl dipropylcarbamate (4ac)



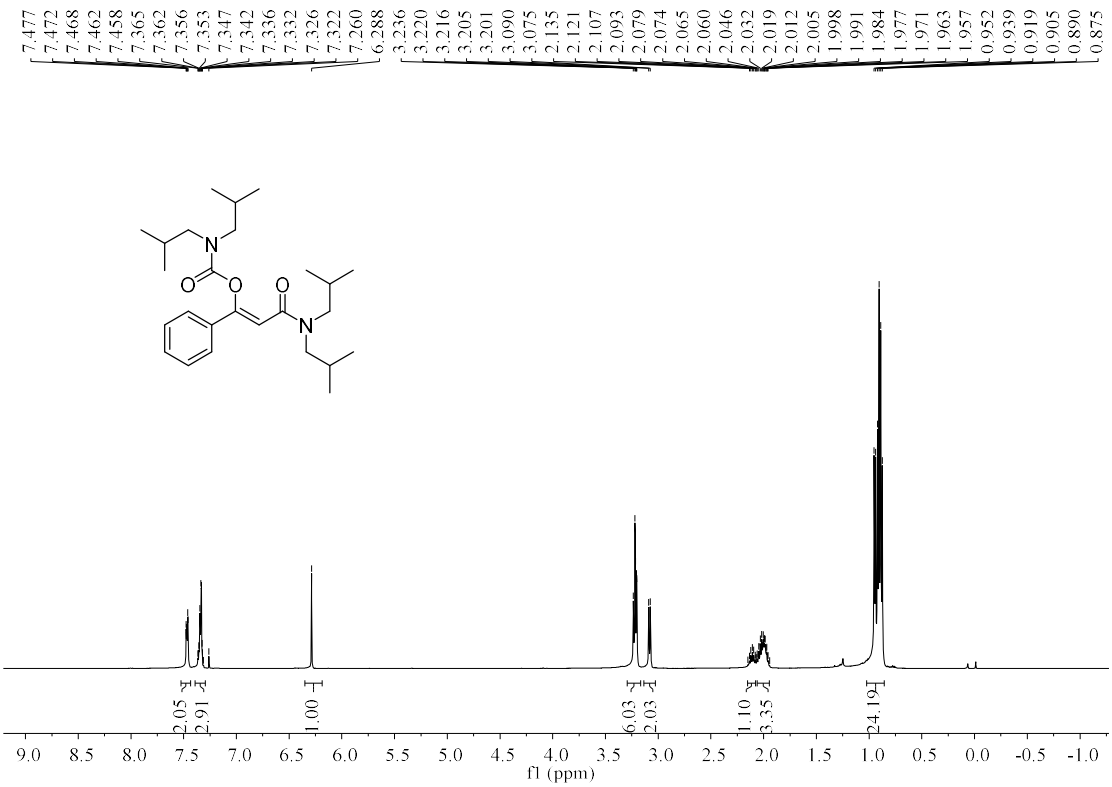


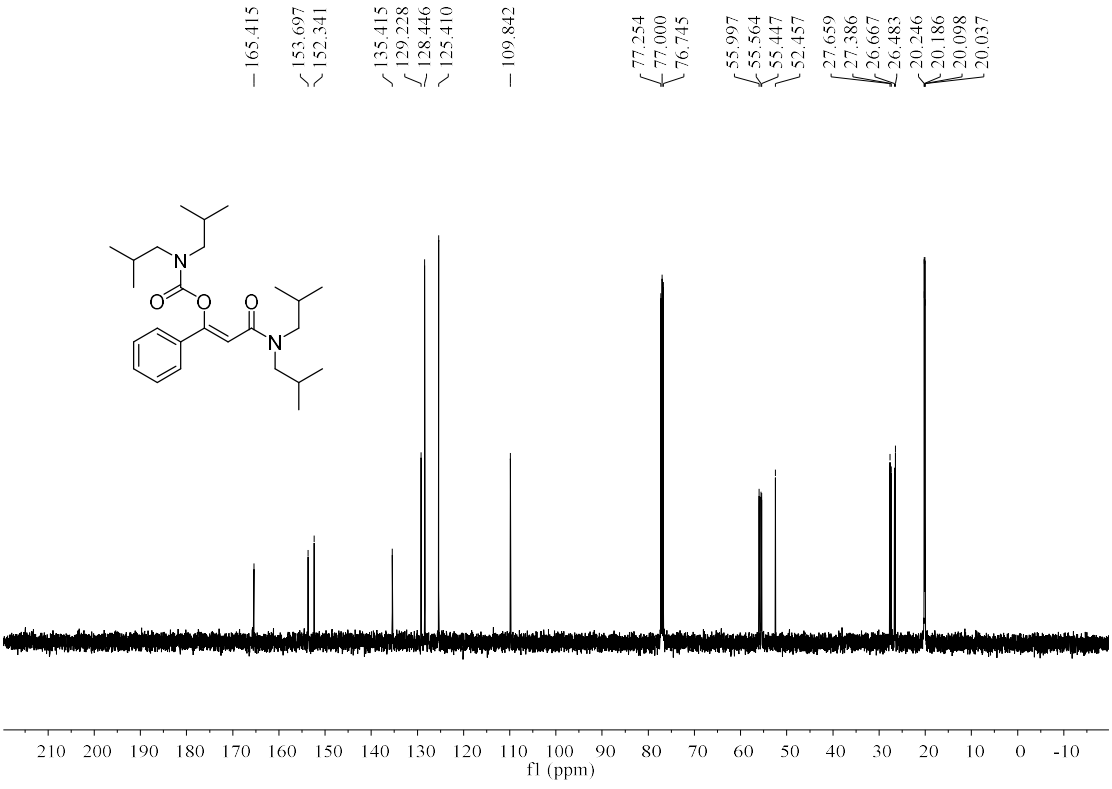
(*Z*)-3-(Dioctylamino)-3-oxo-1-phenylprop-1-en-1-yl dioctylcarbamate (4ad)



