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Electronic Supporting Information for

Dimerizing Cascades of Enallenamides Reveal the Visible-Light-Promoted Activation of Cumulated C-C Double Bonds

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General remarks

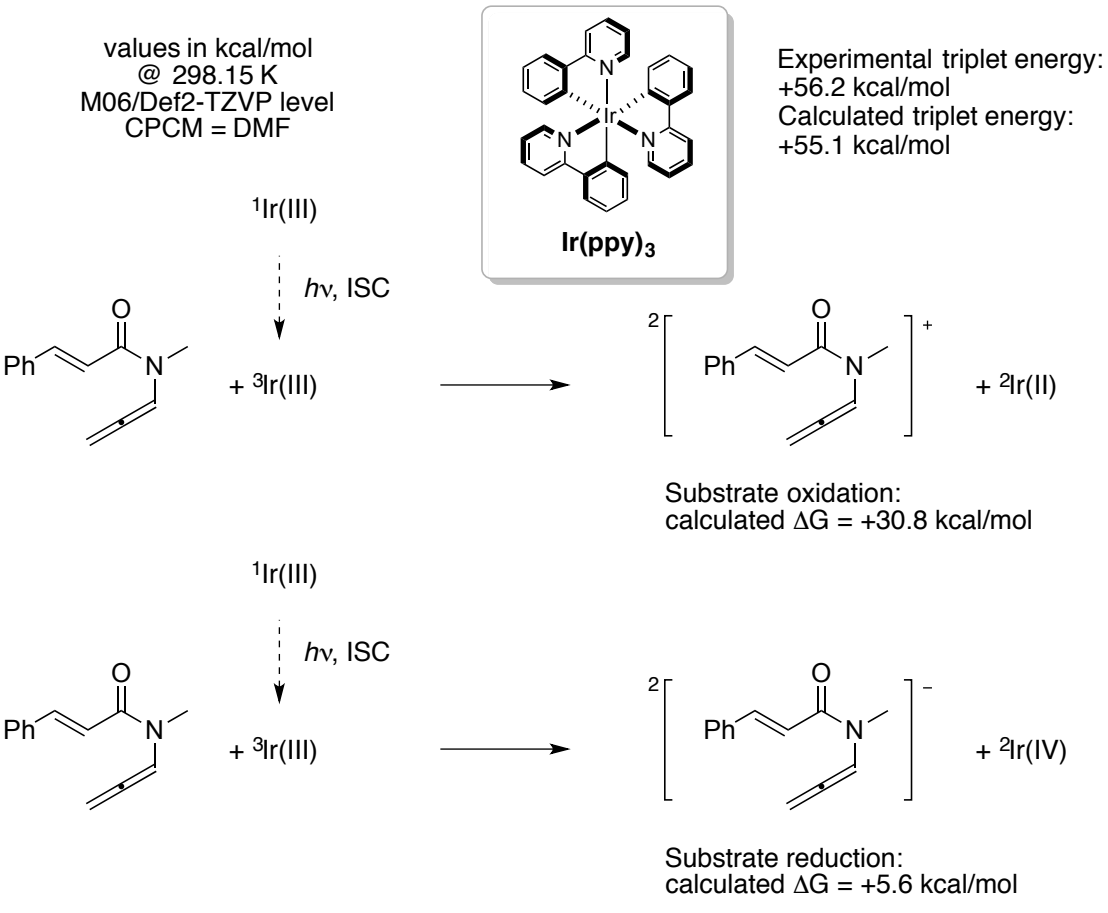
All chemicals those syntheses are not reported hereafter were purchased from commercial sources and used as received. Solvents were dried passing through alumina columns using an Inert® system and were stored under nitrogen. Present visible-light promoted reactions did not required the use of dry solvents but presence of molecular oxygen exerts a negative effect on their rate. Chromatographic purifications were performed under gradient using a Combiflash® system and prepacked disposable silica cartridges or through isocratic flash chromatography using commercial 60 Å silica gel or via preparative TLCs. Melting points were measured with an Electrothermal apparatus and are uncorrected. All reactions that required heating were performed with the use of high-vacuum grade silicon oil. Reactions promoted by visible light were performed into standard 5 mm NMR tubes, surrounded by a commercial strip of 300 RGB household leds (12V). These were put a distance of ca 10 cm and irradiated white light (model SMD5050-300 ip65). The tubes were inside an oil bath fitted with a thermometer to monitor the temperature. Cooling was ensured by two fans recovered by outdated PCs to avoid reproducibility issues. During summer time, solutions are kept at 25 °C through the addition of a rubber spire inside the silicon oil bath. The spire is linked to a chiller that keeps pumping a cooled water/ethylene glycol solution to maintain the desired temperature. ^{1}H and ^{13}C NMR spectra were recorded at 300 K on a Bruker 400 MHz or a Jeol 600 MHz spectrometers using residual non-deuterated solvents as internal standards (7.26 ppm for ^{1}H NMR and 77.00 ppm for ^{13}C-NMR for $CDCl_3$, 2.05 ppm for ^{1} H NMR and 29.84 ppm for ^{13}C NMR for acetone-d6). ^{19}F-NMR spectra were recorded in $CDCl_3$ at 298 K on a Jeol 600 spectrometer fitted with a BBFO probehead at 564 MHz. The terms m, s, d, t, q and quint represent multiplet, singlet, doublet, triplet, quadruplet and quintuplet respectively, and the term br means a broad signal. Reported assignments were based on decoupling, COSY, NOESY, HSQC and HMBC correlation experiments. Mass analyses were recorded on an Infusion Water Acquity Ultra Performance LC HO6UPS-823M instrument equipped with a SQ detector (Electrospray source); high-resolution mass analyses were recorded on a LTQ ORBITRAP XL Thermo Mass Spectrometer (Electrospray source). CCDC 2110024, 2110025, 2120965, 2120966 contain the supplementary crystallographic data for compounds **2a**, and **4a**, respectively. Single crystal Data were collected with a Bruker D8 diffractometer equipped with PhotonII area detector, using a CuKα or a MoKα microfocus 4 radiation source. The data collection strategy covered the sphere of reciprocal space. Absorption corrections were applied using the program SADABS. The structure was solved with the SHELXT code. Fourier analysis and refinement were performed by the full-matrix least-squares methods based on F2 using SHELXL-2014 as implemented in Olex2. All the nonH atoms were refined with anisotropic displacement parameters.

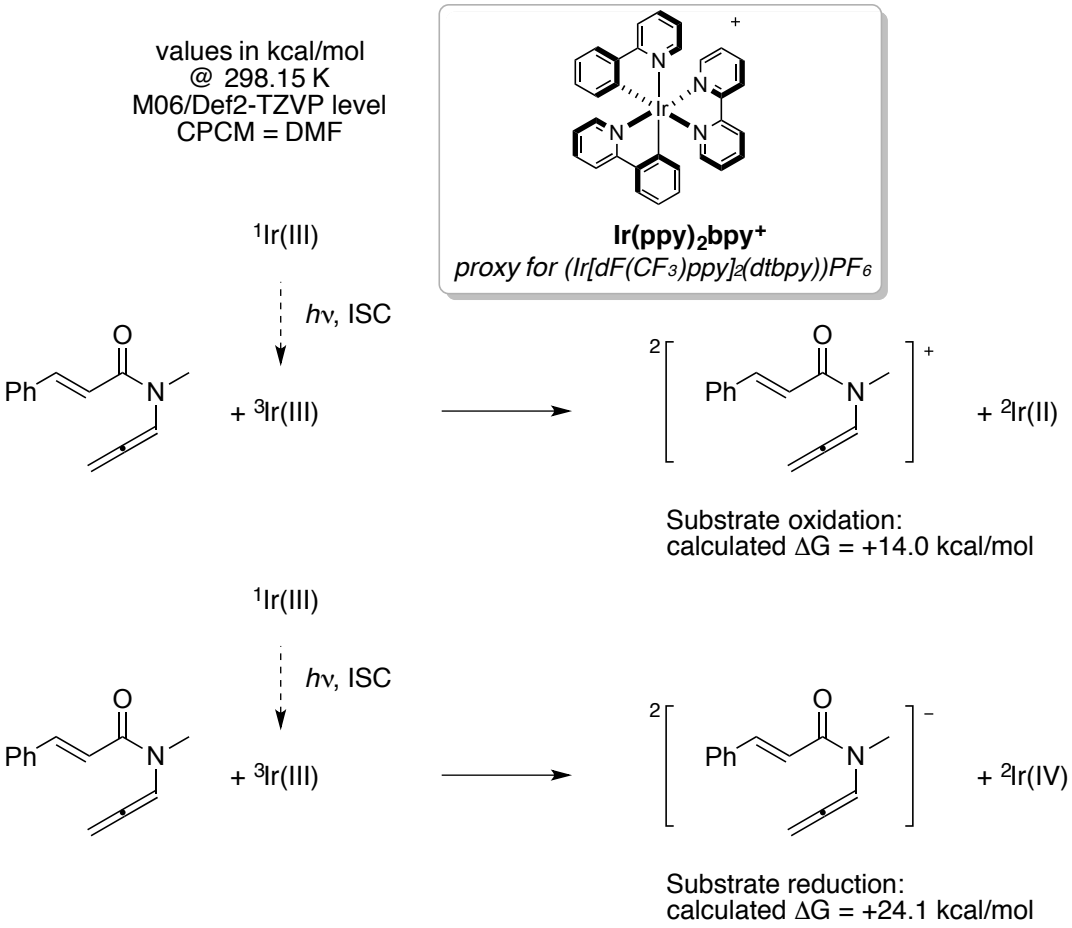
Additional modeling details

Calculations were performed at the DFT level using Gaussian09.[1] The exchange/correlation hybrid M06 functional[2] was used as it proved to afford reliable results in related photochemical cascades involving polyunsaturated substrates and Ir complexes (see ref 4 of the main manuscript). Optimization were performed without any constraint using the Def2-SVP basis set.[3] In order to achieve more precise result, free optimization was then performed again using the Def2-TZVP basis set.[3] The two sets of results were comparable, differences remaining around or below 3 kcal/mol. Together with gas-phase geometries, solvated structures were then modeled using DMF as implicit solvent through the use of the CPCM method.[4] All values and geometries reported hereafter thus refers to freely optimized solvated structures. All intermediates, both in their ground and higher spin states were characterized by the absence of any imaginary frequency in their Hessian matrix.

Calculated redox on substrate 1

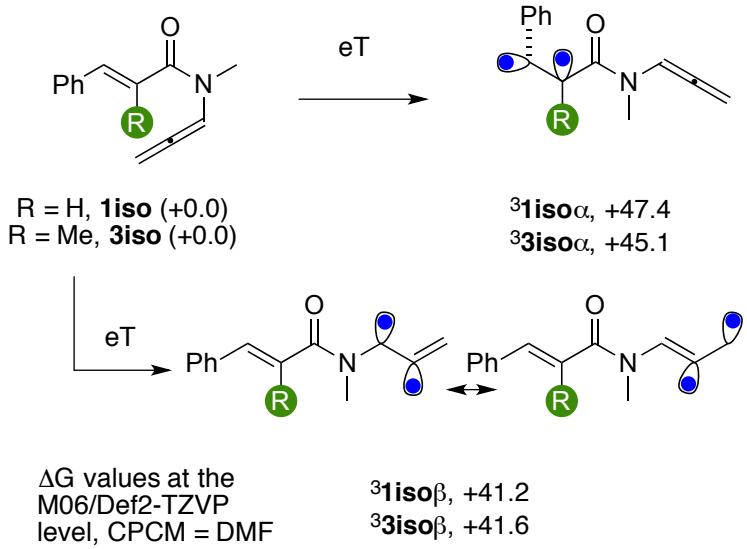
In order to reduce the odds of modeling artefacts, two sets of redoxes were considered, using two different Ir(III) catalysts. In particular, the complex $Ir(ppy)_3$, which is the best one to perform desired cascades, and $Ir(ppy)_2bpy^+$, which was used as proxy for $(Ir[dF(CF_3)ppy]_2(dtbpy))PF_6$ (see Table 1, entry 2, of the main manuscript), were evaluated. Overall, comparable results were obtained in both cases, and the calculated properties of these Ir(III) complexes were in good agreement with their experimental values regarding redox properties and triplet energies (see also references 5a and 5c of the main manuscript).



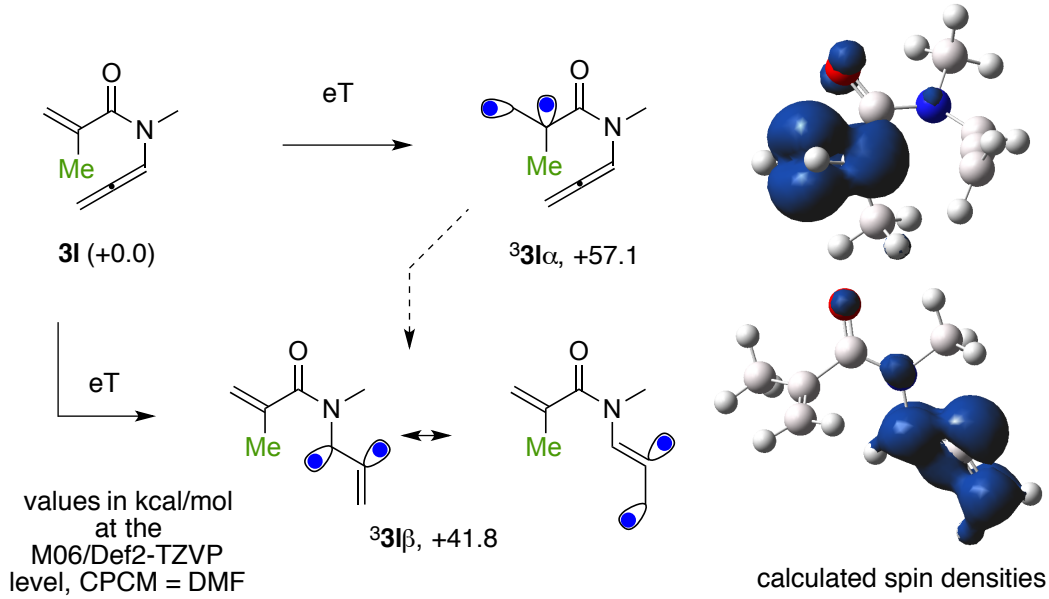


Both the substrate oxidation and reduction via SET from the photoexcited catalyst provide positive variation of the Gibbs free energy, as calculated at 298.15 K. These values for redoxes suggests their reduced likeliness under experimental conditions, in agreement with the literature on related substrates that suggest the higher feasibility of their activation by means of eT in the presence of photoactive Ir(III) complexes as catalyst.

Calculated triplet energies on their rotational isomers of 1 and 3

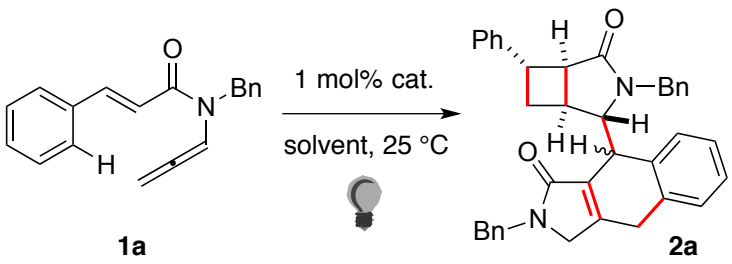


As observed for the isomer of reagent that is prone to cyclization, also those in which the allenyl unit and the cinnamoyl one are far apart show an energetic convenience favoring the localization of the triplet on the three carbon atoms of the former cumulated double bonds rather than on the conjugated alkene. Differences are comparable to those presented in the main manuscript (within 4 and 6 kcal/mol), confirming the main trend described.



This trend is further observed removing the conjugated phenyl ring. The model substrate **3l** was used to this end, and its two corresponding α and β triplets paralleled the above-mentioned results in terms of localization of their spin densities. Regarding their energies, the removal of the conjugated phenyl group had a destabilizing effect on the relative stability of the α triplet, which is ca 12 kcal/mol less stable than its cinnamoyl peer. On the contrary, the relative energy of the β triplet barely moved, in agreement with the absence of any spin density on its acryloyl arm.

Detailed optimization study



1a **2a**

entry	Catalyst (1 mol%)	Solvent (0.1 M)	Yield of **2a**[a]
1	$(Ir[dF(CF_3)ppy]_2(dtbpy))PF_6$	DMF	45%
2[e]	$Ir(ppy)_3$	DMF	47%
3	$(Ir[dF(CF_3)ppy]_2(bpy))PF_6$	DMF	traces
4	$Ru(bpy)_3Cl_2$	DMF	--
5[b]	$Ir(p\text{-}F\text{-}ppy)_3$	DMF	28%
6	2,4,6-Triphenylpyrylium tetrafluoroborate	DMF	--
7	[Ir (dtbbpy) $(ppy_2)_2$]	DMF	--
8[b]	$Ir(ppy)_3$	DMF	54%
9[d]	$Ir(ppy)_3$	DMF	--
10	$Ir(ppy)_3$	DMF	45%
11[c]	$Ir(ppy)_3$	DMF	--
12	Eosin y	DMF	--
13	Riboflavin	CH_3CN	--
14	Thioxanthen-9-one	DMF	--
15	$Ir(ppy)_3$	dioxane	32%
16	$Ir(ppy)_3$	toluene	15%
17	$Ir(ppy)_3$	DCM	25%
18[b]	$Ir(ppy)_3$	MeCN	48%
19	$Ir(ppy)_3$	ETOH	--
20[b]	$Ir(ppy)_3$	DMSO	52%
21	$Ir(ppy)_3$	DMF/DIPA 4:1	31%
22	$Ir(ppy)_3$	DMF/H_20 19:1	52%

Table 1 [a] ^1H NMR yield using 1,2,4,5-tetrachloro-3-nitrobenzene as internal standard, [b] isolated yield, [c] without irradiation, [d] in presence of oxygen, [e] 2 mol % of photocatalyst.

Unsuccessful substrates

Figure S1. Enynes unable to isomerize under standard condition **(GP1-b)**

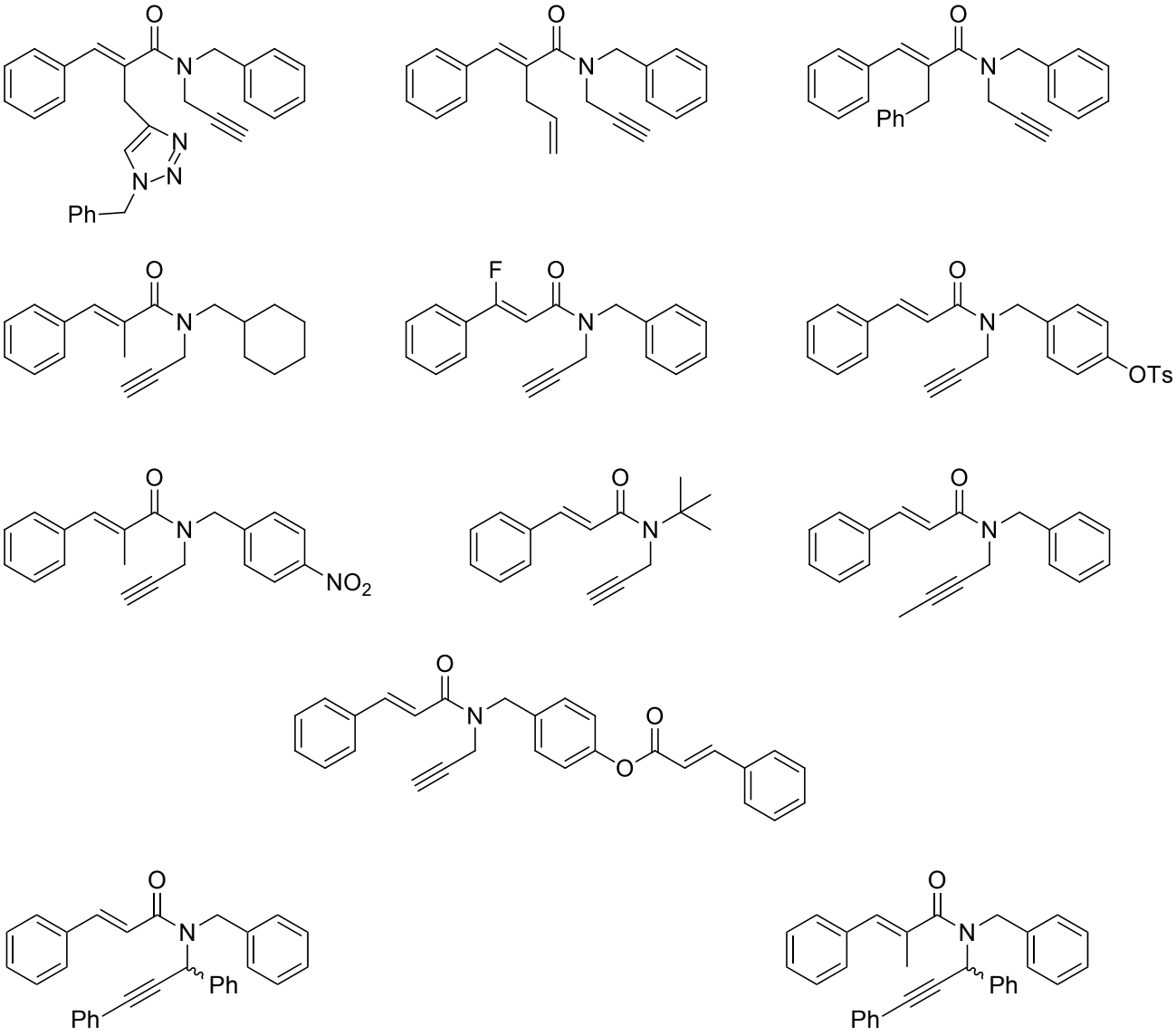
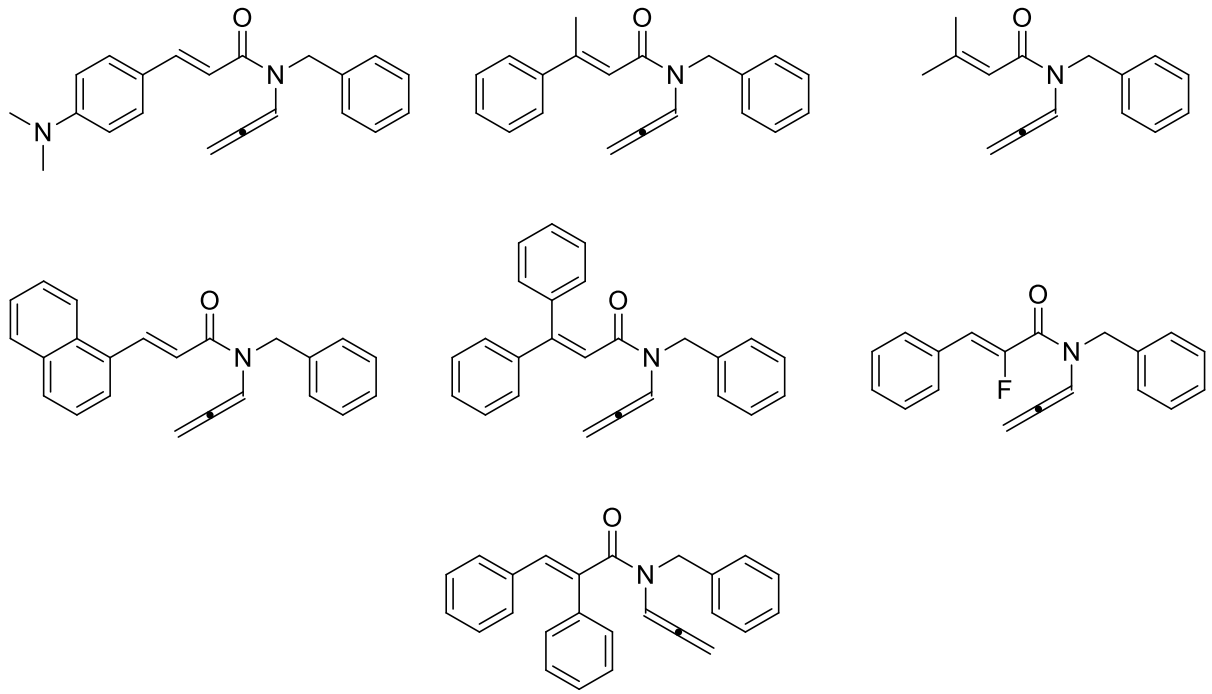


Figure S2. Enallenes that did not afford products **2** or **4** under standard condition (**GP-2**)



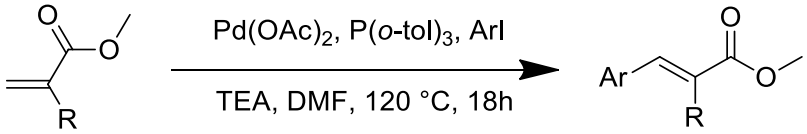
Coil reactor used for scale-up experiments

As mentioned in the main article, reactions performed using 1 gram of starting material were performed in a coil type reactor, adapting a glass condenser, to maintain a high surface/volume ration for the homogeneous, unstirred reaction mixture. Alternatively, the standard 0.2 mmol-scale reaction performed into a 5-mm wide NMR tube can be scaled-up by preparing a stock solution of the catalyst and the desired substrate in DMF, deoxygenate it by means of freezing-thaw, and then split it using a syringe into multiple septum-capped NMR tubes. The number of parallel runs can be tuned to reach the desired overall scale and the all of these samples can be collected together to perform a single purification. This approach carries a minimal practical cost and avoids any loss in the reaction yield.

Figure S3. The coil reactor used for scale-up; from the left: filled with the reaction mixture, with the wrapped LED strip and the cooling water stream, during irradiation.

Synthesis and characterization of substrates

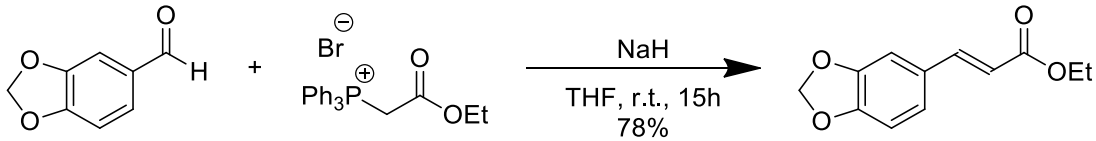
Representative procedure for the preparation of **1h, 1k, 3d, 3f** ester precursors



Precursor of	Ar	R	Yield
1h	4-OMe-C_6H_4	H	80%
1k	3-OMe-C_6H_4	H	99%
3d	4-Cl-C_6H_4	Me	27%
3f	4-OMe-C_6H_4	Me	90%

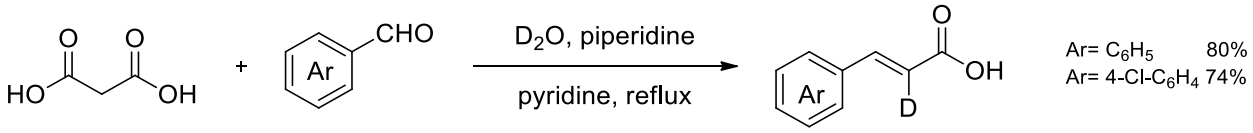
In a Schlenk tube equipped with a magnetic stirring bar under nitrogen atmosphere, were added $Pd(OAc)_2$ (0.02 equiv.), P(*o*-tol)$_3$ (0.04 equiv.), TEA (1.5 equiv.), acrylate (1.3 equiv.) and the aryl halide (1 equiv.) in DMF (1 M). The resulting mixture was stirred at 120 °C for 18 h. After complete conversion as monitored by TLC, the mixture was diluted with EtOAc, washed twice with water and a saturated LiCl solution, dried with Na_2SO_4 and concentrated under reduced pressure. The crude was purified by chromatography on silica gel (*n*-hexane/EtOAc gradient).

Representative procedure for the preparation of **1l** ester precursor



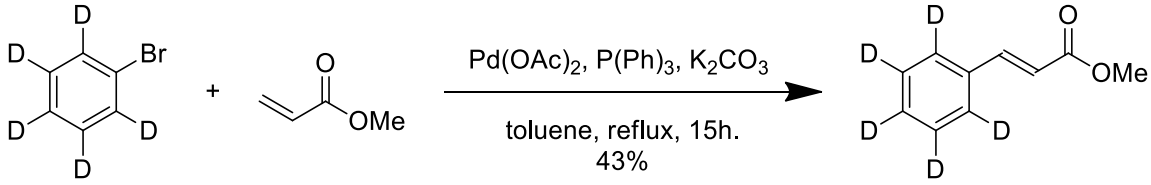
To a solution of triphenylphosphonium salt (1.15 equiv.) in THF (0.87 M) was added NaH (1.15 equiv., 60 % w in paraffin oil) at 0 °C and the resulting mixture was then stirred for 1 h. Then, benzo[d][1,3]dioxole-5-carbaldehyde (1 equiv.) was added and the reaction was mixed at room temperature overnight. After complete conversion as monitored by TLC, the solution was quenched with a saturated NH_4Cl solution, extracted with EtOAc (3 times) and washed with brine. The combined organic phase was finally dried over Na_2SO_4, concentrated under reduced pressure, and purified by chromatography on silica gel (*n*-hexane/EtOAc gradient).

Representative procedure for the preparation of α-deutero-trans-cinnamic acid.



In a 25 mL round bottom flask equipped with magnetic stirring bar connected to a water-cooled-condenser a solution of malonic acid (1 equiv.), piperidine (0.35 equiv.) and D_2O (14 equiv.) in pyridine (1.5 M) were refluxed for 2 hours; the desired aryl aldehyde was then added and the mixture was stirred for additional 3 hours. The resulting mixture was poured in a HCl solution (10% m/V), the precipitate was filtered, washed with water and dried under vacuo affording the the corresponding α-deutero-trans-cinnamic acid (deuterium incorporation: 88%).

Representative procedure for the preparation of (d_5)-methyl cinnamate

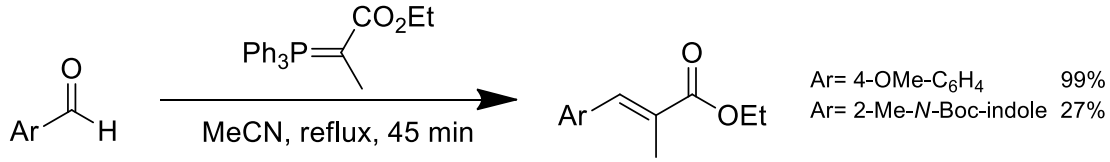


In a Schlenk equipped with a magnetic stirring bar were added bromobenzene-d_5 (1 equiv.), methyl acrylate (1.2 equiv.), K_2CO_3 (1.5 equiv.), $P(Ph)_3$ (0.04 equiv.), $Pd(OAc)_2$ (0.02 equiv.) in toluene (3.3 M) and the resulting mixture was refluxed overnight. After complete conversion as monitored by TLC, the reaction was filtered on celite, diluted with EtOAc and washed with water and brine. The combined organic layers were finally dried over Na_2SO_4, concentrated under reduced pressure, and purified by chromatography on silica gel (*n*-hexane/EtOAc gradient).

Representative procedure for the preparation of **3c** ester precursor[5]

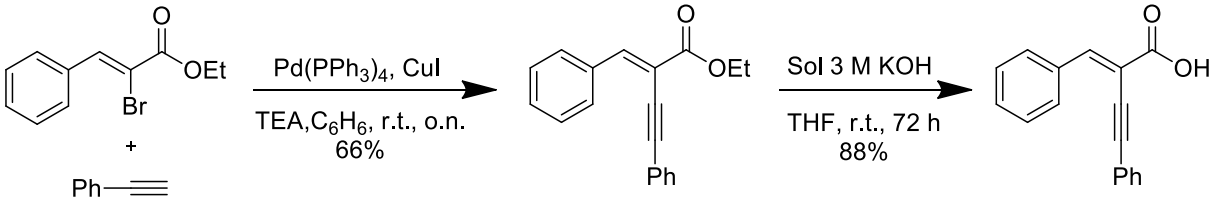
In a three-necked round bottom flask were added freshly distilled benzaldehyde (1 equiv.) and 2-bromoethyl acetate (1.1 equiv.) in DCM (0.67 M). The mixture was stirred for 10 minutes and then $TiCl_4$ (1.2 equiv., 1 M solution in DCM) was added in drops over a period of 10 minutes. The solution was stirred for 30 minutes at room temperature, then NEt_3 (2 equiv.) was added slowly, maintaining the temperature under 30 °C, and the resulting mixture was then stirred for 5 h. After complete conversion as monitored by TLC, the solution was diluted with DCM and washed with a 1 M HCl solution, water and brine. The organic phase was dried over Na_2SO_4, concentrated under reduced pressure and the resulting crude was purified by chromatography on silica gel (*n*-hexane/EtOAc gradient).

Representative procedure for the preparation of **3e**, **3g** ester precursors

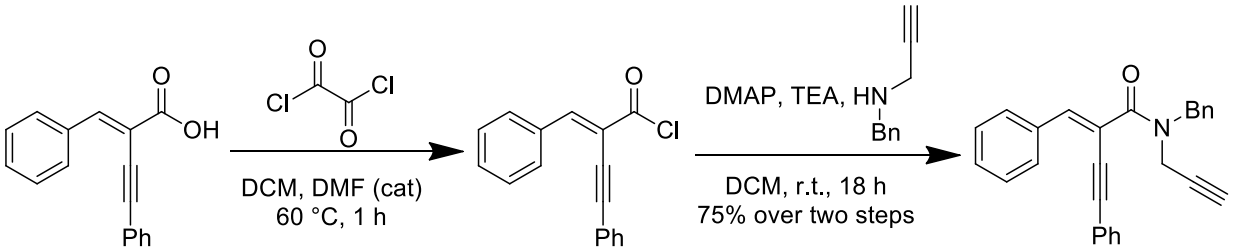


To a solution of phosphonium ylide in MeCN (0.12 M) the desired aryl aldehyde was added. The resulting mixture was refluxed 45 min under stirring. After complete conversion of reagents, the mixture was concentrated under reduced pressure and purified by chromatography on silica gel (*n*-hexane/EtOAc gradient).

Preparation of enyne **3c** precursor



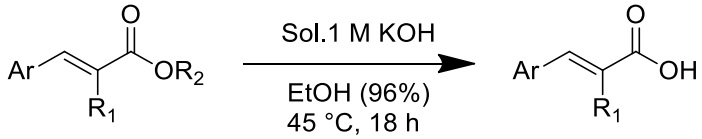
In a Schlenk equipped with a magnetic stirring bar were added (Z)-ethyl 2-bromo-3-phenylacrylate (1 equiv.), ethynylbenzene (1.2 equiv.), $Pd(PPh_3)_4$ (0.05 equiv.), CuI (0.1 equiv.), TEA (2 equiv.) in benzene (0.3 M) and the solution was stirred at room temperature overnight. After complete conversion as monitored by TLC, the mixture was filtered on celite and concentrated under reduced pressure. The crude was then purified by chromatography on silica gel (*n*-hexane/EtOAc gradient).
To a solution of (E)-ethyl 2-benzylidene-4-phenylbut-3-ynoate (1 equiv.) in THF (0.27 M) was added a 3 M solution of KOH (10 equiv.). The biphasic mixture was vigorously stirred at room temperature for 72 h. After complete conversion as monitored by TLC, the mixture was concentrated under reduced pressure and acidified to pH = 1 with a 1 M HCl solution; during the process, the formation of a precipitate was observed. The solid was filtered, washed with water, and dried under high vacuum to afford (E)-2-benzylidene-4-phenylbut-3-ynoic acid.



In a 25 mL round bottom flask equipped with a magnetic stirring bar were added (E)-2-benzylidene-4-phenylbut-3-ynoic acid (1 equiv.), oxalyl chloride (1.5 equiv.), DMF (3 drops) in DCM (0.6 M) and the solution was stirred at 60 °C for 1 h. The mixture was then concentrated under reduced pressure to afford the desired acyl chloride.
To a solution of secondary amine (1 equiv.), TEA (1 equiv.), DMAP (0.02 equiv.) in DCM (0.25 M) was added acyl chloride (1 equiv.) at 0 °C, and the solution was then stirred at room temperature for 18 h. After complete conversion as monitored by TLC, the solution was diluted with DCM and washed with a saturated NH_4Cl solution followed by a saturated $NaHCO_3$ one. The aqueous layers were extracted with DCM (3 times), and the combined organic phase was finally washed with brine,

dried over Na_2SO_4 and concentrated under reduced pressure; the crude was purified by chromatography on silica gel (*n*-hexane/EtOAc gradient).

Representative procedure for the preparation of cinnamic acids from the corresponding esters.

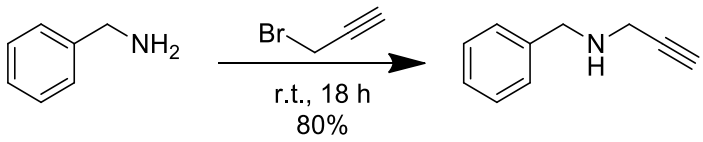


R_1 = H,Me
R_2 = Me, Et

Precursor of	Ar	R^1	R^2	Yield
***d*$_5$-1a**	C_6D_5	H	Me	50%
1k	4-OMe-C_6H_4	H	Me	88%
1l	3,4-methylendioxy-C_6H_3	H	Et	95%
3b	C_6H_5	*n*Pr	Et	85%
3d	4-Cl-C_6H_4	Me	Me	99%
3e	4-OMe-C_6H_4	Me	Me	86%
3f	4-*n*Bu-C_6H_4	Me	Me	68%
3g	2-Me-N-Boc-indole	Me	Et	81%

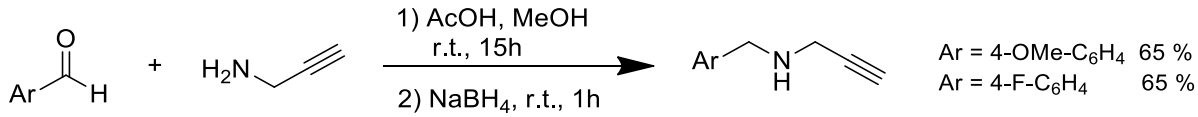
In a round bottom flask equipped with a stir bar were added the desired ester (1 equiv.), EtOH (0.15 M) and a 1 M solution of KOH (2.5 equiv.). The resulting mixture was stirred 18 h at 45 °C. After complete conversion as monitored by TLC, the mixture was concentrated under reduced pressure and acidified to pH = 1 with a 1 M HCl solution. During the process, the formation of a precipitate was observed. The solid was filtered, washed with water and dried under high vacuum to afford the corresponding cinnamic acid.

Representative procedure for the preparation of benzyl propargylamine



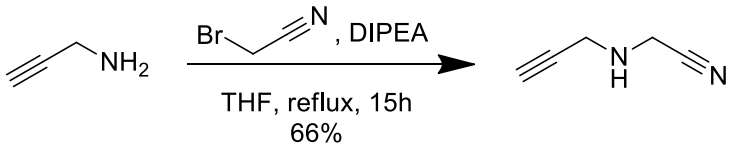
In a round bottom flask equipped with a magnetic stirring bar, propargyl bromide (1 equiv., 80% w in toluene) was added at 0 °C to benzylamine (6 equiv.) and the resulting solution was stirred overnight at room temperature. After complete conversion as monitored by TLC, the mixture was quenched with a saturated $NaHCO_3$ solution and extracted with Et_2O (3 times). The combined organic phase was washed with brine, dried over Na_2SO_4 and concentrated under reduced pressure. The crude was finally purified by chromatography on silica gel (*n*-hexane/EtOAc gradient).

Representative procedure for the preparation of substituted benzyl propargylamine



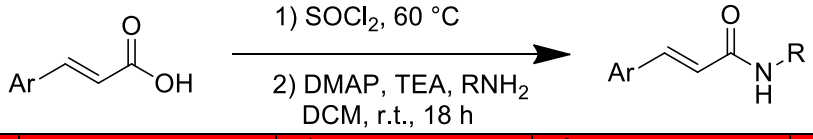
To a solution of propargyl amine (1 equiv.) and aryl aldehyde (1.08 equiv.) in MeOH (0.6 M) was added AcOH (1 drop). The resulting mixture was then stirred overnight at room temperature. $NaBH_4$ (1.5 equiv.) was added at 0 °C and the solution was then stirred for 1 h prior to the evaporation of the solvent. The mixture was diluted with water, extracted with DCM (2 times), and the combined organic layers were then washed with a 1 M HCl solution. Aqueous layers were neutralized, extracted with DCM (2 times), and the resulting organic phase was finally washed with brine, dried over Na_2SO_4, concentrated under reduced pressure, and purified by chromatography on silica gel (DCM/EtOAc gradient).

Representative procedure for the preparation of 2-(prop-2-yn-1-ylamino)acetonitrile.



In a 25 mL round bottom flask equipped with a magnetic stirring bar were added propargyl amine (1 equiv.), 2-bromoacetonitrile (1.2 equiv.), DIPEA (1.2 equiv.) in THF (0.33 M) and the resulting mixture was refluxed overnight. After complete conversion as monitored by TLC, the reaction was diluted with EtOAc and washed with brine. The combined organic phase was dried over Na_2SO_4, concentrated under reduced pressure, and purified by chromatography on silica gel (*n*-hexane/EtOAc gradient).

Representative procedure for preparation of cinnamamide precursors

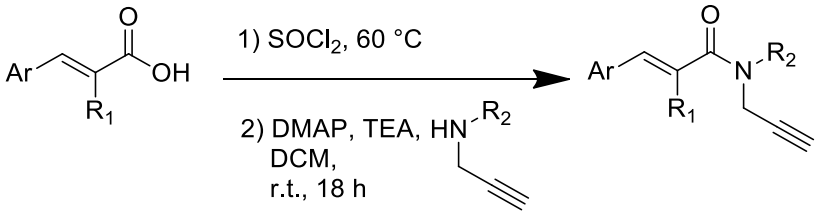


Precursor of	Ar	R^1	R^2	Yield
***d*$_1$-1a**	C_6H_5	D	Bn	92 %
1b	C_6H_5	H	C_9H_{19}	96 %
1e	C_6H_5	H	C_3H_5	94 %
1g	4-Br-C_6H_4	H	Bn	70 %
1i	2-Me-C_6H_4	H	Bn	77 %
3k	C_6H_5	Me	C_3H_5	87 %

In a 25 mL round bottom flask equipped with a magnetic stirring bar, the desired acid was dissolved in $SOCl_2$ (1.67 M) and a catalytic amount of DMF (3 drops) was added. The solution was stirred for 1 h at 60 °C. Then, the mixture was concentrated under reduced pressure to afford the acyl chloride, that was added to a solution of DMAP (0.02 equiv.), TEA (1 equiv.) and primary amine (1 equiv.) in DCM (0.25 M) at 0 °C. The mixture was stirred for 18 h at room temperature. After complete conversion as monitored by TLC, the solution was diluted with DCM and washed with a saturated NH_4Cl solution followed by a saturated $NaHCO_3$ one. The aqueous layers were extracted with DCM

(3 times), and the combined organic phase was finally washed with brine, dried over Na_2SO_4, concentrated under reduced pressure and the crude was purified by chromatography on silica gel (*n*-hexane/EtOAc gradient). Cinnamamide precursors of **1b, 1d, 1e** were directly prepared from commercially available cinnamoyl chloride.

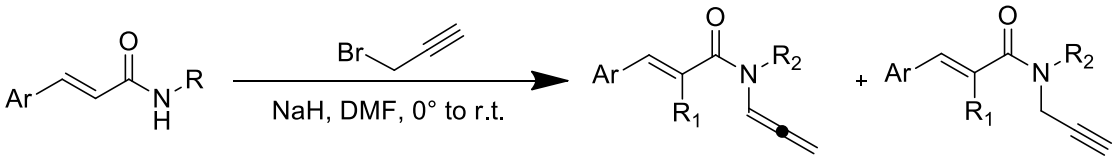
Representative procedure for the preparation of 1,6-enynes



Precursor of	Ar	R^1	R^2	Yield
1a	C_6H_5	H	Bn	71 %
***d*$_5$-1a**	C_6D_5	H	Bn	60 %
1c	C_6H_5	H	CH_2Bn	74 %
1f	4-Cl-C_6H_4	H	CH_2Bn	76 %
1h	4-OMe-C_6H_4	H	Bn	80 %
1j	3-Me-C_6H_4	H	Bn	79 %
1k	3-OMe-C_6H_4	H	Bn	61 %
1l	3,4-methylendioxy-C_6H_3	H	Bn	70 %
1m	4-Cl-C_6H_4	D	Bn	58%
3b	C_6H_5	*n*Pr	Bn	65 %
3d	4-Cl-C_6H_4	Me	Bn	51 %
3e	4-OMe-C_6H_4	Me	Bn	54 %
3f	4-*n*Bu-C_6H_4	Me	Bn	53 %
3g*	2-Me-N-Boc-indole	Me	Bn	55 %
3h	C_6H_5	Me	PMB	68 %
3i	C_6H_5	Me	CH_2-4-F-C_6H_4	78 %
3j	C_6H_5	Me	CH_2CN	72 %

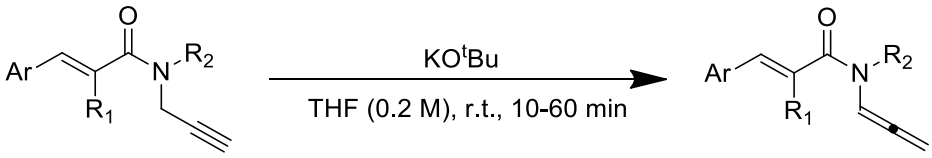
In a 25 mL round bottom flask equipped with a magnetic stirring bar, the desired acid was dissolved in $SOCl_2$ (1.67 M) and a catalytic amount of DMF (3 drops) was added. The solution was stirred for 1 h at 60 °C. Then, the mixture was concentrated under reduced pressure to afford the acyl chloride, that was added to a solution of DMAP (0.02 equiv.), TEA (1 equiv.) and secondary amine (1 equiv.) in DCM (0.25 M) at 0 °C. The mixture was stirred for 18 h at room temperature. After complete conversion as monitored by TLC, the solution was diluted with DCM and washed with a saturated NH_4Cl solution followed by a saturated $NaHCO_3$ one. The aqueous layers were extracted with DCM (3 times), and the combined organic phase was finally washed with brine, dried over Na_2SO_4, concentrated under reduced pressure and the crude was purified by chromatography on silica gel (*n*-hexane/EtOAc gradient). Enyne precursors of **1a, 1c** were directly prepared from commercially available cinnamoyl chloride. Acyl chloride precursor of **3g** was prepared using a solution of oxalyl chloride (1.5 equiv.) in DCM (0.6 M) instead of $SOCl_2$.

Synthesis of 1-6 enallenes [GP-1a]:



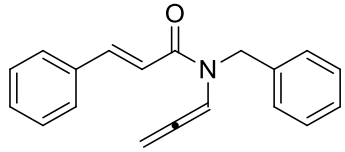
To a solution of acrylamide (1 equiv.) in DMF at 0° C NaH (60% in paraffine oil, 1.3 equiv.) was slowly added and the mixture was stirred 1h. Then a solution of propargyl bromide (80% in toluene, 1.5 equiv.) was slowly added and the reaction was stirred at r.t.. After complete conversion monitoring by TLC, the mixture was quenched with a saturated NH_4Cl solution and extracted with EtOAc (3 times). The combined organic layers were washed with a saturated LiCl solution (3 times), dried over over Na_2SO_4 and concentrated under reduced pressure. The crude was purified by chromatography on silica gel (*n*-hexane/EtOAc gradient) affording the corresponding products **1**.

Synthesis of 1-6 enallenes [GP-1b]:



The desired enyne (1 equiv.) and THF (0.20 M) were sequentially added to a Schlenk tube equipped with a magnetic stirring bar. The resulting mixture was stirred at room temperature for 10 minutes prior to the addition of *t*BuOK (0.2 equiv.). After complete conversion as monitored by TLC, a saturated NH_4Cl solution (15 ml) was added. The mixture was extracted with EtOAc (3 x 15 mL), the organic layers separated and dried over Na_2SO_4. The solution was concentrated under reduced pressure and the crude purified by chromatography on silica gel (*n*-hexane/EtOAc gradient).

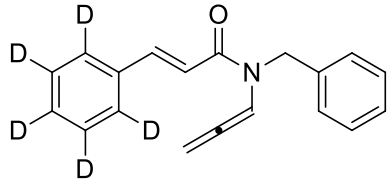
N-benzyl-N-(propa-1,2-dien-1-yl)cinnamamide. 1a



1a

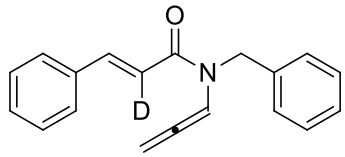
Allene **1a** was prepared following general procedure **GP-1b** from the corresponding enyne (275 mg, 1.0 mmol). Yellow solid (132.7 mg, 48% yield). Two rotamers are observed due to the dynamic amide group. **^{1}H NMR** (400 MHz, Acetone d_6) δ 7.81 – 7.70 (m, 3H RotA, 2H RotB), 7.65 – 7.59 (m, 1H RotA, 1H RotB), 7.48 – 7.24 (m, 9H RotA, 9H RotB), 7.17 (d, J = 15.3 Hz, 1H RotB), 5.38 (d, J = 6.3 Hz, 2H RotA, 2H RotB), 4.99 (s, 2H RotB), 4.84 (s, 2H rotA). **^{13}C NMR** (101 MHz, Acetone) δ 202.7 (Cq, RotB), 202.1 (Cq, RotA), 164.2 (Cq, RotA), 164.1 (Cq, RotB), 143.8 (CH, RotB), 143.4 (CH, RotA), 138.21 (Cq, RotA), 138.18 (Cq, RotB), 135.3 (Cq, RotA), 135.2 (Cq, RotB), 129.9, 128.8, 128.7, 128.2, 128.1, 127.7, 127.2, 126.9, 126.3, 117.4 (CH, RotB), 117.2 (CH, RotA), 100.4 (CH, RotA), 99.5 (CH, RotB), 87.0 (CH_2, RotB), 86.0 (CH_2, RotA), 48.4 (CH_2, RotB), 47.3 (CH_2, RotA). **ESI-MS** calcd for $C_{19}H_{18}NO$ $[M+H]^+$ 276.14, found 276.16.

(*E*)-N-benzyl-3-(2,3,4,5,6-pentadeuterophenyl)-N-(propa-1,2-dien-1-yl)acrylamide. d_5-1a



Allene ***d*$_5$-1a** was prepared following general procedure **GP-1b** from the corresponding enyne (218 mg, 0.78 mmol). Yellow solid (119.8 mg, 55% yield). Two rotamers are observed due to the dynamic amide group. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.79 (apparent dd, J = 10.6, 4.5 Hz, 1H RotA, 2H RotB), 7.41 – 7.20 (m, 5H RotA, 5H RotB), 7.00 (d, J = 15.4 Hz, 1H RotA), 6.91 (t, J = 5.6 Hz, 1H RotA), 6.78 (d, J = 15.8 Hz, 1H RotB), 5.33 (d, J = 6.4 Hz, 2H RotA, 2H RotB), 4.83 (s, 2H RotA, 2H RotB). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 202.7, 202.4, 165.0, 144.6, 143.9, 137.6, 137.2, 134.8, 128.9, 128.8, 128.4, 128.1, 127.5, 127.1, 126.1, 116.9, 100.2, 100.0, 87.7, 86.8, 49.3, 48.2. **ESI-MS** calcd for $C_{19}H_{13}D_5NO$ $[M+H]^+$ 281.17, found 281.28.

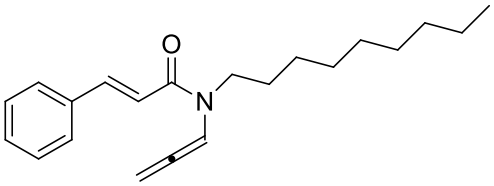
(*E*)-N-benzyl-2-deutero-3-phenyl-N-(propa-1,2-dien-1-yl)acrylamide. d_1-1a



Allene ***d*$_1$-1a** was prepared following general procedure **GP-1b** from the corresponding enyne (354.0 mg, 1.34 mmol). Dark orange solid (188.6 mg, 53% yield). Two rotamers are observed due to the dynamic amide group. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.86 – 7.76 (m, 1H RotA, 1H RotB), 7.63 – 7.18 (m, 8H), 7.03 (d, J = 15.4 Hz, 0.12H RotA), 6.93 (brs, 1H RotA), 6.81 (d, J = 15.4 Hz, 0.12H RotB), 5.36 (d, J = 6.0 Hz, 2H RotA, 2H RotB), 4.89 – 4.82 (m, 2H RotA, 2H RotB). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 202.7, 202.4, 165.0, 144.6, 143.9, 137.6, 137.2, 134.9, 130.0, 128.9, 128.8, 128.4,

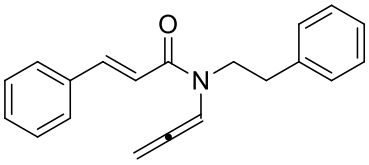
128.0, 127.5, 127.2, 126.1, 116.9, 116.6 (t, J = 24.0 Hz, CD), 100.2, 100.0, 87.7, 86.8, 49.3, 48.2. **ESI-MS** calcd for $C_{19}H_{17}D_1NO$ $[M+H]^+$ 277.15, found 277.40.

***N*-nonyl-*N*-(propa-1,2-dien-1-yl)cinnamamide. 1b**



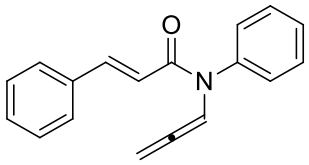
Allene **1b** was directly prepared following general procedure **GP-1a** from the corresponding cinnamamide (1.0 g, 3.65 mmol). Brown oil (306 mg, 31% yield). Two rotamers are observed due to the dynamic amide group. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.78 (d, J = 15.3 Hz, 1H RotB), 7.71 – 7.60 (m, 2H RotA), 7.54 (dd, J = 7.4, 2.0 Hz, 2H RotA, 2H RotB), 7.38 (brs, 2H RotA, 3H RotB), 7.05 – 6.79 (m, 3H RotA, 2H RotB), 5.47 – 5.32 (m, 2H), 3.69 – 3.41 (m, 2H), 1.73 – 1.53 (m, 2H), 1.45 – 1.15 (m, 14H), 0.88 (t, J = 6.8 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 202.6 (Cq), 201.9 (Cq), 164.8 (CH), 164.3 (CH), 144.2 (CH), 143.2 (CH), 135.2 (CH), 129.9 (Cq), 129.8 (Cq), 128.9 (CH), 127.9 (CH), 117.3 (CH), 116.7 (CH), 100.3 (CH), 99.2 (CH), 86.8 (CH_2), 86.1 (CH_2), 45.9 (CH_2), 45.0 (CH_2), 31.9 (CH_2), 29.5 (CH_2), 29.4 (CH_2), 29.3 (CH_2), 29.3 (CH_2), 29.2 (CH_2), 29.0 (CH_2), 26.9 (CH_2), 26.7 (CH_2), 22.7 (CH_2), 14.1 (CH_3). **ESI-MS** calcd for $C_{21}H_{30}NO$ $[M+H]^+$ 312.23, found 312.28.

N-phenethyl-N-(propa-1,2-dien-1-yl)cinnamamide. 1c



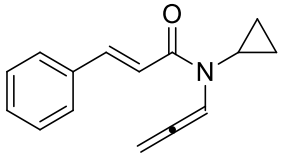
Allene **1c** was prepared following general procedure **GP-1b** from the corresponding enyne (200 mg, 0.69 mmol). Colourless viscous oil (81.3 mg, 40% yield). Two rotamers are observed due to the dynamic amide group. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.78 – 7.63 (m, 1H RotA, 2H RotB), 7.60 – 7.51 (m, 1H RotA, 1H RotB), 7.46 – 7.21 (m, 9H RotA, 9H RotB), 7.03 – 6.85 (m, 2H RotA), 6.60 (d, J = 15.3 Hz, 1H RotB), 5.51 (d, J = 6.5 Hz, 2H RotB), 5.44 (d, J = 5.9 Hz, 2H RotA), 3.83 (t, J = 7.0 Hz, 2H RotA, 2H RotB), 3.06 – 2.85 (m, 2H RotA, 2H RotB). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 202.6 (Cq, RotB), 201.8 (Cq, RotA), 164.7 (Cq, RotA), 164.5 (Cq, RotB), 144.0 (Cq, RotB), 143.5 (Cq, RotA), 138.4 (Cq, RotA), 135.1 (Cq, RotB), 129.9, 128.9, 128.8, 128.5, 127.9, 126.9, 126.4, 117.0 (CH, RotA), 116.6 (CH, RotB), 100.3 (CH, RotA), 98.9 (CH, RotB), 87.1 (CH_2, RotB), 86.5 (CH_2, RotA), 47.6 (CH_2, RotB), 46.7 (CH_2, RotA), 35.0 (CH_2, RotB), 33.7 (CH_2, RotA). **ESI-MS** calcd for $C_{20}H_{19}NNaO$ $[M+Na]^+$ 312.14, found 312.06.

N-phenyl-N-(propa-1,2-dien-1-yl)cinnamamide. 1d



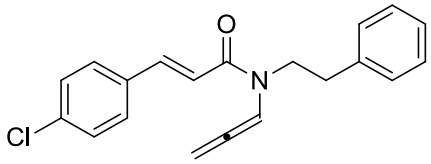
Allene **1d** was prepared following general procedure **GP-1a** from the corresponding cinnamamide (350 mg, 1.34 mmol). Yellow oil (299 mg, 85% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.80 (t, *J* = 6.3 Hz, 1H), 7.73 (d, *J* = 15.5 Hz, 1H), 7.49 – 7.39 (m, 3H), 7.29 (s, 5H), 7.27 – 7.22 (m, 2H), 6.27 (d, *J* = 15.5 Hz, 1H), 5.05 (d, *J* = 6.4 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 203.2 (Cq), 163.9 (Cq), 143.2 (CH), 139.1 (Cq), 134.9 (Cq), 129.9 (CH), 129.4 (2CH), 128.9 (2CH), 128.7 (2CH), 128.6 (CH), 128.0 (2CH), 118.0 (CH), 101.4 (CH), 86.5 (CH_2). **ESI-MS** calcd for $C_{18}H_{15}NNaO$ $[M+Na]^+$ 284.10, found 284.14.

N-cyclopropyl-N-(propa-1,2-dien-1-yl)cinnamamide. 1e



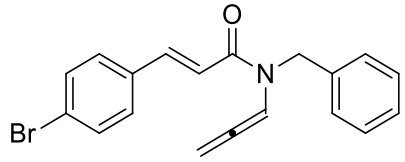
Allene **1e** was prepared following general procedure **GP-1a** from the corresponding cinnamamide (225.3 mg, 1.0 mmol). Yellow liquid (127 mg, 56% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 15.6 Hz, 1H), 7.60 – 7.52 (m, 2H), 7.49 – 7.27 (m, 4H), 5.36 (d, *J* = 6.5 Hz, 1H), 2.76 (tt, *J* = 6.9, 3.9 Hz, 1H), 1.02 (q, *J* = 7.1 Hz, 1H), 0.91 – 0.81 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 203.6 (Cq), 166.2 (Cq), 143.2 (CH), 135.3 (Cq), 129.9 (CH), 128.9 (CH), 128.0 (CH), 118.3 (CH), 99.6 (CH), 85.5 (CH_2), 28.1 (CH), 10.1 ($2CH_2$). **ESI-MS** calcd for $C_{15}H_{16}NO$ $[M+H]^+$ 226.29, found 226.24.

(*E*)-3-(4-chlorophenyl)-N-phenethyl-N-(propa-1,2-dien-1-yl)acrylamide. 1f



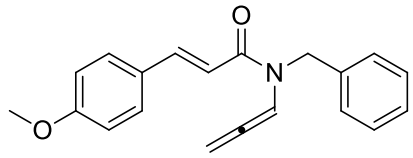
Allene **1f** was prepared following general procedure **GP-1b** from the corresponding enyne (489.1 mg, 1.49 mmol). Orange oil (305 mg, 63% yield). Two rotamers are observed due to the dynamic amide group. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.8 – 7.0 (m, 4H RotA, 5H RotB), 6.9 – 6.8 (m, 2H RotA), 6.5 (d, *J* = 15.3 Hz, 1H RotB), 5.49 (d, *J* = 6.2 Hz, 2H RotA), 5.41 (d, *J* = 6.2 Hz, 2H RotB), 3.9 – 3.7 (m, 2H RotA, 2H RotB), 3.0 – 2.9 (m, 3H RotA, 3H RotB). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 202.6, 201.8, 164.4, 164.3, 162.4, 145.6, 142.4, 142.1, 139.0, 138.4, 138.1, 135.7, 133.6, 129.5, 129.4, 129.1, 129.0, 129.0, 128.9, 128.8, 128.7, 128.5, 126.9, 126.8, 126.4, 117.6, 117.2, 100.2, 98.8, 87.2, 86.6, 47.6, 46.8, 35.0, 33.7. **ESI-MS** calcd for $C_{20}H_{19}ClNO$ $[M+H]^+$ 324.11, found 324.21.

(*E*)-N-benzyl-3-(4-bromophenyl)-N-(propa-1,2-dien-1-yl)acrylamide. 1g



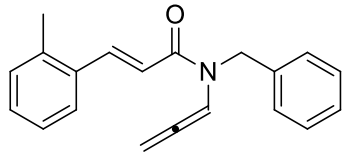
Allene **1g** was directly prepared following general procedure **GP-1a** from the corresponding cinnamamide (700 mg, 2.79 mmol). White solid (263 mg, 37% yield). Two rotamers are observed due to the dynamic amide group. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.80 (t, *J* = 6.3 Hz, 1H RotB), 7.72 (d, *J* = 15.3 Hz, 1H RotA, 1H RotB), 7.58 – 7.24 (m, 9H RotA, 9H RotB), 7.02 (d, *J* = 15.4 Hz, 1H RotA), 6.89 (t, *J* = 6.0 Hz, 1H RotA), 6.77 (d, *J* = 15.3 Hz, 1H RotB), 5.36 (d, *J* = 6.4 Hz, 2H RotA, 2H RotB), 4.84 (d, *J* = 6.5 Hz, 2H RotA, 2H RotB). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 202.6 (Cq, RotB), 202.5 (Cq, RotA), 164.8 (Cq, RotA), 164.7 (Cq, RotB), 143.2 (CH, RotB), 142.6 (CH, RotA), 137.4 (Cq, RotA), 137.1 (Cq, RotB), 132.1, 129.4, 128.9, 127.6, 126.0, 124.2 (Cq RotA, Cq RotB), 117.6, 100.1, 100.0, 87.8, 86.9, 49.3, 48.3. **ESI-MS** calcd for $C_{19}H_{17}BrNO$ $[M+H]^+$ 354.05, found 354.06.

(*E*)-N-benzyl-3-(4-methoxyphenyl)-N-(propa-1,2-dien-1-yl)acrylamide. 1h



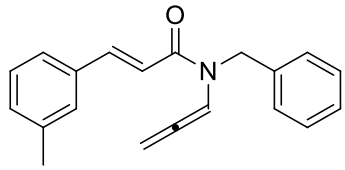
Allene **1h** was prepared following general procedure **GP-1b** from the corresponding enyne (289 mg, 0.94 mmol). White solid (245 mg, 85% yield). Two rotamers are observed due to the dynamic amide group. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.89 – 7.70 (m, 2H RotA, 1H RotB), 7.57 – 7.22 (m, 7H RotA, 7H RotB), 6.98 – 6.82 (m, 3H RotA, 3H RotB), 6.67 (d, *J* = 16.0 Hz, 1H RotB), 5.35 (d, *J* = 6.3 Hz, 2H RotA, 2H RotB), 4.84 (s, 2H RotA, 2H RotB), 3.92 – 3.79 (m, 3H RotA, 3H RotB). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 202.7, 202.4, 165.4, 165.3, 161.2, 144.4, 143.7, 137.7, 137.3, 129.6, 128.9, 128.3, 128.1, 127.7, 127.4, 126.1, 114.4, 114.3, 100.3, 100.1, 87.6, 86.7, 55.4, 49.2, 48.2. **ESI-MS** calcd for $C_{20}H_{20}NO_2$ $[M+H]^+$ 306.38, found 306.24.

(*E*)-N-benzyl-N-(propa-1,2-dien-1-yl)-3-(o-tolyl)acrylamide. 1i



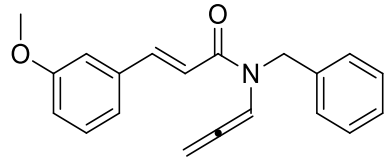
Allene **1i** was prepared following general procedure **GP-1a** from the corresponding cinnamamide (700.0 mg, 2.79 mmol). Orange solid (530.0 mg, 65% yield). Two rotamers are observed due to the dynamic amide group. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 15.3 Hz, 1H RotA, 1H RotB), 7.80 (t, *J* = 6.3 Hz, 1H RotB), 7.57 (d, *J* = 7.1 Hz, 1H RotA), 7.39 – 7.08 (m, 7H RotA, 8H RotB), 6.95 – 6.87 (m, 2H RotA), 6.68 (d, *J* = 15.1 Hz, 1H RotB), 5.34 (d, *J* = 6.4 Hz, 2H RotA, 2H RotB), 4.82 (s, 2H RotA, 2H RotB), 2.45 (s, 3H RotA), 2.40 (s, 3H RotB). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 202.7, 202.4, 165.0, 142.4, 141.8, 137.7, 137.2, 134.1, 130.8, 129.7, 128.9, 128.4, 128.1, 127.5, 126.4, 126.3, 126.2, 126.2, 126.1, 118.2, 100.0, 87.7, 86.8, 49.3, 48.3, 19.9. **ESI-MS** calcd for $C_{20}H_{20}NO$ $[M+H]^+$ 290.15, found 290.26.

(*E*)-N-benzyl-N-(propa-1,2-dien-1-yl)-3-(m-tolyl)acrylamide. 1j



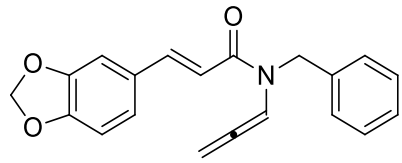
Allene **1j** was prepared following general procedure **GP-1b** from the corresponding enyne (261.3 mg, 0.90 mmol). White solid (187.0 mg, 71% yield). Two rotamers are observed due to the dynamic amide group. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.89 – 7.73 (m, 1H RotA, 2H RotB), 7.45 – 7.13 (m, 9H RotA, 9H RotB), 7.07 – 6.91 (m, 2H RotA), 6.80 (d, *J* = 15.3 Hz, 1H RotB), 5.35 (d, *J* = 6.2 Hz, 2H RotA, 2H RotB), 4.85 (s, 2H RotA, 2H RotB), 2.38 (d, *J* = 18.9 Hz, 3H RotA, 3H RotB). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 202.7, 202.4, 165.2, 165.1, 144.9, 144.2, 138.5, 137.6, 137.2, 135.0, 134.9, 130.8, 128.9, 128.7, 128.6, 128.4, 128.0, 127.5, 127.1, 126.1, 125.2, 125.1, 116.6, 100.3, 100.0, 87.7, 86.8, 49.3, 48.2, 21.3. **ESI-MS** calcd for $C_{20}H_{20}NO$ $[M+H]^+$ 290.15, found 290.26.

(*E*)-N-benzyl-3-(3-methoxyphenyl)-N-(propa-1,2-dien-1-yl)acrylamide. 1k



Allene **1k** was prepared following general procedure **GP-1b** from the corresponding enyne (298 mg, 0.98 mmol). Yellow solid (131.0 mg, 44% yield). Two rotamers are observed due to the dynamic amide group. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.83 – 7.69 (m, 2H RotA, 1H RotB), 7.39 – 7.20 (m, 5H RotA, 5H RotB), 7.15 (d, *J* = 7.4 Hz, 1H RotA), 7.10 – 6.85 (m, 3H RotA, 4H RotB), 6.76 (d, *J* = 15.4 Hz, 1H RotB), 5.34 (d, *J* = 6.4 Hz, 2H RotA, 2H RotB), 4.86 – 4.79 (m, 2H RotA, 2H RotB), 3.84 (s, 3H RotA), 3.79 (s, 3H RotB). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 202.7, 202.4, 165.1, 164.9, 159.9, 159.8, 144.5, 143.9, 137.5, 137.2, 136.4, 136.3, 129.8, 128.9, 128.4, 128.1, 127.5, 127.2, 126.1, 120.6, 117.3, 117.3, 115.6, 113.2, 100.2, 100.0, 87.7, 86.8, 55.3, 53.4, 49.3, 48.2. **ESI-MS** calcd for $C_{20}H_{20}NO_2$ $[M+H]^+$ 306.15, found 306.24.

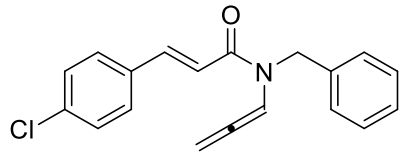
(*E*)-3-(benzo[d][1,3]dioxol-5-yl)-N-benzyl-N-(propa-1,2-dien-1-yl)acrylamide. 1l



Allene **1l** was prepared following general procedure **GP-1b** from the corresponding enyne (250.0 mg, 0.78 mmol). White solid (154 mg, 62% yield). Two rotamers are observed due to the dynamic amide group. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.81 (t, *J* = 6.2 Hz, 1H RotB), 7.71 (d, *J* = 15.2 Hz, 1H RotA, 1H RotB), 7.45 – 7.19 (m, 5H RotA, 5H RotB), 7.13 – 6.76 (m, 5H RotA, 3H RotB), 6.62 (d, *J* = 15.2 Hz, 1H RotB), 6.03 (s, 2H RotA), 6.00 (s, 2H RotB), 5.37 – 5.33 (m, 2H RotA, 2H RotB), 4.83 (brs, 2H RotA, 2H RotB). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 202.7, 202.4, 165.2, 165.1, 149.4, 148.3, 148.2, 144.4, 143.8, 137.5, 137.2, 129.4, 128.9, 128.4, 128.0, 127.5, 127.1, 126.1, 124.4, 124.2, 114.8, 108.6,

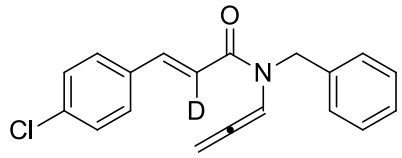
106.4, 101.5, 100.2, 100.1, 87.6, 86.7, 49.2, 48.2. **ESI-MS** calcd for $C_{20}H_{18}NO_3$ $[M+H]^+$ 320.13, found 320.22.

(E)-N-benzyl-3-(4-chlorophenyl)-N-(propa-1,2-dien-1-yl)acrylamide. 1m



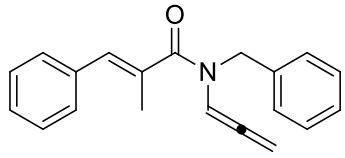
Allene **1m** was prepared following general procedure **GP-1b** from the corresponding enyne (309.7 mg, 1.0 mmol). White solid (184.0 mg, 59% yield). Two rotamers are observed due to the dynamic amide group. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.78 (t, *J* = 6.2 Hz, 1H RotB), 7.72 (d, *J* = 15.3 Hz, 1H RotA, 1H RotB), 7.52 – 7.20 (m, 9H RotA, 9H RotB), 6.98 (d, *J* = 15.4 Hz, 1H RotA), 6.87 (t, *J* = 5.8 Hz, 1H RotA), 6.74 (d, *J* = 15.3 Hz, 1H RotB), 5.37 – 5.30 (m, 2H RotA, 2H RotB), 4.82 (d, *J* = 5.7 Hz, 2H RotA, 2H RotB). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 202.7, 202.5, 164.8, 164.7, 143.2, 142.5, 137.5, 137.1, 135.8, 133.5, 133.4, 129.1, 129.1, 128.9, 128.4, 128.0, 127.5, 127.2, 126.0, 117.5, 100.1, 100.0, 87.8, 86.8, 49.3, 48.3. **ESI-MS** calcd for $C_{19}H_{17}ClNO$ $[M+H]^+$ 310.10, found 310.14.

(*E*)-N-benzyl-2-deutero-3-(4-chlorophenyl)-N-(propa-1,2-dien-1-yl)acrylamide. ***d1*-1m**



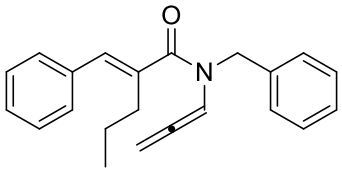
Allene **1m** was prepared following general procedure **GP-1b** from the corresponding enyne (248.1 mg, 0.8 mmol). White solid (126.0 mg, 51% yield). Two rotamers are observed due to the dynamic amide group. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.8 (t, *J* = 6.3 Hz, 1H RotB), 7.8 – 7.7 (m, 1H RotA, 1H RotB), 7.5 – 7.2 (m, 9H RotA, 9H RotB), 7.0 (d, *J* = 15.0 Hz, 0.20H RotA), 6.9 (t, *J* = 5.8 Hz, 1H RotA), 6.8 (d, *J* = 15.3 Hz, 0.20H RotB), 5.4 (d, *J* = 6.3 Hz, 2H RotA, 2H RotB), 4.8 (d, *J* = 6.8 Hz, 2H RotA, 2H RotB). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 202.7, 165.3, 164.7, 143.1, 142.5, 140.1, 137.1, 135.8, 133.4, 129.4, 129.18, 129.11, 129.0, 128.9, 128.8, 128.4, 128.0, 128.0, 127.7, 127.6, 127.2, 126.0, 117.5, 100.0, 87.8, 86.8, 49.3, 48.3. **ESI-MS** calcd for $C_{19}H_{16}DClNO$ $[M+H]^+$ 311.11, found 311.48. (*Slow decomposition during the measurement of the NMR sample was observed*).

(*E*)-N-benzyl-2-methyl-3-phenyl-N-(propa-1,2-dien-1-yl)acrylamide. 3a



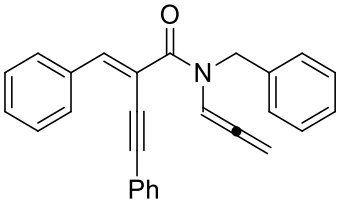
Allene **3a** was prepared following general procedure **GP-1b** from the corresponding enyne (587.0 mg, 2.03 mmol). White solid (475 mg, 80% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.57 – 6.96 (m, 12H), 6.69 (s, 1H), 5.32 (d, *J* = 6.2 Hz, 2H), 4.83 (s, 2H), 2.38 – 2.06 (m, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 201.2, 171.1, 137.6, 135.6, 132.1, 129.1, 128.5, 128.4, 127.7, 127.2, 101.5, 87.3, 47.3, 16.1. **ESI-MS** calcd for $C_{20}H_{20}NO$ $[M+H]^+$ 290.15, found 290.20.

(*E*)-N-benzyl-2-benzylidene-N-(propa-1,2-dien-1-yl)pentanamide. 3b



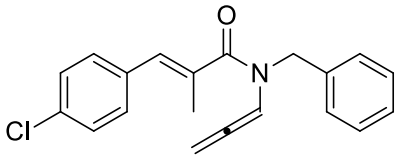
Allene **3b** was prepared following general procedure **GP-1b** from the corresponding enyne (587.0 mg, 1.85 mmol). Viscous oil (354.8 mg, 60% yield).**^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.43 – 7.06 (m, 10H), 6.64 (brs, 1H), 5.30 (brs, 2H), 4.82 (s, 2H), 2.58 (brs, 2H), 1.64 – 1.46 (m, 2H), 0.95 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 200.5 (Cq), 171.2 (Cq), 137.6 (Cq), 137.3 (CH), 135.7 (Cq), 131.7 (Cq), 128.9 (2CH), 128.4 (4CH), 127.9 (2CH), 127.7 (CH), 127.1 (CH), 102.0 (CH), 87.3 (CH_2), 47.1 (CH_2), 31.7 (CH_2), 21.6 (CH_2), 14.2 (CH_3). **ESI-MS** calcd for $C_{22}H_{24}NO$ $[M+H]^+$ 318.18, found 318.26.

(*E*)-N-benzyl-2-benzylidene-4-phenyl-N-(propa-1,2-dien-1-yl)but-3-ynamide. 3c



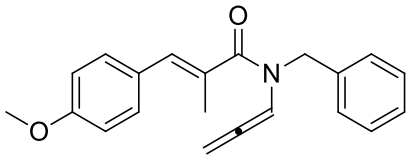
Allene **3c** was prepared following general procedure **GP-1b** from the corresponding enyne (389.0 mg, 0.85 mmol). Red viscous oil (121.3 mg, 60% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.24 – 7.77 (m, 2H), 7.64 – 7.00 (m, 15H), 5.45 – 5.20 (m, 2H), 5.15 – 4.80 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 202.6, 200.8, 166.4, 163.7, 143.9, 141.6, 137.3, 135.0, 131.5, 129.9, 129.5, 129.0, 128.5, 128.4, 128.4, 127.7, 127.1, 126.5, 122.7, 118.5, 116.7, 102.6, 100.3, 99.2, 87.6, 87.3, 85.2, 53.4, 47.9, 47.0. **ESI-MS** calcd for $C_{27}H_{22}NO$ $[M+H]^+$ 376.17, found 376.29.

(*E*)-N-benzyl-3-(4-chlorophenyl)-2-methyl-N-(propa-1,2-dien-1-yl)acrylamide. 3d



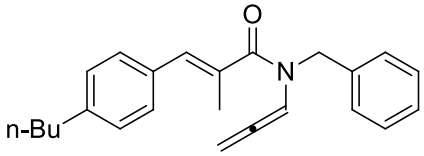
Allene **3d** was prepared following general procedure **GP-1b** from the corresponding enyne (389.0 mg, 0.85 mmol). Red viscous oil (121.3 mg, 60% yield). Two rotamers are observed due to the dynamic amide group. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.4 – 7.2 (m, 9H RotA, 10H RotB), 6.7 (t, *J* = 6.3 Hz, 1H RotA), 6.6 (brs, 1H RotA, 1H RotB), 5.4 – 5.3 (m, 2H RotA, 2H RotB), 4.8 (s, 2H RotA, 2H RotB), 2.2 – 2.0 (m, 3H RotA, 3H RotB). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 202.9, 200.8, 170.6, 169.9, 137.5, 136.5, 134.0, 133.9, 132.8, 132.7, 130.4, 129.0, 129.0, 128.9, 128.6, 128.6, 128.5, 128.4, 128.3, 127.9, 127.3, 127.2, 126.4, 100.5, 98.3, 87.5, 87.5, 49.9, 46.4, 22.1, 16.2. **ESI-MS** calcd for $C_{20}H_{19}ClNO$ $[M+H]^+$ 324.11, found 324.04.

(*E*)-N-benzyl-3-(4-methoxyphenyl)-2-methyl-N-(propa-1,2-dien-1-yl)acrylamide. 3e



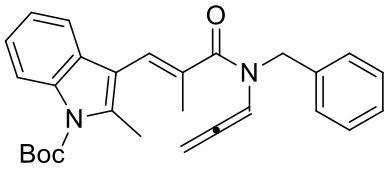
Allene **3e** was prepared following general procedure **GP-1b** from the corresponding enyne (434.4 mg, 1.36 mmol). Colourless viscous oil (334.6 mg, 77% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.36 – 7.20 (m, 8H), 6.95 – 6.85 (m, 2H), 6.62 (brs, 1H), 5.32 – 5.25 (m, 2H), 4.80 (s, 2H), 3.82 (s, 3H), 2.13 (brs, 3H). **^{13}C NMR** (400 MHz, $CDCl_3$) δ 200.9 (Cq), 172.2 (Cq), 159.2 (Cq), 137.7 (CH), 131.8 (Cq), 130.6 (2CH), 130.0 (Cq), 128.5 (2CH), 128.3 (Cq), 127.6 (2CH), 127.1 (CH), 113.8 (2CH), 101.5 (CH), 87.3 (CH_2), 55.3 (CH_3), 47.7 (CH_2), 16.2 (CH_3). **ESI-MS** calcd for $C_{21}H_{22}NO_2$ $[M+H]^+$ 320.16, found 320.20.

(*E*)-N-benzyl-3-(4-butylphenyl)-2-methyl-N-(propa-1,2-dien-1-yl)acrylamide. 3f



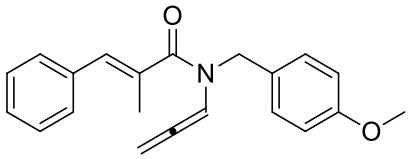
Allene **3f** was prepared following general procedure **GP-1b** from the corresponding enyne (232.0 mg, 0.7 mmol). Colourless oil (152.6 mg, 66% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.50 – 7.11 (m, 10H), 6.67 (s, 1H), 5.31 (d, J = 6.4 Hz, 2H), 4.83 (s, 2H), 2.68 – 2.58 (m, 2H), 2.16 (s, 3H), 1.67 – 1.55 (m, 2H), 1.39 (hex, J = 7.3 Hz, 2H), 0.96 (t, J = 7.3 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 200.9 (Cq), 172.0 (Cq), 142.7 (Cq), 137.6 (Cq), 133.0 (CH), 132.1 (Cq), 131.1 (CH), 129.1 (2CH), 128.5 (4CH), 127.7 (2CH), 127.1 (2CH), 101.9 (CH), 87.3 (CH_2), 47.6 (CH_2), 35.4 (CH_2), 33.5 (CH_2), 22.4 (CH_2), 16.2 (CH_3), 14.0 (CH_3). **ESI-MS** calcd for $C_{24}H_{28}NO$ $[M+H]^+$ 346.22, found 346.25.

(*E*)-tert-butyl 3-(3-(benzyl(propa-1,2-dien-1-yl)amino)-2-methyl-3-oxoprop-1-en-1-yl)-2-methyl-1H-indole-1-carboxylate. 3g



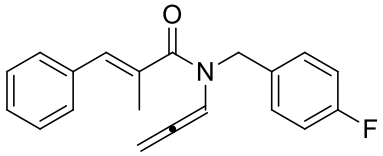
Allene **3g** was prepared following general procedure **GP-1b** from the corresponding enyne (290.0 mg, 0.65 mmol). Red viscous oil (178.0 mg, 61% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.14 (d, J = 8.3 Hz, 1H), 7.50 – 7.10 (m, 9H), 6.68 (brs, 1H), 5.37 – 5.30 (m, 2H), 4.90 (s, 2H), 2.51 (s, 3H), 1.95 (s, 3H), 1.72 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 201.2 (Cq), 171.3 (Cq), 150.6 (Cq), 137.5 (Cq), 135.7 (Cq), 135.3 (Cq), 134.7 (Cq), 128.8 (Cq), 128.5 (2CH), 127.7 (2CH), 127.2 (2CH), 123.8 (CH), 122.8 (CH), 118.8 (CH), 115.5 (CH), 114.8 (Cq), 102.0 (CH), 87.4 (CH_2), 84.1 (Cq), 47.4 (CH_2), 28.3 ($3CH_3$), 17.0 (CH_3), 15.6 (CH_3). **ESI-MS** calcd for $C_{28}H_{30}N_2NaO_3$ $[M+Na]^+$ 465.21, found 465.19.

(*E*)-N-(4-methoxybenzyl)-2-methyl-3-phenyl-N-(propa-1,2-dien-1-yl)acrylamide. 3h



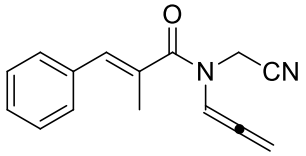
Allene **3h** was prepared following general procedure **GP-1b** from the corresponding enyne (319.4 mg, 1.0 mmol). White solid (163.3 mg, 51% yield). Two rotamers are observed due to the dynamic amide group. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.44 – 7.19 (m, 6H RotA, 6H RotB), 6.95 – 6.71 (m, 2H RotA, 2H RotB), 6.48 (q, *J* = 1.7 Hz, 1H RotB), 6.42 (q, *J* = 2.0 Hz, 1H RotA), 5.35 (d, *J* = 6.1 Hz, 2H RotA), 5.27 (d, *J* = 6.2 Hz, 2H RotB), 4.83 – 4.58 (m, 2H RotA, 2H RotB), 3.84 – 3.82 (m, 3H RotA, 3H RotB), 2.16 (br s, 3H RotA), 2.15 (br s, 3H RotB). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 203.0, 201.0, 171.0, 170.2, 158.8, 158.6, 135.7, 135.4, 132.2, 131.7, 130.0, 129.6, 129.1, 128.9, 128.7, 128.43, 128.38, 127.9, 127.8, 127.74, 127.68, 127.6, 113.8, 113.6, 100.5, 98.3, 87.3, 87.2, 55.33, 55.32, 49.3, 45.8, 22.2, 16.1. **ESI-MS** calcd for $C_{21}H_{22}NO_2$ $[M+H]^+$ 320.16, found 320.09.

(*E*)-N-(4-fluorobenzyl)-2-methyl-3-phenyl-N-(propa-1,2-dien-1-yl)acrylamide. 3i



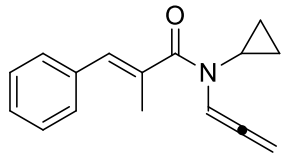
Allene **3i** was prepared following general procedure **GP-1b** from the corresponding enyne (245.9 mg, 0.8 mmol). White solid (192.0 mg, 49% yield). Two rotamers are observed due to the dynamic amide group. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.49 – 7.17 (m, 8H RotA, 8H RotB), 7.14 – 6.89 (m, 2H RotA, 3H RotB), 6.72 (br s, 1H RotA), 5.36 – 5.22 (m, 2H RotA, 2H RotB), 4.79 (s, 2H Rot A, 2H RotB), 2.16 (br s, 3H RotA, 3H RotB). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 200.8, 171.7, 170.2, 162.0 (d, *J* = 245.3 Hz), 135.5, 133.27 (d, *J* = 3.1 Hz), 131.9, 130.26 (d, *J* = 8.0 Hz), 129.3, 129.1, 128.4, 127.8, 127.7, 115.4, 115.2, 115.0, 101.8, 100.6, 87.5, 46.7, 22.1, 16.2. **^{19}F NMR (**565 MHz, $CDCl_3$) δ -115.31 (m). **ESI-MS** calcd for $C_{20}H_{19}FNO$ $[M+H]^+$ 308.14, found 308.24. (*Slow decomposition during the measurement of the NMR sample was observed*).

(*E*)-N-(cyanomethyl)-2-methyl-3-phenyl-N-(propa-1,2-dien-1-yl)acrylamide. 3j



Allene **3j** was prepared following general procedure **GP-1b** from the corresponding enyne (200.0 mg, 0.84 mmol). Pale yellow solid (68.6 mg, 34% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.50 – 7.28 (m, 5H), 7.12 (brs, 1H), 6.81 (brs, 1H), 5.63 (d, *J* = 6.3 Hz, 2H), 4.53 (s, 2H), 2.20 (d, *J* = 1.5 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 199.5, 171.1, 135.0, 134.3, 130.1, 129.3, 128.6, 128.3, 115.2, 100.7, 89.7, 32.3, 16.0. **ESI-MS** calcd for $C_{15}H_{15}N_2O$ $[M+H]^+$ 239.12, found 239.09.

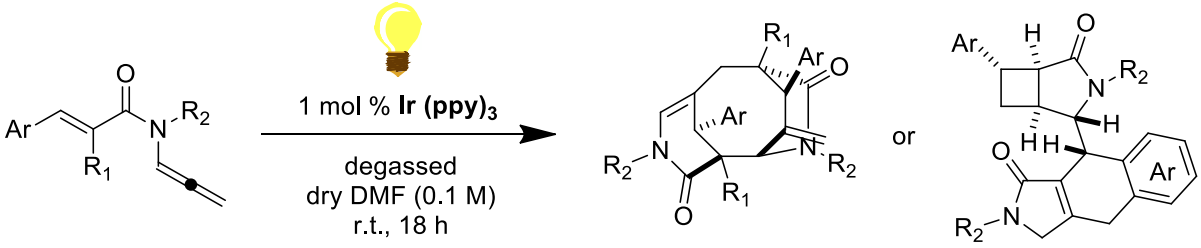
(*E*)-N-cyclopropyl-2-methyl-3-phenyl-N-(propa-1,2-dien-1-yl)acrylamide. 3k



Allene **3k** was prepared following general procedure **GP-1b** from the corresponding enyne (239.2 mg, 1.0 mmol). Pale yellow liquid (123.4 mg, 52% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.52 – 7.18 (m, 6H), 6.78 (s, 1H), 5.38 (d, *J* = 6.4 Hz, 2H), 2.71 (dt, *J* = 6.9, 3.0 Hz, 1H), 2.17 (d, *J* = 1.5 Hz, 3H), 0.95 – 0.88 (m, 2H), 0.77 (ddd, *J* = 3.9, 2.3, 1.3 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 202.8, 172.8, 136.0, 133.1, 132.3, 129.1, 128.4, 127.7, 100.6, 85.8, 29.6, 16.0, 9.8. **ESI-MS** calcd for $C_{16}H_{18}NO$ $[M+H]^+$ 240.14, found 240.19.

Characterization of products

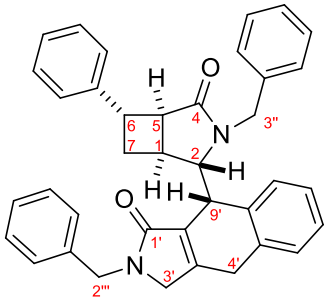
Photocatalytic reactions [GP-2]:



$R_1 \neq H$ $R_1 = H$

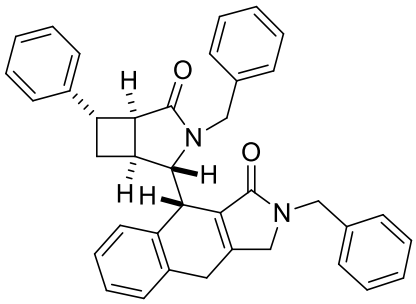
To a vial charged with substrate **1** or **3** (1 equiv., 0.15-0.3 mmol) and **Ir(ppy)$_3$** (1 mol%), dry and degassed DMF (0.1 M) was added through a syringe. The solution was transferred in two NMR tubes capped with a rubber septum and it was then degassed through three freeze-pump cycles. The homogeneous solution was placed in an oil bath kept at 25 °C and irradiated with LED stripes for 18 hours indicatively. Conversion was monitored by TLC and the mixture was then concentrated in vacuo. The residue was purified by chromatography on silica gel; the catalyst was removed using toluene as eluent prior to the separation of desired products (*n*-hexane/EtOAc, under gradient).

(R)-2-benzyl-9-((1S,2S,5R,6S)-3-benzyl-4-oxo-6-phenyl-3-azabicyclo[3.2.0]heptan-2-yl)-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. 2a



2a was isolated following the **GP-2** using **1a** as reagent (55.5 mg, 0.2 mmol). White crystals, m.p. 169-170 °C. Yield **25%** (13.5 mg, 0.024 mmol). The reaction performed in a small Schlenk on 1.0 mmol of **1a** (276 mg) led to the isolation of **2a** in 18% yield (49.7 mg). The reaction conducted in a coil reactor (5 mm inner diameter) using 1.04 g of **3a** allowed to recover 208 mg of **2a** (20%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.49 – 7.03 (m, 19H, Ar-H), 5.32 (d, J = 14.2 Hz, $H_{2'''}$), 4.83 (d, J = 15.1 Hz, $H_{3''}$), 4.47 (d, J = 15.0 Hz, $H_{3''}$), 4.28 – 4.21 (brs, $H_{9'}$), 4.03 – 3.72 (m, H_2, $H_{3'}$, $H_{3'}$, $H_{4'}$, $H_{2'''}$), 3.58 (dd, J = 22.1, 3.0 Hz, $H_{4'}$), 3.44 – 3.31 (m, H_6), 2.68 (q, J = 7.6 Hz, H_1), 2.09 – 1.87 (m, H_5, $2H_7$). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.2 (C_4), 170.1 ($C_{1'}$), 151.1 (Cq), 144.5 (Cq), 137.2 (Cq), 136.8 (Cq), 133.3 (Cq), 132.9 (Cq), 130.5 (Cq), 129.6 (CH), 129.0 (2CH), 128.9 (CH), 128.8 (4CH), 128.5 (2CH), 128.0 (2CH), 127.8 (CH), 127.7 (CH), 127.4 (CH), 127.1 (CH), 126.3 (2CH), 126.2 (CH), 66.2 (C_2), 52.2 ($C_{3'}$), 47.6 (C_5), 46.2 ($C_{3''}$), 45.0 ($C_{2'''}$), 42.8 (C_6), 38.5 ($C_{9'}$), 32.0 (C_7), 31.8 (C_1), 30.3 ($C_{4'}$). **ESI-MS** calcd for $C_{38}H_{34}N_2NaO_2$ $[M+Na]^+$ 573.25, found 573.26. **ESI-HRMS** calcd for $C_{38}H_{34}N_2KO_2$ $[M+K]^+$ 589.2252, found 589.2260.

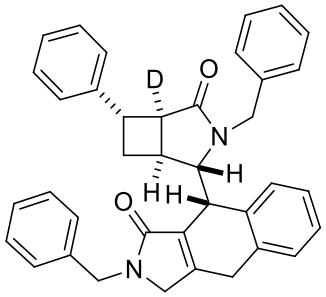
(S)-2-benzyl-9-((1S,2S,5R,6S)-3-benzyl-4-oxo-6-phenyl-3-azabicyclo[3.2.0]heptan-2-yl)-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. 2a'



2a' was isolated following the **GP-2** using **1a** as reagent (55.5 mg, 0.2 mmol). Pale yellow solid, m.p. 106-107 °C. Yield **29%** (16.2 mg, 0.029 mmol). The reaction performed in a small Schlenk on 1.0 mmol of **1a** (276 mg) led to the isolation of **2a** in 21% yield (57.8 mg). The reaction conducted in a coil reactor (5 mm inner diameter) using 1.04 g of **3a** allowed to recover 239 mg of **2a** (23%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.53 – 7.16 (m, 18H), 6.96 (d, J = 7.2 Hz, 1H), 5.52 (d, J = 15.1 Hz, 1H), 4.73 – 4.58 (m, 2H), 4.53 (d, J = 15.1 Hz, 1H), 4.35 (brs, 1H), 3.98 – 3.68 (m, 3H), 3.62 – 3.49 (m, 3H), 2.75 – 2.69 (m, 1H), 2.51 (q, J = 7.6 Hz, 1H), 2.11 – 1.96 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.8 (Cq), 170.0 (Cq), 150.9 (Cq), 144.4 (Cq), 137.5 (Cq), 137.4 (Cq), 134.4 (Cq), 133.4 (Cq), 130.7 (Cq), 129.1 (CH), 129.0 (2CH), 128.9 (CH), 128.9 (2CH), 128.8 (CH), 128.7 (2CH), 128.5 (2CH), 128.2 (2CH), 127.7 (CH), 127.6 (CH), 127.3 (CH), 127.1 (CH), 126.4 (CH), 126.2 (CH), 69.0 (CH), 52.0 (CH_2), 48.2 (CH), 46.2 (CH_2), 45.2 (CH_2), 42.9 (CH), 38.7 (CH), 31.8 (CH_2), 30.6 (CH),

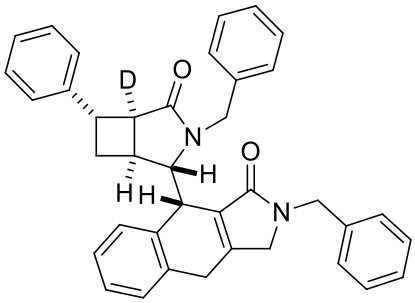
30.5 (CH_2). **ESI-MS** calcd for $C_{38}H_{34}N_2NaO_2$ $[M+Na]^+$ 573.25, found 573.27. **ESI-HRMS** calcd for $C_{38}H_{35}N_2O_2$ $[M+H]^+$ 573.2693, found 573.2697.

(R)-2-benzyl-9-((1S,2S,5R,6S)-3-benzyl-4-oxo-5-deutero-6-phenyl-3-azabicyclo[3.2.0]heptan-2-yl)-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. *d*$_1$-2a



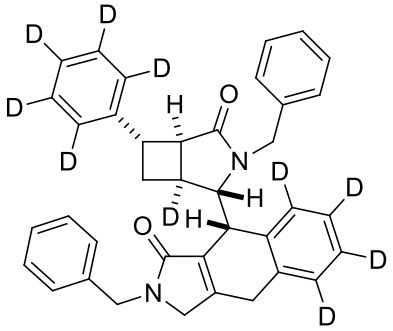
***d*$_1$-2a** was isolated following the **GP-2** using ***d*$_1$-1a** as reagent (55.2 mg, 0.2 mmol). White solid, m.p. 114-115 °C. Yield **22**% (12.3 mg, 0.022 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.52 – 6.99 (m, 19H), 5.31 (d, *J* = 14.2 Hz, 1H), 4.82 (d, *J* = 15.0 Hz, 1H), 4.48 (d, *J* = 15.0 Hz, 1H), 4.25 (brs, 1H), 4.04 – 3.71 (m, 5H), 3.58 (dd, *J* = 22.1, 2.8 Hz, 1H), 3.37 (dd, *J* = 9.1, 3.8 Hz, 1H), 2.69 (t, *J* = 7.9 Hz, 1H), 2.10 – 2.02 (m, 1H), 1.99 – 1.89 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 177.2 (Cq), 170.1 (Cq), 151.1 (Cq), 144.5 (Cq), 137.2 (Cq), 136.8 (Cq), 133.3 (Cq), 133.0 (Cq), 130.5 (Cq), 129.6 (CH), 129.0 (2CH), 128.9 (CH), 128.83 (2CH), 128.82 (2CH), 128.5 (2CH), 128.0 (2CH), 127.8 (CH), 127.7 (CH), 127.4 (CH), 127.1 (CH), 126.3 (2CH), 126.1 (CH), 66.2 (CH), 52.2 (CH_2), 47.6 (CH, residual peak), 46.2 (CH_2), 45.0 (CH_2), 42.7 (CH), 38.5 (CH_2), 32.0 (CH_2), 31.7 (CH), 30.3 (CH_2). **ESI-HRMS** calcd for $C_{38}H_{34}DN_2O_2$ $[M+H]^+$ 552.2756, found 555.2748.

(S)-2-benzyl-9-((1S,2S,5R,6S)-3-benzyl-4-oxo-5-deutero-6-phenyl-3-azabicyclo[3.2.0]heptan-2-yl)-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. *d*$_1$-2a'



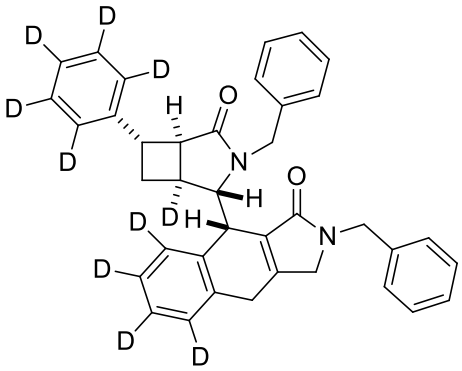
***d*$_1$-2a'** was isolated following the **GP-2** using ***d*$_1$-1a** as reagent (55.2 mg, 0.2 mmol). Pale yellow solid, m.p. 111-112 °C. Yield **29**% (16.1 mg, 0.029 mmol). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 – 7.02 (m, 18H), 6.94 (d, *J* = 7.0 Hz, 1H), 5.50 (d, *J* = 15.1 Hz, 1H), 4.64 (q, *J* = 14.9 Hz, 2H), 4.50 (d, *J* = 15.1 Hz, 1H), 4.33 (brs, 1H), 3.90 (d, *J* = 19.1 Hz, 1H), 3.82 – 3.67 (m, 2H), 3.63 – 3.47 (m, 3H), 2.49 (t, *J* = 7.9 Hz, 1H), 2.10 – 1.95 (m, 2H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 175.7 (Cq), 170.0 (Cq), 150.9 (Cq), 144.4 (Cq), 137.5 (Cq), 137.4 (Cq), 134.5 (Cq), 133.4 (Cq), 130.7 (Cq), 129.1 (CH), 128.9 (2CH), 128.9 (CH), 128.8 (2CH), 128.7 (2CH), 128.5 (2CH), 128.2 (2CH), 127.7 (CH), 127.6 (CH), 127.3 (CH), 127.1 (CH), 126.4 (2CH), 126.2 (CH), 69.0 (CH), 52.0 (CH_2), 48.3 (CH, residual peak), 46.2 (CH_2), 45.2 (CH_2), 42.8 (CH), 38.7 (CH), 31.8 (CH_2), 30.52 (CH), 30.5 (CH_2). **ESI-HRMS** calcd for $C_{38}H_{34}DN_2O_2$ $[M+H]^+$ 552.2756, found 555.2763.

(R)-2-benzyl-9-((1S,2S,5R,6S)-1-deutero-3-benzyl-4-oxo-6-pentadeuterophenyl-3-azabicyclo[3.2.0]heptan-2-yl)-2,3,4,9-tetrahydro-5,6,7,8-tetradeutero-1H-benzo[f]isoindol-1-one. *d_{10}*-2a



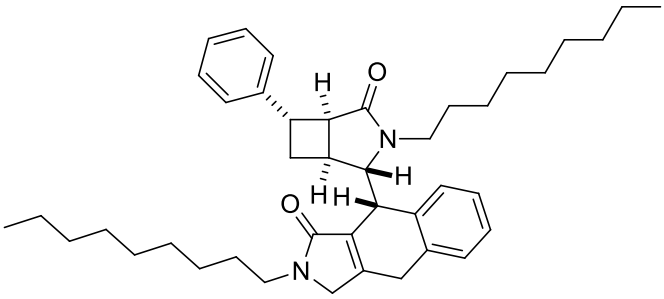
***d_{10}*-2a** was isolated following the **GP-2** using ***d_5*-1a** as reagent (56.0 mg, 0.2 mmol). Pale yellow solid, m.p. 116-117 °C. Yield **26%** (14.8 mg, 0.026 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.50 – 7.15 (m, 10H), 5.31 (d, *J* = 14.2 Hz, 1H), 4.82 (d, *J* = 14.9 Hz, 1H), 4.48 (d, *J* = 15.0 Hz, 1H), 4.25 (s, 1H), 4.06 – 3.71 (m, 5H), 3.58 (dd, *J* = 22.1, 2.9 Hz, 1H), 3.44 – 3.33 (m, 1H), 2.17 – 1.86 (m, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.2 (Cq), 170.1 (Cq), 151.1 (Cq), 144.4 (Cq), 137.2 (Cq), 136.9 (Cq), 133.2 (Cq), 132.9 (Cq), 130.5 (Cq), 129.0 (2CH), 128.8 (2CH), 128.8 (2CH), 128.0 (2CH), 127.8 (CH), 127.7 (CH), 66.1 (CH), 52.2 (CH_2), 47.5 (CH), 46.2 (CH_2), 45.1 (CH_2), 42.8 (CH), 38.5 (CH), 31.9 (CH_2), 31.8 – 31.4 (m, CD), 30.2 (CH_2). **ESI-HRMS** calcd for $C_{38}H_{25}D_{10}N_2O_2$ $[M+H]^+$ 561.3321, found 561.3329.

(S)-2-benzyl-9-((1S,2S,5R,6S)-1-deutero-3-benzyl-4-oxo-6-pentadeuterophenyl-3-azabicyclo[3.2.0]heptan-2-yl)-2,3,4,9-tetrahydro-5,6,7,8-tetradeutero-1H-benzo[f]isoindol-1-one.
***d_{10}*-2a'**



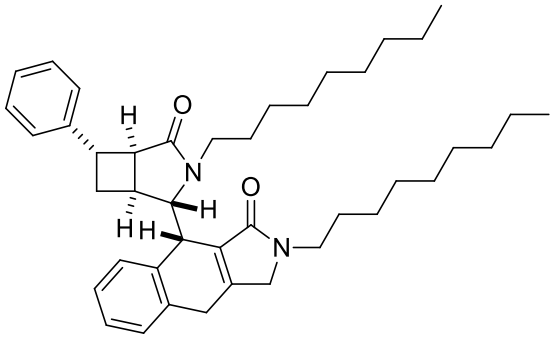
***d_{10}*-2a'** was isolated following the **GP-2** using ***d_5*-1a** as reagent (56.0 mg, 0.2 mmol). Pale yellow solid, m.p. 111-112 °C. Yield **29%** (16.5 mg, 0.029 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.48 – 7.17 (m, 10H), 5.50 (d, *J* = 15.1 Hz, 1H), 4.64 (q, *J* = 14.9 Hz, 2H), 4.50 (d, *J* = 15.5 Hz, 1H), 4.33 (d, *J* = 3.9 Hz, 1H), 3.90 (d, *J* = 19.2 Hz, 1H), 3.80 – 3.67 (m, 2H), 3.62 – 3.46 (m, 3H), 2.71 (s, 1H), 2.08 – 1.93 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.8 (Cq), 170.0 (Cq), 150.9 (Cq), 144.3 (Cq), 137.5 (Cq), 137.4 (Cq), 134.4 (Cq), 133.3 (Cq), 130.8 (Cq), 128.9 (2CH), 128.8 (2CH), 128.7 (2CH), 128.2 (2CH), 127.7 (CH), 127.6 (CH), 68.9 (CH), 52.0 (CH_2), 48.0 (CH), 46.2 (CH_2), 45.3 (CH_2), 42.8 (CH), 38.7 (CH), 31.7 (CH_2), 30.4 (CH_2). **ESI-HRMS** calcd for $C_{38}H_{25}D_{10}N_2O_2$ $[M+H]^+$ 561.3321, found 561.3331.