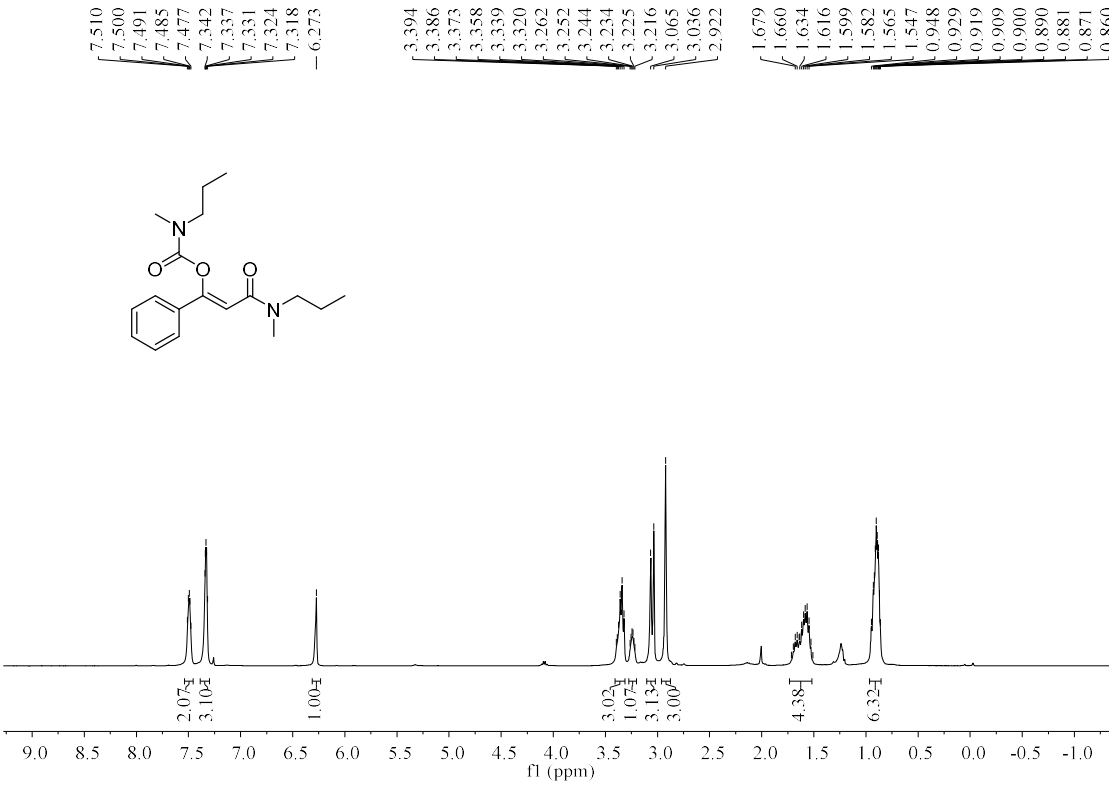


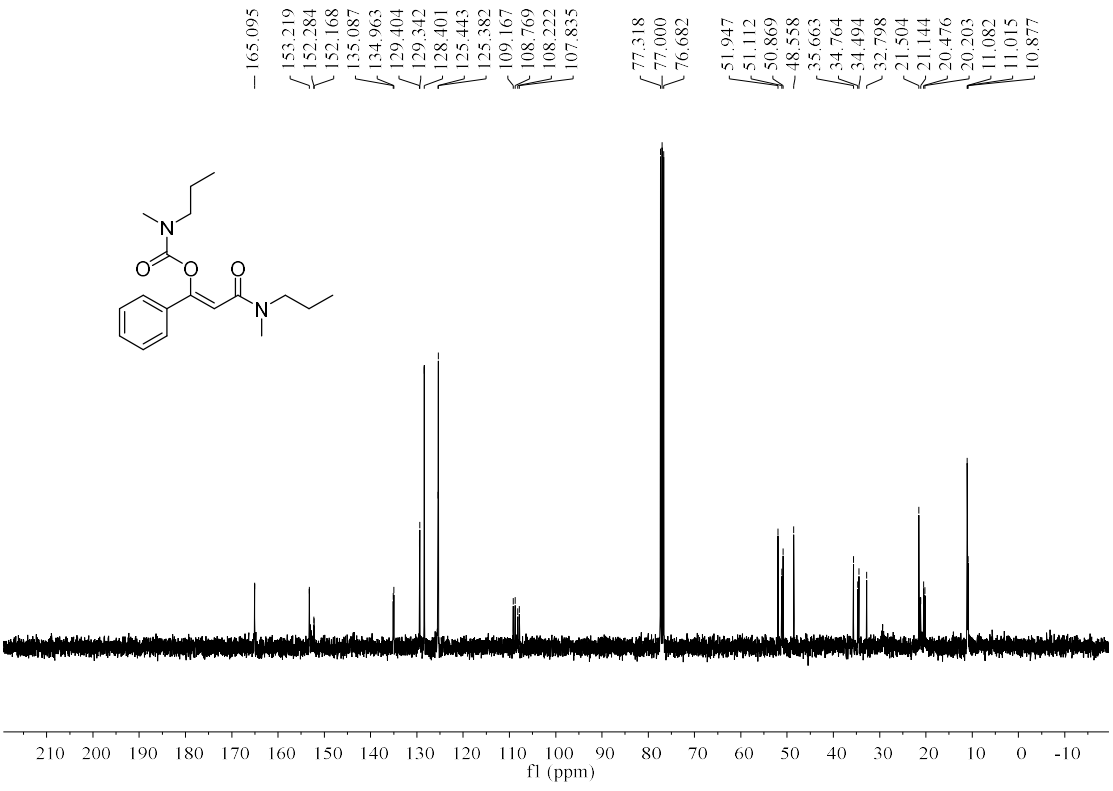
(*Z*)-3-(Diisobutylamino)-3-oxo-1-phenylprop-1-en-1-yl diisobutylcarbamate (4ae)