(R)-2-nonyl-9-((1S,2S,5R,6S)-3-nonyl-4-oxo-6-phenyl-3-azabicyclo[3.2.0]heptan-2-yl)-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. 2b



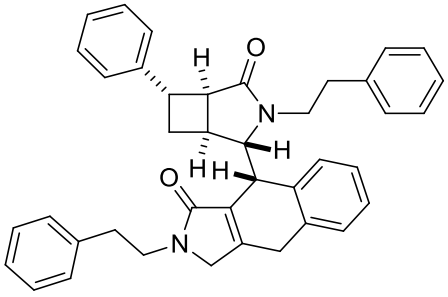
2b was isolated following the **GP-2** using **1b** as reagent (62.3 mg, 0.2 mmol). Pale yellow oil. Yield **15%** (9.3 mg, 0.015 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.42 – 7.12 (m, 6H), 7.11 (d, *J* = 7.3 Hz, 2H), 6.99 (d, *J* = 7.0 Hz, 1H), 4.20 – 4.03 (m, 3H), 4.02 – 3.91 (m, 1H), 3.89 (dd, *J* = 22.1, 3.9 Hz, 1H), 3.68 (dd, *J* = 22.2, 3.2 Hz, 1H), 3.59 (dd, *J* = 14.4, 7.0 Hz, 1H), 3.42 (dt, *J* = 13.9, 7.0 Hz, 2H), 3.19 (ddd, *J* = 13.5, 8.7, 5.2 Hz, 1H), 2.45 (q, *J* = 7.2 Hz, 1H), 2.37 – 2.25 (m, 1H), 2.21 (dtd, *J* = 12.5, 6.9, 3.5 Hz, 1H), 1.93 (d, *J* = 6.7 Hz, 1H), 1.91 – 1.71 (m, 3H), 1.66 – 1.58 (m, 2H), 1.40 – 1.23 (m, 24H), 0.94 – 0.85 (m, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.1 (Cq), 170.1 (Cq), 149.8 (Cq), 144.5 (Cq), 133.0 (Cq), 132.1 (Cq), 130.8 (Cq), 129.5 (CH), 128.9 (CH), 128.4 (2CH), 127.3 (CH), 127.0 (CH), 126.3 (2CH), 126.1 (CH), 66.2 (CH), 52.7 (CH_2), 47.8 (CH), 42.6 (CH), 42.2 (CH_2), 40.7 (CH_2), 37.2 (CH), 32.6 (CH_2), 31.89 (CH_2), 31.85 (CH_2), 31.0 (CH), 30.1 (CH_2), 29.6 (CH_2), 29.5 (CH_2), 29.4 (CH_2), 29.34 (CH_2), 29.29 (CH_2), 29.2 (CH_2), 28.8 (CH_2), 27.3 (CH_2), 27.0 (CH_2), 26.9 (CH_2), 22.71 (CH_2), 22.67 (CH_2), 14.14 (CH_3), 14.12 (CH_3). **ESI-HRMS** calcd for $C_{42}H_{59}N_2O_2$ $[M+H]^+$ 623.4571, found 623.4564.

(S)-2-nonyl-9-((1S,2S,5R,6S)-3-nonyl-4-oxo-6-phenyl-3-azabicyclo[3.2.0]heptan-2-yl)-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. 2b'



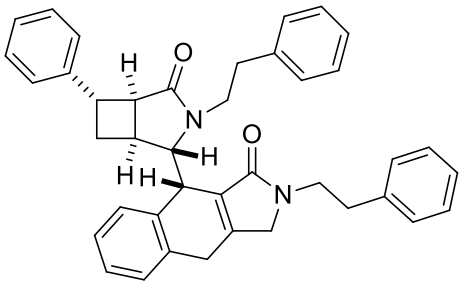
2b' was isolated following the **GP-2** using **1b** as reagent (62.3 mg, 0.2 mmol). Pale yellow oil. Yield **21%** (13.1 mg, 0.021 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.45 – 7.13 (m, 9H), 4.22 (s, 1H), 4.13 – 3.96 (m, 2H), 3.90 – 3.81 (m, 2H), 3.64 (dd, *J* = 21.9, 2.5 Hz, 1H), 3.48 (quint, *J* = 7.4 Hz, 2H), 3.43 – 3.33 (m, 1H), 3.31 – 3.17 (m, 1H), 2.72 (q, *J* = 7.6 Hz, 1H), 2.64 (d, *J* = 6.8 Hz, 1H), 2.23 (t, *J* = 7.4 Hz, 2H), 1.80 – 1.60 (m, 2H), 1.58 – 1.49 (m, 2H), 1.37 – 1.17 (m, 24H), 0.96 – 0.82 (m, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.9 (Cq), 169.8 (Cq), 149.9 (Cq), 144.6 (Cq), 134.5 (Cq), 133.7 (Cq), 131.4 (Cq), 129.1 (CH), 129.0 (CH), 128.5 (2CH), 127.2 (CH), 127.1 (CH), 126.4 (CH), 126.2 (2CH), 69.4 (CH), 52.6 (CH_2), 48.2 (CH), 42.9 (CH), 42.3 (CH_2), 41.2 (CH_2), 39.6 (CH), 32.4 (CH_2), 31.9 (CH), 31.8 (CH_2), 31.6 (CH_2), 30.5 (CH_2), 29.6 (CH_2), 29.5 (CH_2), 29.5 (CH_2), 29.4 (CH_2), 29.3 (CH_2), 29.3 (CH_2), 28.7 (CH_2), 27.3 (CH_2), 27.1 (CH_2), 26.9 (CH_2), 22.7 (CH_2), 22.7 (CH_2), 14.1 (CH_3), 14.1 (CH_3). **ESI-HRMS** calcd for $C_{42}H_{59}N_2O_2$ $[M+H]^+$ 623.4571, found 623.4580.

(R)-9-((1S,2S,5R,6S)-4-oxo-3-phenethyl-6-phenyl-3-azabicyclo[3.2.0]heptan-2-yl)-2-phenethyl-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. 2c



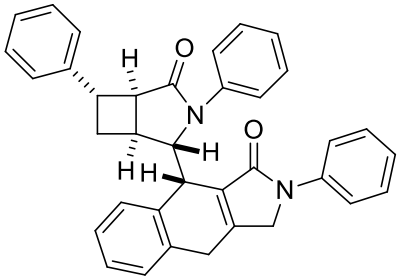
2c was isolated following the **GP-2** using **1c** as reagent (57.9 mg, 0.2 mmol). Colorless oil. Yield **26%** (14.9 mg, 0.026 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.43 (d, *J* = 7.3 Hz, 2H), 7.37 – 7.10 (m, 15H), 7.03 (d, *J* = 7.4 Hz, 2H), 4.47 (dt, *J* = 13.8, 8.3 Hz, 1H), 4.14 (s, 1H), 3.99 (s, 1H), 3.89 – 3.67 (m, 5H), 3.55 (dd, *J* = 22.2, 3.3 Hz, 1H), 3.44 (dt, *J* = 12.2, 5.6 Hz, 1H), 3.28 – 3.21 (m, 2H), 3.16 – 3.07 (m, 1H), 2.99 – 2.91 (m, 2H), 2.28 (q, *J* = 7.2 Hz, 1H), 1.99 (ddt, *J* = 13.0, 7.0, 2.8 Hz, 1H), 1.92 – 1.86 (m, 1H), 1.74 – 1.66 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.2 (Cq), 170.0 (Cq), 149.9 (Cq), 144.5 (Cq), 138.8 (Cq), 138.3 (Cq), 133.0 (Cq), 132.1 (Cq), 130.6 (Cq), 129.4 (CH), 129.1 (2CH), 128.9 (CH), 128.7 (2CH), 128.6 (2CH), 128.5 (2CH), 128.4 (2CH), 127.3 (CH), 127.0 (CH), 126.6 (CH), 126.5 (CH), 126.3 (2CH), 126.1 (CH), 66.3 (CH), 53.4 (CH_2), 47.7 (CH), 43.9 (CH_2), 42.4 (CH), 40.8 (CH_2), 37.2 (CH), 35.1 (CH_2), 32.9 (CH_2), 32.1 (CH_2), 30.6 (CH), 30.0 (CH_2). **ESI-HRMS** calcd for $C_{40}H_{38}N_2NaO_2$ $[M+Na]^+$ 601.2855, found 601.2862.

(S)-9-((1S,2S,5R,6S)-4-oxo-3-phenethyl-6-phenyl-3-azabicyclo[3.2.0]heptan-2-yl)-2-phenethyl-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. 2c'



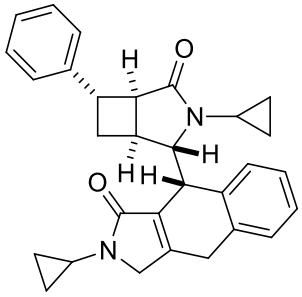
2c' was isolated following the **GP-2** using **1c** as reagent (57.9 mg, 0.2 mmol). Colorless oil. Yield **22%** (12.8 mg, 0.022 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.41 – 7.14 (m, 18H), 7.06 – 7.01 (m, 1H), 4.50 (dt, *J* = 14.1, 6.9 Hz, 1H), 4.16 (brs, 1H), 3.81 – 3.43 (m, 7H), 3.31 (d, *J* = 8.9 Hz, 1H), 3.08 (q, *J* = 7.1 Hz, 2H), 2.86 (t, *J* = 6.8 Hz, 2H), 2.50 (d, *J* = 6.6 Hz, 1H), 2.41 (q, *J* = 7.1 Hz, 1H), 1.95 (tq, *J* = 8.9, 3.2 Hz, 1H), 1.74 (ddd, *J* = 12.8, 9.1, 7.0 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.9 (Cq), 169.8 (Cq), 150.3 (Cq), 144.7 (Cq), 139.3 (Cq), 139.0 (Cq), 134.4 (Cq), 133.5 (Cq), 130.9 (Cq), 129.0 (CH), 128.93 (2CH), 128.92 (CH), 128.8 (2CH), 128.6 (4CH), 128.5 (2CH), 127.2 (CH), 127.0 (CH), 126.5 (CH), 126.40 (CH), 126.38 (2CH), 126.2 (CH), 70.2 (CH), 53.5 (CH_2), 47.8 (CH), 43.8, 42.7 (CH), 41.9 (CH_2), 39.1 (CH), 35.1 (CH_2), 33.9 (CH_2), 31.9 (CH_2), 30.9 (CH), 30.4 (CH_2). **ESI-HRMS** calcd for $C_{40}H_{38}N_2NaO_2$ $[M+Na]^+$ 601.2855, found 601.2861.

(S)-9-((1S,2S,5R,6S)-4-oxo-3,6-diphenyl-3-azabicyclo[3.2.0]heptan-2-yl)-2-phenyl-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. 2d'



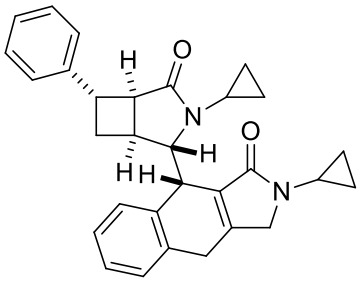
2d' was isolated following the **GP-2** using **1d** as reagent (57.5 mg, 0.22 mmol). Pale yellow solid, m.p. 133-134 °C. Yield **17%** (9.7 mg, 0.022 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 7.9 Hz, 2H), 7.80 (dd, *J* = 8.7, 1.0 Hz, 2H), 7.61 (t, *J* = 8.0 Hz, 2H), 7.45 (t, *J* = 8.0 Hz, 2H). 7.34 – 7.10 (m, 10H), 7.07 (d, *J* = 7.2 Hz, 1H) 5.01 (d, *J* = 2.0 Hz, 1H), 4.64 (d, *J* = 18.2 Hz, 1H), 4.42 (dd, *J* = 18.3, 2.0 Hz, 1H), 4.34 (brs, 1H), 3.99 (dd, *J* = 22.4, 4.1 Hz, 1H), 3.77 (dd, *J* = 22.5, 3.5 Hz, 1H), 3.52 (dt, *J* = 8.5, 4.0 Hz, 1H), 2.54 – 2.42 (m, 2H), 2.42 – 2.32 (m, 1H), 2.18 – 2.11 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.4 (Cq), 169.1 (Cq), 150.0 (Cq), 144.1 (Cq), 139.1 (Cq), 138.2 (Cq), 132.4 (Cq), 131.8 (Cq), 131.7 (Cq), 129.6 (CH), 129.5 (2CH), 129.3 (2CH), 129.0 (CH), 128.5 (2CH), 127.6 (CH), 127.2 (CH), 126.3 (2CH), 125.0 (CH), 124.3 (CH), 122.6 (CH), 121.5 (2CH), 118.8 (2CH), 67.0 (CH), 53.3 (CH_2), 49.1 (CH), 42.6 (CH), 37.0 (CH), 32.8 (CH_2), 30.0 (CH_2), 29.7 (CH). **ESI-HRMS** calcd for $C_{40}H_{38}N_2NaO_2$ $[M+Na]^+$ 545.2199, found 545.2206.

(R)-2-cyclopropyl-9-((1S,2S,5R,6S)-3-cyclopropyl-4-oxo-6-phenyl-3-azabicyclo[3.2.0]heptan-2-yl)-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. 2e



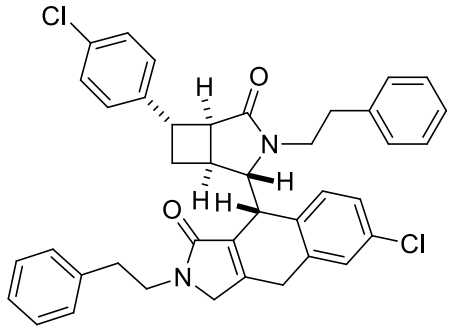
2e was isolated following the **GP-2** using **1e** as reagent (45.1 mg, 0.2 mmol). Pale yellow oil. Yield **24%** (10.8 mg, 0.024 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.50 – 6.99 (m, 9H), 4.25 (brs, 1H), 4.07 (d, *J* = 19.1 Hz, 1H), 3.97 – 3.82 (m, 3H), 3.65 (dd, *J* = 22.2, 3.3 Hz, 1H), 3.38 – 3.27 (m, 1H), 2.93 – 2.85 (m, 1H), 2.83 – 2.73 (m, 1H), 2.42 (q, *J* = 8.0 Hz, 1H), 2.18 (t, *J* = 7.5 Hz, 2H), 1.92 (d, *J* = 8.4 Hz, 1H), 1.21 – 1.12 (m, 2H), 1.03 – 0.70 (m, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 178.5 (Cq), 171.5 (Cq), 150.2 (Cq), 144.4 (Cq), 132.9 (Cq), 132.0 (Cq), 131.1 (Cq), 129.6 (CH), 129.0 (CH), 128.4 (2CH), 127.3 (CH), 127.1 (CH), 126.3 (2CH), 126.1 (CH), 67.9 (CH), 53.4 (CH_2), 48.4 (CH), 42.3 (CH), 38.4 (CH), 32.6 (CH_2), 30.9 (CH), 30.1 (CH_2), 24.7 (CH), 24.6 (CH_2), 7.8 (CH_2), 5.6 (CH_2), 5.4 (CH_2), 5.2 (CH_2). **ESI-HRMS** calcd for $C_{30}H_{30}N_2NaO_2$ $[M+Na]^+$ 473.2199, found 473.2191.

(S)-6-chloro-9-((1S,2S,5R,6S)-6-(4-chlorophenyl)-3-cyclopropyl-4-oxo-3-azabicyclo[3.2.0]heptan-2-yl)-2-cyclopropyl-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. 2e'



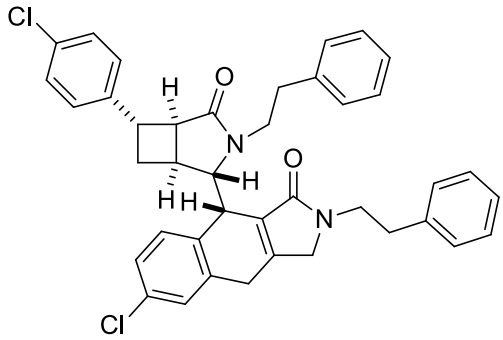
2e' was isolated following the **GP-2** using **1e** as reagent (45.1 mg, 0.2 mmol). Pale yellow oil. Yield **30%** (13.5 mg, 0.030 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.35 – 7.16 (m, 9H), 4.28 (brs, 1H), 3.97 (d, *J* = 19.0 Hz, 1H), 3.83 (d, *J* = 20.4 Hz, 2H), 3.74 (d, *J* = 3.0 Hz, 1H), 3.62 (dd, *J* = 21.9, 2.6 Hz, 1H), 3.41 – 3.31 (m, 1H), 3.12 (tt, *J* = 7.5, 4.1 Hz, 1H), 2.81 – 2.70 (m, 2H), 2.60 (d, *J* = 6.7 Hz, 1H), 2.28 – 2.15 (m, 1H), 2.13 – 2.02 (m, 1H), 1.14 (ddd, *J* = 12.3, 9.6, 6.8 Hz, 2H), 0.97 – 0.64 (m, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.3 (Cq), 171.2 (Cq), 150.1 (Cq), 144.4 (Cq), 134.3 (Cq), 133.6 (Cq), 131.6 (Cq), 129.2 (CH), 129.0 (CH), 128.5 (2CH), 127.2 (CH), 127.2 (CH), 126.4 (CH), 126.3 (2CH), 71.5 (CH), 53.2 (CH_2), 48.8 (CH), 42.6 (CH), 40.5 (CH), 32.4 (CH_2), 31.8 (CH), 30.5 (CH_2), 24.8 (CH), 24.6 (CH), 8.7 (CH_2), 5.8 (CH_2), 5.6 (CH_2), 4.9 (CH_2). **ESI-HRMS** calcd for $C_{30}H_{30}N_2NaO_2$ $[M+Na]^+$ 473.2199, found 473.2208.

(R)-6-chloro-9-((1S,2S,5R,6S)-6-(4-chlorophenyl)-4-oxo-3-phenethyl-3-azabicyclo[3.2.0]heptan-2-yl)-2-phenethyl-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. 2f



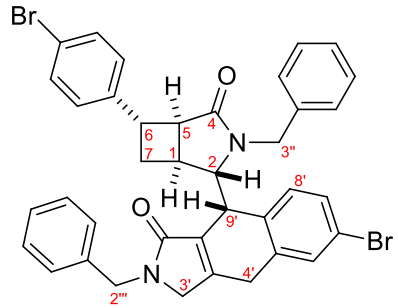
2f was isolated following the **GP-2** using **1f** as reagent (65.0 mg, 0.2 mmol). Colorless oil. Yield **15%** (9.7 mg, 0.015 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.3 Hz, 2H), 7.35 – 7.13 (m, 13H), 6.96 (d, *J* = 8.4 Hz, 2H), 4.47 (dt, *J* = 13.8, 8.3 Hz, 1H), 4.09 (brs, 1H), 3.99 (s, 1H), 3.84 – 3.67 (m, 5H), 3.61 – 3.54 (m, 1H), 3.41 (dt, *J* = 13.1, 6.2 Hz, 1H), 3.23 (t, *J* = 7.6 Hz, 2H), 3.09 – 3.00 (m, 1H), 2.99 – 2.90 (m, 2H), 2.20 (dt, *J* = 13.0, 6.3 Hz, 1H), 2.10 – 1.89 (m, 2H), 1.71 – 1.57 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.8 (Cq), 169.7 (Cq), 149.2 (Cq), 142.7 (Cq), 138.7 (Cq), 138.0 (Cq), 135.0 (Cq), 133.2 (Cq), 131.9 (Cq), 130.7 (Cq), 130.53 (CH), 130.50 (Cq), 129.1 (2CH), 128.9 (CH), 128.67 (2CH), 128.66 (2CH), 128.53 (2CH), 128.50 (2CH), 127.7 (2CH), 127.3 (CH), 126.63 (CH), 126.59 (CH), 66.1 (CH), 53.3 (CH_2), 47.8 (CH), 43.9 (CH_2), 41.9 (CH), 40.7 (CH_2), 36.8 (CH), 35.0 (CH_2), 32.8 (CH_2), 31.9 (CH_2), 30.3 (CH), 29.4 (CH_2). **ESI-HRMS** calcd for $C_{40}H_{37}Cl_2N_2O_2$ $[M+H]^+$ 647.2267, found 647.2274.

(S)-6-chloro-9-((1S,2S,5R,6S)-6-(4-chlorophenyl)-4-oxo-3-phenethyl-3-azabicyclo[3.2.0]heptan-2-yl)-2-phenethyl-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. 2f'



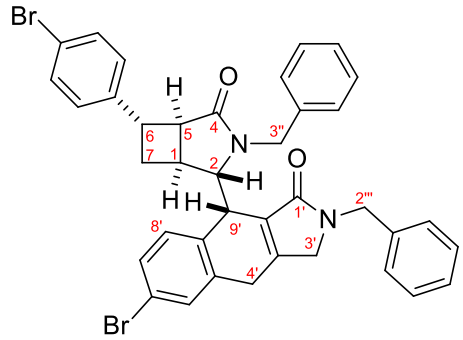
2f' was isolated following the **GP-2** using **1f** as reagent (65.0 mg, 0.2 mmol). Pale yellow oil. Yield **17%** (10.9 mg, 0.017 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.43 – 7.06 (m, 16H), 6.92 (d, *J* = 8.4 Hz, 1H), 4.51 (dt, *J* = 13.8, 6.6 Hz, 1H), 4.13 (s, 1H), 3.84 – 3.73 (m, 1H), 3.72 – 3.53 (m, 5H), 3.53 – 3.42 (m, 2H), 3.30 (d, *J* = 7.9 Hz, 1H), 3.16 – 2.98 (m, *J* = 6.6 Hz, 2H), 2.88 (t, *J* = 6.6 Hz, 2H), 2.47 (d, *J* = 7.1 Hz, 1H), 2.34 (q, *J* = 7.2 Hz, 1H), 1.95 (t, *J* = 10.6 Hz, 1H), 1.83 – 1.68 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.7 (Cq), 169.4 (Cq), 149.6 (Cq), 142.8 (Cq), 139.3 (Cq), 138.8 (Cq), 135.3 (Cq), 132.9 (Cq), 132.8 (Cq), 132.0 (Cq), 130.7 (Cq), 130.2 (CH), 128.9 (2CH), 128.8 (CH), 128.7 (2CH), 128.7 (2CH), 128.63 (2CH), 128.62 (2CH), 127.8 (2CH), 127.5 (CH), 126.6 (CH), 126.5 (CH), 70.2 (CH), 53.4 (CH_2), 47.8 (CH), 43.8 (CH_2), 42.2 (CH), 42.0 (CH_2), 38.5 (CH), 35.0 (CH_2), 33.9 (CH_2), 31.7 (CH_2), 30.7 (CH), 30.2 (CH_2). **ESI-HRMS** calcd for $C_{40}H_{37}Cl_2N_2O_2$ $[M+H]^+$ 647.2267, found 647.2259.

(*R*)-2-benzyl-9-((1S,2S,5R,6S)-3-benzyl-6-(4-bromophenyl)-4-oxo-3-azabicyclo[3.2.0]heptan-2-yl)-6-bromo-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. 2g



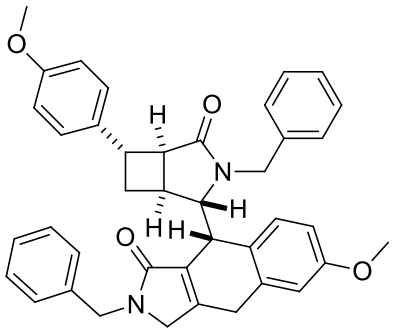
2g was isolated with traces of **2g'** following the **GP-2** using **1g** as reagent (59.2 mg, 0.167 mmol). Pale yellow solid, m.p. 124-125 °C. Yield **17%** (10.9 mg, 0.014 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.51 – 7.29 (m, 12H), 7.24 (dd, *J* = 7.5, 1.8 Hz, 2H), 7.03 (d, *J* = 8.4 Hz, 2H), 6.96 (d, *J* = 8.2 Hz, $H_{8'}$), 5.31 (d, *J* = 14.2 Hz, $H_{3''}$), 4.83 (d, *J* = 14.9 Hz, $H_{2'''}$), 4.50 (d, *J* = 14.9 Hz, $H_{2'''}$), 4.21 (brs, $H_{9'}$), 4.05 – 3.74 (m, H_2, $H_{3''}$, $H_{3'}$, $H_{3'}$, $H_{4'}$), 3.57 (dd, *J* = 22.2, 2.8 Hz, $H_{4'}$), 3.36 (dt, *J* = 6.5, 3.1 Hz, H_6), 2.62 (q, *J* = 7.5 Hz, H_1), 2.13 – 2.01 (m, H_5, H_7), 2.02 – 1.90 (m, H_7). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.8 (C_4), 169.7 ($C_{1'}$), 150.3 (Cq), 143.2 (Cq), 137.0 (Cq), 136.5 (Cq), 135.6 (Cq), 131.9 (Cq), 131.8 (CH), 131.6 (2CH), 131.0 ($C_{8'}$), 130.3 (Cq), 130.2 (CH), 129.0 (2CH), 128.9 (2CH), 128.9 (2CH), 128.1 (2CH), 128.0 (2CH), 128.0 (CH), 127.8 (CH), 121.4 (Cq), 120.0 (Cq), 66.0 (C_2), 52.1 ($C_{3'}$), 47.6 (C_5), 46.2 ($C_{2'''}$), 45.2 ($C_{3''}$), 42.3 (C_6), 38.1 ($C_{9'}$), 31.8 (C_7), 31.5 (C_1), 30.0 ($C_{4'}$). **ESI-MS** calcd for $C_{38}H_{32}Br_2N_2NaO_2$ $[M+Na]^+$ 731.07, found 731.14. **ESI-HRMS** calcd for $C_{38}H_{32}{}^{79}Br_2N_2KO_2$ $[M+K]^+$ 745.0462, found 745.0455.

(S)-2-benzyl-9-((1S,2S,5R,6S)-3-benzyl-6-(4-bromophenyl)-4-oxo-3-azabicyclo[3.2.0]heptan-2-yl)-6-bromo-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. 2g'



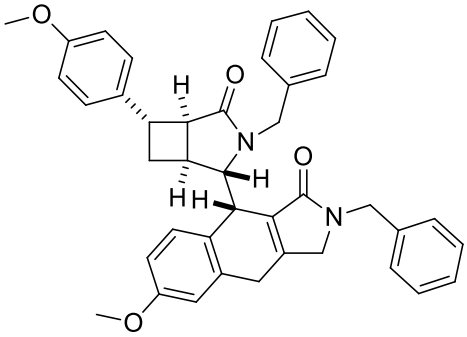
2g' was isolated following the **GP-2** using **1g** as reagent (59.2 mg, 0.167 mmol). Pale yellow solid, m.p. 113-114 °C. Yield **27%** (16.0 mg, 0.022 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.51 – 7.21 (m, 14H), 7.08 (d, *J* = 8.3 Hz, 2H), 6.79 (d, *J* = 8.3 Hz, H_8), 5.50 (d, *J* = 15.1 Hz, $H_{3''}$), 4.71 – 4.58 (m, $2H_{2'''}$), 4.51 (d, *J* = 15.2 Hz, $H_{3''}$), 4.32 – 4.25 (m, $H_{9'}$), 3.91 (d, *J* = 19.2 Hz, H_3), 3.80 – 3.68 (m, H_4, H_3), 3.58 – 3.47 (m, H_6, H_4, H_2), 2.63 (d, *J* = 6.6 Hz, H_5), 2.42 (q, *J* = 7.3 Hz, H_1), 2.11 – 1.96 (m, $2H_7$). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.4 (C_4), 169.6 ($C_{1'}$), 150.1 (Cq), 143.1 (Cq), 137.3 (Cq), 137.1 (Cq), 136.4 (Cq), 135.6 (Cq), 133.4 (Cq), 131.7 (CH), 131.6 (2CH), 130.5 (CH), 130.5 (CH), 129.0 (2CH), 128.9 (2CH), 128.7 (2CH), 128.2 (2CH), 128.2 (2CH), 127.8 (CH), 127.7 (CH), 120.9 (Cq), 120.0 (Cq), 68.8 (C_2), 51.9 ($CH_{3'}$), 48.2 (C_5), 46.2 ($C_{2'''}$), 45.3 ($C_{3''}$), 42.4 (C_6), 38.3 ($C_{9'}$), 31.5 (C_7), 30.5 (C_1), 30.2 ($C_{4'}$). **ESI-HRMS** calcd for $C_{38}H_{32}{}^{79}Br_2N_2NaO_2$ $[M+Na]^+$ 729.0723, found 745.0717.

(R)-2-benzyl-9-((1S,2S,5R,6S)-3-benzyl-6-(4-methoxyphenyl)-4-oxo-3-azabicyclo[3.2.0]heptan-2-yl)-6-methoxy-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. 2h



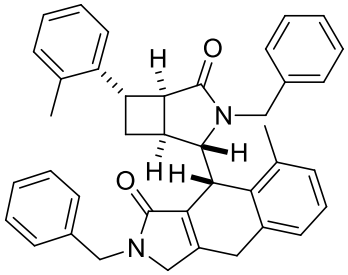
2h was isolated following the **GP-2** using **1h** as reagent (61.1 mg, 0.2 mmol). White crystals, m.p. 169 °C (dec.). Yield **18%** (11.0 mg, 0.018 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.2 Hz, 2H), 7.42 (t, *J* = 7.5 Hz, 2H), 7.37 – 7.21 (m, 6H), 7.07 (d, *J* = 8.6 Hz, 2H), 7.02 (d, *J* = 8.6 Hz, 1H), 6.86 – 6.78 (m, 3H), 6.76 (d, *J* = 2.6 Hz, 1H), 5.34 (d, *J* = 13.6 Hz, 1H), 4.85 (d, *J* = 15.0 Hz, 1H), 4.49 (d, *J* = 15.0 Hz, 1H), 4.22 (brs, 1H), 4.04 (d, *J* = 14.2 Hz, 1H), 3.95 (d, *J* = 19.1 Hz, 1H), 3.88 (d, *J* = 2.2 Hz, 1H), 3.85 – 3.75 (m, 8H), 3.55 (dd, *J* = 22.1, 2.8 Hz, 1H), 3.35 (dt, *J* = 6.4, 3.1 Hz, 1H), 2.60 (q, *J* = 7.5 Hz, 1H), 2.16 – 1.91 (m, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.2 (Cq), 170.1 (Cq), 158.7 (Cq), 157.9 (Cq), 150.7 (Cq), 137.2 (Cq), 136.9 (Cq), 136.7 (Cq), 134.6 (Cq), 130.9 (Cq), 130.5 (CH), 129.0 (2CH), 128.8 (4CH), 128.0 (2CH), 127.8 (CH), 127.7 (CH), 127.3 (2CH), 124.8 (Cq), 114.4 (CH), 113.8 (2CH), 112.3 (CH), 66.2 (CH), 55.3 ($2CH_3$), 52.2 (CH_2), 48.0 (CH), 46.2 (CH_2), 45.0 (CH_2), 42.2 (CH), 37.5 (CH), 32.2 (CH_2), 31.5 (CH), 30.5 (CH_2). **ESI-HRMS** calcd for $C_{40}H_{39}N_2O_4$ $[M+H]^+$ 611.2904, found 611.2897.

(S)-2-benzyl-9-((1S,2S,5R,6S)-3-benzyl-6-(4-methoxyphenyl)-4-oxo-3-azabicyclo[3.2.0]heptan-2-yl)-6-methoxy-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. 2h'



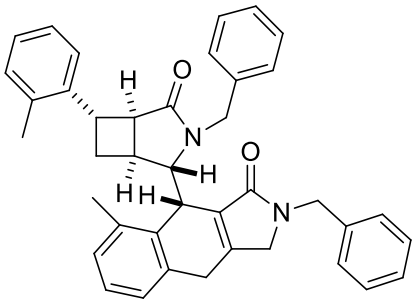
2h' was isolated with traces of **2h** following the **GP-2** using **1h** as reagent (61.1 mg, 0.2 mmol). White solid, m.p. 128-129 °C. Yield **29%** (17.6 mg, 0.029 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.51 – 7.27 (m, 9H), 7.25 – 7.20 (m, 2H), 7.12 (d, *J* = 8.6 Hz, 2H), 6.88 – 6.80 (m, 2H), 6.75 – 6.70 (m, 2H), 5.50 (d, *J* = 15.1 Hz, 1H), 4.75 – 4.55 (m, 2H), 4.50 (d, *J* = 15.2 Hz, 1H), 4.28 (brs, 1H), 3.88 (d, *J* = 18.9 Hz, 1H), 3.81 – 3.68 (m, 8H), 3.60 – 3.46 (m, 3H), 2.67 (d, *J* = 6.8 Hz, 1H), 2.51 (q, *J* = 7.4 Hz, 1H), 2.12 – 1.91 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.9 (Cq), 170.0 (Cq), 158.4 (Cq), 158.0 (Cq), 150.6 (Cq), 137.5 (Cq), 137.4 (Cq), 136.6 (Cq), 134.6 (Cq), 131.1 (Cq), 129.9 (CH), 128.9 (2CH), 128.8 (2CH), 128.7 (2CH), 128.2 (2CH), 127.7 (CH), 127.6 (CH), 127.4 (2CH), 126.5 (Cq), 113.9 (CH), 113.7 (2CH), 113.2 (CH), 68.9 (CH), 55.3 (CH_3), 55.3 (CH_3), 52.0 (CH_2), 48.5 (CH), 46.2 (CH_2), 45.3 (CH_2), 42.3 (CH), 38.0 (CH), 32.0 (CH_2), 30.7 (CH), 30.7(CH_2). **ESI-HRMS** calcd for $C_{40}H_{39}N_2O_4$ $[M+H]^+$ 611.2904, found 611.2910.

(R)-2-benzyl-9-((1S,2S,5R,6S)-3-benzyl-4-oxo-6-(o-tolyl)-3-azabicyclo[3.2.0]heptan-2-yl)-8-methyl-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. 2i



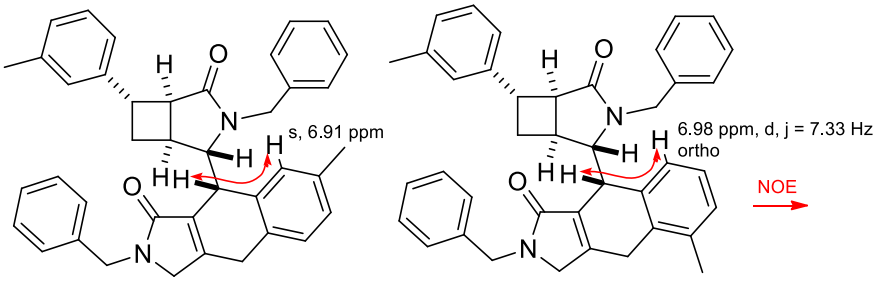
2i was isolated with traces of an additional isomer following the **GP-2** using **1i** as reagent (59.7 mg, 0.206 mmol). Colorless oil. Yield **25%** (14.9 mg, 0.025 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.48 – 7.07 (m, 15H), 6.87 – 6.82 (m, 2H), 5.00 (d, *J* = 14.1 Hz, 1H), 4.74 (d, *J* = 14.8 Hz, 1H), 4.49 (d, *J* = 14.9 Hz, 1H), 4.29 (s, 1H), 3.98 (d, *J* = 19.2 Hz, 1H), 3.79 – 3.63 (m, 3H), 3.61 – 3.45 (m, 3H), 2.66 – 2.52 (m, 2H), 2.37 (s, 3H), 2.24 (s, 3H), 2.13 – 2.06 (m, 1H), 1.83 – 1.73 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 178.1 (Cq), 170.5 (Cq), 153.6 (Cq), 142.0 (Cq), 137.4 (Cq), 136.6 (Cq), 136.6 (Cq), 135.8 (Cq), 135.5 (Cq), 134.7 (Cq), 131.0 (Cq), 130.2 (CH), 129.5 (CH), 128.82 (2CH), 128.79 (2CH), 128.5 (2CH), 128.0 (2CH), 127.8 (CH), 127.6 (CH), 127.4 (CH), 126.9 (CH), 126.4 (CH), 126.2 (CH), 124.3 (CH), 64.2 (CH), 52.1 (CH_2), 47.2 (CH), 46.3 (CH_2), 46.1 (CH_2), 40.1 (CH), 40.0 (CH), 33.5 (CH), 31.3 (CH_2), 29.9 (CH_2), 19.7 (CH_3), 19.6 (CH_3). **ESI-HRMS** calcd for $C_{40}H_{39}N_2O_2$ $[M+H]^+$ 579.3006, found 579.3011.

(S)-2-benzyl-9-((1S,2S,5R,6S)-3-benzyl-4-oxo-6-(o-tolyl)-3-azabicyclo[3.2.0]heptan-2-yl)-8-methyl-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. 2i'



2i' was isolated following the **GP-2** using **1i** as reagent (59.7 mg, 0.206 mmol). Colorless oil. Yield **36%** (21.6 mg, 0.037 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.51 – 7.03 (m, 17H), 5.60 (d, *J* = 15.5 Hz, 1H), 4.75 – 4.58 (m, 3H), 4.56 (brs, 1H), 3.92 (d, *J* = 19.1 Hz, 1H), 3.84 – 3.66 (m, 3H), 3.61 – 3.45 (m, 2H), 2.67 (d, *J* = 6.6 Hz, 1H), 2.52 (dt, *J* = 16.3, 8.1 Hz, 1H), 2.32 (s, 3H), 2.16 (s, 3H), 2.13 – 2.01 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.0 (Cq), 170.1 (Cq), 151.1 (Cq), 141.5 (Cq), 137.6 (Cq), 137.5 (Cq), 136.8 (Cq), 136.3 (Cq), 134.1 (Cq), 133.2 (Cq), 131.8 (Cq), 130.6 (CH), 129.5 (CH), 128.8 (2CH), 128.8 (2CH), 128.6 (2CH), 128.0 (2CH), 127.6 (2CH), 127.04 (CH), 126.95 (CH), 126.3 (CH), 125.8 (CH), 123.4 (CH), 66.4 (CH), 51.9 (CH_2), 47.0 (CH), 46.2 (CH_2), 45.0 (CH_2), 40.2 (CH), 35.5 (CH), 31.6 (CH_2), 30.6 (CH), 30.2 (CH_2), 19.6 (CH_3), 19.5 (CH_3). **ESI-HRMS** calcd for $C_{40}H_{39}N_2O_2$ $[M+H]^+$ 579.3006, found 579.3013.

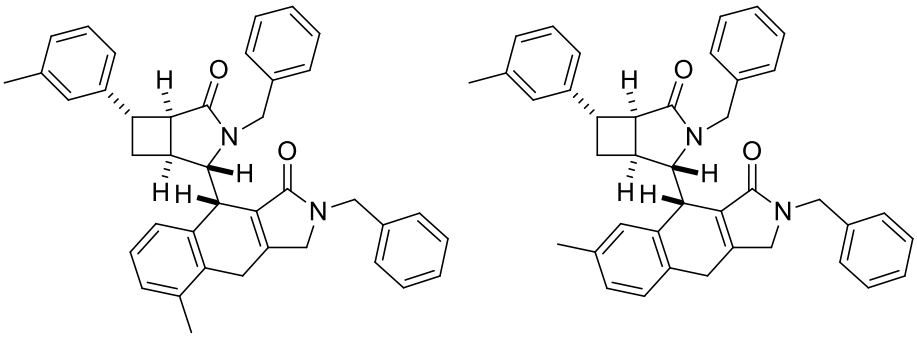
(R)-2-benzyl-9-((1S,2S,5R,6S)-3-benzyl-4-oxo-6-(m-tolyl)-3-azabicyclo[3.2.0]heptan-2-yl)-5-methyl-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one (A) compound with **(R)-2-benzyl-9-((1S,2S,5R,6S)-3-benzyl-4-oxo-6-(m-tolyl)-3-azabicyclo[3.2.0]heptan-2-yl)-7-methyl-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one (B). 2j$_A$/2j$_B$**



A B

2j$_A$/2j$_B$ mixture was isolated following the **GP-2** using **1j** as reagent (58.1 mg, 0.20 mmol). Colorless oil. Yield **25%** (14.5 mg, 0.025 mmol, ^{1}H NMR ratio: 1:0.65). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.54 – 6.84 (m, 17H$_A$, 17H$_B$), 5.35 – 5.22 (m, 1H$_A$, 1H$_B$), 4.86 (d, *J* = 15.0 Hz, 1H$_B$), 4.82 (d, *J* = 15.0 Hz, 1H$_A$), 4.57 – 4.45 (m, 1H$_A$, 1H$_B$), 4.28 (brs, 1H$_B$), 4.20 (brs, 1H$_A$), 4.05 – 3.72 (m, 5H$_A$, 4H$_B$), 3.65 – 3.46 (m, 1H$_A$, 2H$_B$), 3.41 – 3.32 (m, 1H$_A$, 1H$_B$), 2.80 (q, *J* = 7.7 Hz, 1H$_A$), 2.70 (q, *J* = 7.5 Hz, 1H$_B$), 2.41 – 2.26 (m, 6H$_A$, 6H$_B$), 2.25 – 1.84 (m, 3H$_A$, 3H$_B$). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.33 (Cq), 177.32 (Cq), 170.23 (Cq), 170.18 (Cq), 151.5 (Cq), 150.7 (Cq), 144.6 (Cq), 144.5 (Cq), 138.03 (Cq), 138.00 (Cq), 137.3 (Cq), 137.2 (Cq), 137.0 (Cq), 136.9 (Cq), 136.7 (Cq), 136.2 (Cq), 133.1 (Cq), 132.8 (Cq), 131.9 (Cq), 130.5 (Cq), 130.4 (Cq), 130.3 (CH), 130.2 (Cq), 129.04 (CH), 128.99 (CH), 128.82 (CH), 128.78 (CH), 128.7 (CH), 128.6 (CH), 128.40 (CH), 128.37 (CH), 128.1 (CH), 128.0 (CH), 127.77 (CH), 127.75 (CH), 127.65 (CH), 127.64 (CH), 127.4 (CH), 127.3 (CH), 126.9 (CH), 126.86 (CH), 126.84 (CH), 123.2 (CH), 123.1 (CH), 66.4 (CH), 66.3 (CH), 52.3 (CH_2), 52.2 (CH_2), 47.6 (CH), 47.5 (CH), 46.19 (CH_2), 46.18 (CH_2), 45.2 (CH_2), 45.0 (CH_2), 42.9 (CH), 42.7 (CH), 38.9 (CH_2), 38.7 (CH_2), 32.01 (CH), 31.96 (CH_2), 31.93 (CH_2), 31.89 (CH), 29.9 (CH_2), 28.2 (CH_2), 21.47 (CH_3), 21.46 (CH_3), 21.1 (CH_3), 19.9 (CH_3). **ESI-HRMS** calcd for $C_{40}H_{39}N_2O_2$ $[M+H]^+$ 579.3006, found 579.3012.

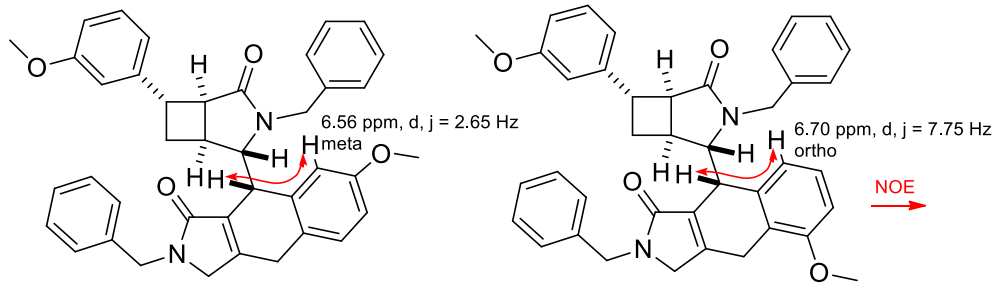
(S)-2-benzyl-9-((1S,2S,5R,6S)-3-benzyl-4-oxo-6-(m-tolyl)-3-azabicyclo[3.2.0]heptan-2-yl)-5-methyl-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one compound with **(S)-2-benzyl-9-((1S,2S,5R,6S)-3-benzyl-4-oxo-6-(m-tolyl)-3-azabicyclo[3.2.0]heptan-2-yl)-7-methyl-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. 2j'$_A$/2j'$_B$**



A B

2j'$_A$/2j'$_B$ mixture was isolated following the **GP-2** using **1j** as reagent (58.1 mg, 0.20 mmol). Colorless oil. Yield **29%** (16.7 mg, 0.029 mmol, ^{1}H NMR ratio: 0.91:1). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.57 – 6.90 (m, 16H$_A$, 16H$_B$), 6.78 (dd, *J* = 6.8, 1.9 Hz, 1H$_B$), 6.71 (s, 1H$_A$), 5.51 (d, *J* = 15.1 Hz, 1H$_A$, 1H$_B$), 4.71 – 4.57 (m, 2H$_A$, 2H$_B$), 4.59 – 4.46 (m, 1H$_A$, 1H$_B$), 4.34 (brs, 1H$_B$), 4.27 (s, 1H$_A$), 3.96 – 3.81 (m, 1H$_A$, 1H$_B$), 3.77 – 3.62 (m, 2H$_A$, 1H$_B$), 3.58 – 3.43 (m, 3H$_A$, 4H$_B$), 2.74 – 2.63 (m, 1H$_A$, 1H$_B$), 2.52 – 2.37 (m, 1H$_A$, 1H$_B$), 2.34 – 1.91 (m, 8H$_A$, 8H$_B$). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.84 (Cq), 175.82 (Cq), 170.1 (Cq), 170.0 (Cq), 151.1 (Cq), 150.5 (Cq), 144.33 (Cq), 144.28 (Cq), 138.07 (Cq), 138.05 (Cq), 137.6 (2Cq), 137.5 (Cq), 137.4 (Cq), 136.8 (Cq), 136.2 (Cq), 134.4 (Cq), 134.3 (Cq), 131.9 (Cq), 130.7 (Cq), 130.4 (Cq), 130.3 (Cq), 129.6 (CH), 128.91 (CH), 128.88 (CH), 128.83 (CH), 128.82 (CH), 128.78 (CH), 128.75 (CH), 128.69 (CH), 128.6 (CH), 128.40 (CH), 128.37 (CH), 128.19 (CH), 128.16 (CH), 127.9 (CH), 127.64 (CH), 127.62 (CH), 127.58 (CH), 127.56 (CH), 127.49 (CH), 127.47 (CH), 127.0 (CH), 126.91 (CH), 126.89 (CH), 126.87 (CH), 123.1 (CH), 69.4 (CH), 69.1 (CH), 52.1 (CH_2), 52.0 (CH_2), 48.2 (CH), 48.1 (CH), 46.2 (CH_2), 45.3 (CH_2), 45.2 (CH_2), 42.8 (CH), 42.7 (CH), 38.7 (CH), 38.6 (CH), 31.7 (CH_2), 31.6 (CH_2), 30.6 (CH), 30.4 (CH), 30.1 (CH_2), 28.3 (CH_2), 21.5 (2CH_3), 21.0 (CH_3), 19.9 (CH_3). **ESI-HRMS** calcd for $C_{40}H_{39}N_2O_2$ $[M+H]^+$ 579.3006, found 579.3000.

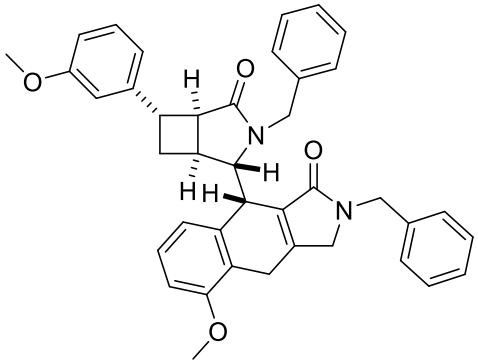
(R)-2-benzyl-9-((1S,2S,5R,6S)-3-benzyl-6-(3-methoxyphenyl)-4-oxo-3-azabicyclo[3.2.0]heptan-2-yl)-5-methoxy-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one compound with **(R)-2-benzyl-9-((1S,2S,5R,6S)-3-benzyl-6-(3-methoxyphenyl)-4-oxo-3-azabicyclo[3.2.0]heptan-2-yl)-7-methoxy-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. $2k_A/2k_B$**



A B

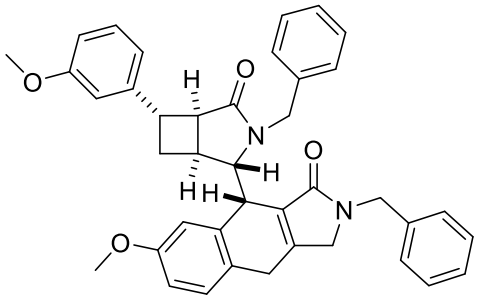
$2k_A/2k_B$ mixture was isolated following the **GP-2** using **1k** as reagent (61.1 mg, 0.20 mmol). Pale yellow oil. Yield **28%** (17.0 mg, 0.028 mmol, ^{1}H NMR ratio: 1:1). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.51 – 7.44 (m, $2H_A$, $2H_B$), 7.39 (t, J = 7.6 Hz, $2H_A$, $2H_B$), 7.35 – 7.08 (m, $8H_A$, $8H_B$), 6.84 – 6.76 (m, $1H_A$, $1H_B$), 6.75 – 6.63 (m, $4H_A$, $3H_B$), 6.57 (d, J = 2.6 Hz, H_B), 5.30 (d, J = 14.2 Hz, H_A), 5.26 (d, J = 14.1 Hz, H_B), 4.84 (d, J = 7.6 Hz, H_A), 4.80 (d, J = 7.6 Hz, H_B), 4.49 (d, J = 8.0 Hz, H_B), 4.45 (d, J = 8.1 Hz, H_A), 4.25 (s, H_A), 4.18 (s, H_B), 4.11 – 3.40 (m, $12H_A$, $12H_B$), 3.35 (t, J = 7.8 Hz, H_A, H_B), 2.76 – 2.59 (m, H_A, H_B), 2.13 – 1.86 (m, $3H_A$, $3H_B$). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.24 (Cq), 177.21 (Cq), 170.3 (Cq), 170.2 (Cq), 159.69 (Cq), 159.68 (Cq), 158.2 (Cq), 156.9 (Cq), 151.6 (Cq), 151.2 (Cq), 146.2 (2Cq), 137.3 (Cq), 137.2 (Cq), 136.88 (Cq), 136.85 (Cq), 134.1 (Cq), 134.0 (Cq), 130.2 (Cq), 129.8 (Cq), 129.7 (CH), 129.49 (CH), 129.45 (CH), 129.1 (2CH), 129.0 (2CH), 128.83 (2CH), 128.82 (2CH), 128.81 (4CH), 127.99 (2CH), 127.94 (2CH), 127.84 (CH), 127.79 (CH), 127.67 (CH), 127.64 (CH), 127.63 (CH), 125.1 (Cq), 122.3 (Cq), 121.7 (CH), 118.8 (CH), 118.7 (CH), 114.5 (CH), 113.5 (CH), 112.1 (CH), 111.8 (CH), 111.7 (CH), 111.6 (CH), 108.6 (CH), 66.4 (CH), 66.1 (CH), 55.5 (CH_3), 55.4 (CH_3), 55.2 (CH_3), 55.1 (CH_3), 52.4 (CH_2), 52.2 (CH_2), 47.70 (CH), 47.66 (CH), 46.19 (CH_2), 46.16 (CH_2), 45.2 (CH_2), 45.0 (CH_2), 42.93 (CH), 42.88 (CH), 38.7 (CH), 38.1 (CH), 32.1 (CH_2), 32.0 (CH), 31.7 (CH), 29.5 (CH_2), 25.1 (CH_2). **ESI-HRMS** calcd for $C_{40}H_{39}N_2O_4$ $[M+H]^+$ 611.2904, found 611.2895.

(S)-2-benzyl-9-((1S,2S,5R,6S)-3-benzyl-6-(3-methoxyphenyl)-4-oxo-3-azabicyclo[3.2.0]heptan-2-yl)-5-methoxy-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. 2k'$_A$



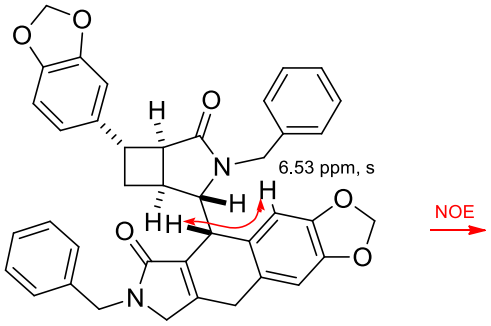
2k'$_A$ was isolated following the **GP-2** using **1k** as reagent (61.1 mg, 0.20 mmol). Pale yellow solid, m.p. 145-147 °C. Yield **17%** (10.3 mg, 0.017 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.57 – 7.43 (m, 4H), 7.43 – 7.17 (m, 7H), 7.12 (d, *J* = 8.5 Hz, 1H), 6.87 – 6.72 (m, 4H), 6.39 (d, *J* = 2.6 Hz, 1H), 5.53 (d, *J* = 15.1 Hz, 1H), 4.72 – 4.55 (m, 3H), 4.29 (brs, 1H), 4.01 – 3.63 (m, 9H), 3.65 – 3.45 (m, 3H), 2.72 (d, *J* = 6.7 Hz, 1H), 2.47 (q, *J* = 7.5 Hz, 1H), 2.19 – 1.99 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.6 (Cq), 170.0 (Cq), 159.7 (Cq), 158.5 (Cq), 151.3 (Cq), 146.1 (Cq), 137.5 (Cq), 137.3 (Cq), 135.8 (Cq), 130.3 (Cq), 129.7 (CH), 129.5 (CH), 128.92 (2CH), 128.86 (2CH), 128.8 (2CH), 128.1 (2CH), 127.7 (CH), 127.6 (CH), 125.2 (Cq), 118.6 (CH), 113.6 (CH), 113.2 (CH), 112.5 (CH), 111.3 (CH), 69.2 (CH), 55.3 (CH_3), 55.2 (CH_3) , 52.0 (CH_2), 48.2 (CH), 46.2 (CH_2), 45.3 (CH_2), 43.0 (CH), 38.7 (CH), 31.9 (CH_2), 30.6 (CH), 29.7 (CH_2). **ESI-HRMS** calcd for $C_{40}H_{39}N_2O_4$ $[M+H]^+$ 611.2904, found 611.2908.

(S)-2-benzyl-9-((1S,2S,5R,6S)-3-benzyl-6-(3-methoxyphenyl)-4-oxo-3-azabicyclo[3.2.0]heptan-2-yl)-7-methoxy-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. 2k'$_B$



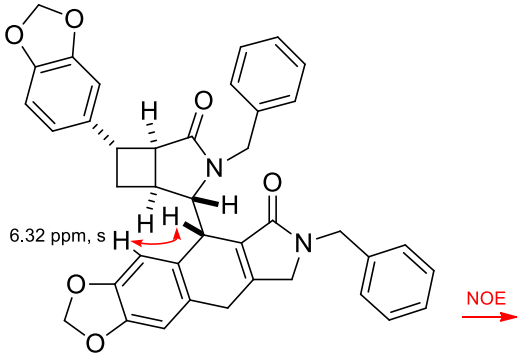
2k'$_B$ was isolated following the **GP-2** using **1k** as reagent (61.1 mg, 0.20 mmol). Pale yellow solid, m.p. 122-123 °C. Yield **18%** (10.9 mg, 0.018 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.52 – 7.30 (m, 8H), 7.27 – 7.12 (m, 4H), 6.84 – 6.72 (m, 4H), 6.55 (d, *J* = 7.7 Hz, 1H), 5.52 (d, *J* = 15.2 Hz, 1H), 4.74 – 4.52 (m, 3H), 4.36 (brs, 1H), 3.94 (d, *J* = 19.2 Hz, 1H), 3.89 – 3.62 (m, 8H), 3.59 – 3.50 (m, 2H), 3.42 (dd, *J* = 22.9, 3.5 Hz, 1H), 2.72 (d, *J* = 6.5 Hz, 1H), 2.51 (q, *J* = 7.3 Hz, 1H), 2.13 – 1.94 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.7 (Cq), 170.1 (Cq), 159.7 (Cq), 156.9 (Cq), 151.0 (Cq), 146.2 (Cq), 137.6 (Cq), 137.4 (Cq), 135.7 (Cq), 130.0 (Cq), 129.5 (CH), 128.9 (2CH), 128.8 (2CH), 128.7 (2CH), 128.1 (2CH), 127.9 (CH), 127.7 (CH), 127.5 (CH), 122.4 (Cq), 120.9 (CH), 118.6 (CH), 112.5 (CH), 111.4 (CH), 108.2 (CH), 69.2 (CH), 55.3 (CH_3), 55.2 (CH_3), 52.2 (CH_2), 48.2 (CH), 46.2 (CH_2), 45.2 (CH_2), 43.0 (CH), 38.4 (CH), 31.9 (CH_2), 30.6 (CH), 25.2 (CH_2). **ESI-HRMS** calcd for $C_{40}H_{39}N_2O_4$ $[M+H]^+$ 611.2904, found 611.2910.

(R)-5-((1S,2S,5R,6S)-6-(benzo[d][1,3]dioxol-5-yl)-3-benzyl-4-oxo-3-azabicyclo[3.2.0]heptan-2-yl)-7-benzyl-7,8-dihydro-5H-[1,3]dioxolo[4',5':4,5]benzo[1,2-f]isoindol-6(9H)-one. 2l



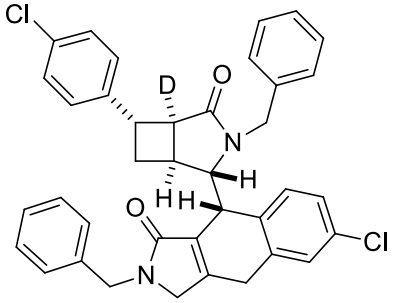
2l was isolated following the **GP-2** using **1n** as reagent (63.7 mg, 0.2 mmol). Pale yellow solid, m.p. 131-132 °C. Yield **26%** (16.7 mg, 0.026 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.53 – 7.18 (m, 11H), 6.70 (d, *J* = 8.0 Hz, 1H), 6.65 (d, *J* = 2.4 Hz, 1H), 6.59 (dd, *J* = 8.1, 1.8 Hz, 1H), 6.51 (s, 1H), 5.96 – 5.92 (m, 2H), 5.90 (s, 2H), 5.28 (d, *J* = 14.8 Hz, 1H), 4.81 (d, *J* = 15.0 Hz, 1H), 4.47 (d, *J* = 15.0 Hz, 1H), 4.15 – 4.09 (m, 1H), 4.03 – 3.65 (m, 5H), 3.50 (td, *J* = 22.7, 21.9, 3.1 Hz, 1H), 3.34 – 3.25 (m, 1H), 2.63 (q, *J* = 7.4 Hz, 1H), 2.20 – 2.14 (m, 1H), 2.03 – 1.85 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.0 (Cq), 170.0 (Cq), 151.0 (Cq), 147.8 (Cq), 147.1 (Cq), 146.8 (Cq), 145.8 (Cq), 138.6 (Cq), 137.2 (Cq), 136.8 (Cq), 130.5 (Cq), 129.0 (2CH), 128.8 (2CH), 128.8 (2CH), 128.0 (2CH), 127.8 (CH), 127.7 (CH), 126.5 (Cq), 126.0 (Cq), 119.3 (CH), 109.2 (CH), 108.4 (CH), 108.1 (CH), 106.9 (CH), 101.3 (CH_2), 100.9 (CH_2), 66.3 (CH), 52.1 (CH_2), 48.0 (CH), 46.2 (CH_2), 45.1 (CH_2), 42.9 (CH), 38.5 (CH_2), 32.3 (CH_2), 31.5 (CH), 30.5 (CH_2). **ESI-HRMS** calcd for $C_{40}H_{34}N_2NaO_6$ $[M+Na]^+$ 661.2309, found 661.2313.

(S)-5-((1S,2S,5R,6S)-6-(benzo[d][1,3]dioxol-5-yl)-3-benzyl-4-oxo-3-azabicyclo[3.2.0]heptan-2-yl)-7-benzyl-7,8-dihydro-5H-[1,3]dioxolo[4',5':4,5]benzo[1,2-f]isoindol-6(9H)-one. 2l'



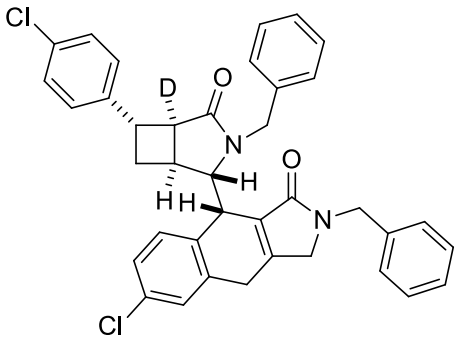
2l' was isolated following the **GP-2** using **1n** as reagent (63.7 mg, 0.206 mmol). Pale yellow solid, m.p. 99-101 °C. Yield **35%** (22.1 mg, 0.035 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.48 – 7.29 (m, 8H), 7.25 – 7.21 (m, 2H), 6.74 – 6.67 (m, 2H), 6.66 – 6.61 (m, 2H), 6.31 (s, 1H), 5.95 – 5.88 (m, 4H), 5.48 (d, *J* = 15.1 Hz, 1H), 4.68 – 4.56 (m, 2H), 4.53 (d, *J* = 15.4 Hz, 1H), 4.21 (brs, 1H), 3.87 (d, *J* = 19.1 Hz, 1H), 3.75 – 3.62 (m, 2H), 3.53 – 3.39 (m, 3H), 2.60 (d, *J* = 7.7 Hz, 1H), 2.40 (q, *J* = 7.6 Hz, 1H), 2.00 (ddt, *J* = 14.1, 8.4, 4.0 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.5 (Cq), 169.9 (Cq), 150.7 (Cq), 147.8 (Cq), 146.9 (Cq), 146.9 (Cq), 145.9 (Cq), 138.5 (Cq), 137.5 (Cq), 137.3 (Cq), 130.5 (Cq), 129.0 (2CH), 128.8 (2CH), 128.7 (2CH), 128.2 (2CH), 127.8 (CH), 127.6 (CH), 127.5 (Cq), 126.4 (Cq), 119.3 (CH), 108.4 (CH), 108.4 (CH), 108.1 (CH), 106.9 (CH), 101.3 (CH_2), 100.9 (CH_2), 68.9 (CH), 51.9 (CH_2), 48.5 (CH), 46.2 (CH_2), 45.2 (CH_2), 42.9 (CH), 38.5 (CH), 32.2 (CH_2), 30.7 (CH_2), 30.3 (CH). **ESI-HRMS** calcd for $C_{40}H_{34}N_2NaO_6$ $[M+Na]^+$ 661.2309, found 661.2301.

(R)-2-benzyl-9-((1S,2S,5R,6S)-3-benzyl-5-deutero-6-(4-chlorophenyl)-4-oxo-3-azabicyclo[3.2.0]heptan-2-yl)-6-chloro-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. 2m



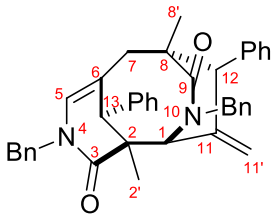
2m was isolated following the **GP-2** using **1m** as reagent (63.6 mg, 0.2 mmol). Pale yellow solid, m.p. 126-127 °C. Yield **20%** (12.4 mg, 0.019 mmol).**^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.54 – 7.17 (m, 15H), 7.07 (d, *J* = 8.4 Hz, 2H), 7.02 (d, *J* = 8.0 Hz, 1H), 5.32 (d, *J* = 14.2 Hz, 1H), 4.84 (d, *J* = 14.9 Hz, 1H), 4.50 (d, *J* = 15.0 Hz, 1H), 4.23 (brs, 1H), 4.05 – 3.94 (m, 2H), 3.90 (d, *J* = 2.4 Hz, 1H), 3.87 – 3.74 (m, 2H), 3.57 (dd, *J* = 22.2, 2.9 Hz, 1H), 3.37 (dd, *J* = 9.0, 3.9 Hz, 1H), 2.67 – 2.56 (m, 1H), 2.07 (ddt, *J* = 13.0, 9.0, 4.1 Hz, 1H), 2.01 – 1.91 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.9 (Cq), 169.8 (Cq), 150.4 (Cq), 142.6 (Cq), 137.0 (Cq), 136.5 (Cq), 135.2 (Cq), 133.3 (Cq), 132.0 (Cq), 130.7 (Cq), 130.4 (Cq), 129.0 (2CH), 128.9 (2CH), 128.9 (CH), 128.9 (2CH), 128.6 (2CH), 128.3 (CH), 128.0 (CH), 128.0 (2CH), 127.8 (CH), 127.7 (2CH), 127.3 (CH), 66.1 (CH), 52.2 (CH_2), 47.6 (CH, residual peak), 46.3 (CH_2), 45.2 (CH_2), 42.2 (CH), 38.0 (CH), 31.8 (CH_2), 31.4 (CH), 30.1 (CH_2). **ESI-HRMS** calcd for $C_{38}H_{32}Cl_2N_2NaO_2$ $[M+Na]^+$ 642.1796, found 642.1802.

(S)-2-benzyl-9-((1S,2S,5R,6S)-3-benzyl-5-deutero-6-(4-chlorophenyl)-4-oxo-3-azabicyclo[3.2.0]heptan-2-yl)-6-chloro-2,3,4,9-tetrahydro-1H-benzo[f]isoindol-1-one. 2m'



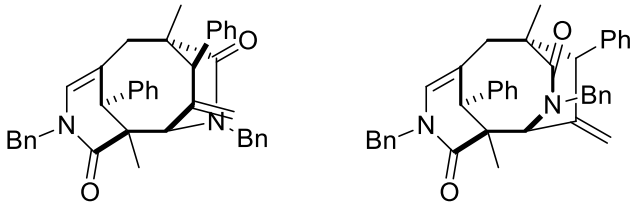
2m' was isolated following the **GP-2** using **1m** as reagent (63.6 mg, 0.2 mmol). Colorless oil. Yield **17%** (11.1 mg, 0.017 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.51 – 7.00 (m, 16H), 6.83 (d, *J* = 8.3 Hz, 1H), 5.48 (d, *J* = 15.2 Hz, 1H), 4.61 (s, 2H), 4.50 (d, *J* = 14.8 Hz, 1H), 4.28 (s, 1H), 3.89 (d, *J* = 19.2 Hz, 1H), 3.81 – 3.65 (m, 2H), 3.58 – 3.43 (m, 3H), 2.46 – 2.36 (m, 1H), 2.14 – 1.90 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.5 (Cq), 169.7 (Cq), 150.3 (Cq), 142.5 (Cq), 137.3 (Cq), 137.0 (Cq), 135.2 (Cq), 132.9 (Cq), 132.8 (Cq), 132.0 (Cq), 130.5 (Cq), 130.2 (CH), 129.0 (2CH), 128.9 (2CH), 128.8 (CH), 128.7 (2CH), 128.6 (2CH), 128.2 (2CH), 127.9 (CH), 127.7 (2CH), 127.7 (CH), 127.6 (CH), 68.9 (CH), 51.9 (CH_2), 48.3 (CH, residual peak), 46.2 (CH_2), 45.4 (CH_2), 42.2 (CH), 38.2 (CH), 31.5 (CH_2), 30.3 (CH), 30.3 (CH_2). **ESI-HRMS** calcd for $C_{38}H_{32}Cl_2N_2NaO_2$ $[M+Na]^+$ 642.1796, found 642.1805.

(1R,2S,8R,12R,13R)-4,10-dibenzyl-2,8-dimethyl-11-methylene-12,13-diphenyl-4,10-diazatricyclo[6.2.2.12,6]tridec-5-ene-3,9-dione. 4a



4a was isolated via recrystallization from the **4a/4a'** mixture. White crystals, m.p. 221 °C (dec.). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.50 (dd, *J* = 7.5, 1.9 Hz, 2H), 7.43 – 7.35 (m, 8H), 7.20 – 6.98 (m, 8H), 6.74 – 6.44 (m, 2H), 6.12 (s, H_5), 5.65 (d, *J* = 14.0 Hz, $H_{10'}$), 5.18 (d, *J* = 14.0 Hz, $H_{4'}$), 4.82 (s, $H_{11'}$), 4.65 (s, H_1), 4.27 (d, *J* = 14.0 Hz, $H_{4'}$), 4.22 (d, *J* = 14.0 Hz, $H_{10'}$), 3.43 (s, H_{12}), 3.26 (s, H_{13}), 2.79 (d, *J* = 12.7 Hz, H_7), 2.21 (d, *J* = 12.8 Hz, H_7), 1.41 (s, $3H_{2'}$), 0.88 (s, $3H_{8'}$). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.6 (C_9), 172.9 (C_3), 146.6 (C_{11}), 145.2 (Cq Ar), 136.1 (C_3), 136.0 (Cq), 135.7 (Cq), 130.0 (2CH), 129.7 (2CH), 129.3 (2CH), 128.9 (C_5), 128.7 (2CH), 128.7 (2CH), 128.25 (4CH), 128.20 (2CH), 128.1 (2CH), 127.2 (CH), 126.2 (CH), 118.2 (C_6), 115.7 ($C_{11'}$), 71.0 (C_1), 56.2 (C_{12}), 54.6 (C_2), 53.9 ($C_{10'}$), 50.1 ($C_{4'}$), 49.0 (C_7), 46.4 (C_{13}), 46.2 (C_8), 26.5 ($C_{8'}$), 24.2 ($C_{2'}$). **ESI-MS** calcd for $C_{40}H_{39}N_2O_2$ $[M+H]^+$ 579.30, found 579.26. **ESI-HRMS** calcd for $C_{40}H_{39}N_2O_2$ $[M+H]^+$ 579.3006, found 579.3011.

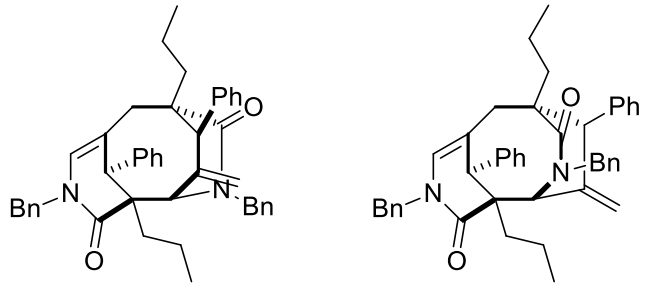
(1R,2S,8R,12R,13R)-4,10-dibenzyl-2,8-dimethyl-11-methylene-12,13-diphenyl-4,10-diazatricyclo[6.2.2.12,6]tridec-5-ene-3,9-dione compound with **(1S,2S,8S,12S,13R)-4,10-dibenzyl-2,8-dimethyl-11-methylene-12,13-diphenyl-4,10-diazatricyclo[6.2.2.12,6]tridec-5-ene-3,9-dione 4a/4a'**



4a/4a' mixture was isolated following the **GP-2** using **3a** as reagent (28.9 mg, 0.1 mmol). White solid. Yield **64%** (18.5 mg, 0.032 mmol, dr 55:45). The reaction performed in a small Schlenk on 1.0 mmol of 3a (289 mg) led to the isolation of the mixture in 63% yield (182 mg). The reaction conducted in a coil reactor (5 mm inner diameter) using 1.03 g of **3a** allowed to recover 422 mg of polycycles (41%). **^{1}H NMR** (400 MHz,$_3$ $CDCl_3$) δ 7.54 – 6.90 (m, $18H_A$, $18H_B$), 6.73 – 6.42 (m, $2H_A$, $2H_B$) 6.31 (s, $1H_A$), 6.12 (s, $1H_B$), 5.65 (d, *J* = 14.0 Hz, $1H_B$), 5.39 (d, *J* = 13.8 Hz, $1H_A$), 5.32 (d, *J* = 14.2 Hz, $1H_A$), 5.18 (d, *J* = 14.0 Hz, $1H_B$), 5.03 (d, *J* = 2.3 Hz, $1H_A$), 4.82 (s, $1H_B$), 4.78 (d, *J* = 2.0 Hz, $1H_A$), 4.65 (s, $1H_B$), 4.49 – 4.38 (m, $1H_A$, $1H_B$), 4.28 (d, *J* = 14.1 Hz, $1H_A$, $1H_B$), 4.22 (d, *J* = 14.0 Hz, $1H_B$), 3.98 (s, $1H_A$), 3.51 (d, *J* = 14.2 Hz, $1H_a$), 3.47 – 3.40 (m, $1H_A$, $1H_B$), 3.26 (s, $1H_B$), 2.79 (d, *J* = 12.7 Hz, 1 H_B), 2.66 (d, *J* = 12.7 Hz, 1H), 2.46 (d, *J* = 12.7 Hz, 1H), 2.21 (d, *J* = 12.7 Hz, $1H_B$), 1.41 (s, $3H_B$), 1.21 (s, $3H_A$), 0.88 (s, $3H_B$), 0.86 (s, $3H_A$). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.6 (Cq), 174.1 (Cq), 173.7 (Cq), 172.9 (Cq), 146.7 (Cq), 146.6 (Cq), 145.2 (Cq), 144.9 (Cq), 136.9 (Cq), 136.09 (Cq), 136.08 (Cq), 136.0 (Cq), 135.9 (Cq), 135.7 (Cq), 130.0 (2CH), 129.9 (2CH), 129.7 (2CH), 129.32 (2CH), 129.28 (2CH), 129.0 (2CH), 128.9 (CH), 128.8 (4CH), 128.72 (2CH), 128.67 (2CH), 128.5 (2CH), 128.24 (brs, 6CH), 128.20 (2CH), 128.19 (CH), 128.11 (2CH), 128.07 (2CH), 127.8 (CH), 127.4 (CH), 127.2 (CH), 127.1 (CH), 126.3 (CH), 126.2 (CH), 121.0 (CH_2), 119.0 (Cq), 118.2 (Cq), 115.7 (CH_2), 72.1 (CH), 71.0 (CH), 57.9 (CH), 56.2 (CH), 54.6 (Cq), 53.9 (CH_2), 50.9 (CH_2),

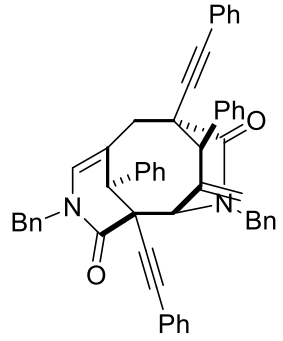
50.8 (CH_2), 50.2 (CH_2), 50.1 (CH_2), 50.0 (Cq), 49.0 (CH_2), 48.9 (Cq), 47.4 (CH), 46.4 (CH), 46.2 (Cq), 26.7 (CH_3), 26.5 (CH_3), 24.2 (CH_3), 21.6 (CH_3). **ESI-MS** calcd for $C_{40}H_{39}N_2O_2$ $[M+H]^+$ 579.30, found 579.26.

(1R,2S,8R,12R,13R)-4,10-dibenzyl-11-methylene-12,13-diphenyl-2,8-dipropyl-4,10-diazatricyclo[6.2.2.12,6]tridec-5-ene-3,9-dione compound with **(1S,2S,8S,12S,13R)-4,10-dibenzyl-11-methylene-12,13-diphenyl-2,8-dipropyl-4,10-diazatricyclo[6.2.2.12,6]tridec-5-ene-3,9-dione. 4b/4b'**



4b/4b' mixture was isolated following the **GP-2** using **3b** as reagent (65.5 mg, 0.206 mmol). White solid. Yield **54%** (35.1 mg, 0.055 mmol, dr 61:39). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.59 – 6.80 (m, 20H_A, 18H_B), 6.64 – 6.39 (m, 2H_B) 6.24 (s, 1H_A), 6.03 (s, 1H_B), 5.43 (d, *J* = 13.8 Hz, 1H_B), 5.35 (d, *J* = 13.7 Hz, 1H_A), 5.29 (d, *J* = 13.9 Hz, 1H_A), 5.18 (d, *J* = 13.9 Hz, 1H_B), 4.96 (s, 1H_B), 4.91 (d, *J* = 6.5 Hz, 1H_A, 1H_B), 4.86 (d, *J* = 1.5 Hz, 1H_B), 4.74 (s, 1H_B), 4.43 (s, 1H_B), 4.28 – 4.20 (m, 1H_A, 1H_B), 4.11 (d, *J* = 13.8 Hz, 1H_A), 3.98 (s, 1H_A), 3.51 – 3.43 (m, 1H_A, 1H_B), 3.32 (s, 1H_A), 3.19 (s, 1H_B), 2.60 – 2.39 (m, 2H_A, 2H_B), 2.09 – 1.87 (m, 3H), 1.80 – 1.12 (m, 10H), 1.05 – 0.93 (m, 3H), 0.92 – 0.80 (m, 6H_B), 0.57 – 0.45 (m, 6H_A). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.2 (Cq), 174.5 (Cq), 173.7 (Cq), 172.7 (Cq), 146.7 (Cq), 146.4 (Cq), 144.9 (Cq), 144.7 (Cq), 136.55 (Cq), 136.53 (Cq), 136.4 (Cq), 136.12 (Cq), 136.07 (Cq), 135.9 (Cq), 129.9 (2CH), 129.74 (2CH), 129.72 (2CH), 129.6 (2CH), 129.4 (2CH), 129.3 (2CH), 128.9, 128.8 (2CH), 128.7 (4CH), 128.6 (2CH), 128.23 (10CH), 128.16 (2CH), 128.1 (2CH), 127.93 (2CH), 127.89 (CH), 127.23 (CH), 127.16 (CH), 127.0 (CH), 126.04 (CH), 126.02 (CH), 119.17 (Cq), 119.15 (CH_2), 118.6 (Cq), 114.7 (CH_2), 65.8 (CH), 65.1 (CH), 56.8 (CH_2), 55.6 (CH), 54.4 (CH), 52.4 (CH_2), 51.8 (CH_2), 51.3 (CH_2), 50.9 (CH_2), 50.2 (CH_2), 50.1 (CH_2), 49.0 (CH), 48.4 (CH_2), 47.6 (CH), 47.0 (CH_2), 43.9 (CH_2), 39.3 (CH_2), 38.7 (CH_2), 38.6 (CH_2), 37.1 (CH_2), 19.9 (CH_2), 19.1 (CH_2), 16.9 (CH_2), 15.6 (CH_2), 14.93 (CH_3), 14.86 (CH_3), 14.5 (CH_3), 14.4 (CH_3). **ESI-HRMS** calcd for $C_{44}H_{46}N_2NaO_2$ $[M+Na]^+$ 657.3451, found 657.3458.

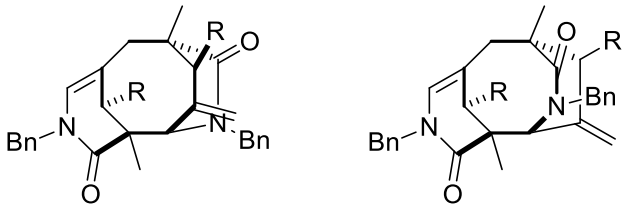
(1S,2R,8S,12S,13R)-4,10-dibenzyl-11-methylene-12,13-diphenyl-2,8-bis(phenylethynyl)-4,10-diazatricyclo[6.2.2.12,6]tridec-5-ene-3,9-dione 4c



4c was isolated following the **GP-2** using **3c** as reagent (60.5 mg, 0.16 mmol). White solid, m.p. 122-123 °C. Yield **34%** (20.8 mg, 0.028 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.60 – 7.54 (m, 2H), 7.48

– 6.96 (m, 26H), 6.84 – 6.77 (m, 2H), 6.23 (s, 1H), 5.94 (d, *J* = 14.1 Hz, 1H), 5.29 (s, 1H), 5.08 (d, *J* = 14.2 Hz, 1H), 5.02 (d, *J* = 14.1 Hz, 1H), 4.96 (s, 1H), 4.49 (s, 1H), 4.39 (d, *J* = 14.3 Hz, 1H), 3.78 (s, 1H), 3.75 (s, 1H), 3.46 (d, *J* = 13.0 Hz, 1H), 2.90 (d, *J* = 13.2 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 171.1 (Cq), 168.0 (Cq), 144.7 (Cq), 142.4 (Cq), 135.7 (Cq), 135.5 (Cq), 134.9 (Cq), 131.7 (CH), 131.6 (CH), 130.8 (CH), 130.2 (CH), 129.5 (CH), 129.2 (CH), 128.8 (CH), 128.74 (CH), 128.71 (CH), 128.68 (CH), 128.4 (CH), 128.2 (CH), 128.0 (CH), 127.94 (CH), 127.88 (CH), 127.8 (CH), 127.4 (CH), 126.6 (CH), 123.0 (Cq), 122.4 (Cq), 117.4 (CH_2), 115.7 (Cq), 90.5 (Cq), 89.8 (Cq), 89.5 (Cq), 87.7 (Cq), 67.1 (CH), 56.8 (Cq), 55.5 (CH), 50.6 (Cq), 50.3 (CH_2), 50.2 (CH_2), 48.8 (CH_2), 45.8 (CH). **ESI-HRMS** calcd for $C_{54}H_{43}N_2O_2$ $[M+H]^+$ 751.3319, found 751.3326.

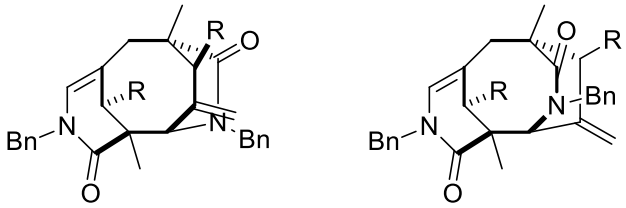
(1S,2S,8S,12S,13R)-4,10-dibenzyl-12,13-bis(4-chlorophenyl)-2,8-dimethyl-11-methylene-4,10-diazatricyclo[6.2.2.12,6]tridec-5-ene-3,9-dione compound with (1R,2S,8R,12S,13R)-4,10-dibenzyl-12,13-bis(4-chlorophenyl)-2,8-dimethyl-11-methylene-4,10-diazatricyclo[6.2.2.12,6]tridec-5-ene-3,9-dione. 4d/4d'



R= 4-Cl-C_6H_4

4d/4d' mixture was isolated following the **GP-2** using (Ir[dF(CF_3)ppy]$_2$(dtbpy))PF_6 instead of Ir(ppy)$_3$ and **3d** as reagent (65.3 mg, 0.202 mmol, dr 50:50). White solid. Yield **31%** (20.5 mg, 0.029 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.49 – 7.13 (m, 14H_A, 14H_B), 7.00 (d, *J* = 8.5 Hz, 2H_B), 6.96 (d, *J* = 8.5 Hz, 2H_A), 6.86 (d, *J* = 8.5 Hz, 2H_B), 6.79 (d, *J* = 8.5 Hz, 2H_A), 6.28 (s, 1H_A), 6.09 (s, 1H_B), 5.61 (d, *J* = 13.9 Hz, 1H_B), 5.40 (d, *J* = 13.8 Hz, 1H_A), 5.30 (d, *J* = 14.1 Hz, 1H_A), 5.20 (d, *J* = 14.0 Hz, 1H_B), 5.02 (d, *J* = 2.1 Hz, 1H_A), 4.81 (s, 1H_B), 4.74 (d, *J* = 2.0 Hz, 1H_A), 4.63 (s, 1H_B), 4.40 (d, *J* = 10.6 Hz, 1H_A, 1H_B), 4.20 – 4.09 (m, 1H_A, 2H_B), 3.90 (s, 1H_A), 3.47 (d, *J* = 14.1 Hz, 1H_A), 3.38 (s, 1H_B), 3.33 (s, 1H_A), 3.19 (s, 1H_B), 2.72 (d, *J* = 12.8 Hz, 1H_B), 2.63 (d, *J* = 12.8 Hz, 1H_A), 2.39 (d, *J* = 12.8 Hz, 1H_A), 2.17 (d, *J* = 12.8 Hz, 1H_B), 1.38 (s, 3H_B), 1.16 (s, 3H_A), 0.83 (d, *J* = 2.0 Hz, 3H_A, 3H_B). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.1 (Cq), 173.7 (Cq), 173.2 (Cq), 172.4 (Cq), 146.3 (Cq), 145.2 (Cq), 144.5 (Cq), 143.6 (Cq), 136.7 (Cq), 136.0 (Cq), 135.82 (Cq), 135.76 (Cq), 134.3 (Cq), 134.0 (Cq), 133.18 (Cq), 133.14 (Cq), 132.2 (Cq), 132.1 (Cq), 130.7 (2CH), 130.6 (2CH), 130.0 (2CH), 129.8 (2CH), 129.6 (2CH), 129.2 (CH), 129.1 (2CH), 128.9 (2CH), 128.8 (4CH), 128.8 (2CH), 128.7 (CH), 128.6 (2CH), 128.4 (CH), 128.37 (CH), 128.33 (2CH), 128.2 (2CH), 128.0 (CH), 127.8 (CH), 127.73 (CH), 127.66 (2CH), 126.5 (CH), 123.0 (Cq), 121.4 (CH_2), 117.8 (Cq), 116.0 (CH_2), 71.8 (CH), 71.0 (CH), 57.1 (CH), 55.6 (CH), 54.6 (Cq), 54.0 (CH_2), 50.9 (CH_2), 50.6 (CH_2), 50.3 (CH_2), 50.2 (CH_2), 50.0 (Cq), 48.8 (Cq), 48.7 (CH_2), 46.8 (CH), 46.1 (Cq), 45.8 (CH), 26.8 (CH_3), 26.5 (CH_3), 24.2 (CH_3), 21.6 (CH_3). **ESI-HRMS** calcd for $C_{40}H_{36}Cl_2N_2NaO_2$ $[M+Na]^+$ 669.2046, found 669.2039.

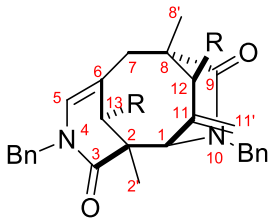
(1S,2S,8S,12S,13R)-4,10-dibenzyl-12,13-bis(4-methoxyphenyl)-2,8-dimethyl-11-methylene-4,10-diazatricyclo[6.2.2.12,6]tridec-5-ene-3,9-dione compound with (1R,2S,8R,12S,13R)-4,10-dibenzyl-12,13-bis(4-methoxyphenyl)-2,8-dimethyl-11-methylene-4,10-diazatricyclo[6.2.2.12,6]tridec-5-ene-3,9-dione 4e/4e'



R= 4-OMe-C_6H_4

4e/4e' mixture was isolated following the **GP-2** using **3e** as reagent (65.2 mg, 0.204 mmol). White solid. Yield **41%** (27.0 mg, 0.041 mmol, dr 53:47). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.50 – 7.28 (m, $12H_A$, $12H_B$), 6.88 (d, *J* = 8.7 Hz, $2H_B$), 6.81 (d, *J* = 8.7 Hz, $2H_A$), 6.68 – 6.43 (m, $4H_A$, $4H_B$), 6.26 (s, $1H_A$), 6.06 (s, $1H_B$), 5.61 (d, *J* = 14.0 Hz, $1H_B$), 5.36 (d, *J* = 13.8 Hz, $1H_A$), 5.28 (d, *J* = 14.3 Hz, $1H_A$), 5.16 (d, *J* = 14.0 Hz, $1H_B$), 4.99 (d, *J* = 2.2 Hz, $1H_A$), 4.83 – 4.72 (m, $1H_A$, $1H_B$), 4.61 (s, $1H_B$), 4.39 (s, $1H_A$, $1H_B$), 4.29 – 4.12 (m, $2H_A$, $1H_B$), 3.90 (d, *J* = 6.3 Hz, $1H_A$), 3.78 – 3.68 (m, $6H_A$, $6H_B$), 3.47 (d, *J* = 14.2 Hz, $1H_A$), 3.35 (d, *J* = 6.7 Hz, $1H_A$, $1H_B$), 3.17 (s, $1H_B$), 2.74 (d, *J* = 12.7 Hz, $1H_B$), 2.61 (d, *J* = 12.7 Hz, $1H_A$), 2.40 (d, *J* = 12.6 Hz, $1H_A$), 2.16 (d, *J* = 12.7 Hz, $1H_B$), 1.37 (s, $3H_B$), 1.17 (s, $3H_A$), 0.85 (s, $3H_B$), 0.83 (s, $3H_A$). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.7 (Cq), 174.2 (Cq), 173.7 (Cq), 172.9 (Cq), 158.73 (Cq), 158.66 (Cq), 158.0 (Cq), 157.9 (Cq), 147.1 (Cq), 145.2 (Cq), 139.1 (Cq), 137.6 (Cq), 137.0 (Cq), 136.2 (Cq), 136.1 (Cq), 136.0 (Cq), 130.34 (2CH), 130.32 (2CH), 130.0 (3CH), 129.9 (2CH), 129.7 (2CH), 129.3 (2CH), 129.2 (2CH), 129.0 (2CH), 128.8 (2CH), 128.72 (4CH), 128.67 (2CH), 128.5 (3CH), 128.1 (CH), 128.04 (2CH), 127.97 (Cq), 127.7 (CH), 127.6 (Cq), 127.2 (CH), 120.8 (CH_2), 119.4 (Cq), 118.6 (Cq), 115.4 (CH_2), 113.5 (2CH), 113.4 (2CH), 72.0 (CH), 71.0 (CH), 57.1 (CH), 55.4 (CH_2), 55.20 (CH_3), 55.19 (CH_3), 55.18 (CH_3), 55.1 (CH_3), 54.7 (Cq), 53.9 (CH_2), 50.8 ($2CH_2$), 50.2 (CH_2), 50.14 (CH_2), 50.14 (Cq), 49.2 (Cq), 48.9 (CH_2), 46.6 (CH), 46.4 (Cq), 45.6 (CH), 26.8 (CH_3), 26.6 (CH_3), 24.2 (CH_3), 21.6 (CH_3). **ESI-HRMS** calcd for $C_{42}H_{43}N_2O_4$ $[M+H]^+$ 639.3217, found 639.3211.

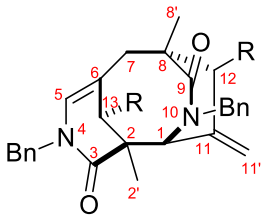
(1S,2S,8S,12S,13R)-4,10-dibenzyl-12,13-bis(4-butylphenyl)-2,8-dimethyl-11-methylene-4,10-diazatricyclo[6.2.2.12,6]tridec-5-ene-3,9-dione 4f



R= 4-*n*Bu-C_6H_4

4f was isolated following the **GP-2** using **3f** as reagent (66.3 mg, 0.20 mmol). White solid, m.p. 175-176 °C. Yield **22%** (14.5 mg, 0.022 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.51 – 7.32 (m, 12H), 7.01 – 6.37 (m, 6H), 6.05 (s, H_5), 5.61 (d, *J* = 14.0 Hz, $H_{10'}$), 5.12 (d, *J* = 14.0 Hz, $H_{4'}$), 4.77 (s, $H_{11'}$), 4.60 (s, H_1), 4.40 – 4.33 (m, $H_{11'}$), 4.27 (d, *J* = 14.1 Hz, $H_{4'}$), 4.20 (d, *J* = 14.0 Hz, $H_{10'}$), 3.36 (s, H_{12}), 3.19 (s, H_{13}), 2.75 (d, *J* = 12.7 Hz, H_7), 2.60 – 2.42 (m, 4H), 2.16 (d, *J* = 12.8 Hz, H_7), 1.52 (tdd, *J* = 15.3, 11.0, 7.5 Hz, 4H), 1.38 – 1.25 (m, 4H + 3$H_{2'}$), 1.00 – 0.87 (m, 6H), 0.84 (s, 3$H_{8'}$). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.8 (C_9), 173.1 (C_3), 146.8 (C_{11}), 142.5 (Cq), 141.8 (Cq), 140.7 (Cq), 136.1 (Cq), 136.0 (Cq), 132.9 (Cq), 130.0 (2CH), 129.7 (2CH), 129.1 (2CH), 128.7 (2CH), 128.67 (C_5), 128.6 (2CH), 128.21 (2CH), 128.15 (brs, 4CH) 128.0 (2CH), 118.5 (C_6), 115.5 ($C_{11'}$), 70.9 (C_1), 55.8 (C_{12}), 54.6 (Cq), 53.8 (C_{10}), 50.1 ($C_{4'}$), 49.0 (C_7), 46.3 (Cq), 46.1 (C_{13}), 35.11 (CH_2), 35.09 (CH_2), 33.5 (CH_2), 33.4 (CH_2), 26.6 ($C_{8'}$), 24.2 ($C_{2'}$), 22.39 (CH_2), 22.37 (CH_2), 14.1 (CH_3), 14.0 (CH_3). **ESI-HRMS** calcd for $C_{49}H_{55}N_2O_2$ $[M+H]^+$ 691.4258, found 691.4265.

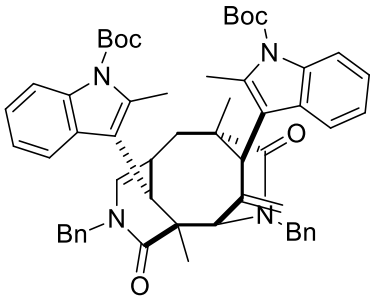
(1R,2S,8R,12S,13R)-4,10-dibenzyl-12,13-bis(4-butylphenyl)-2,8-dimethyl-11-methylene-4,10-diazatricyclo[6.2.2.12,6]tridec-5-ene-3,9-dione 4f'



R= 4-*n*Bu-C_6H_4

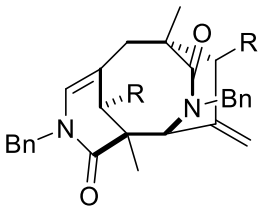
4f' was isolated following the **GP-2** using **3f** as reagent (66.3 mg, 0.20 mmol). White solid, m.p. 146-147 °C. Yield **20%** (13.5 mg, 0.020 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.51 – 7.31 (m, 12H), 7.03 – 6.72 (m, 6H), 6.27 (s, H_5), 5.36 (d, *J* = 13.8 Hz, $H_{4'}$), 5.30 (d, *J* = 14.3 Hz, $H_{10'}$), 5.01 (d, *J* = 2.2 Hz, $H_{11'}$), 4.79 (d, *J* = 1.9 Hz, $H_{11'}$), 4.41 (s, $H_{1'}$), 4.28 (d, *J* = 13.8 Hz, $H_{4'}$), 3.94 (s, H_{12}), 3.50 (d, *J* = 14.2 Hz, $H_{10'}$), 3.40 (s, H_{13}), 2.63 (d, *J* = 12.7 Hz, H_7), 2.54 (td, *J* = 8.0, 2.8 Hz, 4H), 2.44 (d, *J* = 12.7 Hz, H_7), 1.55 (dtt, *J* = 12.5, 7.8, 3.4 Hz, 4H), 1.44 – 1.24 (m, 4H), 1.21 (s, 3$H_{2'}$), 1.02 – 0.89 (m, 6H), 0.84 (s, 3$H_{8'}$). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 174.3 (Cq), 173.9 (Cq), 145.0 (Cq), 143.9 (Cq), 141.8 (Cq), 140.9 (Cq), 136.9 (Cq), 135.9 (Cq), 133.2 (Cq), 129.9 (2CH), 129.1 (4CH), 129.0 (2CH), 128.7 (4CH), 128.5 (2CH), 128.14 (CH), 128.13 (2CH), 127.7 (CH), 127.1 (C_5), 120.9 ($C_{11'}$), 119.3 (C_6), 72.1 (C_1), 57.5 (C_{12}), 50.9 (C_7), 50.8 ($C_{10'}$), 50.2 ($C_{4'}$), 50.0 (Cq), 49.0 (Cq), 47.0 (C_{13}), 35.2 (CH_2), 35.1 (CH_2), 33.5 (2CH_2), 26.7 ($C_{8'}$), 22.40 (CH_2), 22.36 (CH_2), 21.6 ($C_{2'}$), 14.0 (2CH_3). **ESI-HRMS** calcd for $C_{49}H_{55}N_2O_2$ $[M+H]^+$ 691.4258, found 691.4254.

di-tert-butyl 3,3'-((1S,2S,8S,12R,13S)-4,10-dibenzyl-2,8-dimethyl-11-methylene-3,9-dioxo-4,10-diazatricyclo[6.2.2.12,6]tridec-5-ene-12,13-diyl)bis(2-methyl-1H-indole-1-carboxylate) 4g



4g was isolated following the **GP-2** using **3g** as reagent (65.0 mg, 0.147 mmol). White solid, m.p. 195 °C (dec.). Yield **31%** (20.6 mg, 0.023 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 8.1 Hz, 1H), 7.94 (d, *J* = 8.4 Hz, 1H), 7.51 – 7.19 (m, 12H), 7.13 (d, *J* = 6.9 Hz, 1H), 7.08 – 7.01 (m, 1H), 6.70 (d, *J* = 7.7 Hz, 1H), 6.61 (t, *J* = 7.5 Hz, 1H), 6.16 (s, 1H), 5.66 (d, *J* = 14.3 Hz, 1H), 5.44 (d, *J* = 13.8 Hz, 1H), 4.77 (s, 1H), 4.66 (s, 1H), 4.29 (d, *J* = 14.4 Hz, 1H), 4.21 – 4.08 (m, 2H), 3.84 (s, 1H), 3.72 (s, 1H), 2.93 (d, *J* = 12.5 Hz, 1H), 2.72 (s, 3H), 2.24 (s, 3H), 1.97 (d, *J* = 12.6 Hz, 1H), 1.69 (s, 9H), 1.69 (s, 9H), 1.37 (s, 3H), 0.92 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 178.1 (Cq), 174.2 (Cq), 150.7 (Cq), 150.4 (Cq), 141.7 (Cq), 136.6 (Cq), 136.2 (Cq), 135.5 (2Cq), 135.4 (Cq), 134.5 (Cq), 130.2 (2CH), 130.1 (2CH), 128.9 (2CH), 128.7 (2CH), 128.2 (CH), 128.0 (CH), 127.6 (CH), 127.53 (Cq), 126.6 (CH), 123.2 (2CH), 122.6 (Cq), 122.5 (CH), 121.0 (Cq), 120.2 (CH), 120.1(CH), 118.3 (CH_2), 116.1 (2Cq), 115.2 (CH), 115.0 (CH), 84.1 (Cq), 83.8 (Cq), 71.3 (CH), 53.4 (CH_2), 52.9 (Cq), 50.9 (CH_2), 49.2 (CH_2), 44.2 (Cq), 44.1 (CH), 38.1 (CH), 28.34 ($3CH_3$), 28.30 ($3CH_3$), 25.1 (CH_3), 24.0 (CH_3), 15.1 (CH_3), 13.8 (CH_3). **ESI-HRMS** calcd for $C_{56}H_{60}N_4NaO_6$ $[M+Na]^+$ 907.4405 found 907.4418.

di-tert-butyl 3,3'-((1R,2S,8R,12R,13S)-4,10-dibenzyl-2,8-dimethyl-11-methylene-3,9-dioxo-4,10-diazatricyclo[6.2.2.12,6]tridec-5-ene-12,13-diyl)bis(2-methyl-1H-indole-1-carboxylate). 4g'

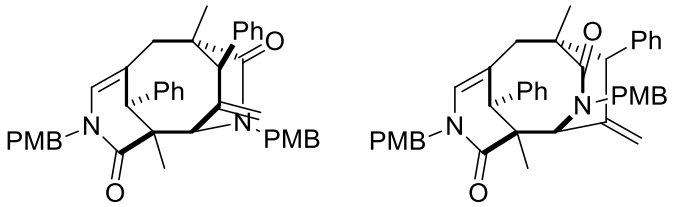


R = 2-Me-N-Boc-indole

4g' was isolated as a mixture of atropisomers following the **GP-2** using **3g** as reagent (65.0 mg, 0.147 mmol). White solid, m.p. 162 °C (dec.). Yield **12%** (7.7 mg, 0.087 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.09 (dd, *J* = 8.4, 3.8 Hz, 1H), 7.97 (d, *J* = 8.4 Hz, 1H), 7.56 (d, *J* = 7.7 Hz, 2H), 7.46 – 7.33 (m, 8H), 7.21 – 7.13 (m, 2H), 7.10 – 7.03 (m, 2H), 6.79 (d, *J* = 3.5 Hz, 1H), 6.53 (t, *J* = 7.2 Hz, 1H), 6.40 (s, 1H), 6.29 (d, *J* = 7.8 Hz, 1H), 5.64 (d, *J* = 14.5 Hz, 1H), 4.99 – 4.93 (m, 2H), 4.90 – 4.70 (m, 4H), 4.56 (s, 1H), 4.12 (d, *J* = 14.6 Hz, 1H), 2.68 – 2.48 (m, 8H), 1.71 (s, 9H), 1.70 (s, 9H), 1.28 (s, 3H), 0.91 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 173.9 (Cq), 172.9 (Cq), 150.7 (Cq), 150.5 (Cq), 144.4 (Cq), 136.3 (Cq), 136.1 (Cq), 135.9 (Cq), 135.8 (Cq), 135.5 (Cq), 135.1 (Cq), 134.6 (Cq), 130.4 (2CH), 130.0 (CH), 129.9 (2CH), 128.9 (2CH), 128.8 (CH), 128.6 (2CH), 128.4 (CH), 128.0 (CH), 127.8 (CH), 127.4 (Cq), 127.0 (Cq), 123.3 (CH), 122.43 (CH), 122.41 (CH), 120.8 (Cq), 120.5 (CH), 120.1 (CH_2), 117.6 (Cq), 114.98 (CH), 114.95 (CH), 83.91 (Cq), 83.89 (Cq), 73.4 (CH), 52.0

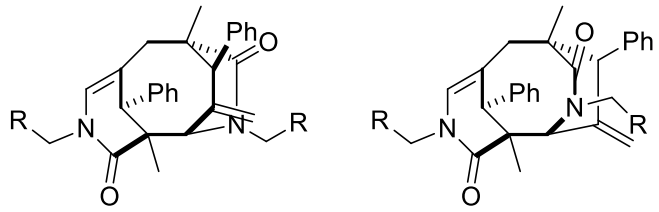
(CH_2), 51.45 (Cq), 51.43 (CH_2), 51.0 (CH_2), 48.5 (Cq), 48.2 (CH), 43.2 (CH), 28.3 ($3CH_3$), 28.3 ($3CH_3$), 24.6 (CH_3), 20.1 (CH_3), 14.0 (CH_3), 13.6 (CH_3). **ESI-HRMS** calcd for $C_{56}H_{60}N_4NaO_6$ $[M+Na]^+$ 907.4405 found 907.4440.

(1S,2S,8S,12R,13R)-4,10-bis(4-methoxybenzyl)-2,8-dimethyl-11-methylene-12,13-diphenyl-4,10-diazatricyclo[6.2.2.12,6]tridec-5-ene-3,9-dione compound with **(1R,2S,8R,12S,13R)-4,10-bis(4-methoxybenzyl)-2,8-dimethyl-11-methylene-12,13-diphenyl-4,10-diazatricyclo[6.2.2.12,6]tridec-5-ene-3,9-dione 4h/4h'**



4h/4h' mixture was isolated following the **GP-2** using **2h** as reagent (63.8 mg, 0.20 mmol). White solid. Yield **39%** (25.2 mg, 0.039 mmol, dr 53:47). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.44 – 7.28 (m, $4H_A$, $4H_B$), 7.20 – 6.86 (m, $14H_A$, $12H_B$), 6.71 – 6.38 (m, $2H_B$), 6.25 ($1H_A$), 6.07 ($1H_B$), 5.60 (d, *J* = 14.0 Hz, $1H_B$), 5.34 – 5.24 (m, $2H_A$), 5.07 (d, *J* = 14.0 Hz, $1H_B$), 5.00 (d, *J* = 2.1 Hz, $1H_A$), 4.78 (s, $1H_A$), 4.75 (d, *J* = 1.9 Hz, $1H_B$), 4.60 (s, $1H_B$), 4.41 – 4.38 (m, $1H_A$, $1H_B$), 4.27 – 4.15 (m, $1H_A$, $1H_B$), 4.11 (d, *J* = 14.0 Hz, $1H_B$), 3.93 (brs, $1H_A$), 3.87 – 3.78 (m, $6H_A$, $6H_B$), 3.47 – 3.36 (m, $2H_A$, $1H_B$), 3.22 (s, $1H_B$), 2.75 (d, *J* = 12.7 Hz, $1H_B$), 2.62 (d, *J* = 12.7 Hz, $1H_A$), 2.42 (d, *J* = 12.7 Hz, $1H_A$), 2.17 (d, *J* = 12.8 Hz, $1H_B$), 1.38 (s, $3H_B$), 1.18 (s, $3H_A$), 0.85 (s, $3H_B$), 0.83 (s, $3H_A$). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.5 (Cq), 174.0 (Cq), 173.6 (Cq), 172.8 (Cq), 159.5 (Cq), 159.41 (Cq), 159.36 (Cq), 159.2 (Cq), 146.8 (Cq), 146.7 (Cq), 145.3 (Cq), 145.0 (Cq), 136.2 (Cq), 135.8 (Cq), 131.3 (4CH), 131.1 (2CH), 131.0 (2CH), 130.4 (2CH), 129.33 (2CH), 129.29 (2CH), 129.0 (Cq), 128.8 (CH), 128.3 (Cq), 128.2 (6CH), 128.18 (Cq), 128.16 (Cq), 128.1 (4CH), 127.4 (CH), 127.2 (CH), 127.1 (CH), 126.3 (CH), 126.2 (CH), 120.9 (CH_2), 118.9 (Cq), 118.1 (Cq), 115.6 (CH_2), 114.1 (2CH), 114.00 (2CH), 113.98 (2CH), 113.8 (2CH), 71.6 (CH), 70.6 (CH), 57.9 (CH), 56.2 (CH), 55.37 (CH_3), 55.35 (CH_3), 55.34 (CH_3), 55.28 (CH_3), 54.6 (Cq), 53.2 (CH_2), 50.8 (CH_2), 50.1 (CH_2), 50.0 (Cq), 49.5 (CH_2), 49.4 (CH_2), 49.0 (CH_2), 48.9 (Cq), 47.4 (CH), 46.4 (CH), 46.2 (Cq), 26.7 (CH_3), 26.5 (CH_3), 24.2 (CH_3), 21.6 (CH_3). **ESI-HRMS** calcd for $C_{42}H_{43}N_2O_4$ $[M+H]^+$ 639.3217, found 639.3215.