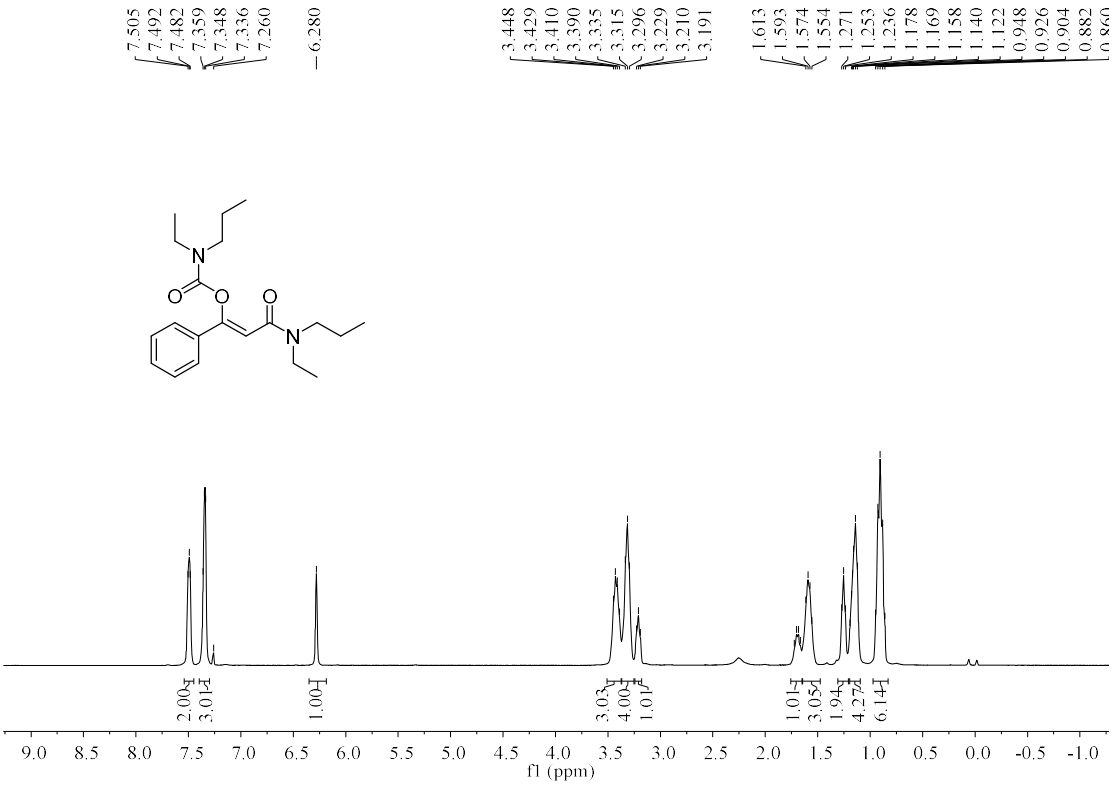


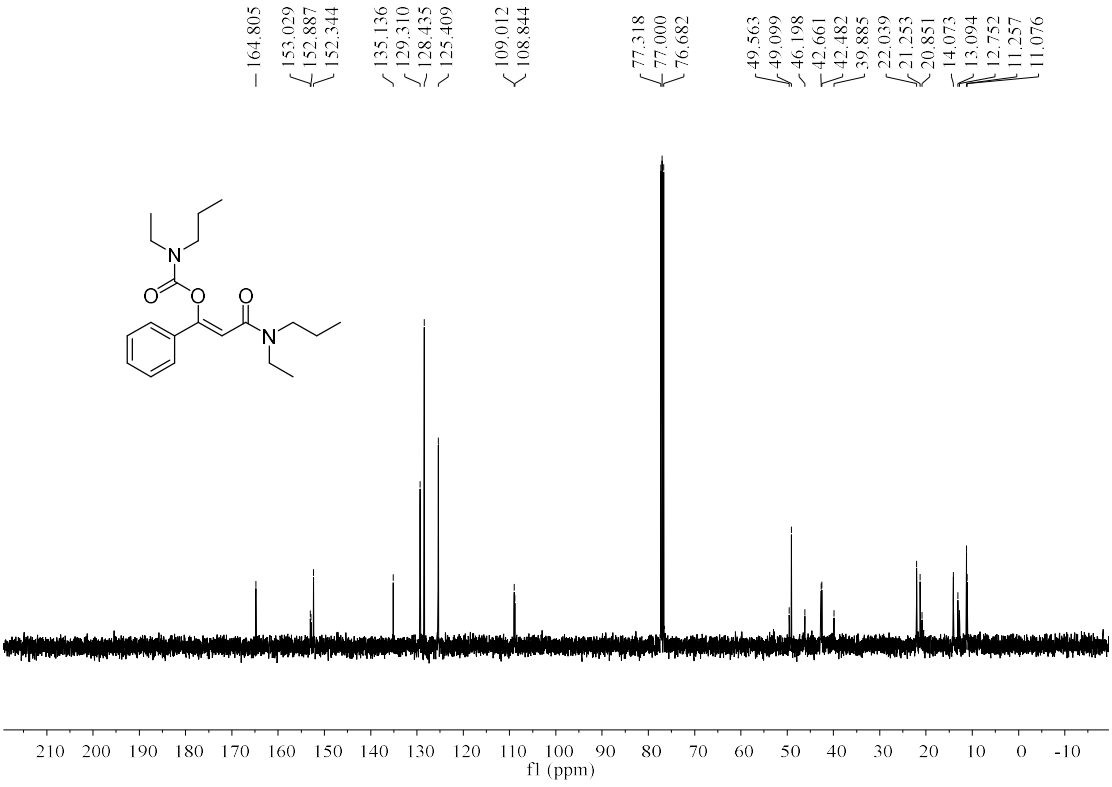
(*Z*)-3-(Methyl(propyl)amino)-3-oxo-1-phenylprop-1-en-1-yl methyl(propyl)carbamate (4af)