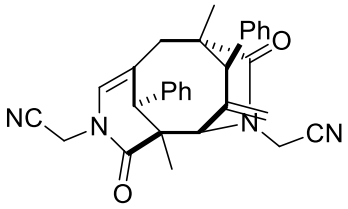
(1S,2S,8S,12S,13R)-4,10-bis(4-fluorobenzyl)-2,8-dimethyl-11-methylene-12,13-diphenyl-4,10-diazatricyclo[6.2.2.12,6]tridec-5-ene-3,9-dione compound with **(1R,2S,8R,12S,13R)-4,10-bis(4-fluorobenzyl)-2,8-dimethyl-11-methylene-12,13-diphenyl-4,10-diazatricyclo[6.2.2.12,6]tridec-5-ene-3,9-dione. 4i/4i'**



R=4-F-C_6H_4

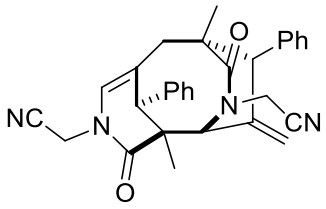
4i/4i' mixture was isolated following the **GP-2** using **2i** as reagent (67.2 mg, 0.22 mmol). White solid. Yield **49%** (32.6 mg, 0.053 mmol, dr 48:52). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.51 – 7.31 (m, $4H_A$, $4H_B$), 7.20 – 6.88 (m, $14H_A$, $14H_B$), 6.24 (s, $1H_A$), 6.07 (s, $1H_B$), 5.57 (d, *J* = 14.0 Hz, $1H_B$), 5.32 (d, *J* = 13.9 Hz, $1H_A$), 5.24 (d, *J* = 14.2 Hz, $1H_A$), 5.13 (d, *J* = 14.1 Hz, $1H_B$), 5.03 (d, *J* = 2.1 Hz, $1H_A$), 4.82 – 4.75 (m, $1H_A$, $1H_B$), 4.60 (s, $1H_B$), 4.43 – 4.36 (m, $1H_A$, $1H_B$), 4.27 – 4.18 (m, $1H_A$, $1H_B$), 4.15 (d, *J* = 14.0 Hz, $1H_B$), 3.95 (s, $1H_A$), 3.50 – 3.37 (m, $2H_A$, $1H_B$), 3.22 (s, $1H_B$), 2.77 (d, *J* = 12.7 Hz, $1H_B$), 2.63 (d, *J* = 12.8 Hz, $1H_A$), 2.45 (d, *J* = 12.7 Hz, $1H_A$), 2.19 (d, *J* = 12.8 Hz, $1H_B$), 1.38 (s, $3H_B$), 1.19 (s, $3H_A$), 0.85 (s, $3H_B$), 0.83 (s, $3H_A$). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.6 (Cq), 174.2 (Cq), 173.8 (Cq), 172.9 (Cq), 162.6 (d, *J* = 246.8 Hz, Cq), 162.54 (d, *J* = 246.8 Hz, Cq), 162.51 (d, *J* = 246.7 Hz, Cq) 162.4 (d, *J* = 245.9 Hz, Cq), 146.7 (Cq), 146.6 (Cq), 145.1 (Cq), 144.8 (Cq), 135.9 (Cq), 135.6 (Cq), 132.7 (d, *J* = 3.3 Hz, Cq), 132.1 (d, *J* = 3.4 Hz, Cq), 131.9 (d, *J* = 3.3 Hz, Cq), 131.8 (d, *J* = 3.3 Hz, Cq), 131.8 (d, *J* = 8.4 Hz, 2CH), 131.6 (d, *J* = 8.2 Hz, 2CH), 131.4 (d, *J* = 8.2 Hz, 2CH), 130.8 (d, *J* = 8.1 Hz, 2CH), 129.2 (2CH), 129.2 (2CH), 128.9 (CH), 128.3 (brs, 6CH), 128.2 (4CH), 128.1 (2CH), 127.3 (CH), 127.3 (CH), 127.2 (CH), 126.4 (CH), 126.4 (CH), 121.2 (CH_2), 119.2 (Cq), 118.4 (Cq), 115.7 (CH_2), 115.6 (d, *J* = 21.6 Hz, 2CH), 115.53 (d, *J* = 21.5 Hz, 2CH), 115.53 (d, *J* = 21.5 Hz, 2CH), 115.4 (d, *J* = 21.5 Hz, 2CH), 72.0 (CH), 71.4 (CH), 57.8 (CH), 56.2 (CH), 54.5 (Cq), 53.4 (CH_2), 50.8 (CH_2), 50.1 (CH_2), 50.0 (Cq), 49.5 (CH_2), 49.5 (CH_2), 48.93 (Cq), 48.90 (CH_2), 47.3 (CH), 46.4 (CH), 46.2 (Cq), 26.7 (CH_3), 26.5 (CH_3), 24.2 (CH_3), 21.6 (CH_3). **^{19}F NMR** (565 MHz, $CDCl_3$) δ -113.6 (tt, *J* = 8.7, 5.3 Hz), -113.7 – -113.8 (m), -114.3 (tt, *J* = 8.7, 5.4 Hz). **ESI-HRMS** calcd for $C_{40}H_{37}F_2N_2O_2$ $[M+H]^+$ 615.2818, found 615.2823.

2,2'-((1S,2S,8S,12S,13R)-2,8-dimethyl-11-methylene-3,9-dioxo-12,13-diphenyl-4,10-diazatricyclo[6.2.2.12,6]tridec-5-ene-4,10-diyl)diacetonitrile 4j



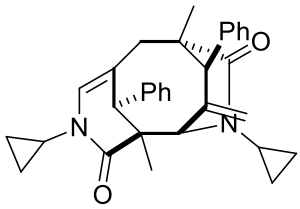
4j was isolated with traces of **4j'** following the **GP-2** using **3j** as reagent (42.0 mg, 0.18 mmol). White solid, m.p. 147-149 °C. Yield **38%** (16.0 mg, 0.034 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.39 – 7.15 (m, 8H), 6.91 (d, *J* = 6.5 Hz, 2H), 6.24 (s, 1H), 4.93 (s, 1H), 4.82 (s, 1H), 4.64 (d, *J* = 17.3 Hz, 1H), 4.59 (d, *J* = 16.8 Hz, 1H), 4.47 (s, 1H), 4.40 (d, *J* = 17.3 Hz, 1H), 4.27 (d, *J* = 16.7 Hz, 1H), 3.62 (s, 1H), 3.26 (s, 1H), 2.86 (d, *J* = 13.0 Hz, 1H), 2.38 (d, *J* = 13.0 Hz, 1H), 1.43 (s, 3H), 0.96 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.5 (Cq), 172.3 (Cq), 145.6 (Cq), 144.4 (Cq), 133.7 (Cq), 129.1 (2CH), 128.9 (brs, 4CH), 128.8 (2CH), 127.9 (CH), 127.5 (CH), 127.0 (CH), 119.9 (Cq), 116.9 (CH_2), 114.8 (Cq), 114.2 (Cq), 73.5 (CH), 56.2 (CH), 53.8 (Cq), 48.2 (CH_2), 46.6 (Cq), 46.2 (CH), 40.1 (CH_2), 33.0 (CH_2), 25.8 (CH_3), 22.6 (CH_3). **ESI-HRMS** calcd for $C_{30}H_{28}N_4NaO_2$ $[M+Na]^+$ 499.2104, found 499.2098.

2,2'-((1R,2S,8R,12R,13R)-2,8-dimethyl-11-methylene-3,9-dioxo-12,13-diphenyl-4,10-diazatricyclo[6.2.2.12,6]tridec-5-ene-4,10-diyl)diacetonitrile 4j'



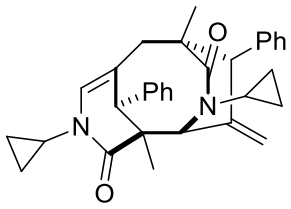
4j' was isolated, with traces of **4j**, following the **GP-2** using **3j** as reagent (42.0 mg, 0.18 mmol). White solid. Yield **20%** (8.4 mg, 0.018 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.5 – 7.1 (m, 10H), 6.15 (s, 1H), 5.31 (d, *J* = 2.0 Hz, 1H), 5.05 (d, *J* = 2.1 Hz, 1H), 4.72 (d, *J* = 17.3 Hz, 1H), 4.63 (d, *J* = 16.8 Hz, 1H), 4.42 (s, 1H), 4.38 (d, *J* = 17.3 Hz, 1H), 4.09 (s, 1H), 3.90 (d, *J* = 16.8 Hz, 1H), 3.60 (s, 1H), 2.73 (d, *J* = 12.9 Hz, 1H), 2.61 (d, *J* = 12.9 Hz, 1H), 1.27 (s, 3H), 0.91 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 174.7 (Cq), 174.0 (Cq), 145.8 (Cq), 143.5 (Cq), 134.5 (Cq), 129.0 (2CH), 128.8 (brs,4CH), 128.7 (2CH), 127.9 (CH), 127.0 (CH), 125.3 (CH), 122.7 (CH_2), 121.6 (Cq), 114.8 (Cq), 114.2 (Cq), 74.3 (CH), 58.0 (CH), 50.6 (Cq), 49.9 (CH_2), 48.8 (Cq), 47.3 (CH), 37.5 (CH_2), 33.5 (CH_2), 26.4 (CH), 21.5 (CH). **ESI-HRMS** calcd for $C_{30}H_{28}N_4NaO_2$ $[M+Na]^+$ 499.2104, found 499.2099.

(1S,2S,8S,12S,13R)-4,10-dicyclopropyl-2,8-dimethyl-11-methylene-12,13-diphenyl-4,10-diazatricyclo[6.2.2.12,6]tridec-5-ene-3,9-dione 4k



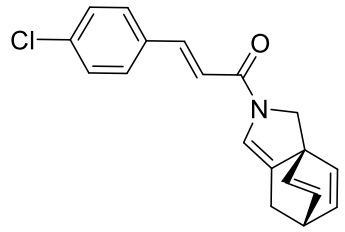
4k was isolated following the **GP-2** using **3k** as reagent (47.9 mg, 0.20 mmol). Colorless viscous oil. Yield **29%** (13.9 mg, 0.029 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.23 – 7.10 (m, 6H), 7.05 (dd, *J* = 7.5, 1.9 Hz, 2H), 6.93 – 6.74 (m, 2H), 6.10 (s, 1H), 4.91 (s, 1H), 4.66 (s, 1H), 4.47 (s, 1H), 3.52 (s, 1H), 3.12 (s, 1H), 3.04 – 2.92 (m, 1H), 2.91 – 2.72 (m, 2H), 2.26 (d, *J* = 12.7 Hz, 1H), 1.42 (s, 3H), 1.06 – 0.56 (m, 11H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 178.8 (Cq), 174.6 (Cq), 147.7 (Cq), 145.7 (Cq), 135.9 (Cq), 130.1 (CH), 129.1 (2CH), 128.4 (brs, 4CH), 128.1 (2CH), 127.2 (CH), 126.5 (CH), 117.0 (Cq), 114.8 (CH_2), 70.8 (CH), 55.5 (CH), 55.4 (CH_2), 49.5 (Cq), 46.6 (Cq), 45.6 (CH), 33.4 (CH), 29.1 (CH), 25.9 (CH_3), 22.6 (CH_3), 12.3 (CH_2), 6.7 (CH_2), 6.4 (CH_2), 4.9 (CH_2). **ESI-HRMS** calcd for $C_{32}H_{34}N_2NaO_2$ $[M+Na]^+$ 501.2512, found 501.2503.

(1R,2S,8R,12R,13R)-4,10-dicyclopropyl-2,8-dimethyl-11-methylene-12,13-diphenyl-4,10-diazatricyclo[6.2.2.12,6]tridec-5-ene-3,9-dione 4k'



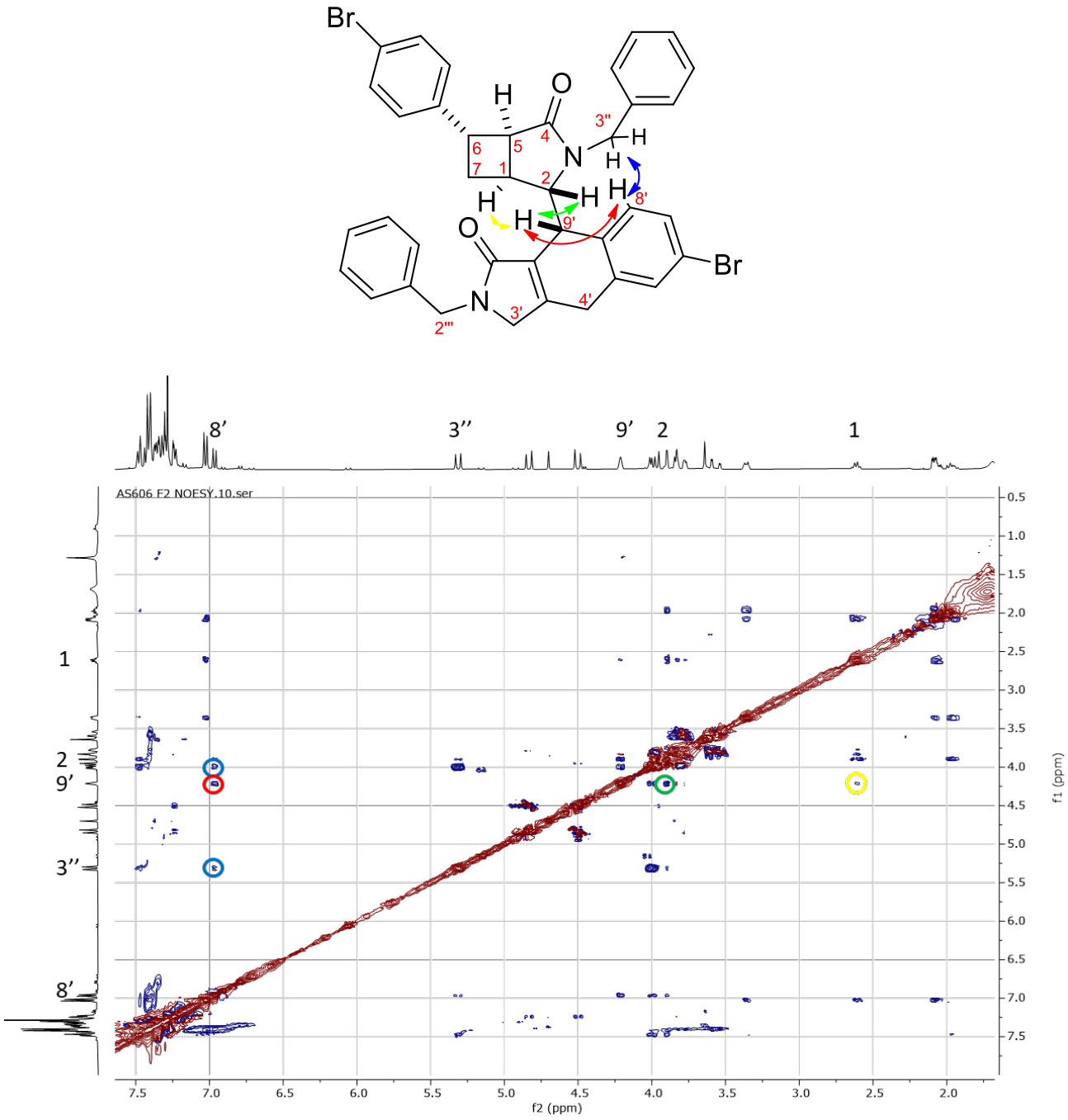
4k' was isolated following the **GP-2** using **3k** as reagent (47.9 mg, 0.20 mmol). Colorless viscous oil. Yield **26%** (12.6 mg, 0.026 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.24 – 7.12 (m, 6H), 7.08 (dd, *J* = 7.7, 1.6 Hz, 2H), 7.00 – 6.77 (m, 2H), 6.22 (s, 1H), 5.17 (d, *J* = 2.2 Hz, 1H), 4.87 (d, *J* = 2.0 Hz, 1H), 4.40 (s, 1H), 3.93 (s, 1H), 3.40 (s, 1H), 2.89 (ddd, *J* = 9.6, 6.8, 4.5 Hz, 1H), 2.63 (d, *J* = 12.7 Hz, 1H), 2.53 – 2.46 (m, 1H), 2.43 (d, *J* = 12.7 Hz, 1H), 1.19 (s, 3H), 1.00 – 0.91 (m, 2H), 0.90 – 0.76 (m, 7H), 0.74 – 0.65 (m, 1H), 0.64 – 0.57 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 176.2 (Cq), 175.5 (Cq), 147.2 (Cq), 145.7 (Cq), 136.5 (Cq), 129.1 (2CH), 128.5 (brs, 4CH), 128.1 (2CH), 127.2 (CH), 127.2 (CH), 126.4 (CH), 120.5 (CH_2), 118.2 (Cq), 73.3 (CH), 56.8 (CH), 51.2 (Cq), 51.0 (CH_2), 49.1 (Cq), 46.9 (CH), 31.7 (CH), 28.9 (CH), 26.3 (CH_3), 21.8 (CH_3), 11.7 (CH_2), 6.6 (CH_2), 6.6 (CH_2), 5.0 (CH_2). **ESI-HRMS** calcd for $C_{32}H_{34}N_2NaO_2$ $[M+Na]^+$ 501.2512, found 501.2505.

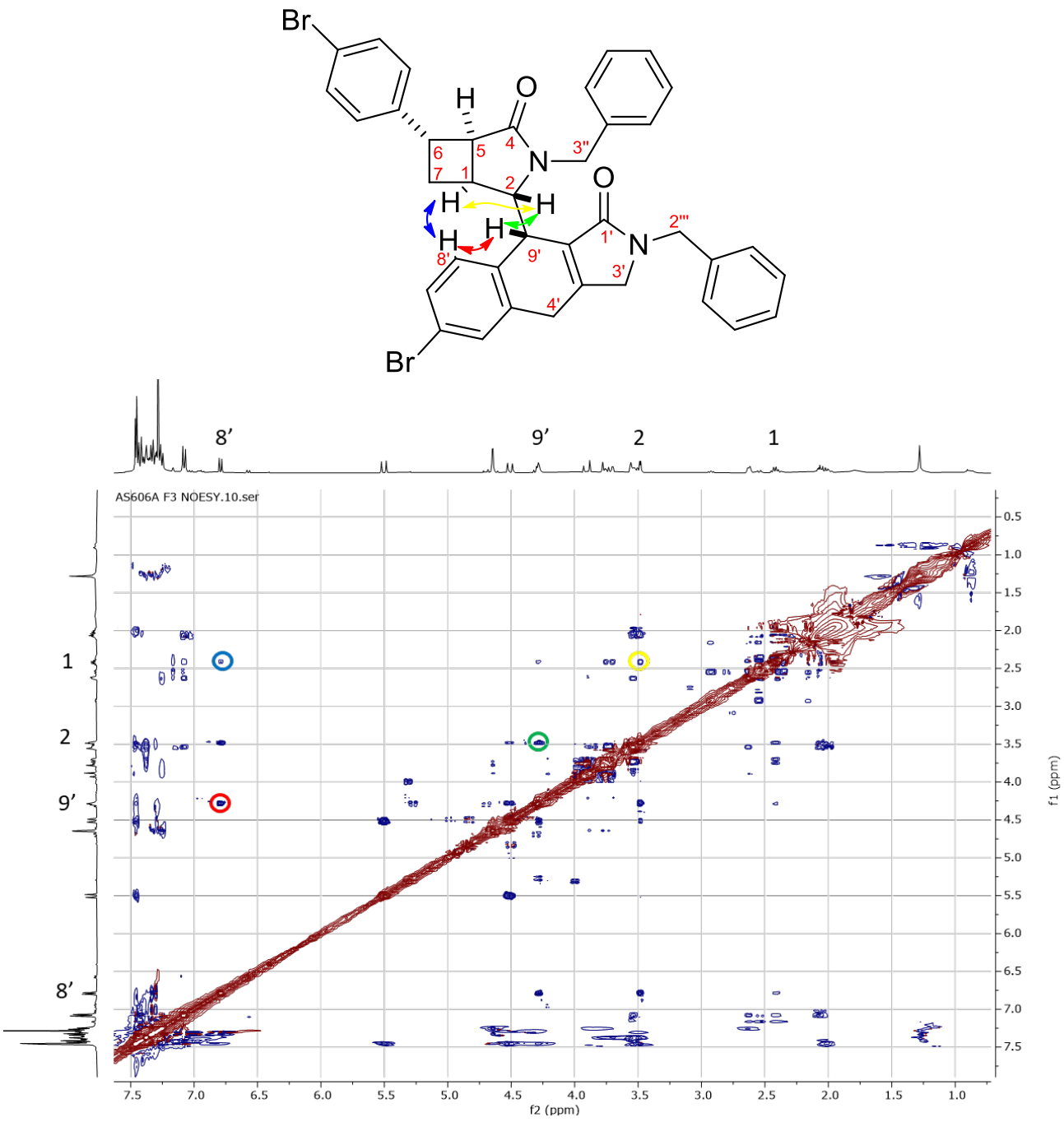
(E)-3-(4-chlorophenyl)-1-((3ar,6r)-6,7-dihydro-3a,6-ethenoisoindol-2(3H)-yl)prop-2-en-1-one. 2'''m

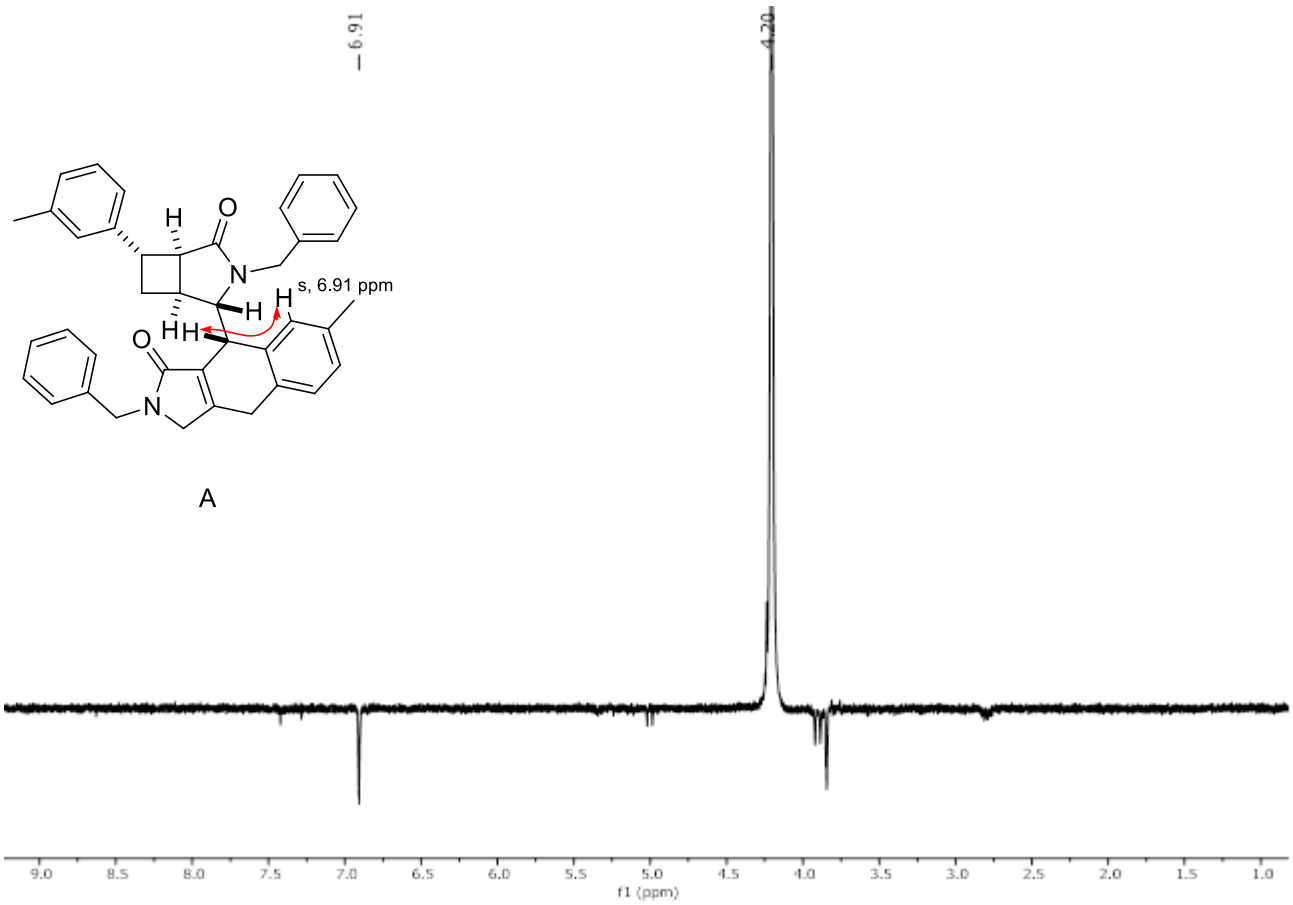


Tetraene **2'''m** was prepared following general procedure **GP-2** using **1m** as reagent. (62.3 mg, 0.20 mmol). White crystals, m.p. 123-124 °C. Yield 14% (9.0 mg, 0.03 mmol). Two rotamers are observed due to the dynamic amide group. **^{1}H NMR** (400 MHz, Acetone) δ .78 – 7.69 (m, 1H RotA, 1H RotB), 7.66 – 7.55 (1H RotA, 1H RotB), 7.50 – 7.37 (m, 2H RotA, 2H RotB), 7.19 (d, *J* = 15.4 Hz, 1H RotB), 7.10 (d, *J* = 15.4 Hz, 1H RotA), 6.86 (t, *J* = 1.8 Hz, 1H RotB), 6.65 (t, *J* = 1.8 Hz, 1H RotA), 6.44 – 6.28 (m, 4H RotA, 4H RotB), 4.61 (s, 2H RotA), 4.31 (s, 2H RotB), 3.97 – 3.89 (m, 1H RotA, 1H RotB), 2.11 – 2.07 (m, 2H RotA, 2H RotB). **^{13}C NMR** (101 MHz, Acetone) δ = 160.7 (Cq), 160.2 (Cq), 139.8 (CH), 139.5 (CH), 138.4 (2CH), 138.3 (2CH), 134.7 (Cq), 134.6 (Cq), 134.47 (Cq), 134.45 (Cq), 133.64 (2CH), 133.63 (2CH), 129.6 (2CH), 129.5 (2CH), 128.9 (2CH), 128.82 (2CH), 128.76 (2Cq), 119.9 (CH), 119.4 (CH), 117.0 (CH), 116.9 (CH), 58.0 (Cq), 55.6 (Cq), 53.64 (CH_2), 53.57 (CH_2), 40.0 (CH), 39.9 (CH), 27.72 (CH_2), 27.67 (CH_2). **ESI-HRMS** calcd for $C_{19}H_{16}ClNNaO$ $[M+Na]^+$ 332,0813, found 332,0817.

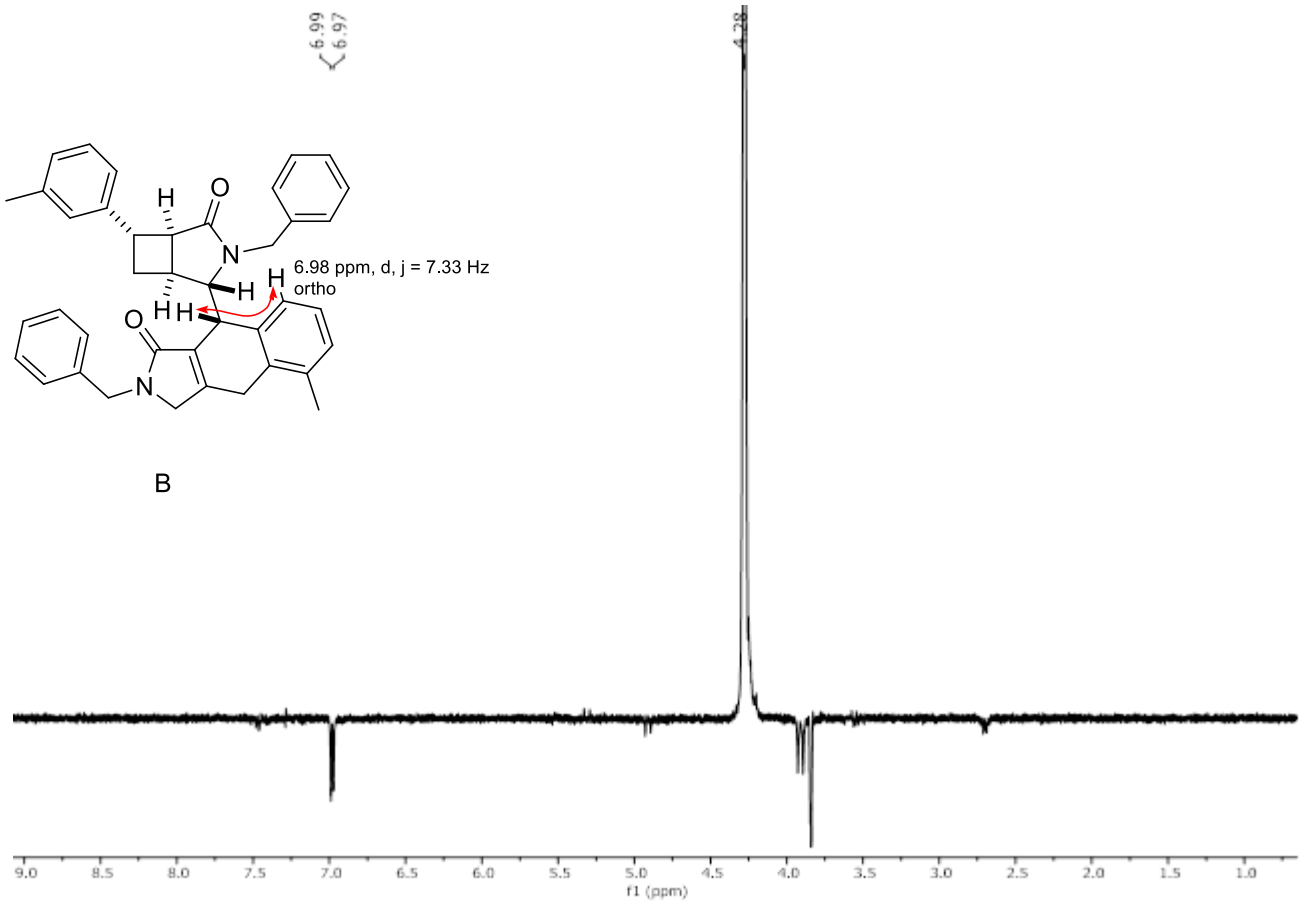
Selected correlation NMR experiments



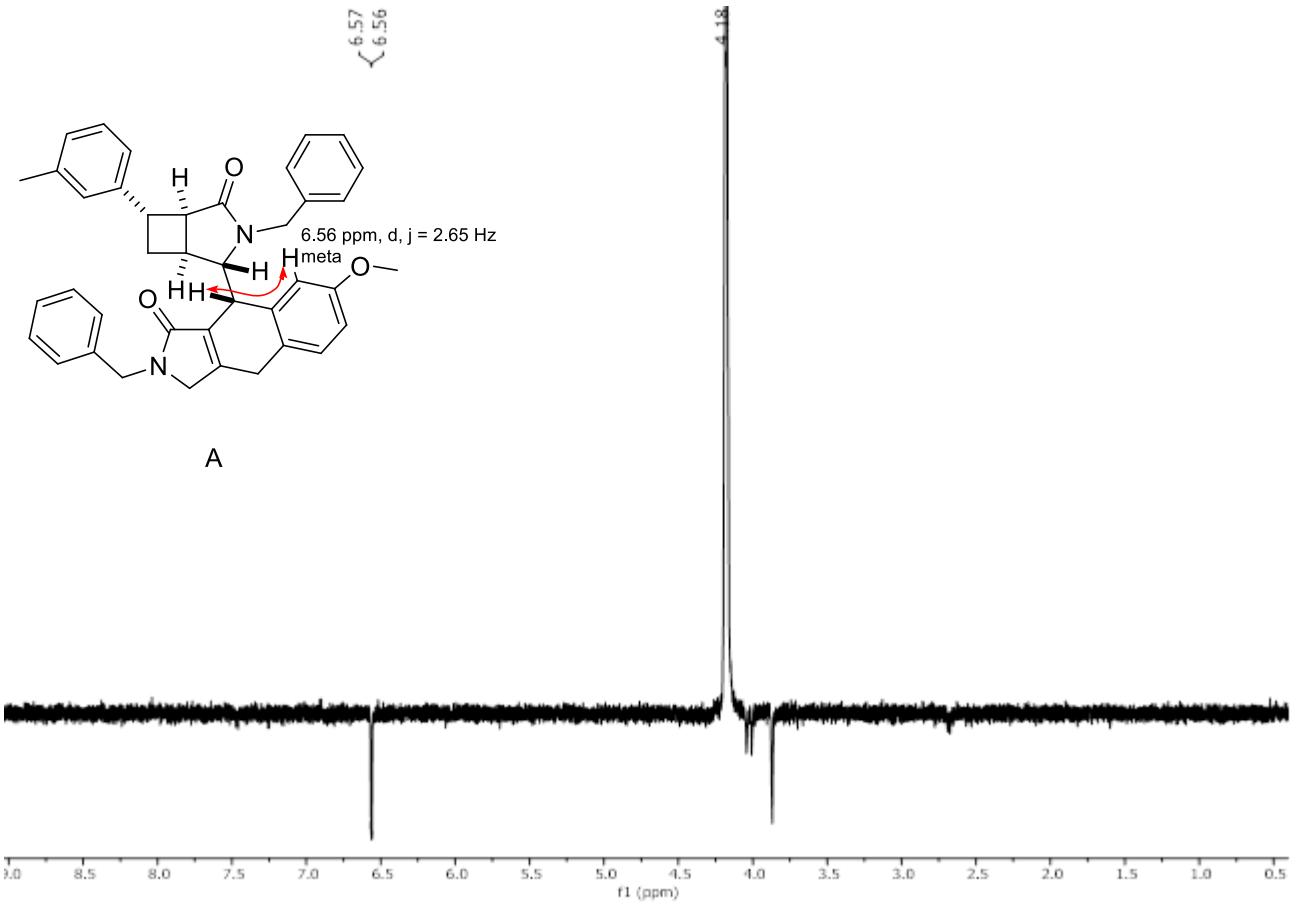

Br
O
H
4
3"
N
6
5
7
1
2
O
H
H
H
1'
2'''
N
8'
9'
3'
4'
Br
8'
9'
2
1
AS606A F3 NOESY.10.ser
1
2
9'
8'
f2 (ppm)
f1 (ppm)


6.91
4.20
s, 6.91 ppm
f1 (ppm)

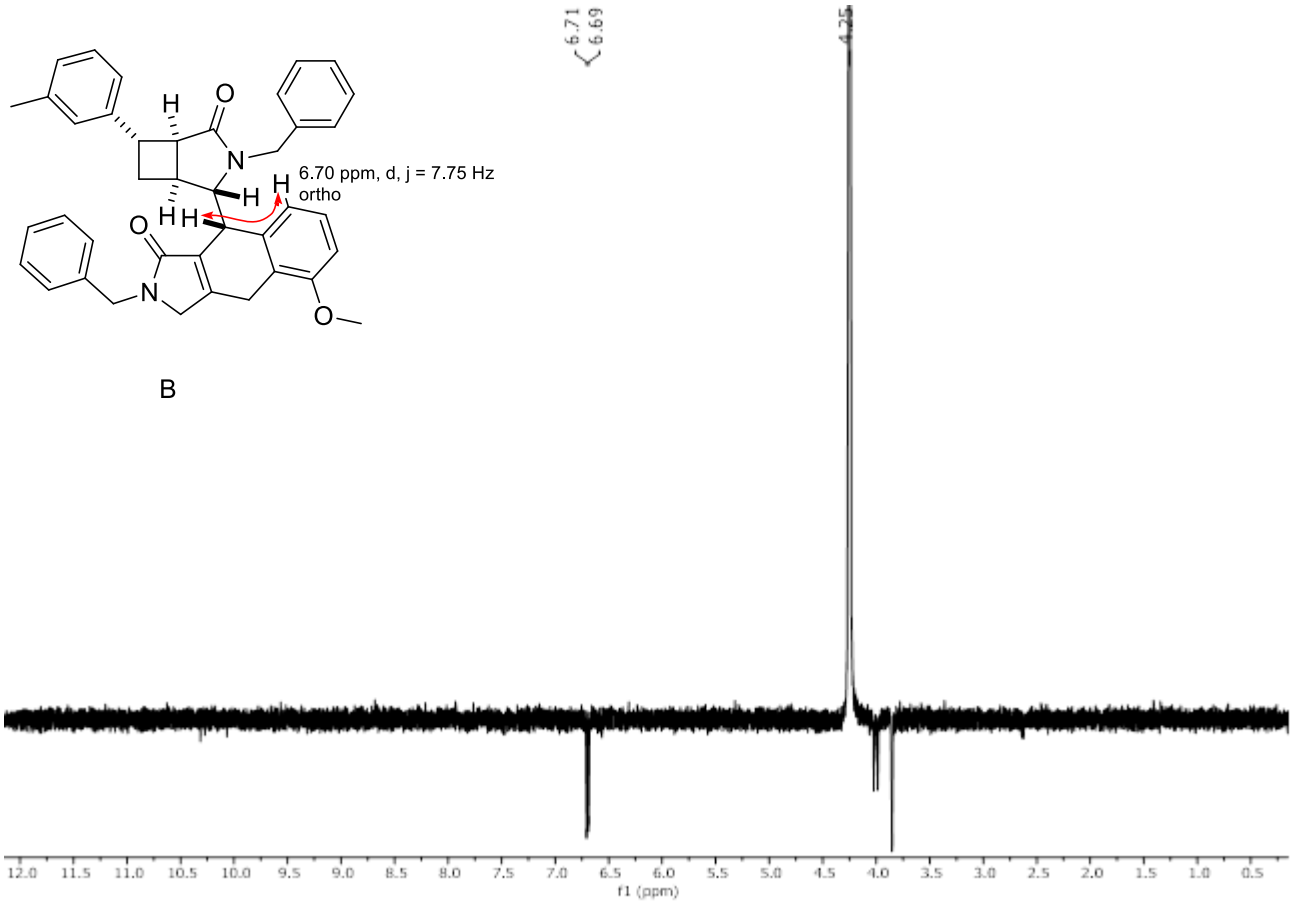
A


6.99
6.97
4.28
6.98 ppm, d, j = 7.33 Hz
ortho
f1 (ppm)

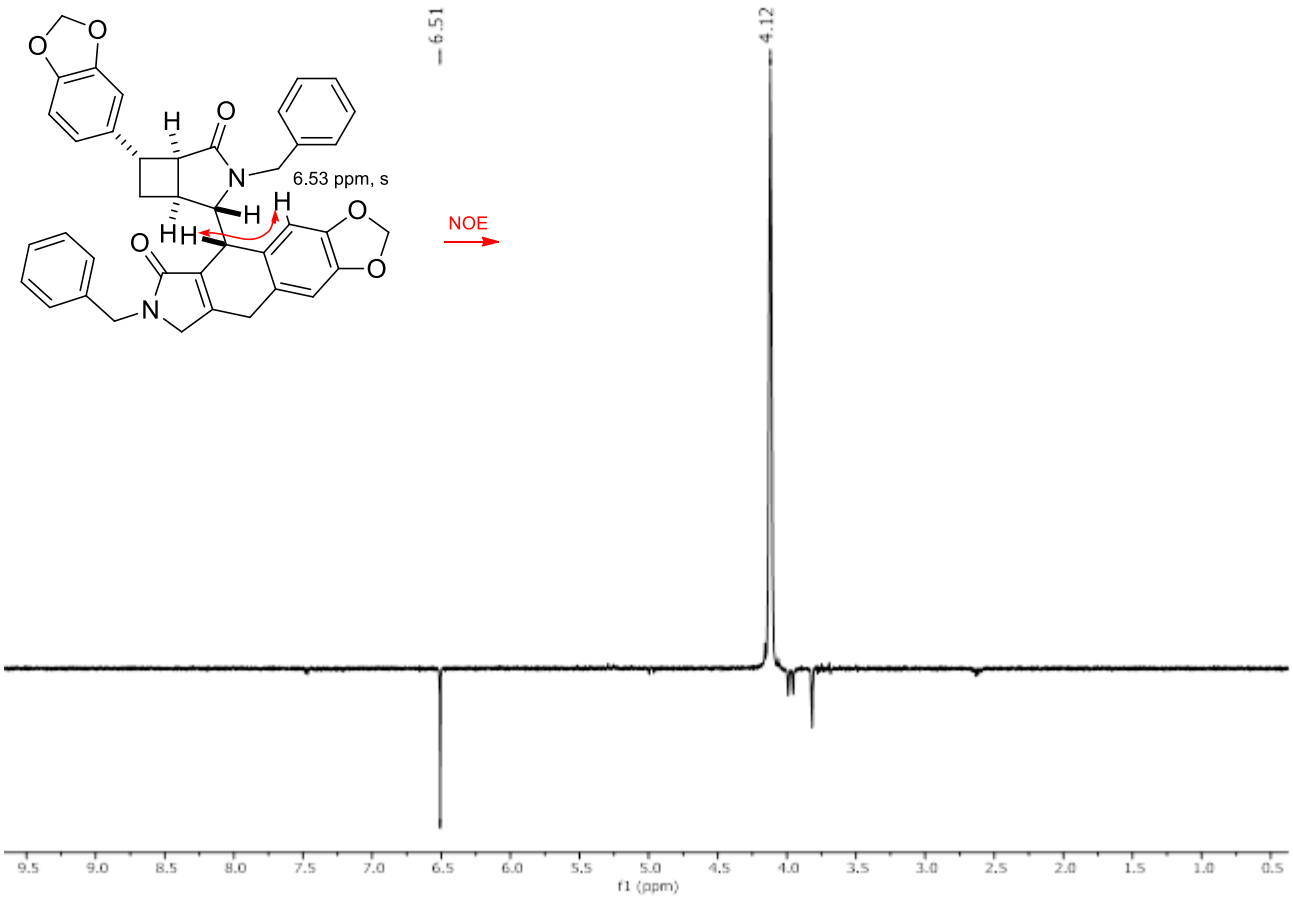
B

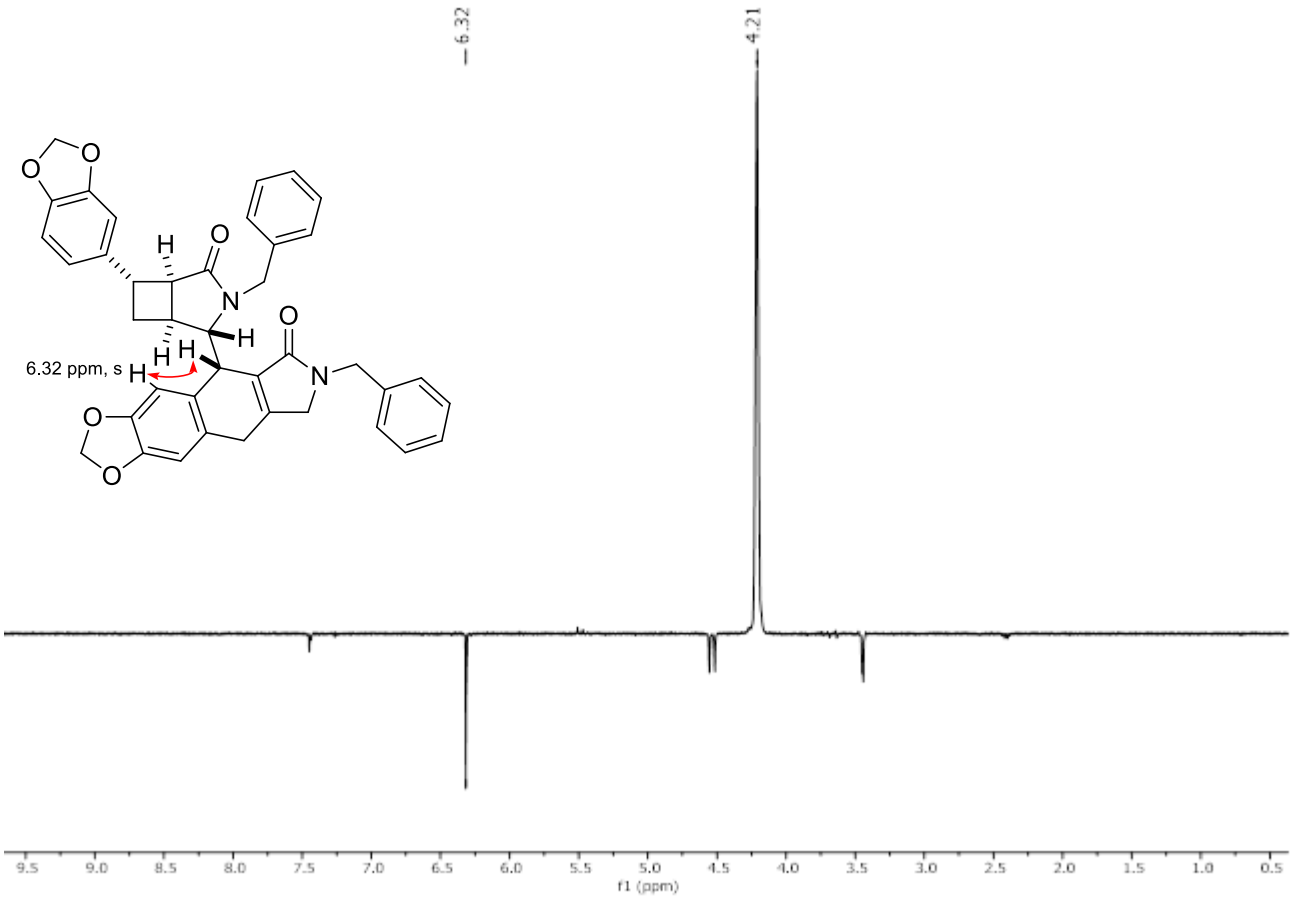

6.57
6.56
4.18
6.56 ppm, d, j = 2.65 Hz
meta
f1 (ppm)

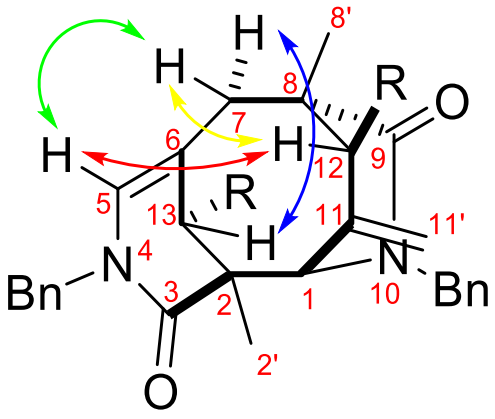
A


6.71
6.69
4.25
6.70 ppm, d, j = 7.75 Hz
ortho
f1 (ppm)

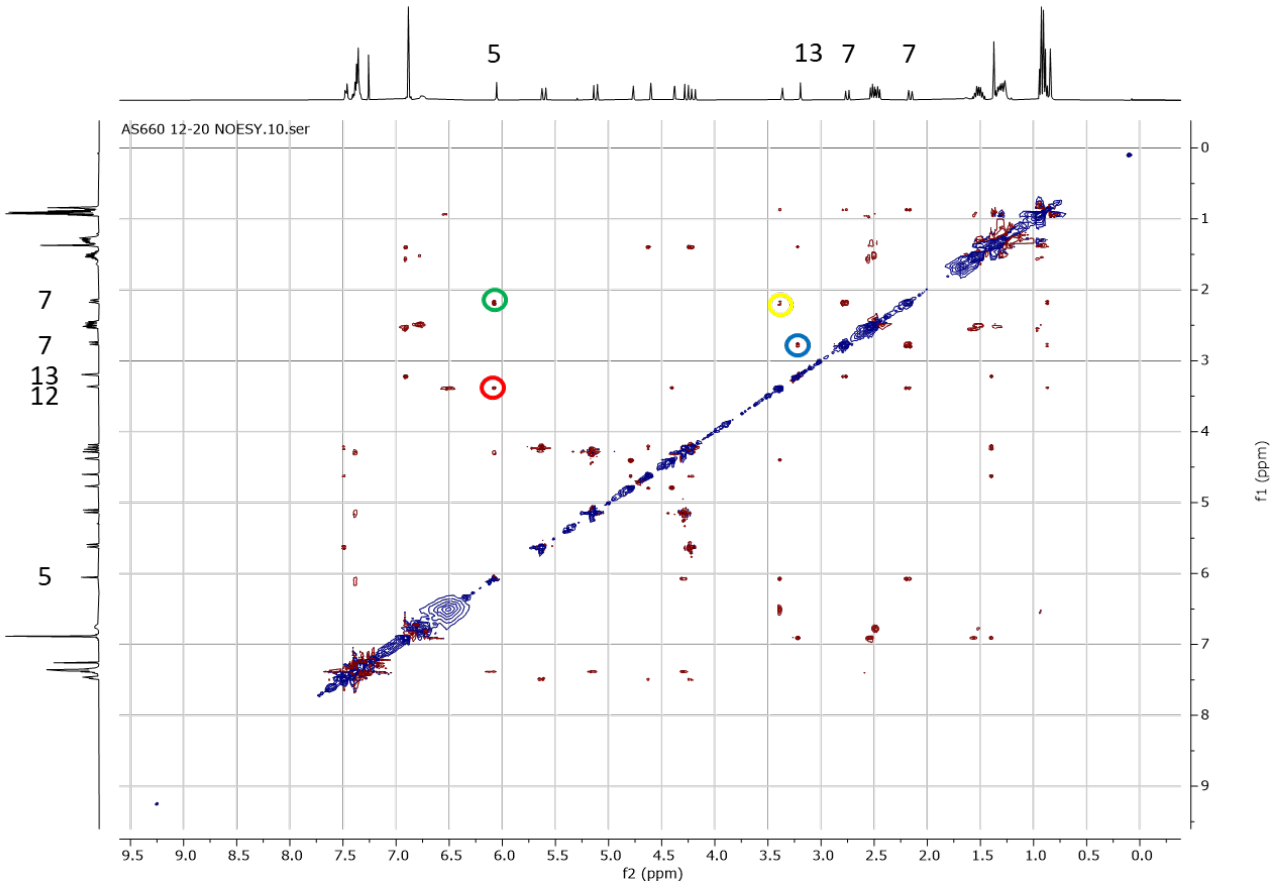
B

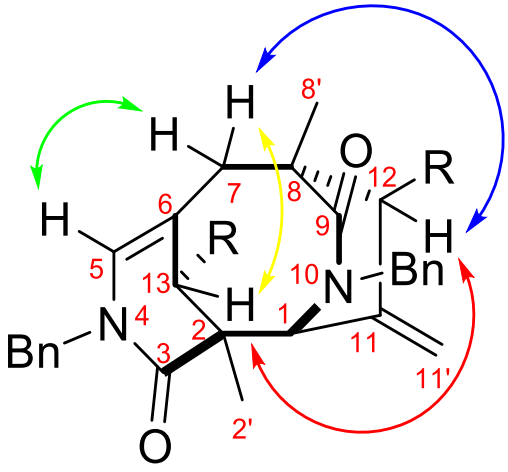

6.53 ppm, s
NOE
6.51
4.12
f1 (ppm)


6.32 ppm, s
6.32
4.21
f1 (ppm)

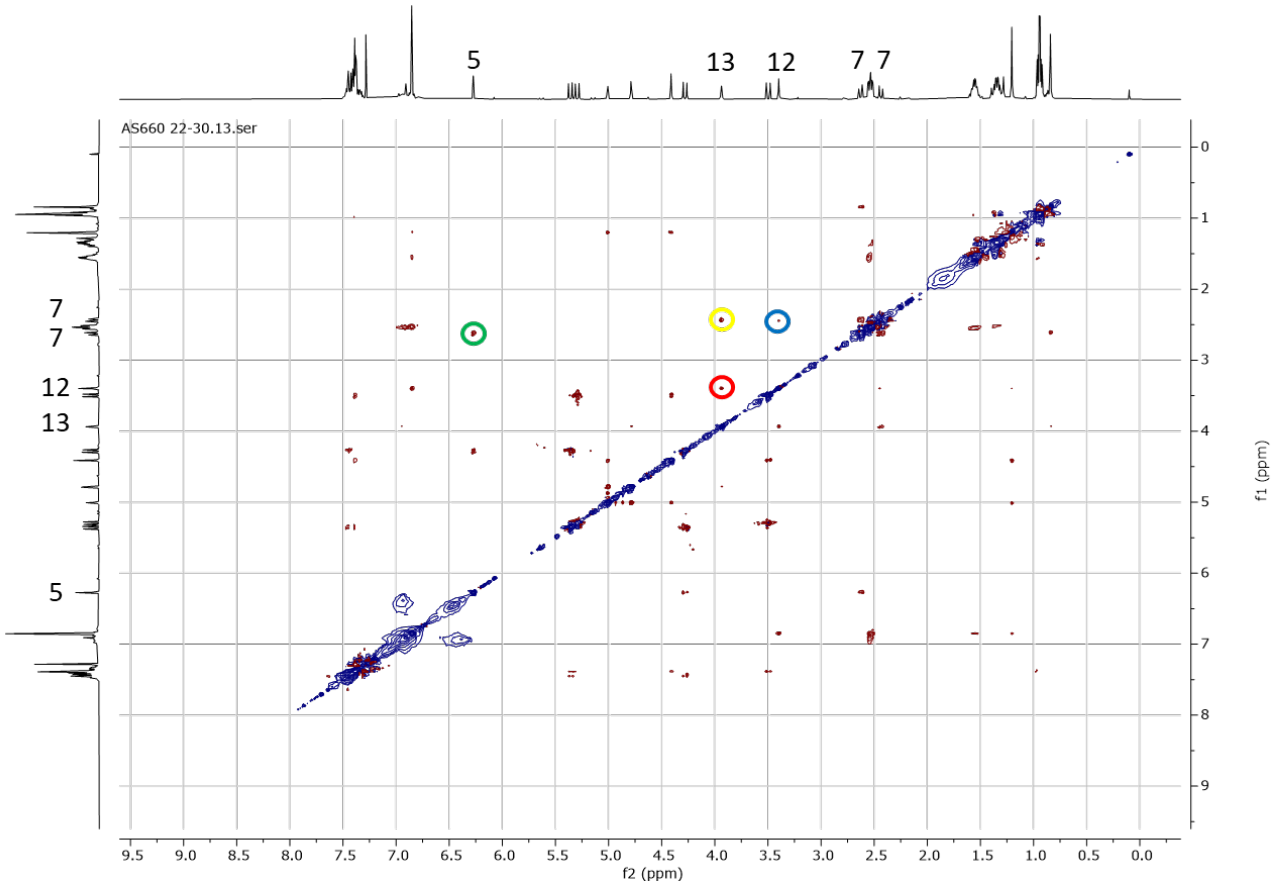

H
8'
H
8
R
O
7
6
H
12
9
H
5
13
R
11
11'
H
N
4
N
Bn
3
2
1
10
Bn
2'
O

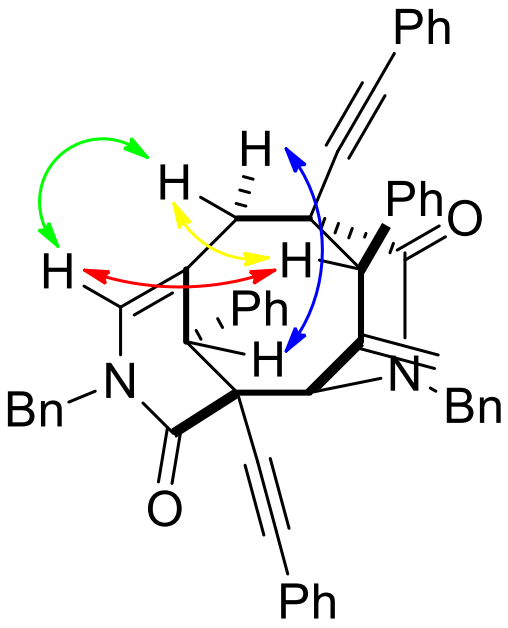
R = 4-nBu-C_6H_4

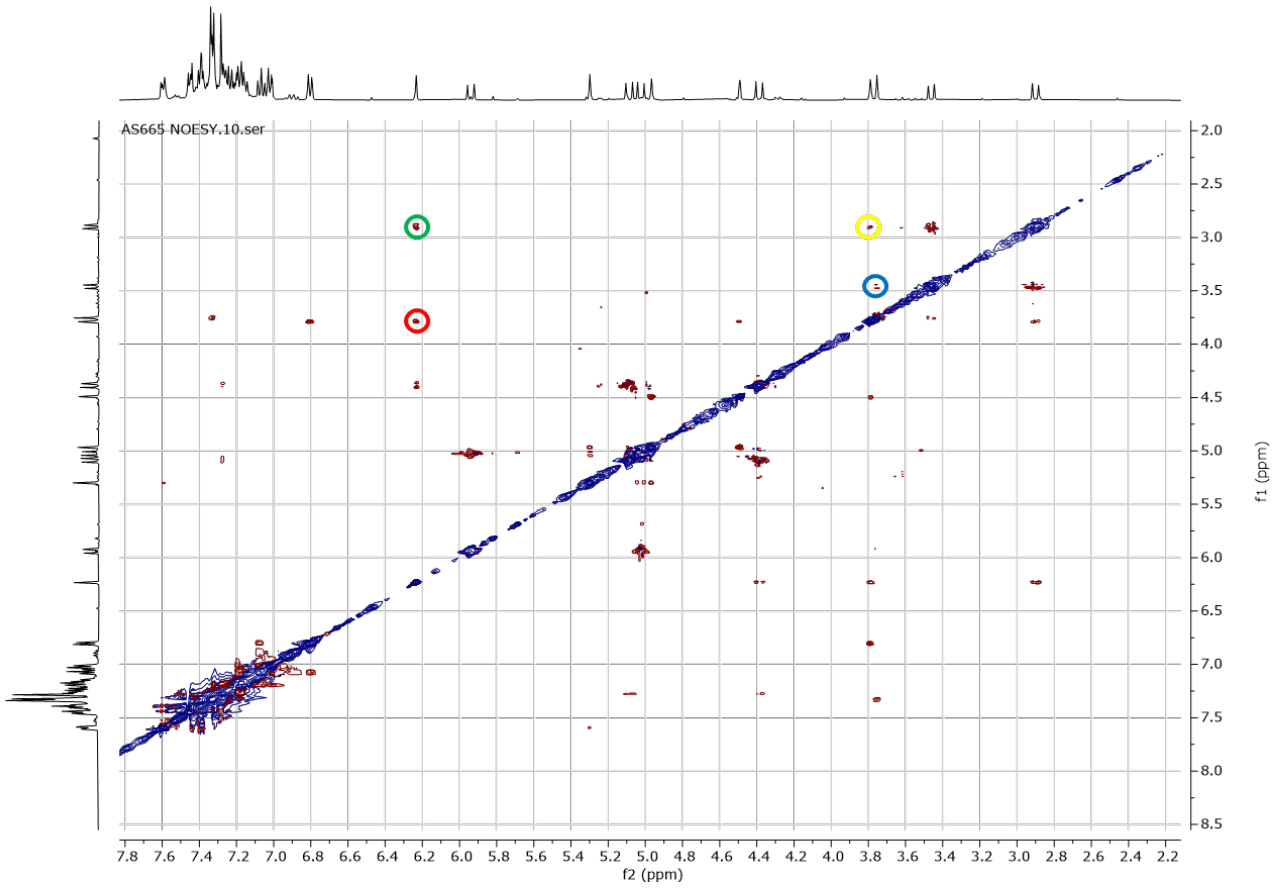

5
13
7
7
AS660 12-20 NOESY.10.ser
7
7
13
12
5
f2 (ppm)
f1 (ppm)


H
8'
H
O
12
R
7
8
6
9
H
H
R
5
13
10
N
Bn
H
1
N
4
2
Bn
3
11
11'
2'
O

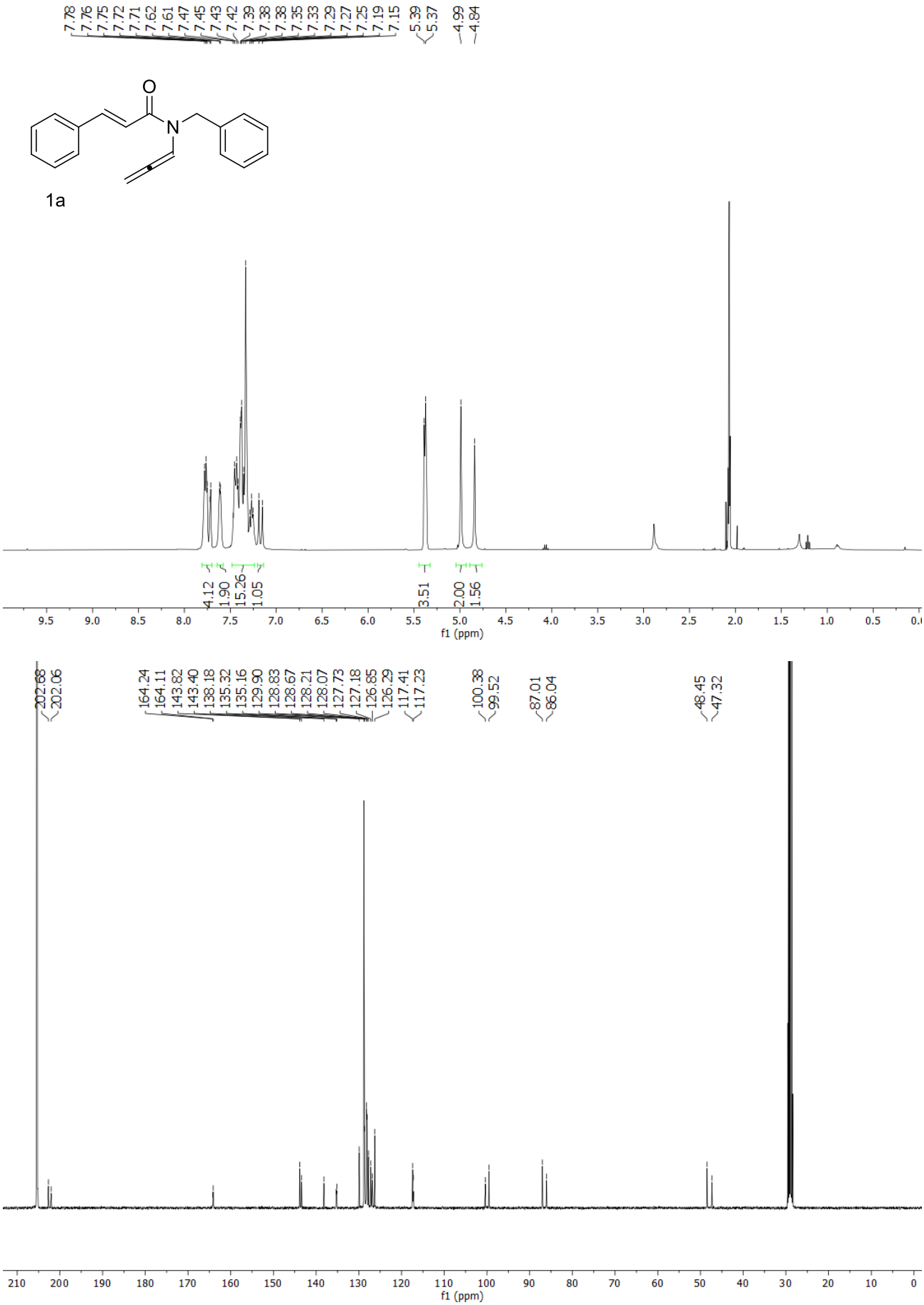
R = 4-nBu-C_6H_4

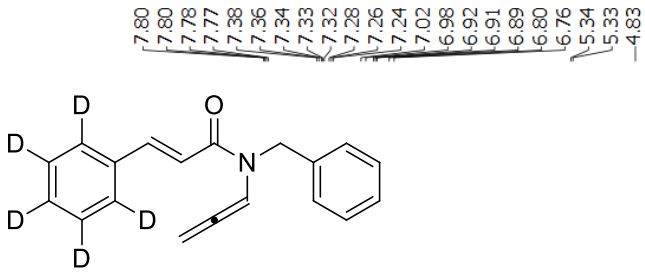

5
13
12
7
7
AS660 22-30.13.ser
7
7
12
13
5
f2 (ppm)
f1 (ppm)


Ph
H
H
Ph
O
H
H
Ph
H
N
Bn
N
Bn
O
Ph


AS665 NOESY.10.ser
f2 (ppm)
f1 (ppm)

Copies of NMR spectra

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7.80
7.78
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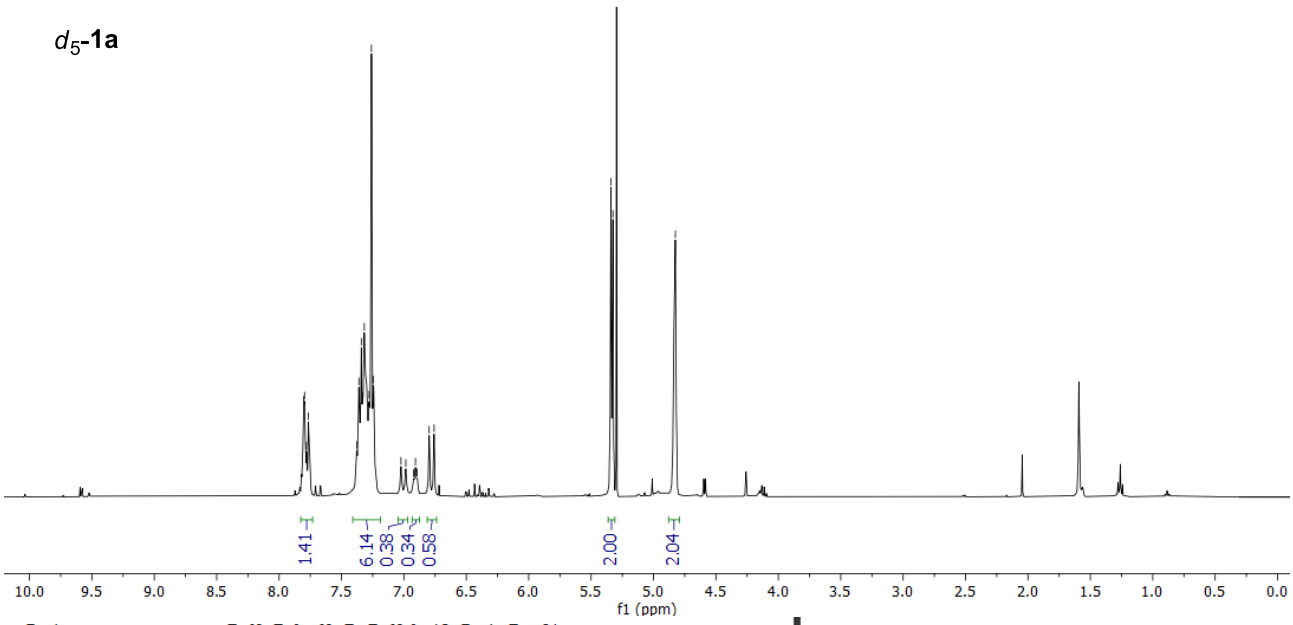
7.38
7.36
7.34
7.33
7.32
7.28
7.26
7.24
7.02
6.98
6.92
6.91
6.89
6.80
6.76
5.34
5.33
4.83
D
O
D
N
D
D
D

d$_5$-**1a**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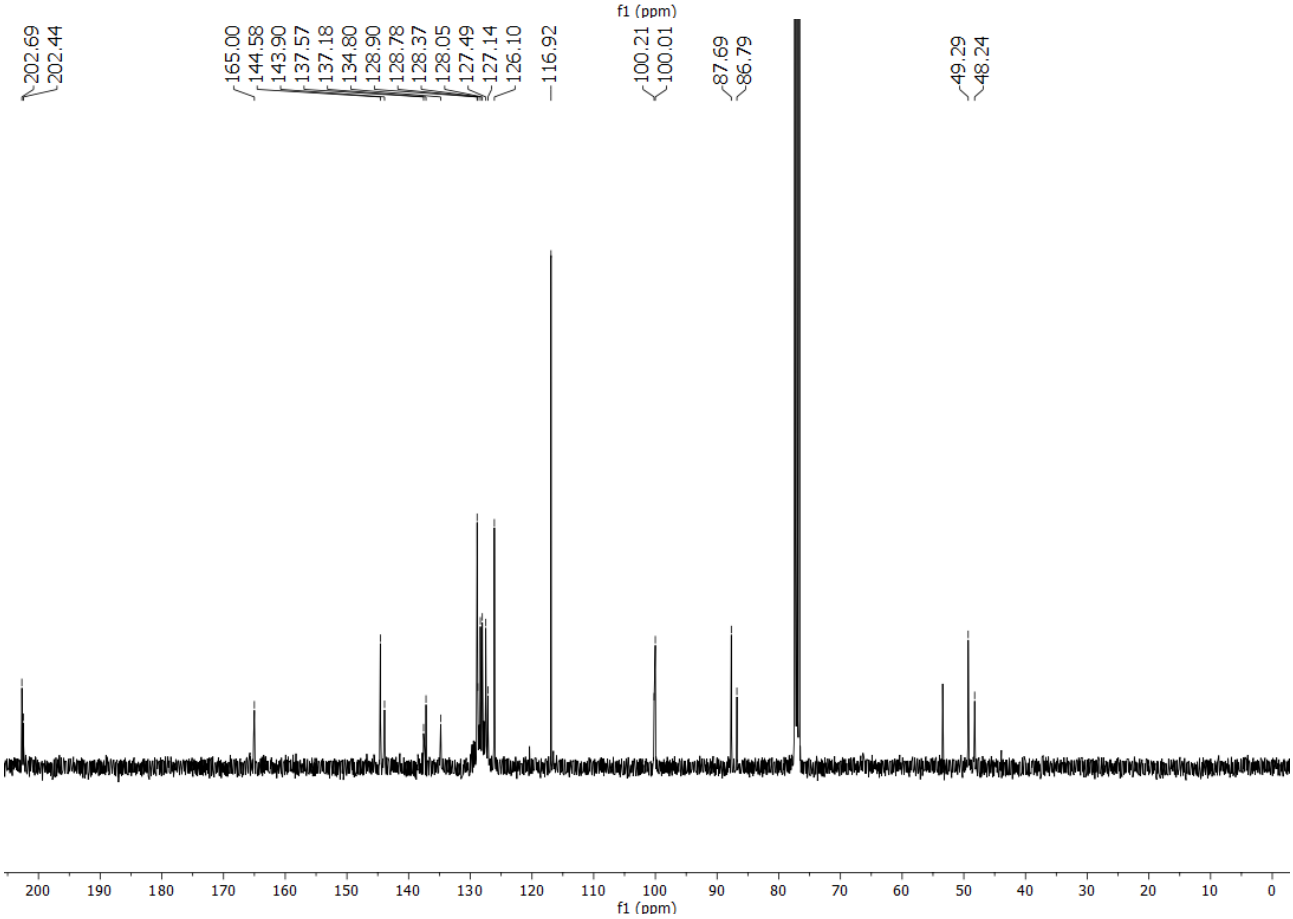
6.14
0.38
0.34
0.58
2.00
2.04
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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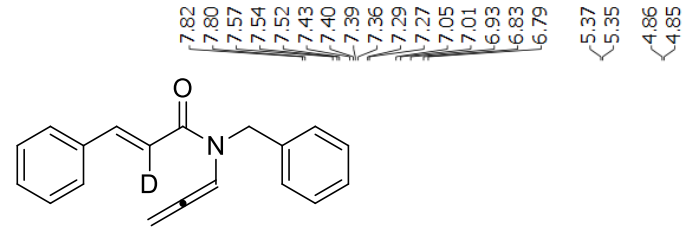
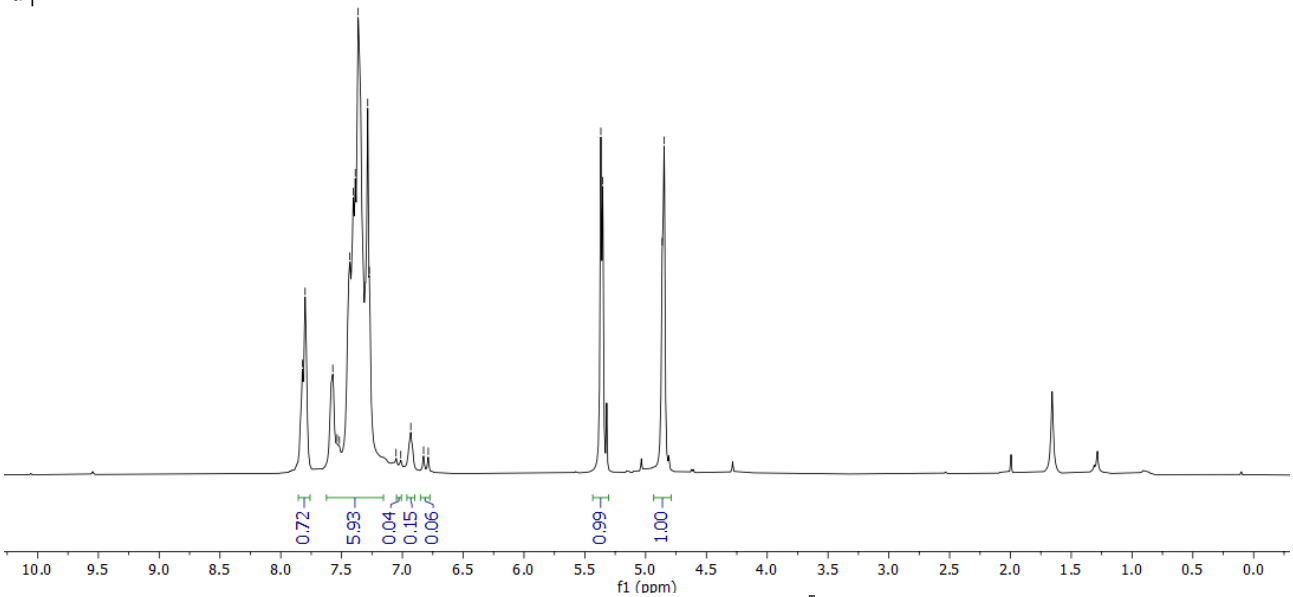
202.44
165.00
144.58
143.90
137.57
137.18
134.80
128.90
128.78
128.37
128.05
127.49
127.14
126.10
116.92
100.21
100.01
87.69
86.79
49.29
48.24
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.82
7.80
7.57
7.54
7.52
7.43
7.40
7.39
7.36
7.29
7.27
7.05
7.01
6.93
6.83
6.79
5.37
5.35
4.86
4.85
O
N
D

d_1-**1a**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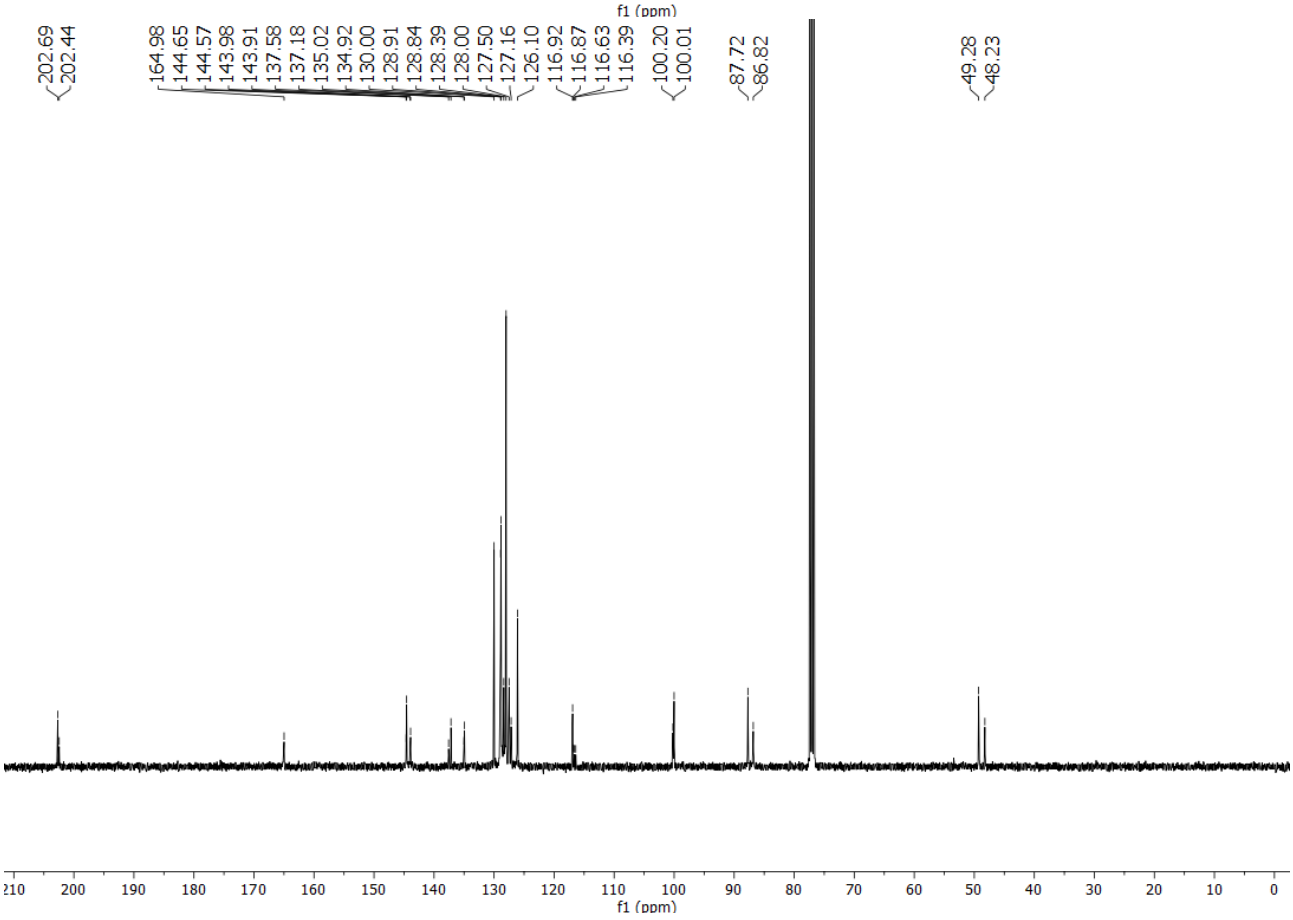
5.93
0.04
0.15
0.06
0.99
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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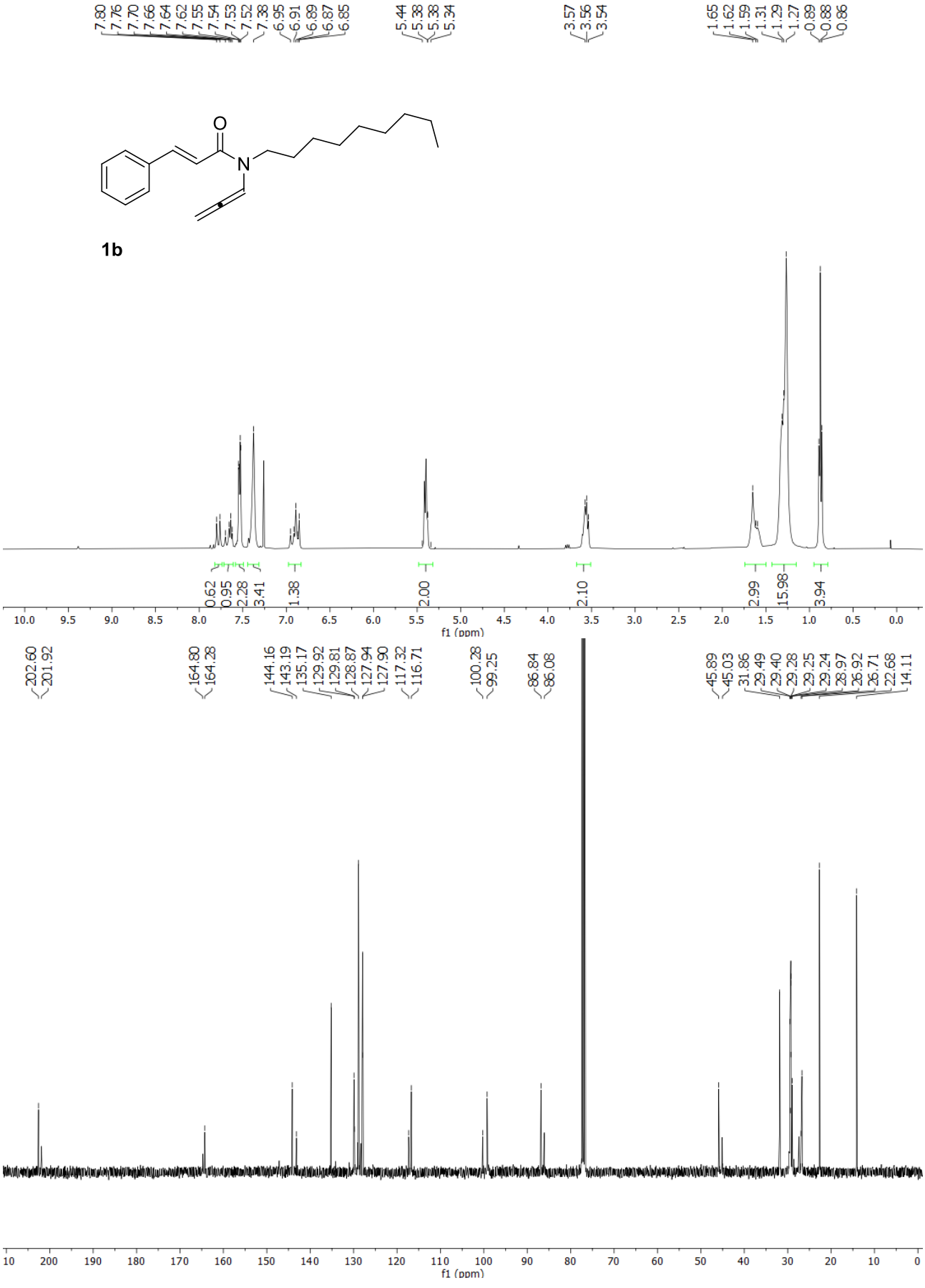
202.44
164.98
144.65
144.57
143.98
143.91
137.58
137.18
135.02
134.92
130.00
128.91
128.84
128.39
128.00
127.50
127.16
126.10
116.92
116.87
116.63
116.39
100.20
100.01
87.72
86.82
49.28
48.23
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.76
7.70
7.66
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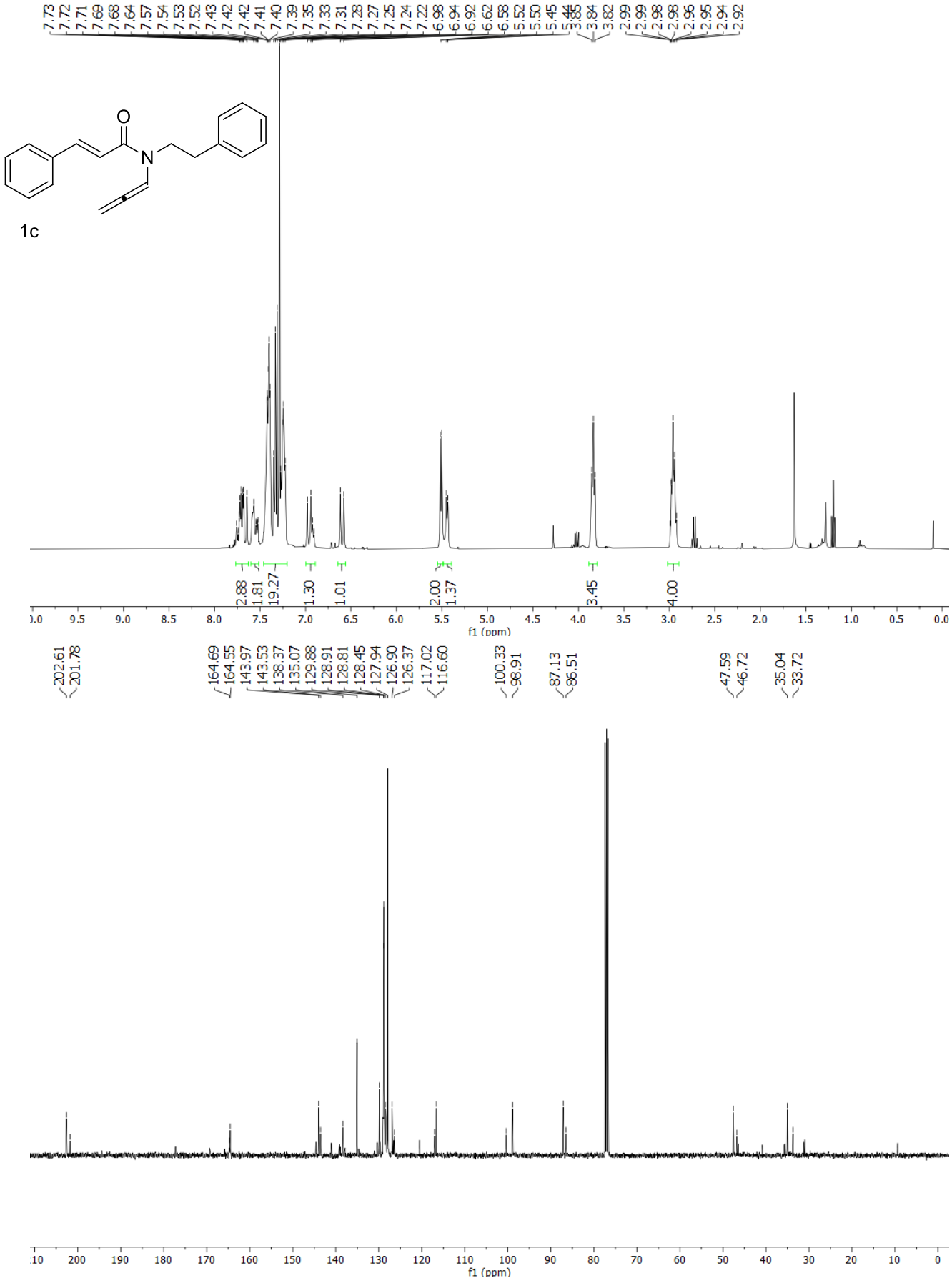
7.62
7.55
7.54
7.53
7.52
7.38
6.95
6.91
6.89
6.87
6.85
5.44
5.38
5.33
5.34
3.57
3.56
3.54
1.65
1.62
1.59
1.31
1.29
1.27
0.89
0.88
0.86
O
N
1b
0.62
0.95
2.28
3.41
1.38
2.00
2.10
2.99
15.98
3.94
f1 (ppm)
202.60
201.92
164.80
164.28
144.16
143.19
135.17
129.92
129.81
128.87
127.94
127.90
117.32
116.71
100.28
99.25
86.84
86.08
45.89
45.03
31.86
29.49
29.40
29.28
29.25
29.24
28.97
26.92
26.71
22.68
14.11
f1 (ppm)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7.64
7.57
7.54
7.53
7.52
7.43
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7.42
7.41
7.40
7.39
7.35
7.33
7.31
7.28
7.27
7.25
7.24
7.22
6.98
6.94
6.92
6.62
6.58
5.52
5.50
5.45
3.84
3.82
2.99
2.98
2.98
2.96
2.95
2.94
2.92
O
N
1c
2.88
1.81
19.27
1.30
1.01
2.00
1.37
3.45
4.00
f1 (ppm)
202.61
201.78
164.69
164.55
143.97
143.53
138.37
135.07
129.88
128.91
128.81
128.45
127.94
126.90
126.37
117.02
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100.33
98.91
87.13
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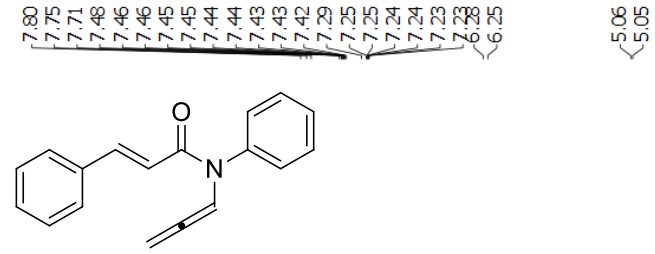
46.72
35.04
33.72
f1 (ppm)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7.44
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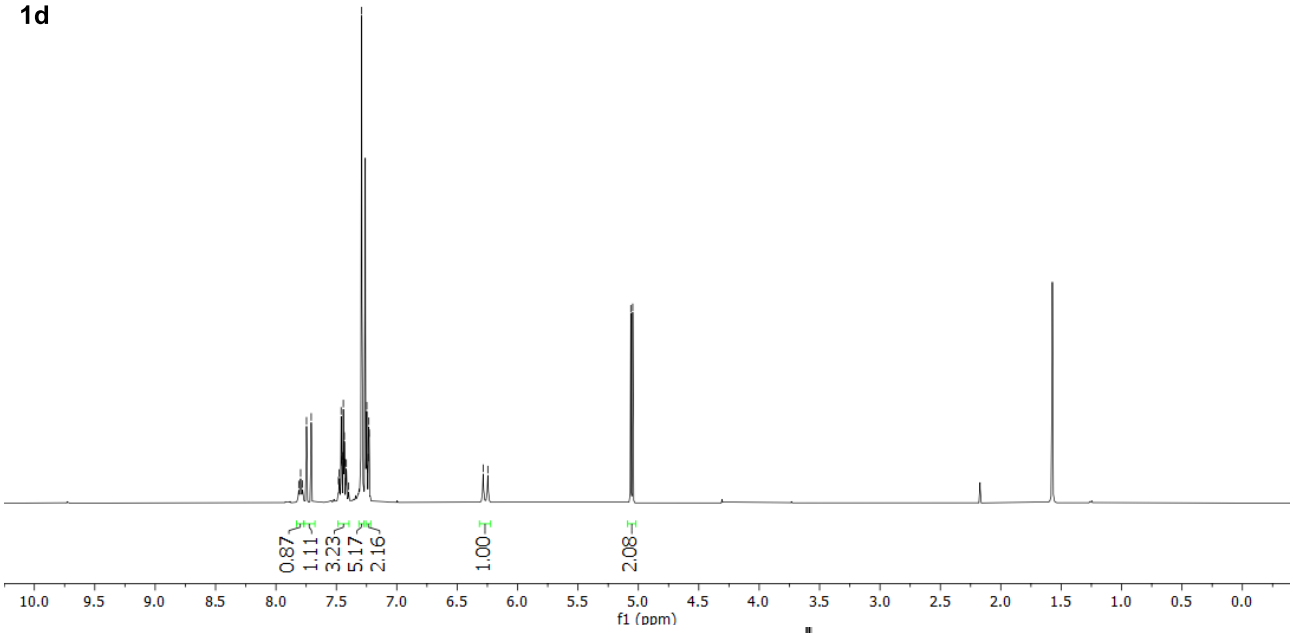
7.43
7.43
7.42
7.29
7.25
7.25
7.24
7.24
7.23
7.23
6.28
6.25
5.06
5.05
O
N

1d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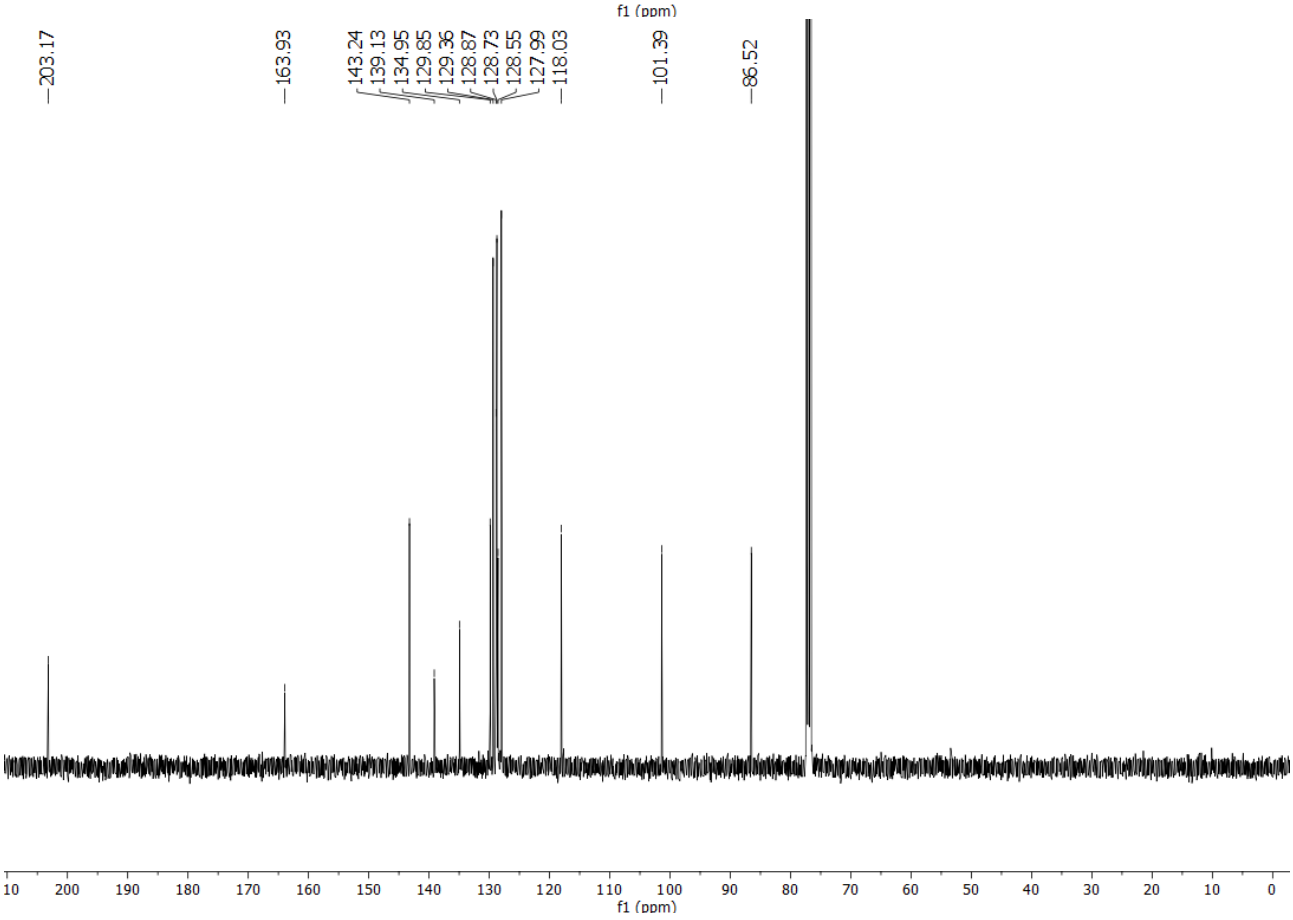
3.23
5.17
2.16
1.00
2.08
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


203.17
163.93
143.24
139.13
134.95
129.85
129.36
128.87
128.73
128.55
127.99
118.03
101.39
86.52
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.73
7.70
7.57
7.56
7.55
7.55
7.55
7.44
7.44
7.43
7.42
7.41
7.41
7.40
7.39
7.39
7.38
7.38
7.37
7.36
7.35
7.35
7.31
7.27
5.37
5.35
2.79
2.78
2.77
2.76
2.75
2.74
2.73
1.05
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1.00
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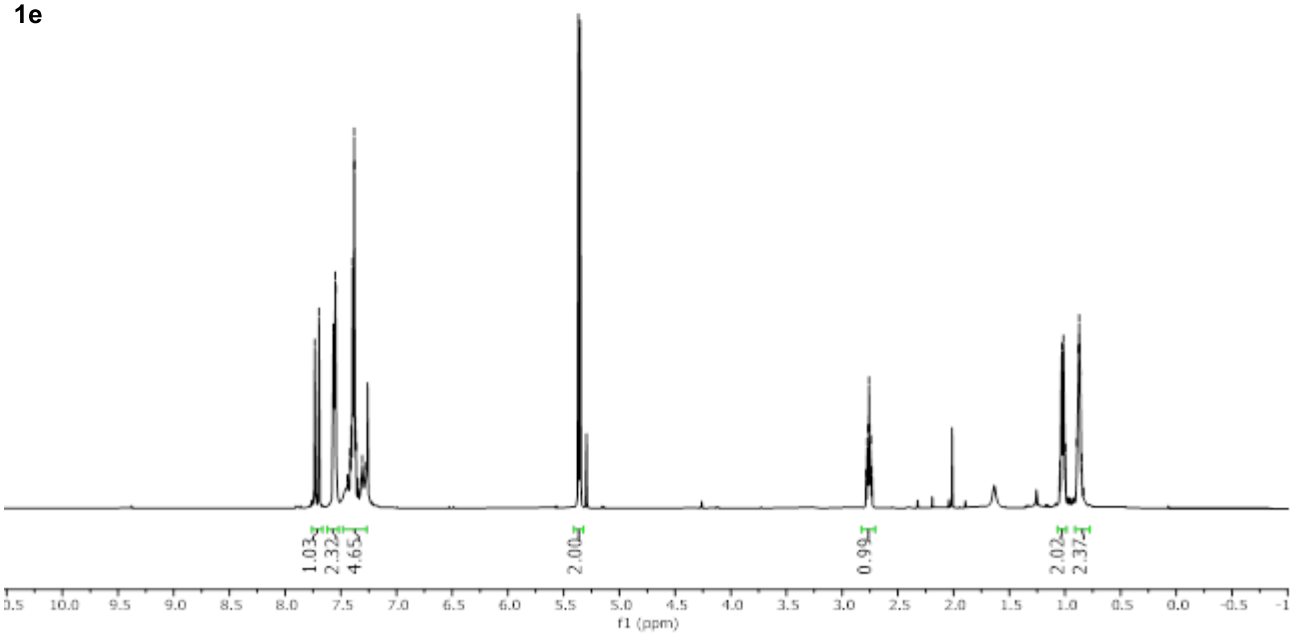
0.86
0.85
0.83

O
N

1e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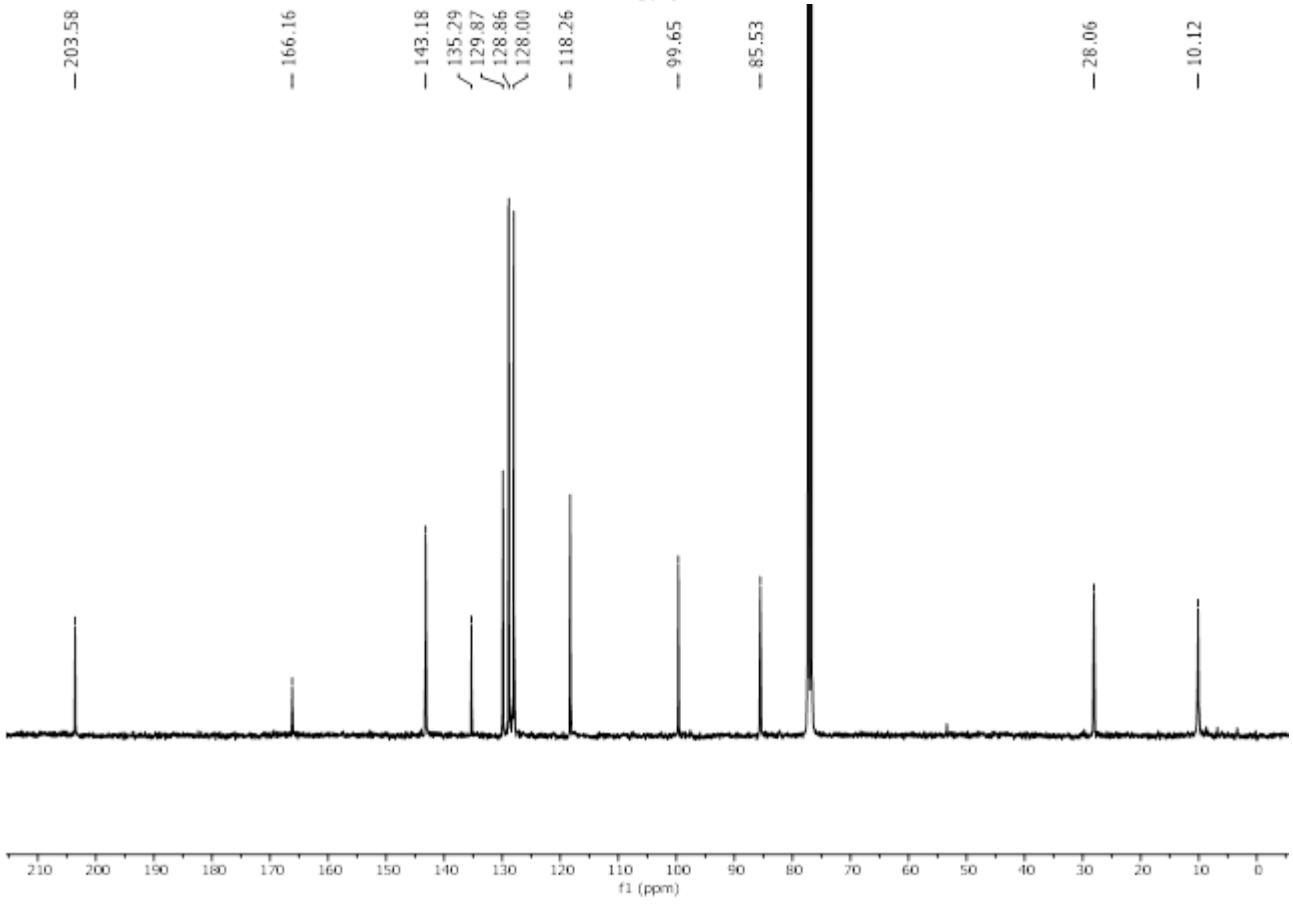
0.99
2.02
2.37
f1 (ppm)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166.16
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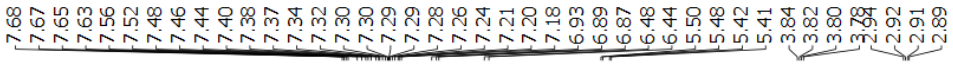
135.29
129.87
128.86
128.00
118.26
99.65
85.53
28.06
10.12
f1 (ppm)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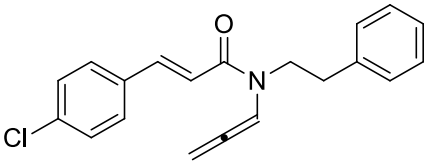
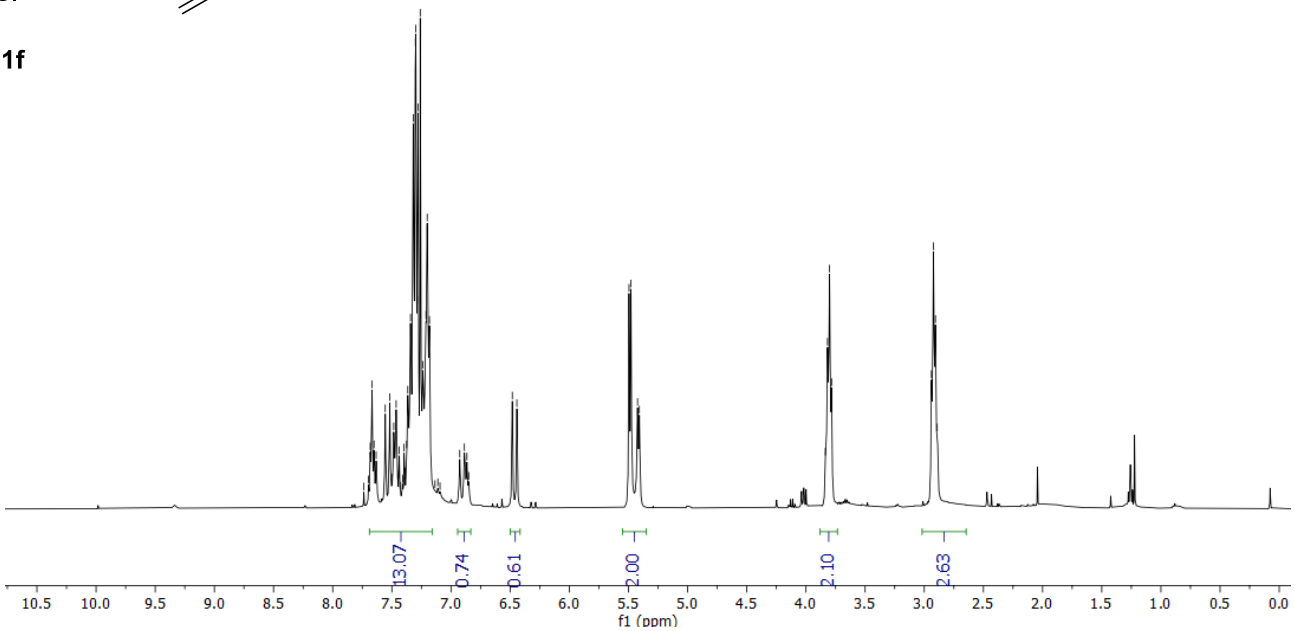
7.34
7.32
7.30
7.30
7.29
7.29
7.28
7.26
7.24
7.21
7.20
7.18
6.93
6.89
6.87
6.48
6.44
5.50
5.48
5.42
5.41
3.84
3.82
3.80
2.94
2.92
2.91
2.89


O
N
Cl

1f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10.0
9.5
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8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.5
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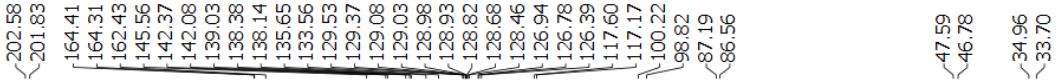
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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201.83
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164.31
162.43
145.56
142.37
142.08
139.03
138.38
138.14
135.65
133.56
129.53
129.37
129.08
129.03
128.98
128.93
128.82
128.68
128.46
126.94
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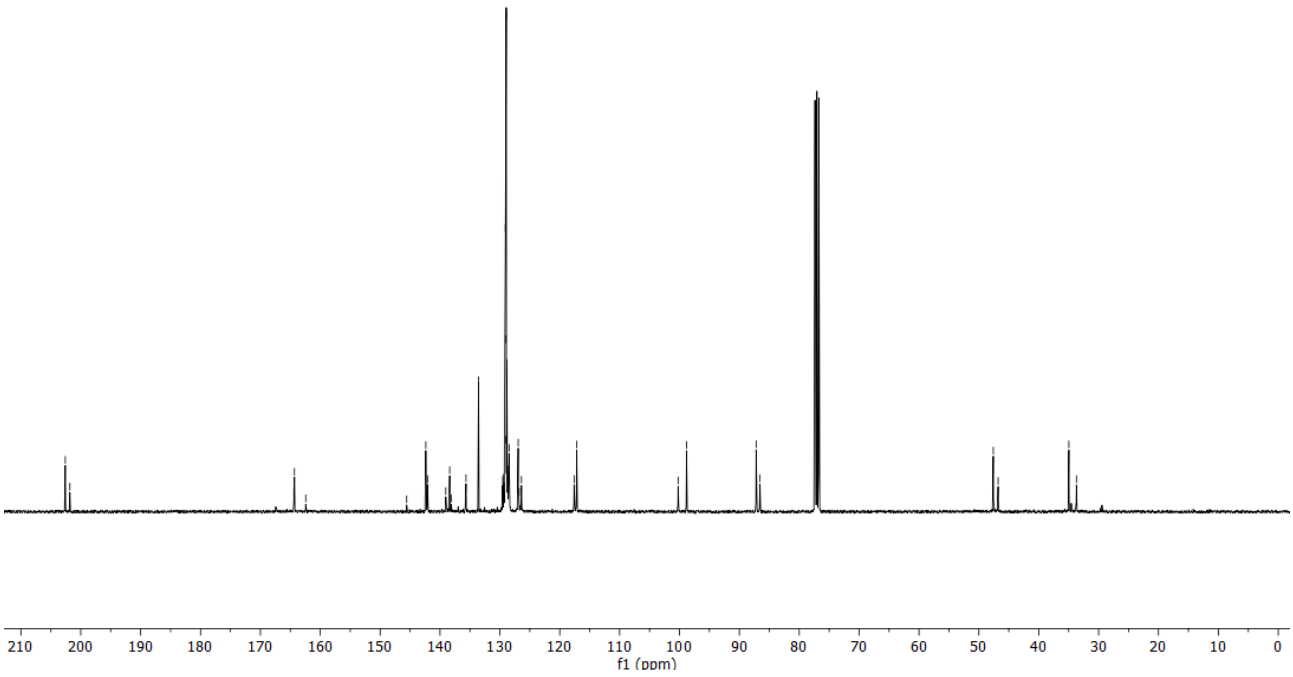
46.78
34.96
33.70