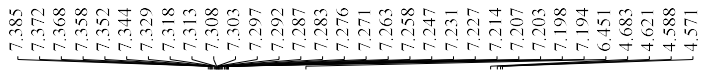


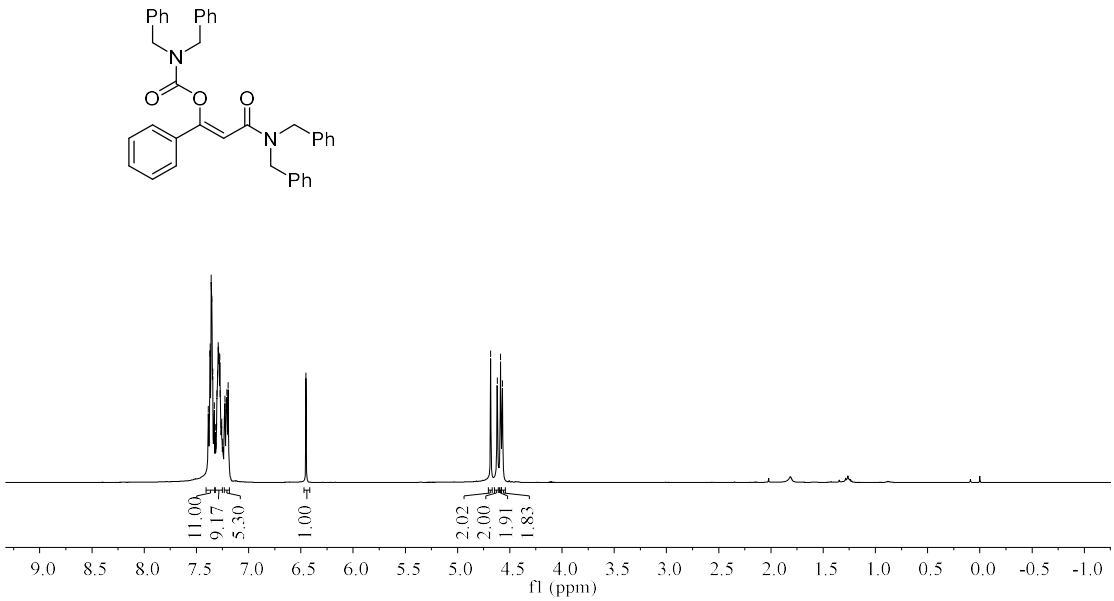
(*Z*)-3-(Methyl(propyl)amino)-3-oxo-1-phenylprop-1-en-1-yl ethyl(propyl)carbamate (4ag)

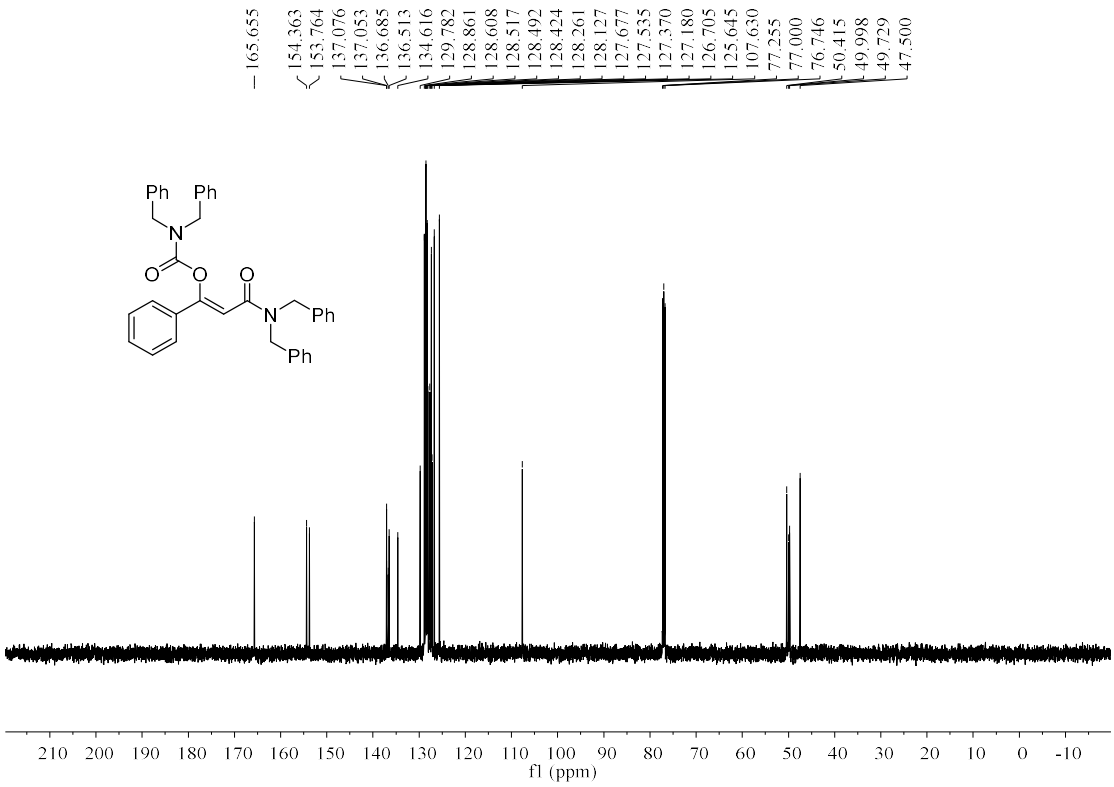




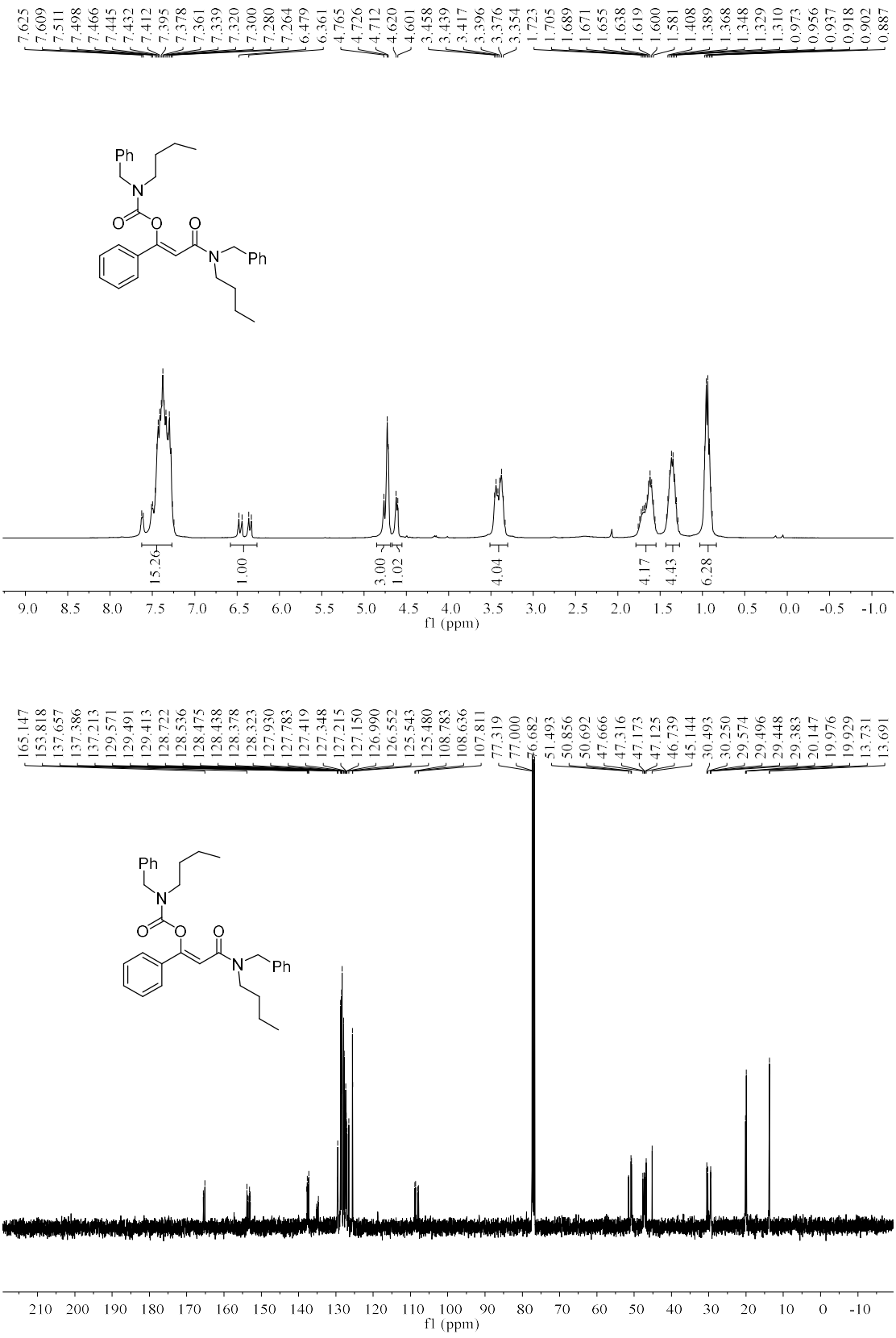
(*Z*)-3-(Dibenzylamino)-3-oxo-1-phenylprop-1-en-1-yl dibenzylcarbamate (4ah)