210
200
190
180
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140
130
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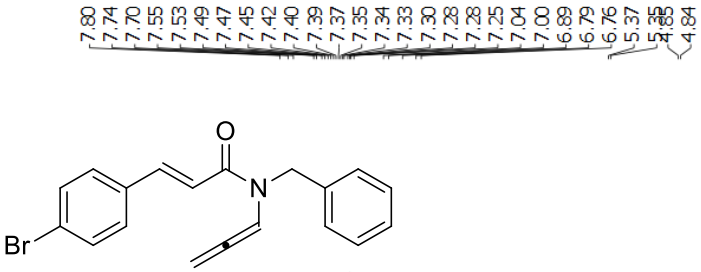
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


O
N
Br

1g

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7.47
7.45
7.42
7.40
7.39
7.37
7.35
7.34
7.33
7.30
7.28
7.28
7.25
7.04
7.00
6.89
6.79
6.76
5.37
4.85
4.84
0.53
0.97
9.52
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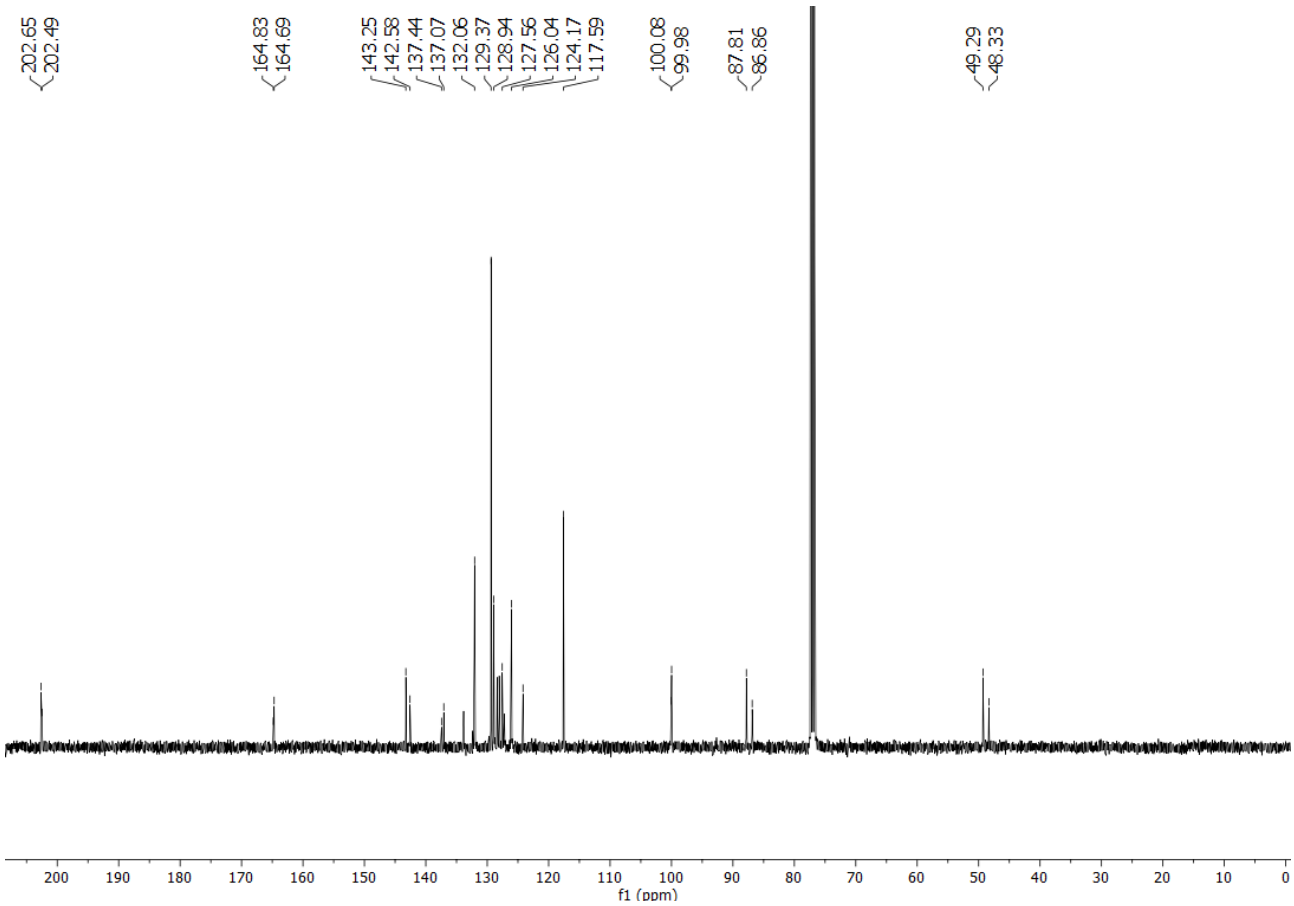
0.37
0.59
1.95
2.00
f1 (ppm)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142.58
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132.06
129.37
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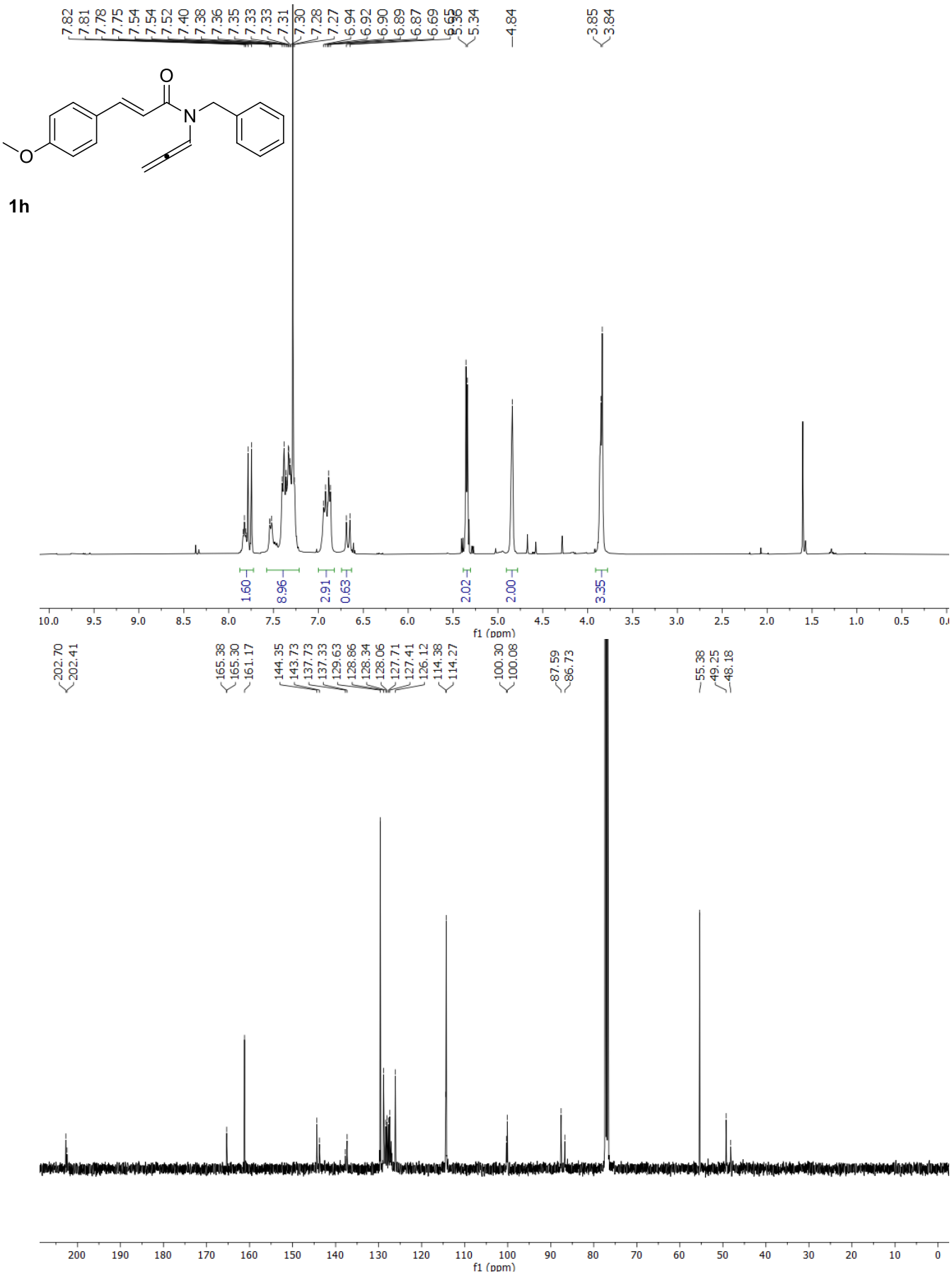
127.56
126.04
124.17
117.59
100.08
99.98
87.81
86.86
49.29
48.33
f1 (ppm)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7.40
7.38
7.36
7.35
7.33
7.33
7.31
7.30
7.28
7.27
6.94
6.92
6.90
6.89
6.87
6.69
6.65
5.38
5.34
4.84
3.85
3.84
O
N
O
1h
1.60
8.96
2.91
0.63
2.02
2.00
3.35
f1 (ppm)
202.70
202.41
165.38
165.30
161.17
144.35
143.73
137.73
137.33
129.63
128.86
128.34
128.06
127.71
127.41
126.12
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114.27
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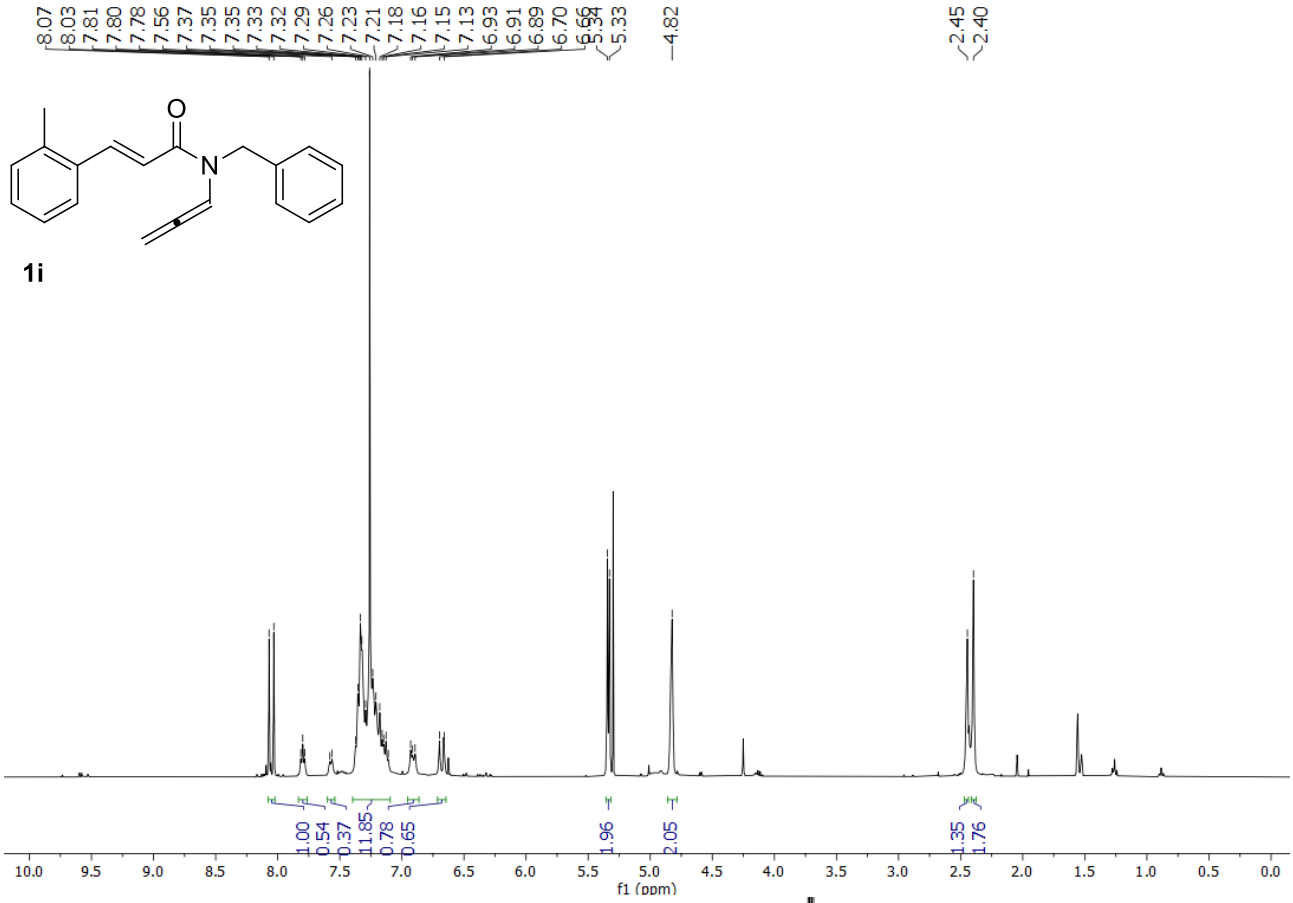
100.08
87.59
86.73
55.38
49.25
48.18
f1 (ppm)


8.07
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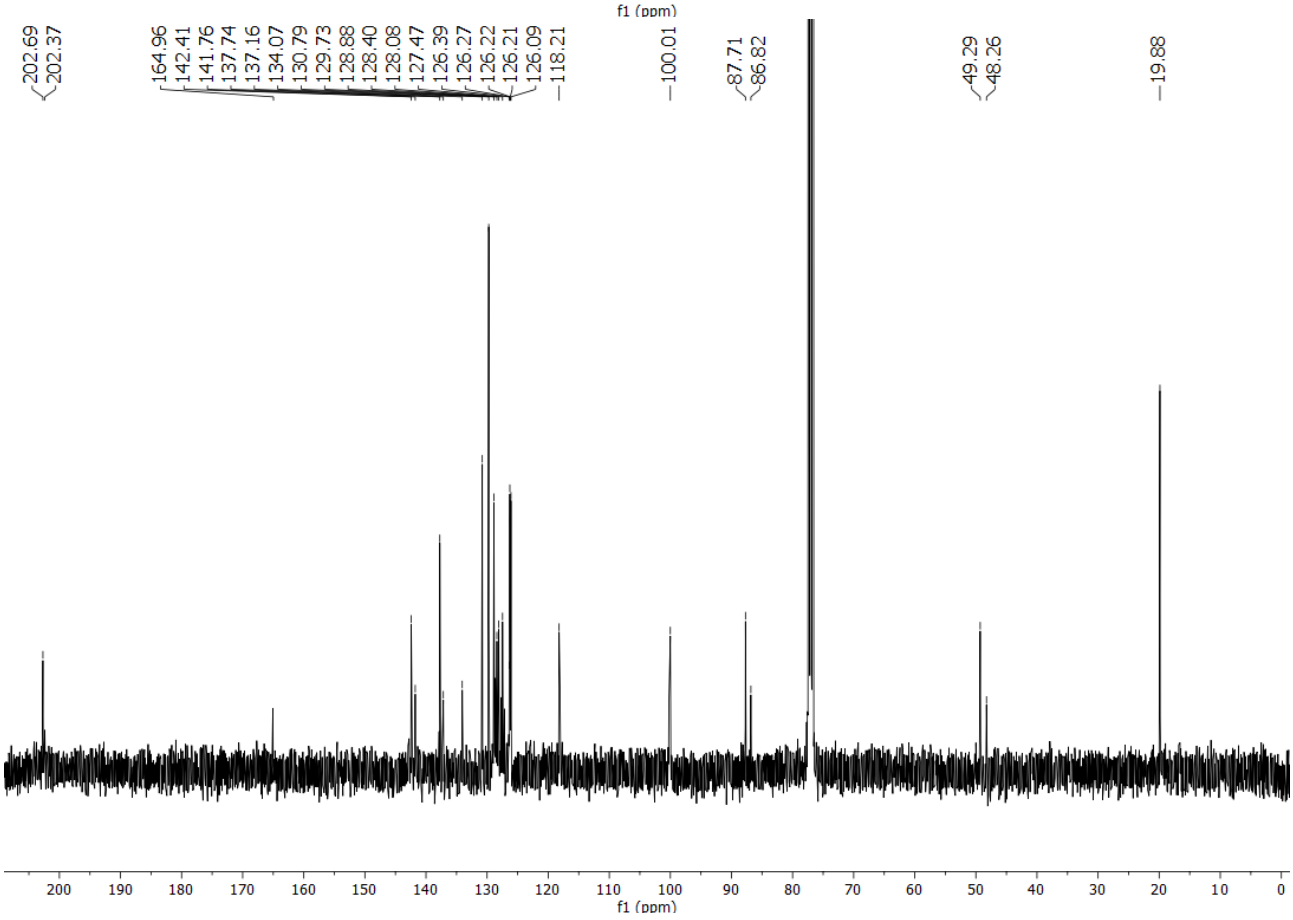
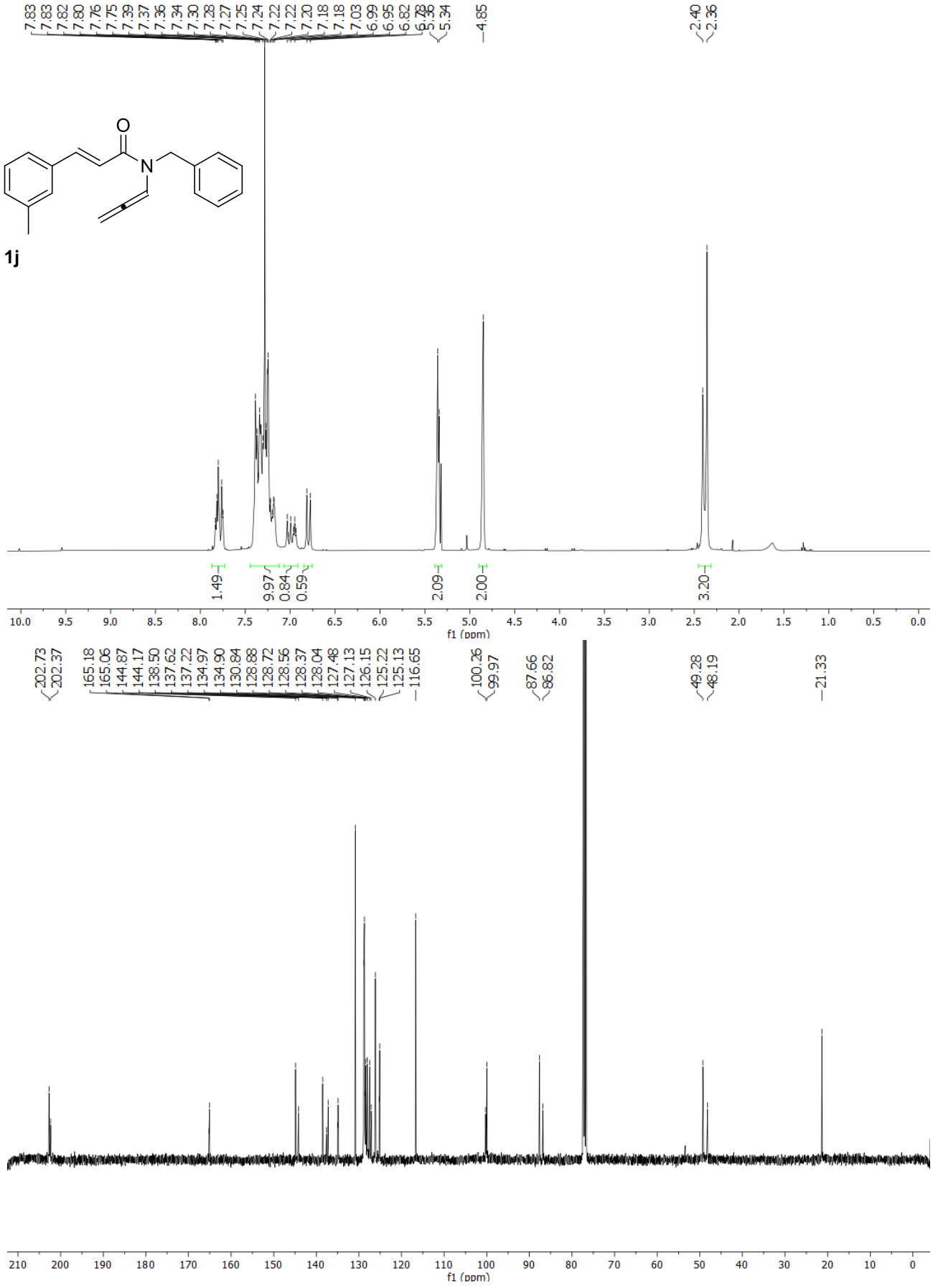
7.80
7.78
7.56
7.37
7.35
7.35
7.33
7.32
7.29
7.26
7.23
7.21
7.18
7.16
7.15
7.13
6.93
6.91
6.89
6.70
6.66
5.34
5.33
4.82
2.45
2.40
O
N
1i
1.00
0.54
0.37
11.85
0.78
0.65
1.96
2.05
1.35
1.76
f1 (ppm)


202.69
202.37
164.96
142.41
141.76
137.74
137.16
134.07
130.79
129.73
128.88
128.40
128.08
127.47
126.39
126.27
126.22
126.21
126.09
118.21
100.01
87.71
86.82
49.29
48.26
19.88
f1 (ppm)


7.83
7.83
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7.80
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7.75
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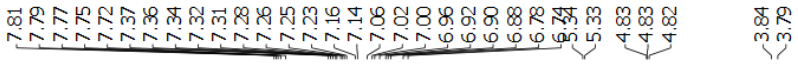
7.37
7.36
7.34
7.30
7.28
7.27
7.25
7.24
7.22
7.22
7.20
7.18
7.18
7.03
6.99
6.95
6.82
6.78
5.36
5.34
4.85
2.40
2.36
O
N
1j
1.49
9.97
0.84
0.59
2.09
2.00
3.20
f1 (ppm)
202.73
202.37
165.18
165.06
144.87
144.17
138.50
137.62
137.22
134.97
134.90
130.84
128.88
128.72
128.56
128.37
128.04
127.48
127.13
126.15
125.22
125.13
116.65
100.26
99.97
87.66
86.82
49.28
48.19
21.33
f1 (ppm)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7.79
7.77
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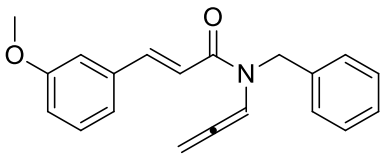
7.72
7.37
7.36
7.34
7.32
7.31
7.28
7.26
7.25
7.23
7.16
7.14
7.06
7.02
7.00
6.96
6.92
6.90
6.88
6.78
6.74
5.34
5.33
4.83
4.83
4.82
3.84
3.79


O
O
N

1k

0.52
0.99
6.73
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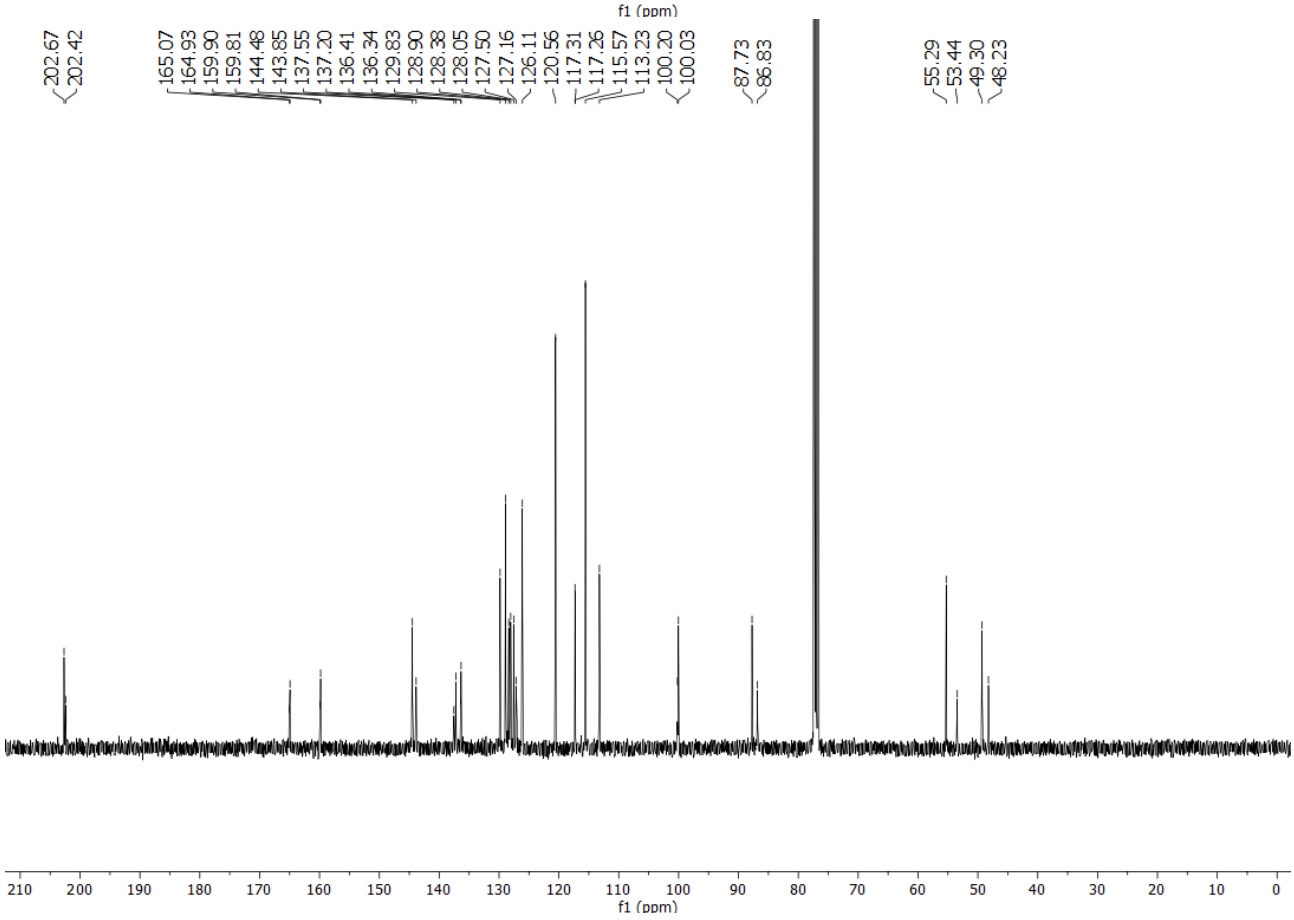
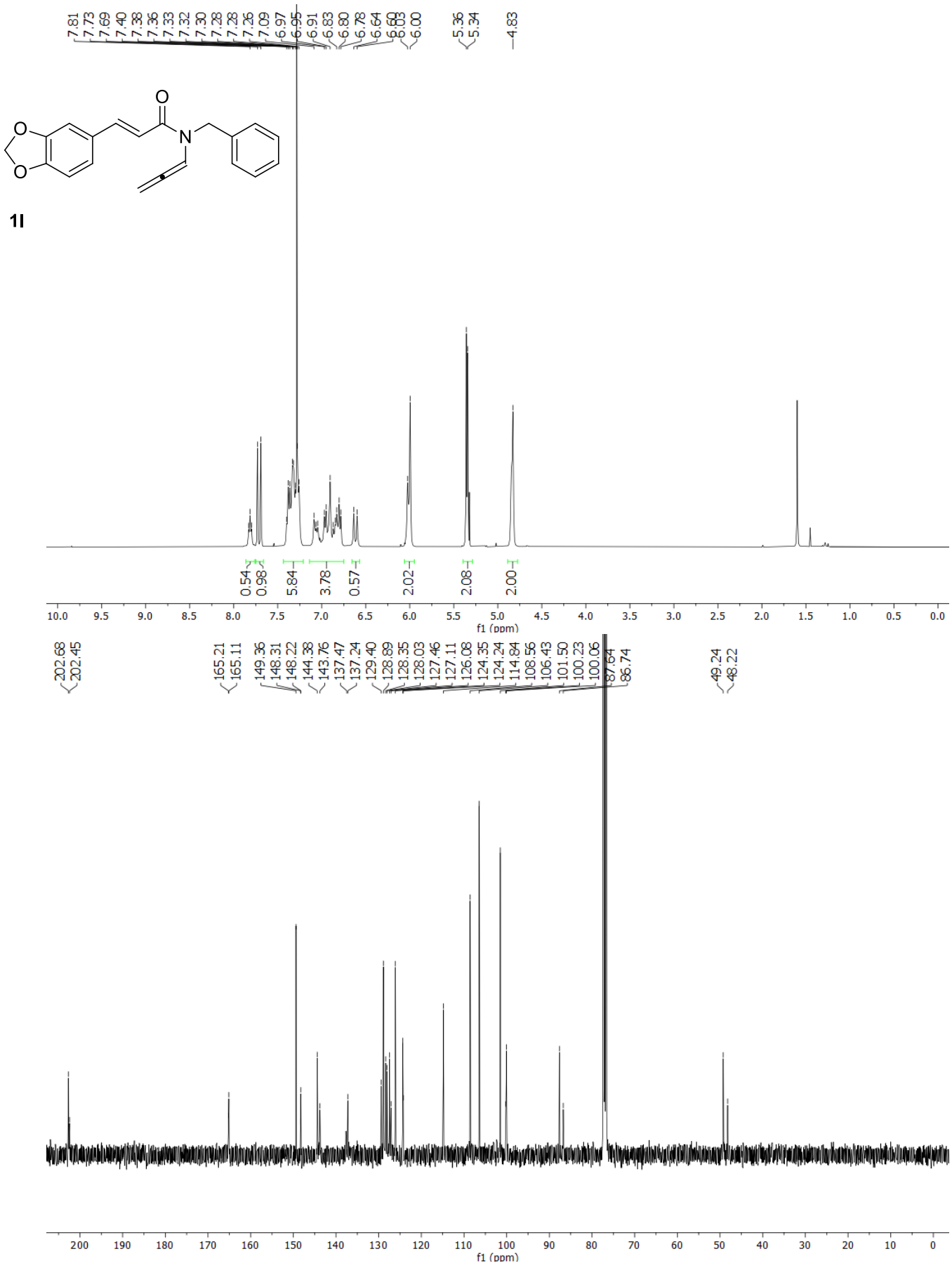
3.52
0.62
2.03
2.01
3.18
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


202.67
202.42
165.07
164.93
159.90
159.81
144.48
143.85
137.55
137.20
136.41
136.34
129.83
128.90
128.38
128.05
127.50
127.16
126.11
120.56
117.31
117.26
115.57
113.23
100.20
100.03
87.73
86.83
55.29
53.44
49.30
48.23
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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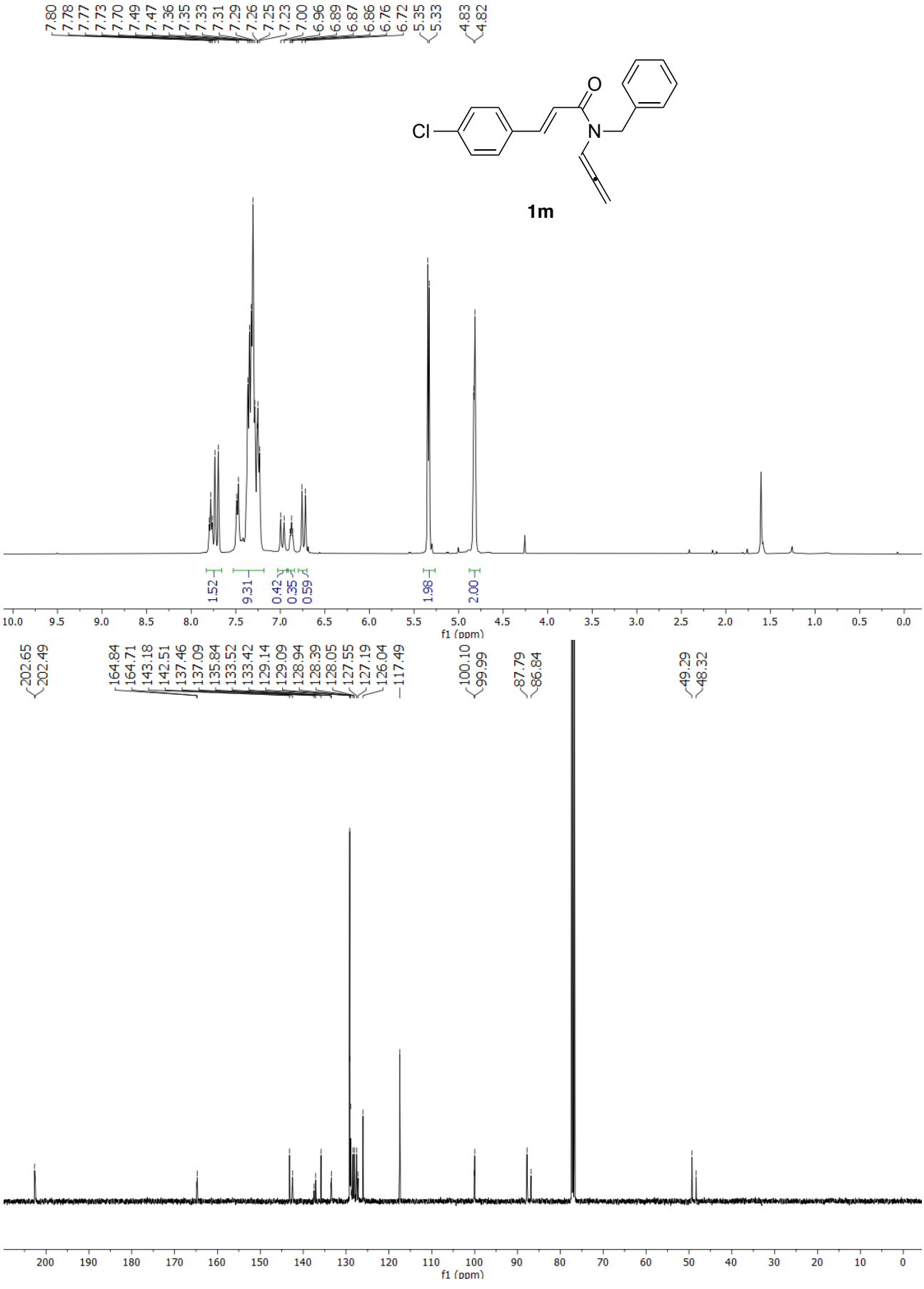
7.73
7.69
7.40
7.38
7.36
7.33
7.32
7.30
7.28
7.28
7.26
7.09
6.97
6.95
6.91
6.83
6.80
6.78
6.64
6.63
6.60
6.00
5.36
5.34
4.83
O
O
O
N
0.54
0.98
5.84
3.78
0.57
2.02
2.08
2.00
f1 (ppm)
202.68
202.45
165.21
165.11
149.36
148.31
148.22
144.38
143.76
137.47
137.24
129.40
128.89
128.35
128.03
127.46
127.11
126.08
124.35
124.24
114.84
108.56
106.43
101.50
100.23
100.06
87.64
86.74
49.24
48.22
f1 (ppm)

1l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7.78
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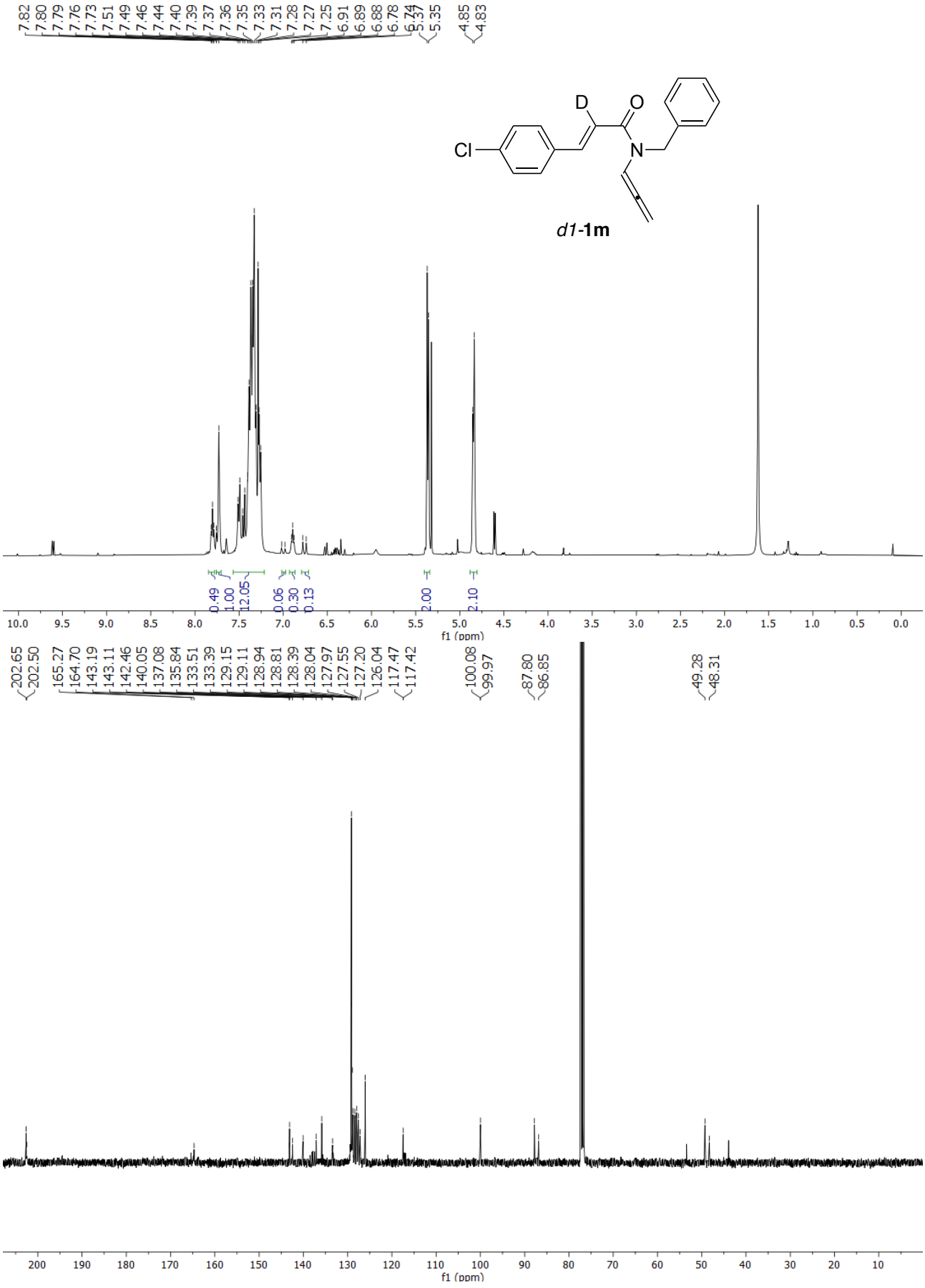
7.73
7.70
7.49
7.47
7.36
7.35
7.33
7.31
7.29
7.26
7.25
7.23
7.00
6.96
6.89
6.87
6.86
6.76
6.72
5.35
5.33
4.83
4.82
Cl
O
N
1m
1.52
9.31
0.42
0.35
0.59
1.98
2.00
f1 (ppm)
202.65
202.49
164.84
164.71
143.18
142.51
137.46
137.09
135.84
133.52
133.42
129.14
129.09
128.94
128.39
128.05
127.55
127.19
126.04
117.49
100.10
99.99
87.79
86.84
49.29
48.32
f1 (ppm)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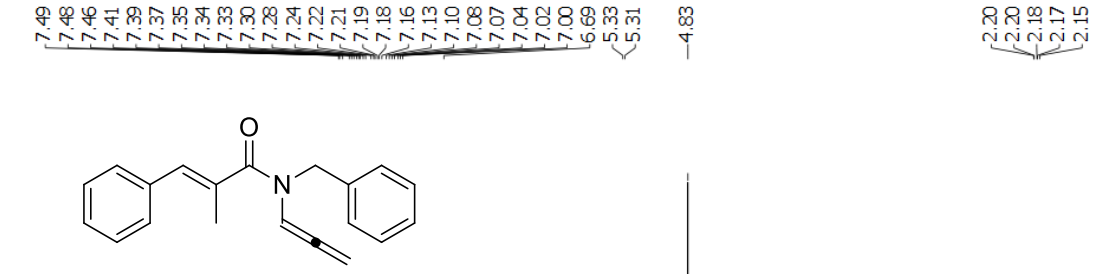
7.80
7.79
7.76
7.73
7.51
7.49
7.46
7.44
7.40
7.39
7.37
7.36
7.35
7.33
7.31
7.28
7.27
7.25
6.91
6.89
6.88
6.78
6.74
5.37
5.35
4.85
4.83
D
O
Cl
N
0.49
1.00
12.05
0.06
0.30
0.13
2.00
2.10
f1 (ppm)
202.65
202.50
165.27
164.70
143.19
143.11
142.46
140.05
137.08
135.84
133.51
133.39
129.15
129.11
128.94
128.81
128.39
128.04
127.97
127.55
127.20
126.04
117.47
117.42
100.08
99.97
87.80
86.85
49.28
48.31
f1 (ppm)

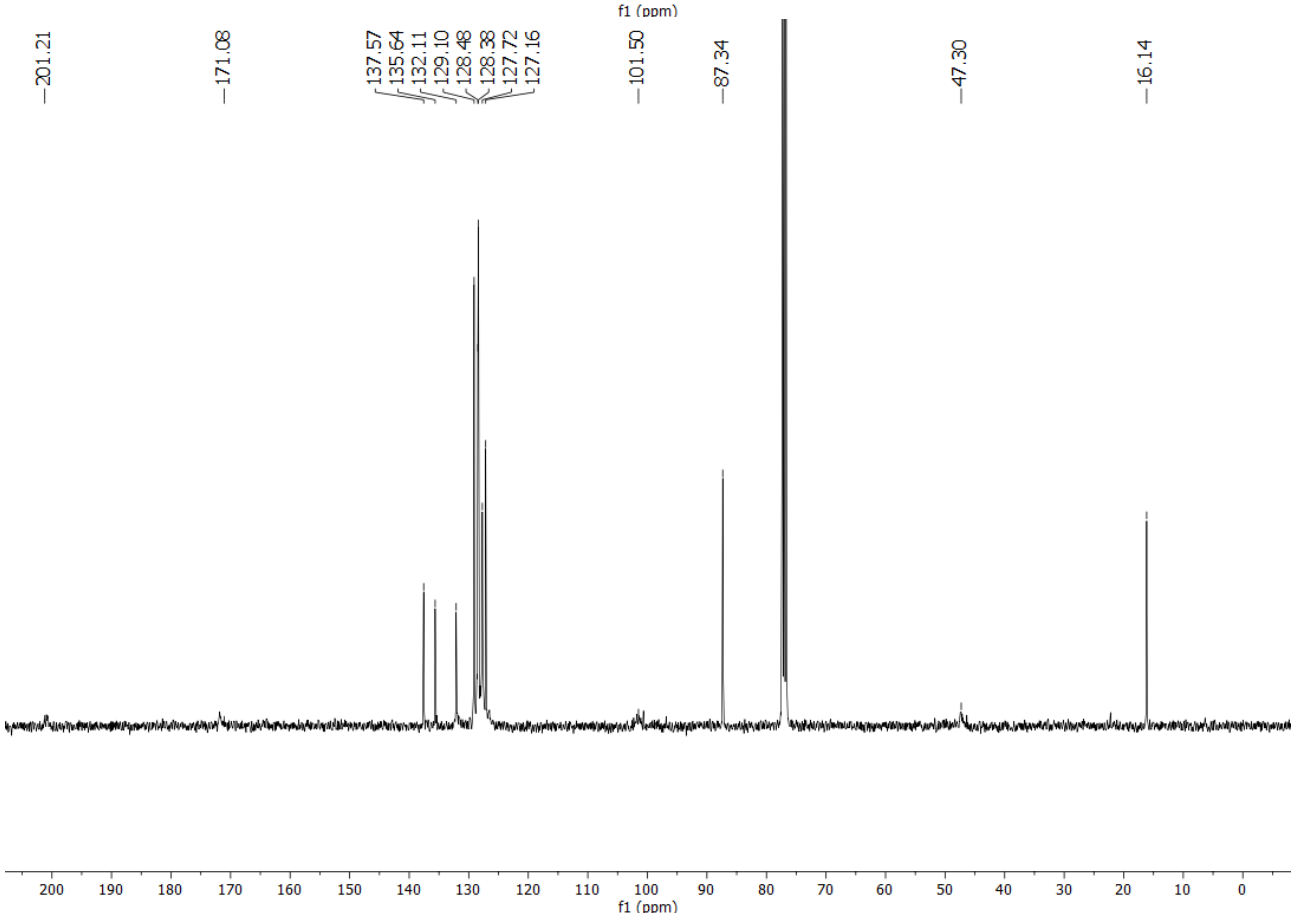
d1-**1m**

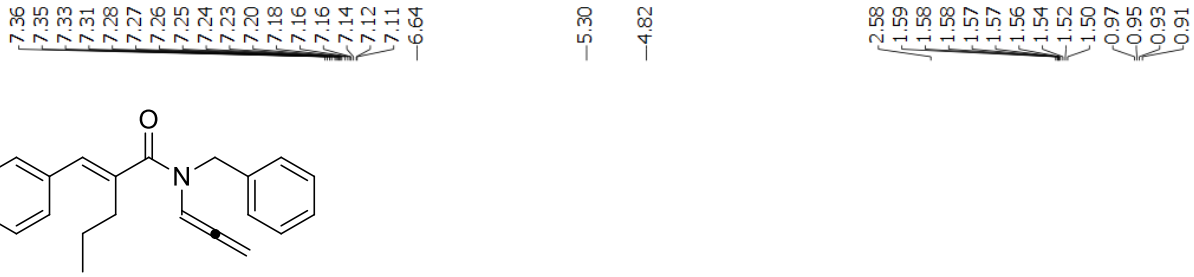

7.49
7.48
7.46
7.41
7.39
7.37
7.35
7.34
7.33
7.30
7.28
7.24
7.22
7.21
7.19
7.18
7.16
7.13
7.10
7.08
7.07
7.04
7.02
7.00
6.69
5.33
5.31
4.83
2.20
2.20
2.18
2.17
2.15

O
N

3a

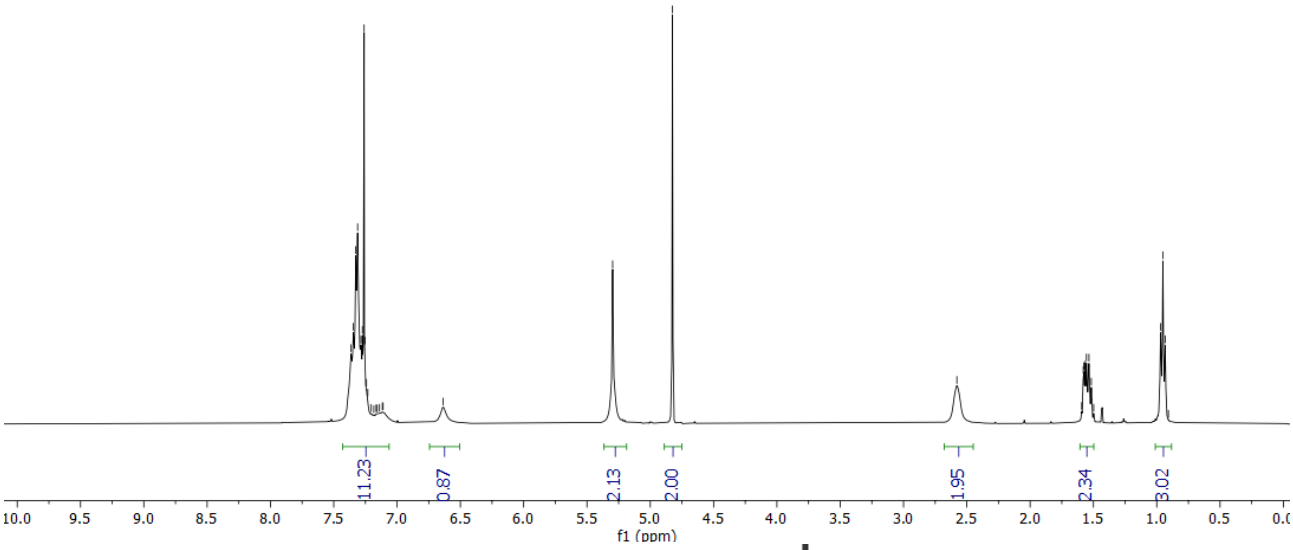
12.98
0.97
2.00
2.20
3.03
f1 (ppm)

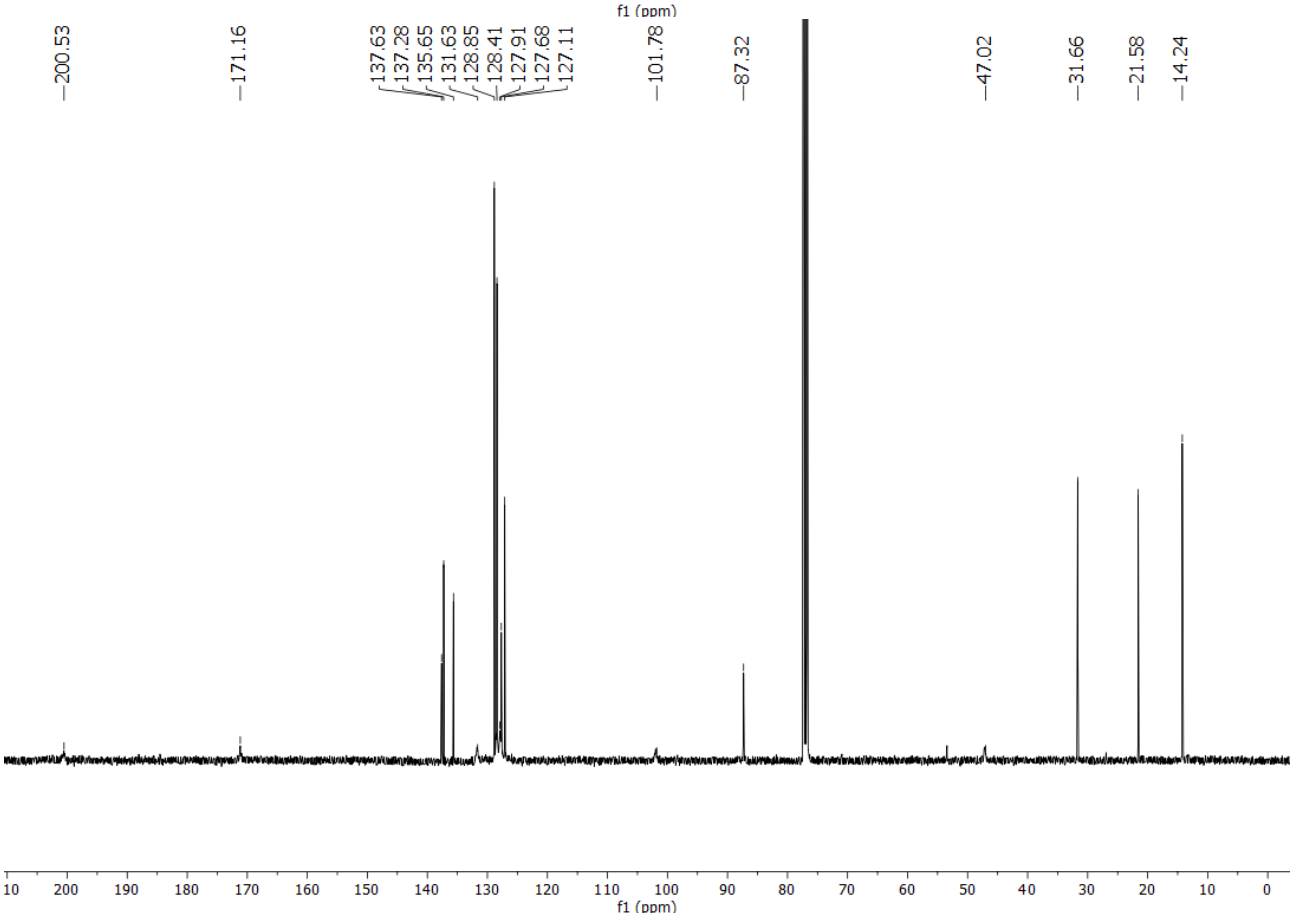

201.21
171.08
137.57
135.64
132.11
129.10
128.48
128.38
127.72
127.16
101.50
87.34
47.30
16.14
f1 (ppm)

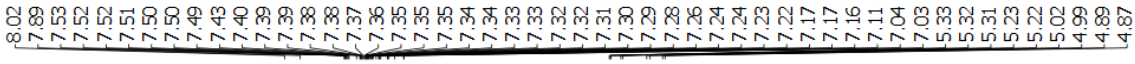

7.36
7.35
7.33
7.31
7.28
7.27
7.26
7.25
7.24
7.23
7.20
7.18
7.16
7.16
7.14
7.12
7.11
6.64
5.30
4.82
2.58
1.59
1.58
1.58
1.57
1.57
1.56
1.54
1.52
1.50
0.97
0.95
0.93
0.91