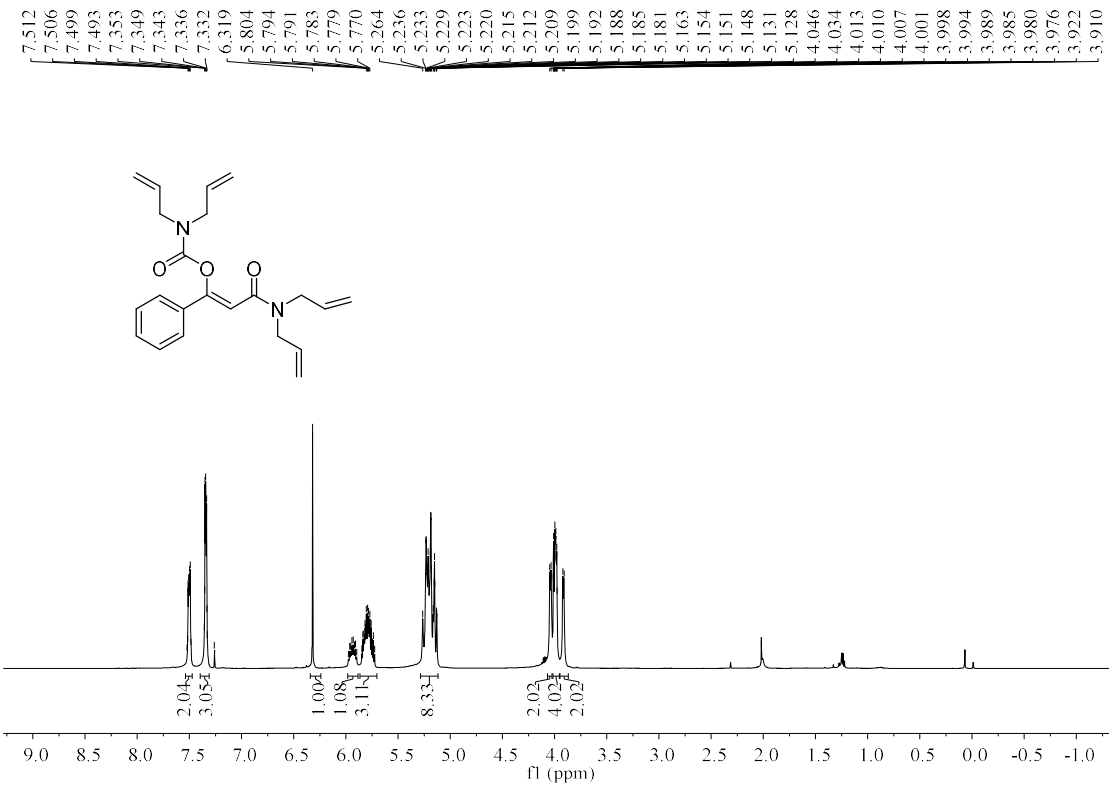


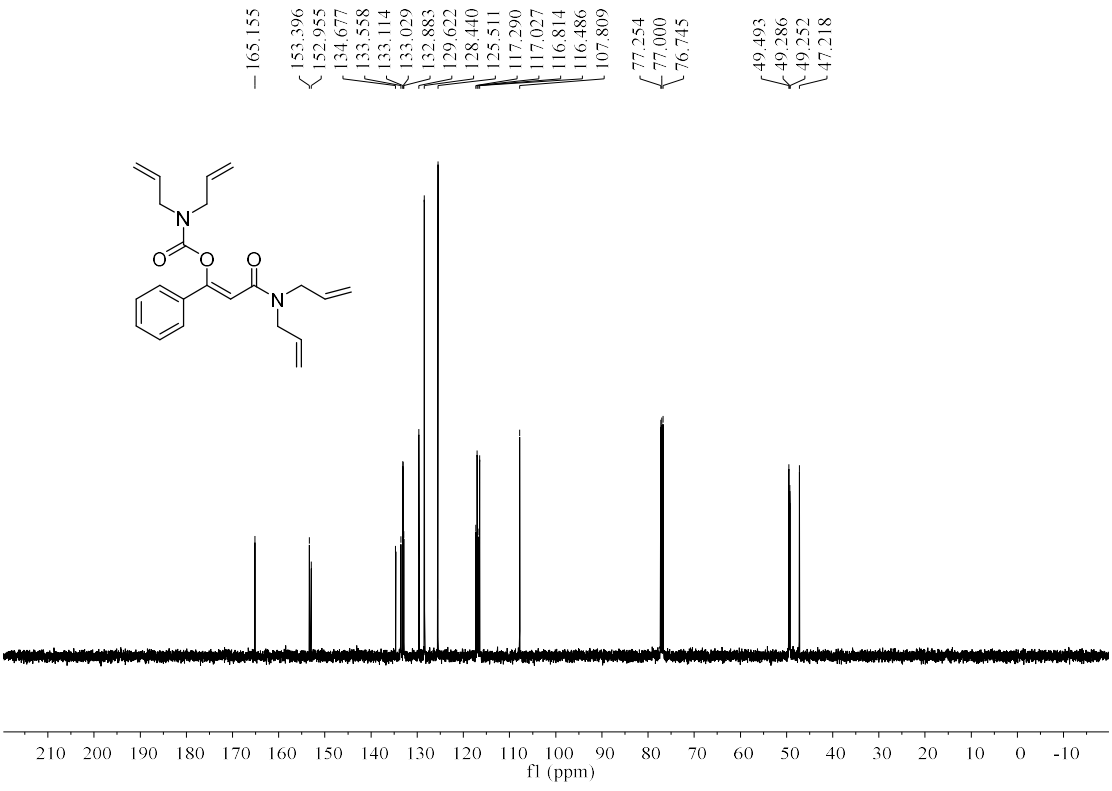


(*Z*)-3-(Benzyl(butyl)amino)-3-oxo-1-phenylprop-1-en-1-yl benzyl(butyl)carbamate (4ai)

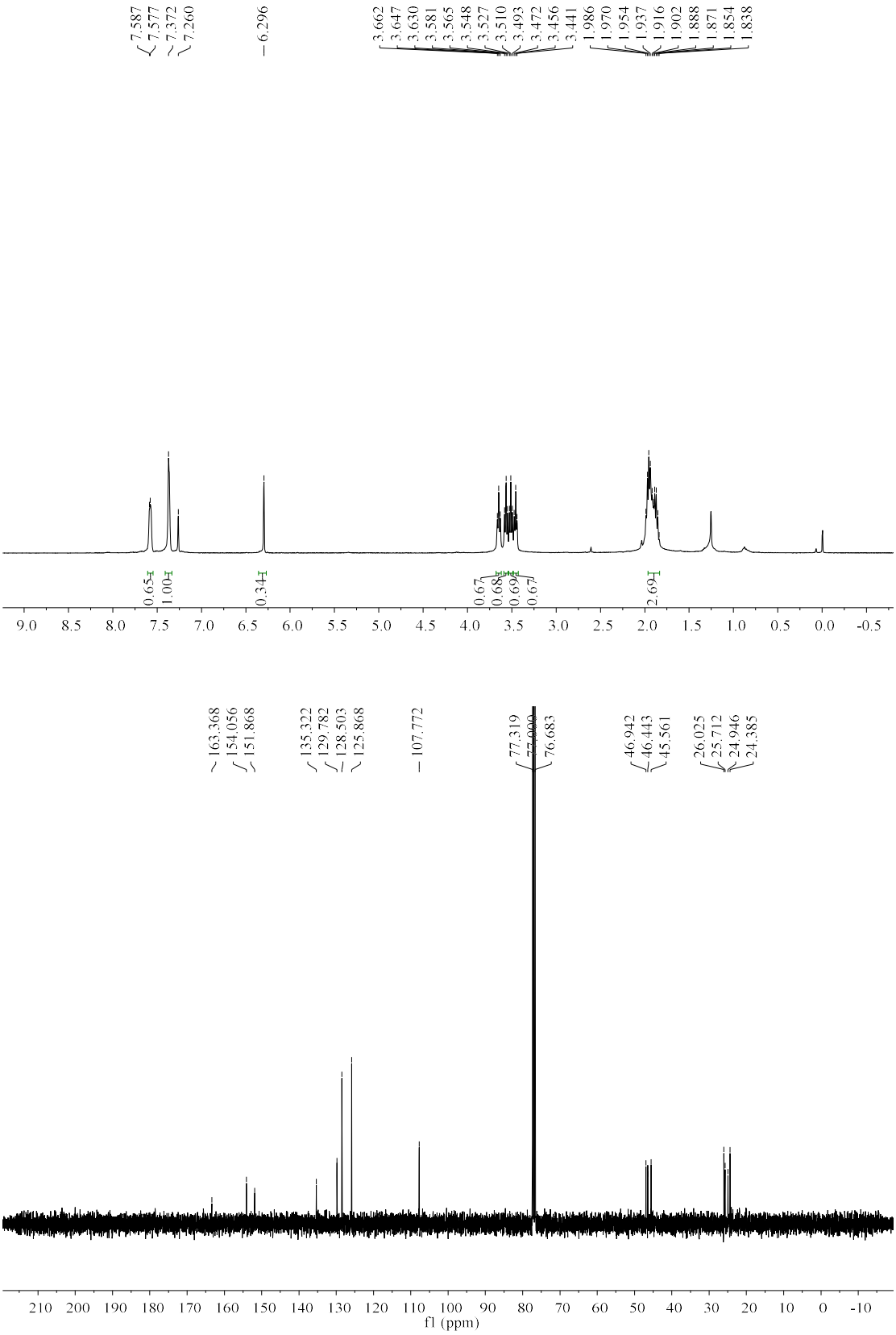


(*Z*)-3-(Diallylamino)-3-oxo-1-phenylprop-1-en-1-yl diallylcarbamate (4aj)

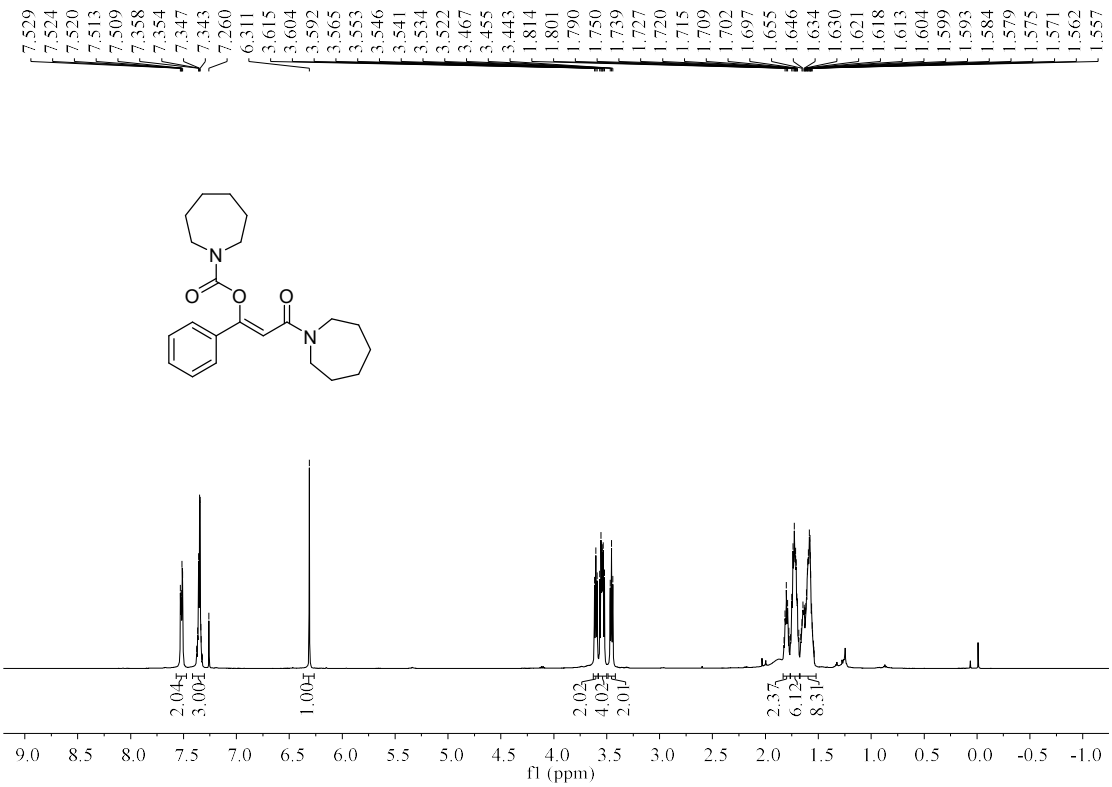


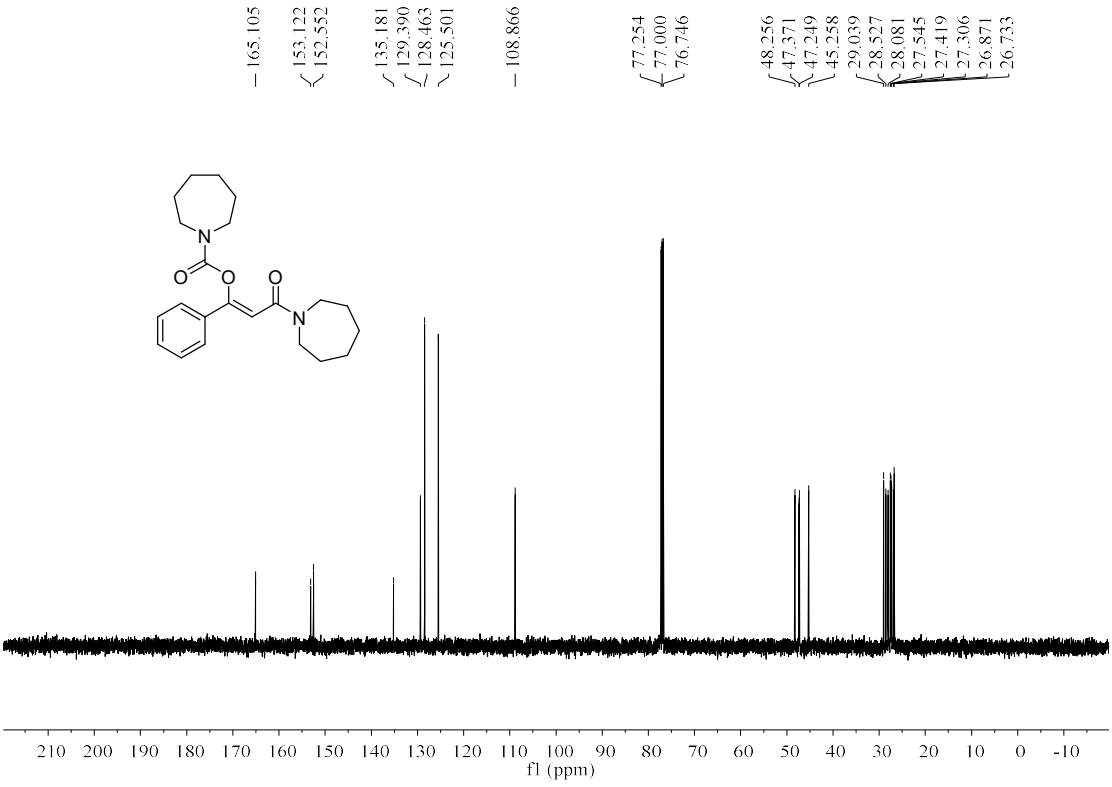


(*Z*)-3-Oxo-1-phenyl-3-(pyrrolidin-1-yl)prop-1-en-1-yl pyrrolidine-1-carboxylate (4ak)



(*Z*)-3-(Azepan-1-yl)-3-oxo-1-phenylprop-1-en-1-yl azepane-1-carboxylate (4al)





(*Z*)-3-Morpholino-3-oxo-1-phenylprop-1-en-1-yl morpholine-4-carboxylate (4am)