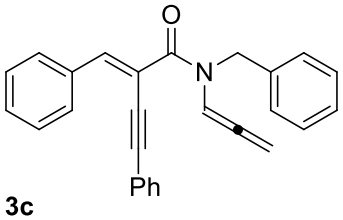
O
N

3b

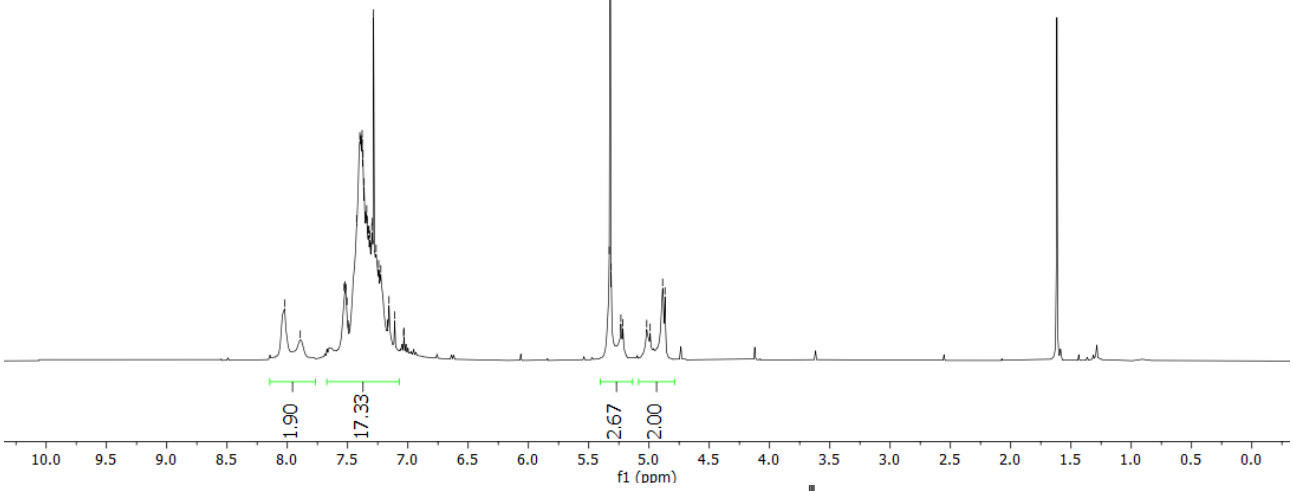

11.23
0.87
2.13
2.00
1.95
2.34
3.02
f1 (ppm)


200.53
171.16
137.63
137.28
135.65
131.63
128.85
128.41
127.91
127.68
127.11
101.78
87.32
47.02
31.66
21.58
14.24
f1 (ppm)


8.02
7.89
7.53
7.52
7.52
7.51
7.50
7.50
7.49
7.43
7.40
7.39
7.39
7.38
7.37
7.36
7.35
7.35
7.35
7.34
7.34
7.33
7.33
7.32
7.32
7.31
7.30
7.29
7.28
7.26
7.24
7.24
7.23
7.22
7.17
7.17
7.16
7.11
7.04
7.03
5.33
5.32
5.31
5.23
5.22
5.02
4.99
4.89
4.87


O
N
Ph

3c


1.90
17.33
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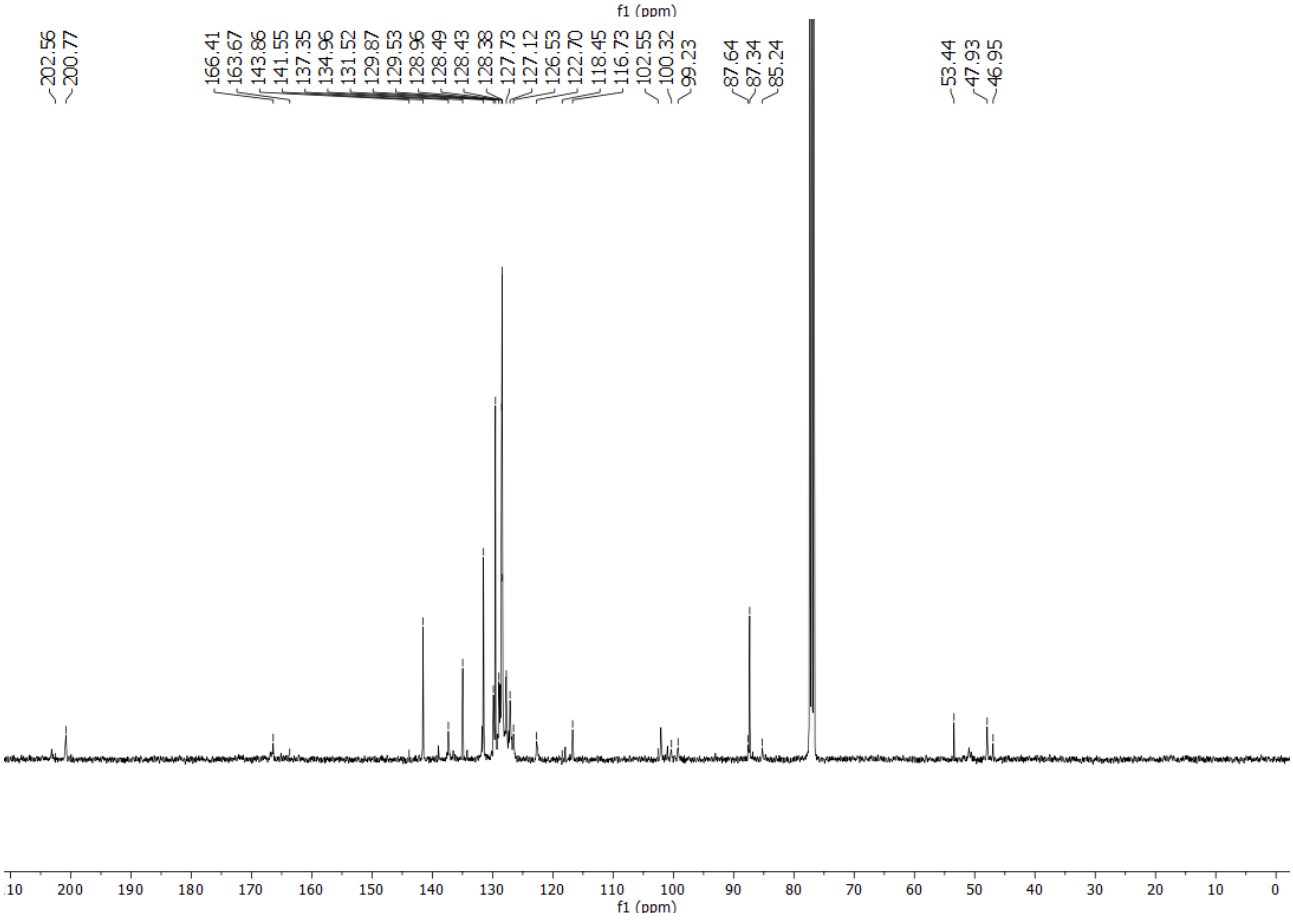
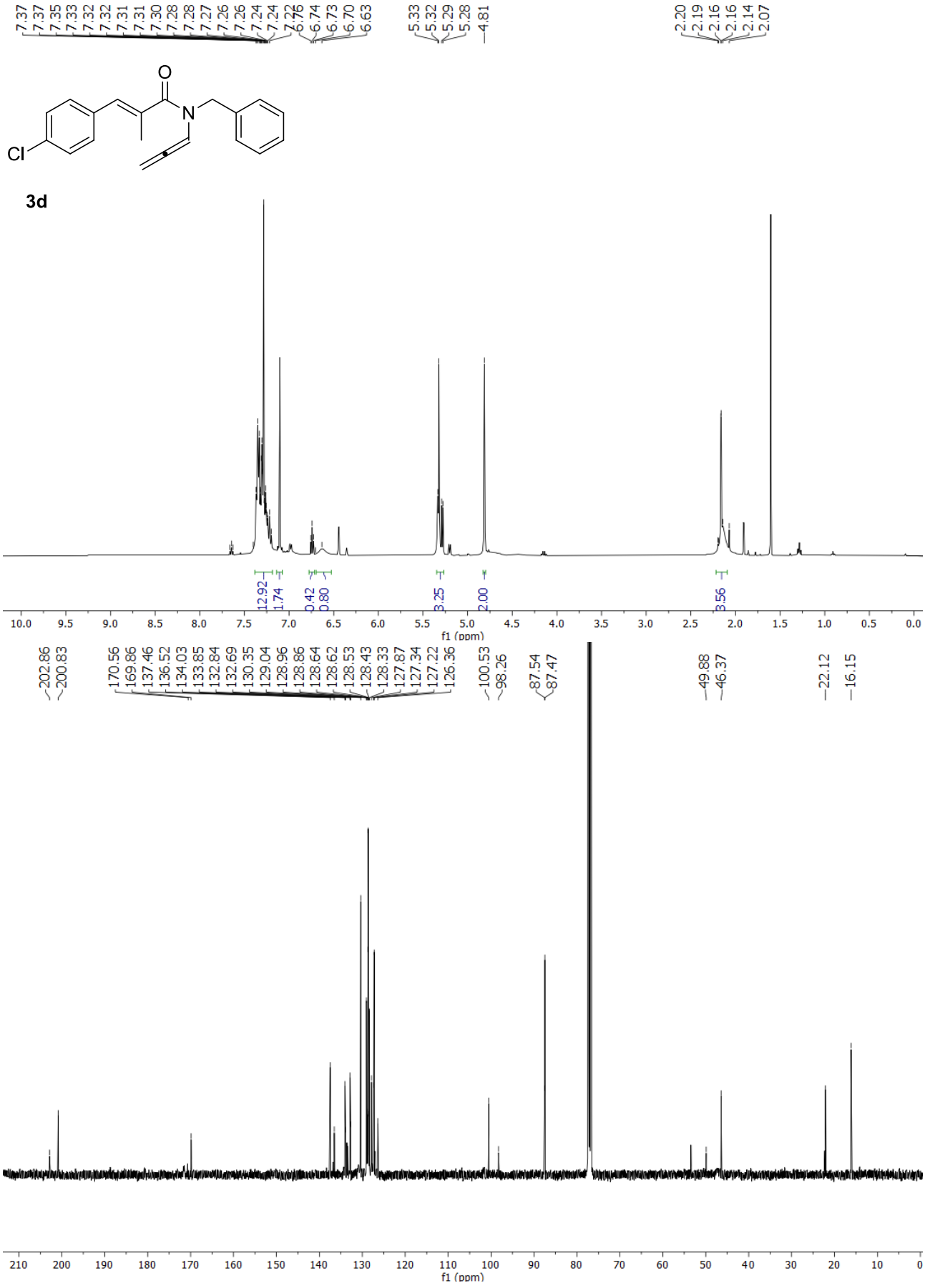
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


202.56
200.77
166.41
163.67
143.86
141.55
137.35
134.96
131.52
129.87
129.53
128.96
128.49
128.43
128.38
127.73
127.12
126.53
122.70
118.45
116.73
102.55
100.32
99.23
87.64
87.34
85.24
53.44
47.93
46.95
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.37
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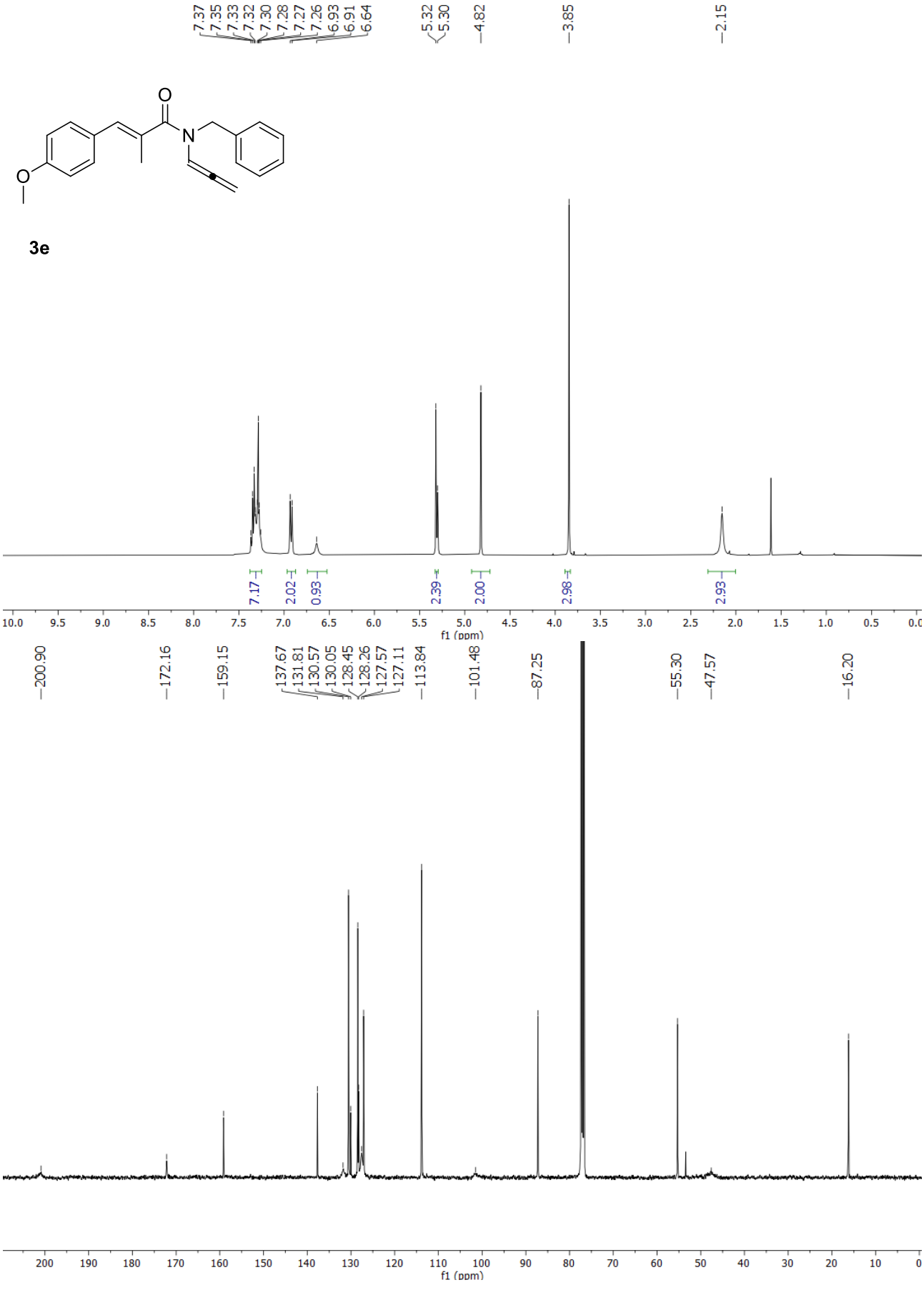
7.32
7.31
7.31
7.30
7.28
7.28
7.27
7.26
7.26
7.24
7.24
7.22
6.76
6.74
6.73
6.70
6.63
5.33
5.32
5.29
5.28
4.81
2.20
2.19
2.16
2.16
2.14
2.07
O
N
Cl
3d
12.92
1.74
0.42
0.80
3.25
2.00
3.56
f1 (ppm)
202.86
200.83
170.56
169.86
137.46
136.52
134.03
133.85
132.84
132.69
130.35
129.04
128.96
128.86
128.64
128.62
128.53
128.43
128.33
127.87
127.34
127.22
126.36
100.53
98.26
87.54
87.47
49.88
46.37
22.12
16.15
f1 (ppm)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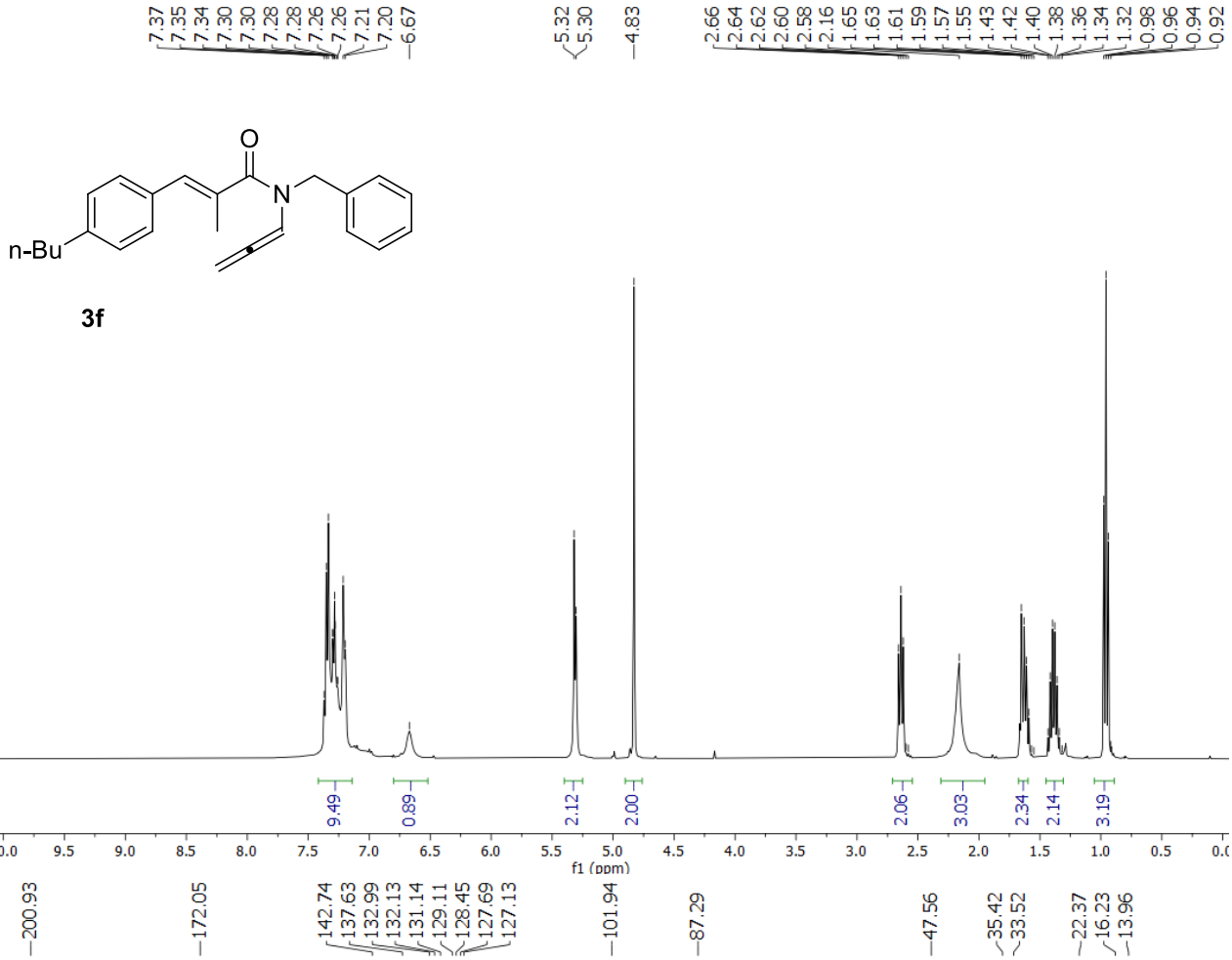
7.35
7.33
7.32
7.30
7.28
7.27
7.26
6.93
6.91
6.64
5.32
5.30
4.82
3.85
2.15
O
N
O
7.17
2.02
0.93
2.39
2.00
2.98
2.93
f1 (ppm)
200.90
172.16
159.15
137.67
131.81
130.57
130.05
128.45
128.26
127.57
127.11
113.84
101.48
87.25
55.30
47.57
16.20
f1 (ppm)

3e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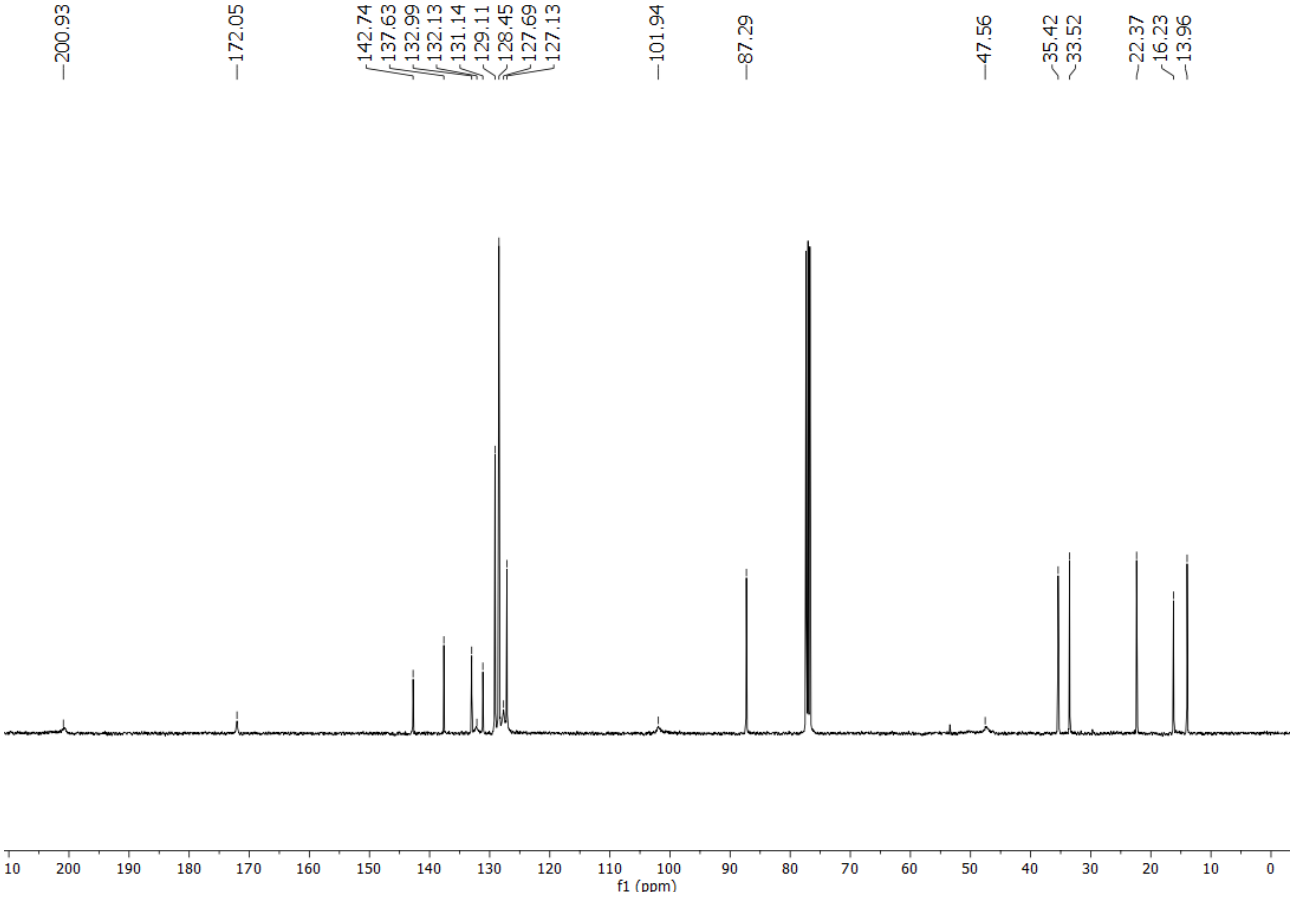
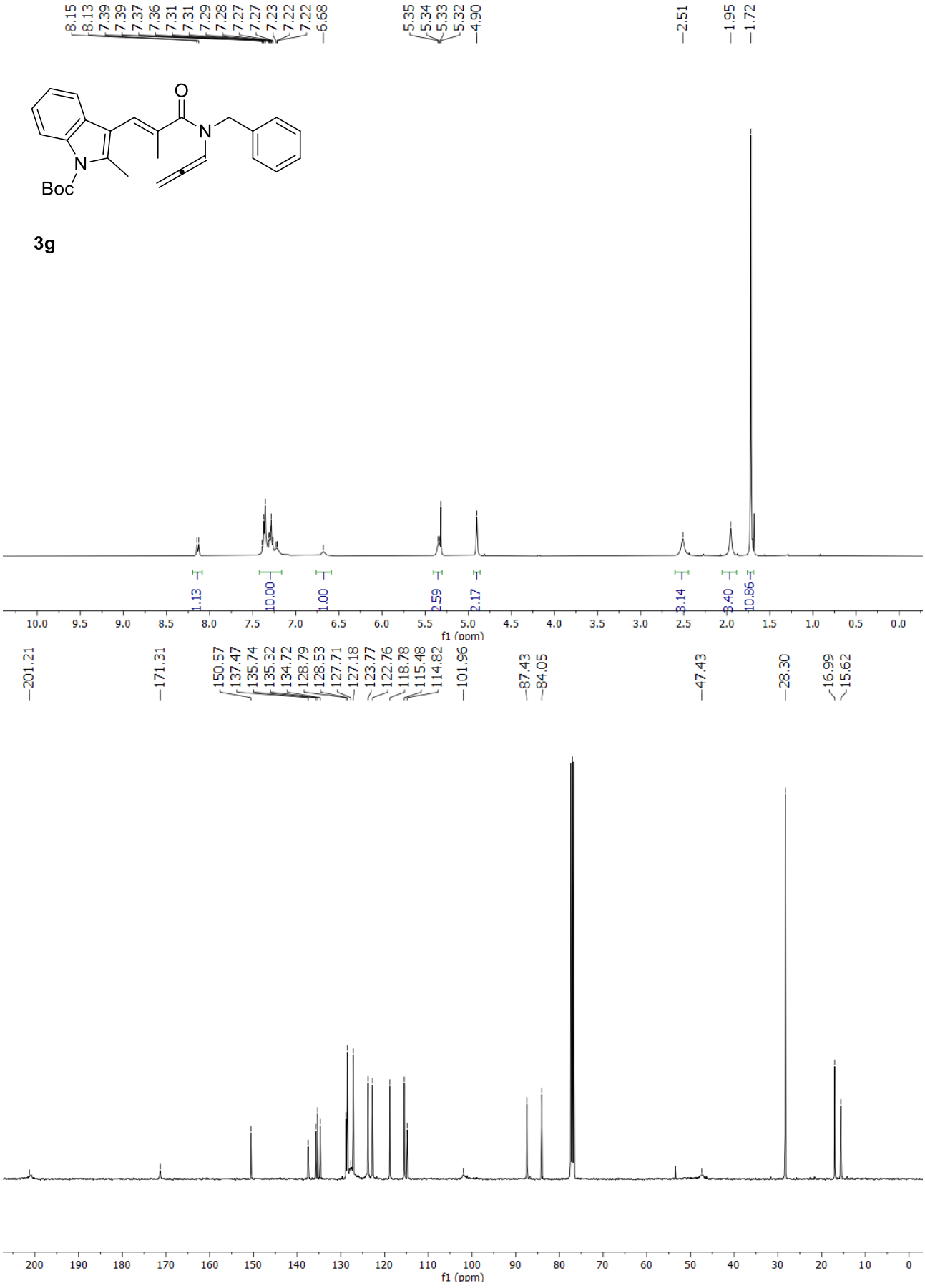
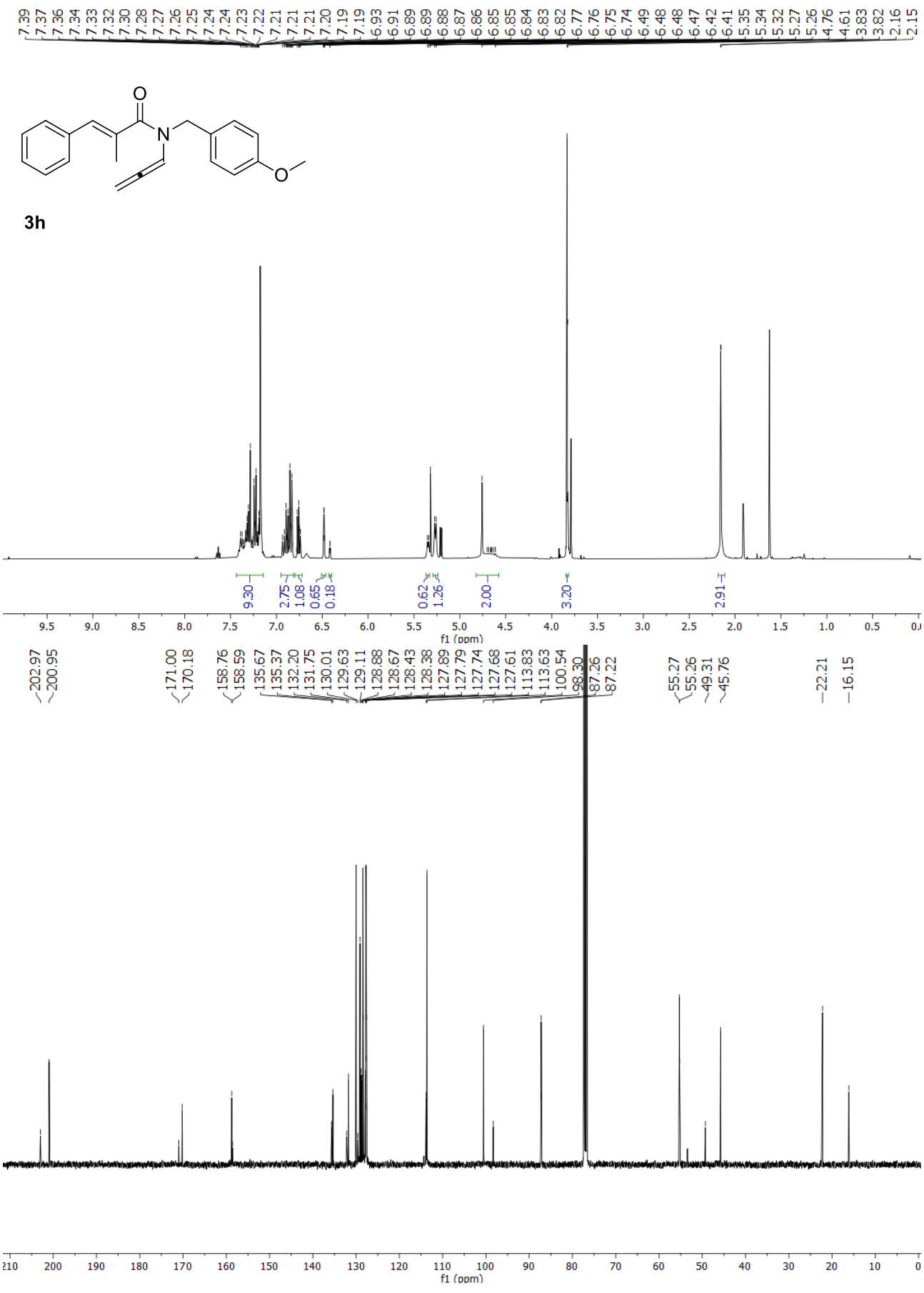
7.35
7.34
7.30
7.30
7.28
7.26
7.26
7.21
7.20
6.67
5.32
5.30
4.83
2.66
2.64
2.62
2.60
2.58
2.16
1.65
1.63
1.61
1.59
1.57
1.55
1.43
1.42
1.40
1.38
1.36
1.34
1.32
0.98
0.96
0.94
0.92
O
N
n-Bu
9.49
0.89
2.12
2.00
2.06
3.03
2.34
2.14
3.19
f1 (ppm)

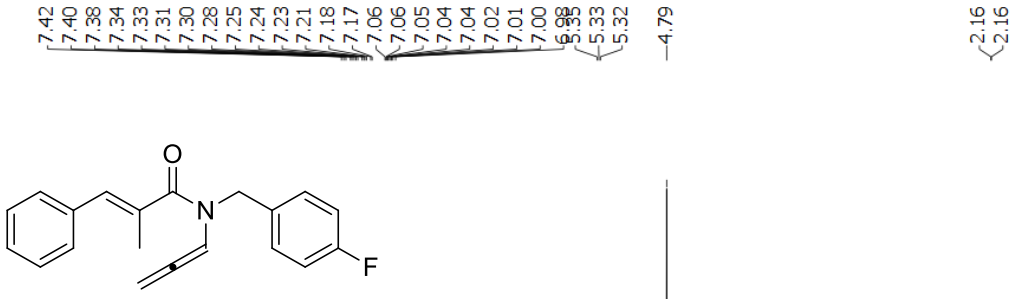
3f


200.93
172.05
142.74
137.63
132.99
132.13
131.14
129.11
128.45
127.69
127.13
101.94
87.29
47.56
35.42
33.52
22.37
16.23
13.96
f1 (ppm)


8.15
8.13
7.39
7.39
7.37
7.36
7.31
7.31
7.29
7.28
7.27
7.27
7.23
7.22
7.22
6.68
5.35
5.34
5.33
5.32
4.90
2.51
1.95
1.72
O
N
N
Boc
1.13
10.00
1.00
2.59
2.17
3.14
3.40
10.86
f1 (ppm)
201.21
171.31
150.57
137.47
135.74
135.32
134.72
128.79
128.53
127.71
127.18
123.77
122.76
118.78
115.48
114.82
101.96
87.43
84.05
47.43
28.30
16.99
15.62
f1 (ppm)

3g


7.39 7.37 7.36 7.34 7.33 7.32 7.30 7.28 7.27 7.26 7.25 7.24 7.24 7.23 7.22 7.21 7.21 7.21 7.20 7.19 7.19 6.93 6.91 6.89 6.89 6.88 6.87 6.86 6.85 6.85 6.84 6.83 6.82 6.77 6.76 6.75 6.74 6.49 6.48 6.47 6.42 6.41 5.35 5.34 5.32 5.27 5.26 4.76 4.61 3.83 3.82 2.16 2.15
O
N
O
3h
9.30 2.75 1.08 0.65 0.18 0.62 1.26 2.00 3.20 2.91
f1 (ppm)
202.97 200.95 171.00 170.18 158.76 158.59 135.67 135.37 132.20 131.75 130.01 129.63 129.11 128.88 128.67 128.43 128.38 127.89 127.79 127.74 127.68 127.61 113.83 113.63 100.54 98.30 87.26 87.22 55.27 55.26 49.31 45.76 22.21 16.15
f1 (ppm)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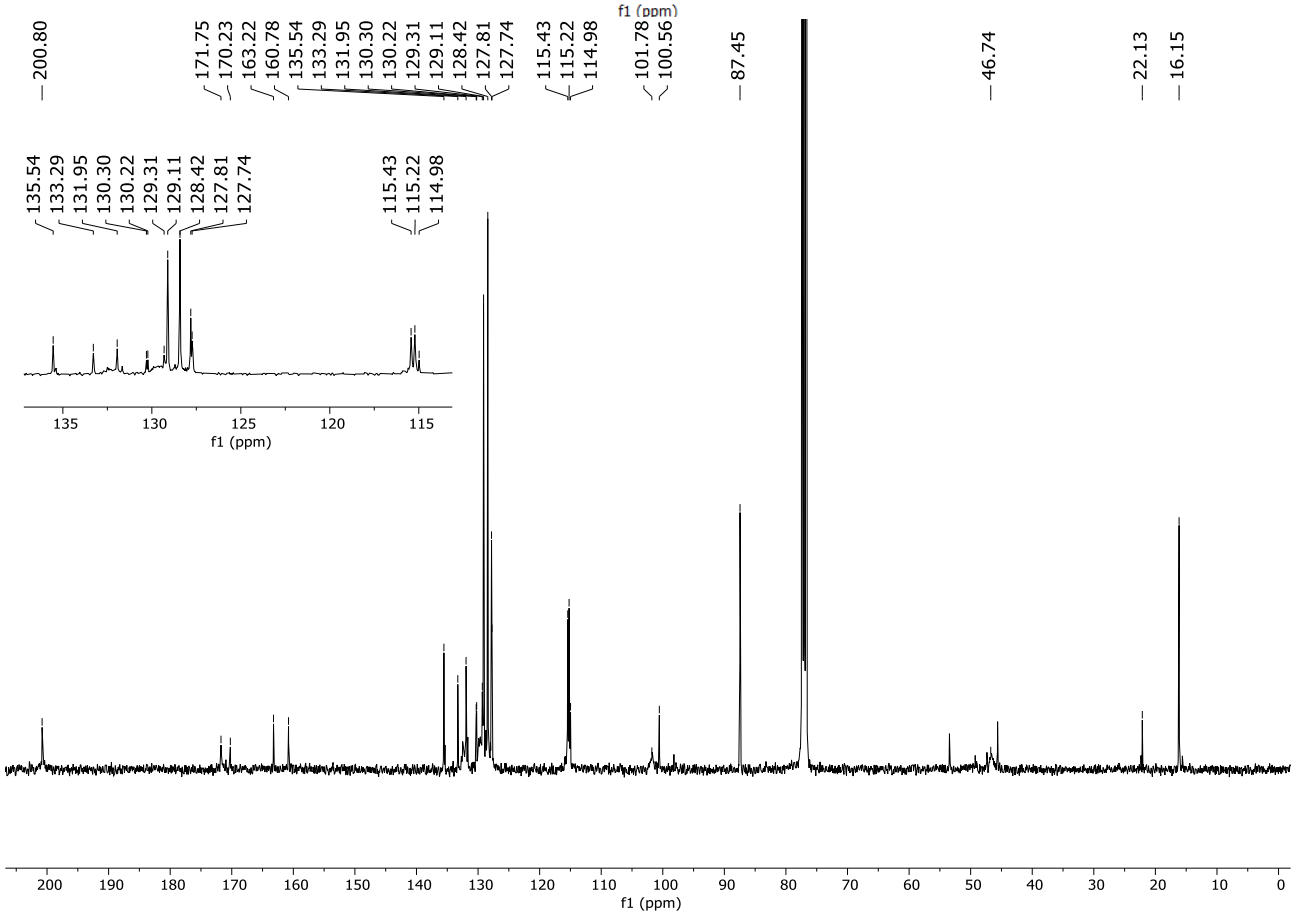
7.31
7.30
7.28
7.25
7.24
7.23
7.21
7.18
7.17
7.06
7.06
7.05
7.04
7.04
7.02
7.01
7.00
6.98
5.35
5.33
5.32
4.79
2.16
2.16

O
N
F

3i

9.17
2.83
0.82
2.27
1.95
3.08
f1 (ppm)


200.80
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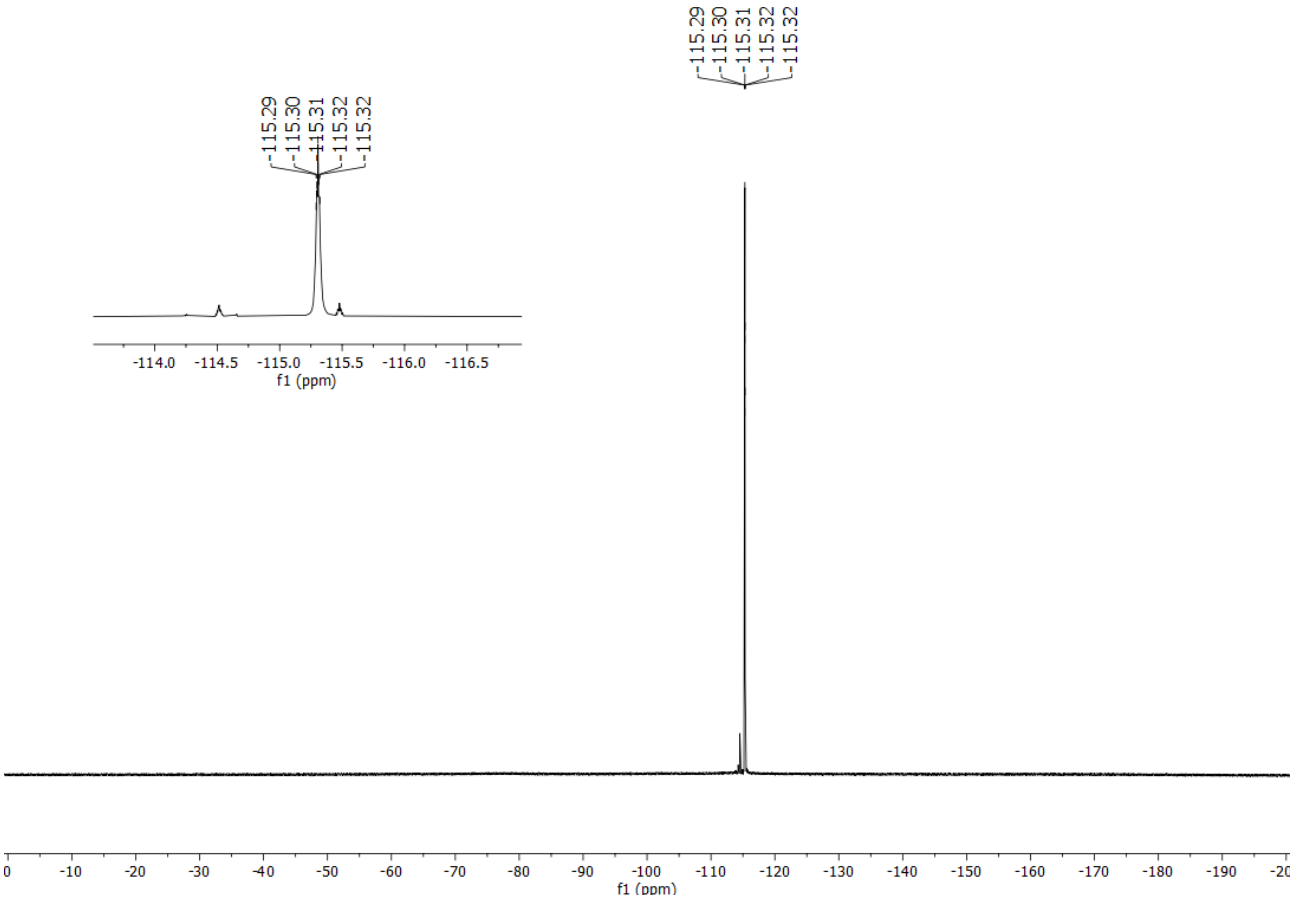
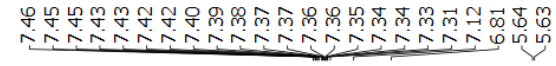
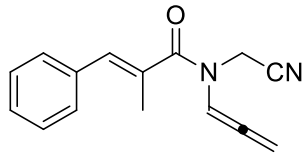
170.23
163.22
160.78
135.54
133.29
131.95
130.30
130.22
129.31
129.11
128.42
127.81
127.74
115.43
115.22
114.98
101.78
100.56
87.45
46.74
22.13
16.15
f1 (ppm)

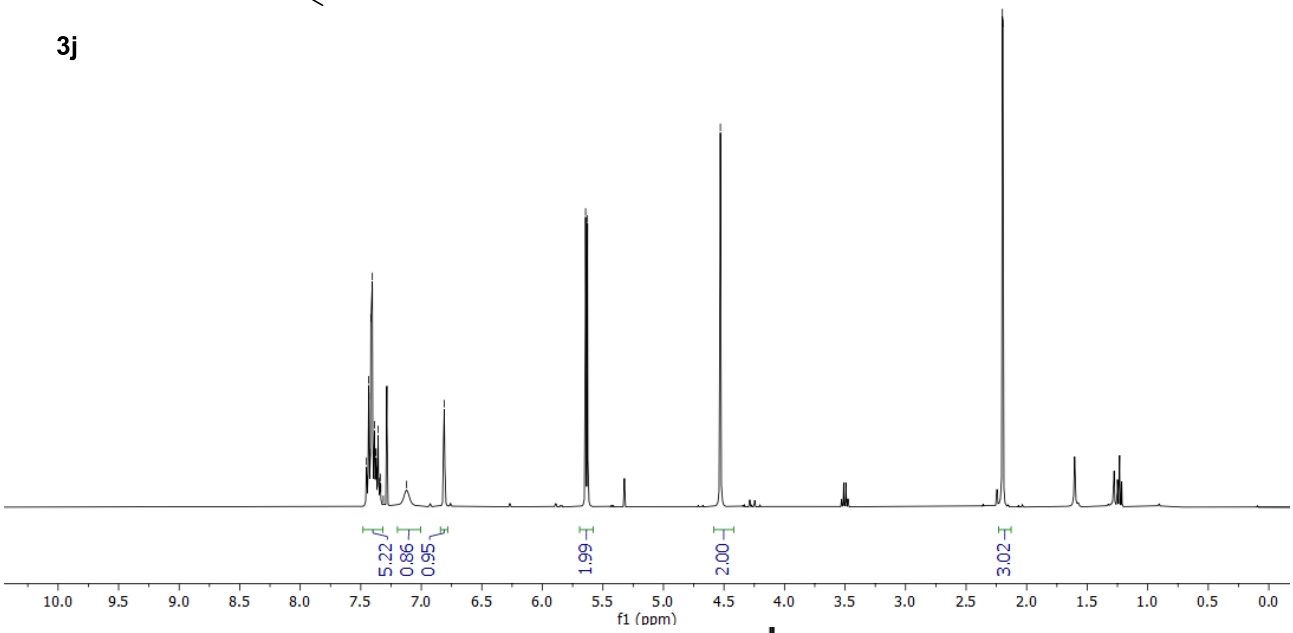
135.54
133.29
131.95
130.30
130.22
129.31
129.11
128.42
127.81
127.74
115.43
115.22
114.98
135
130
125
120
115
f1 (ppm)

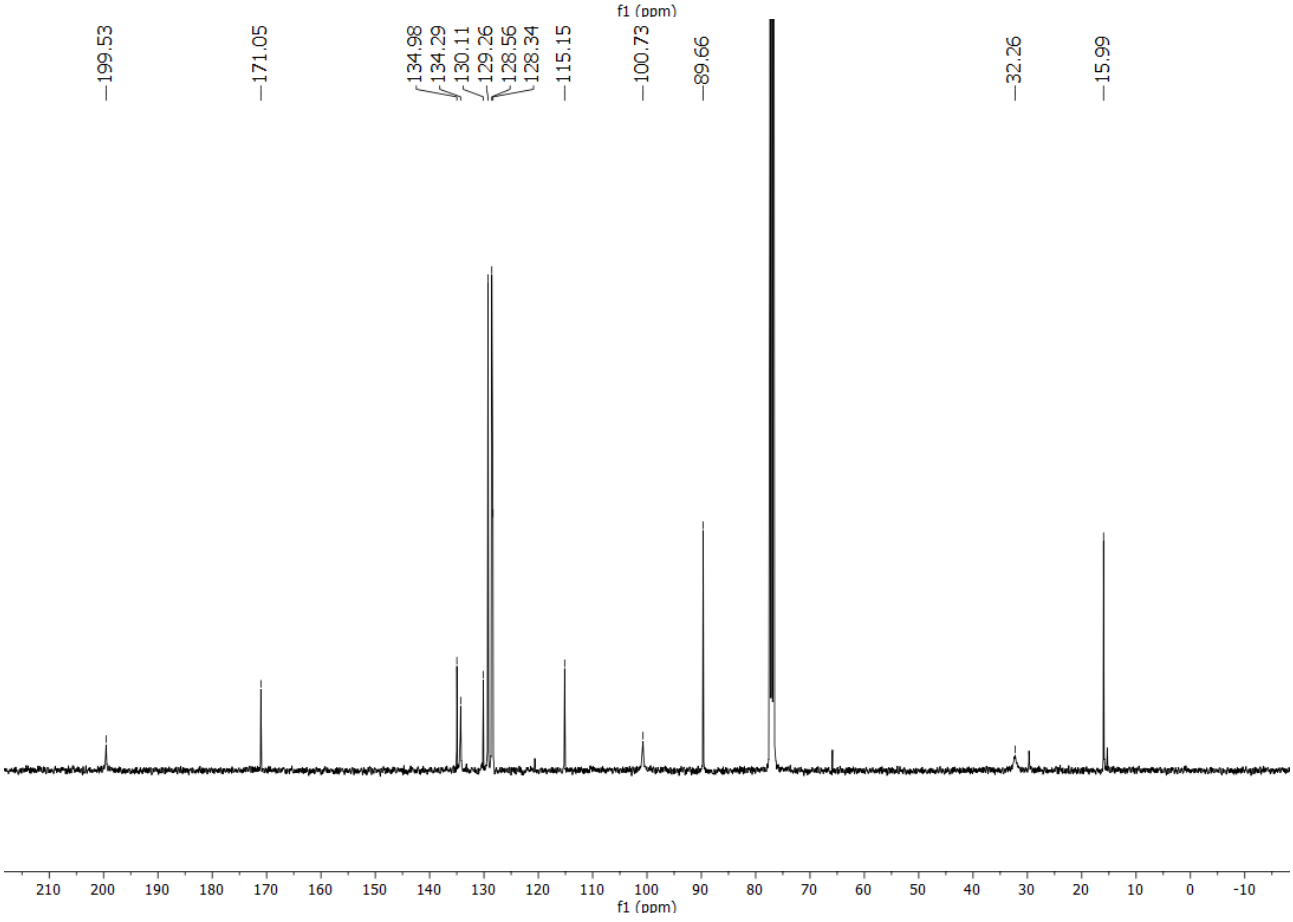

-115.29
-115.30
-115.31
-115.32
-115.32
-114.0
-114.5
-115.0
-115.5
-116.0
-116.5
f1 (ppm)
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

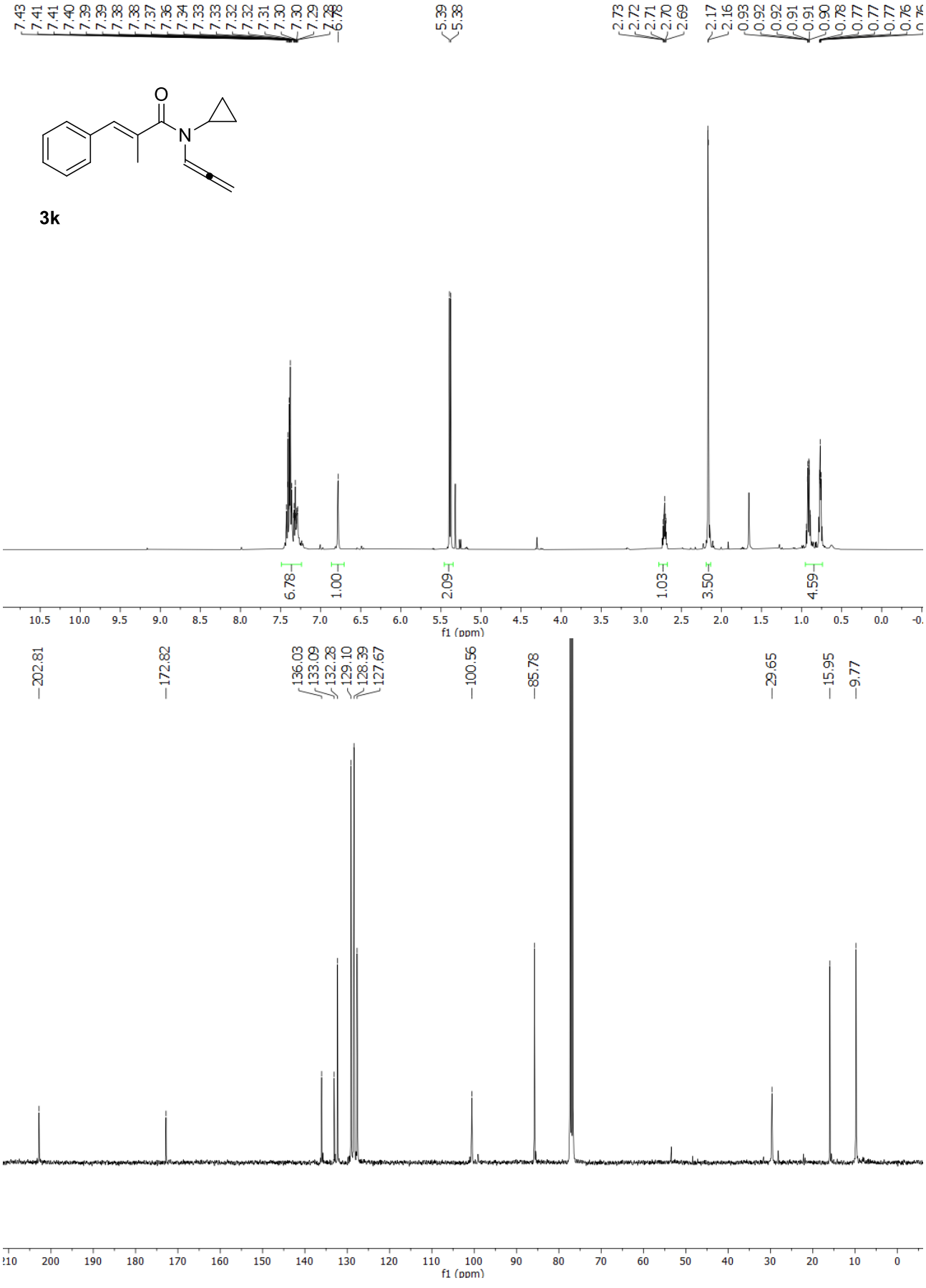

7.46
7.45
7.45
7.43
7.43
7.42
7.42
7.40
7.39
7.38
7.37
7.37
7.36
7.36
7.35
7.34
7.34
7.33
7.31
7.12
6.81
5.64
5.63
4.53
2.20
2.20

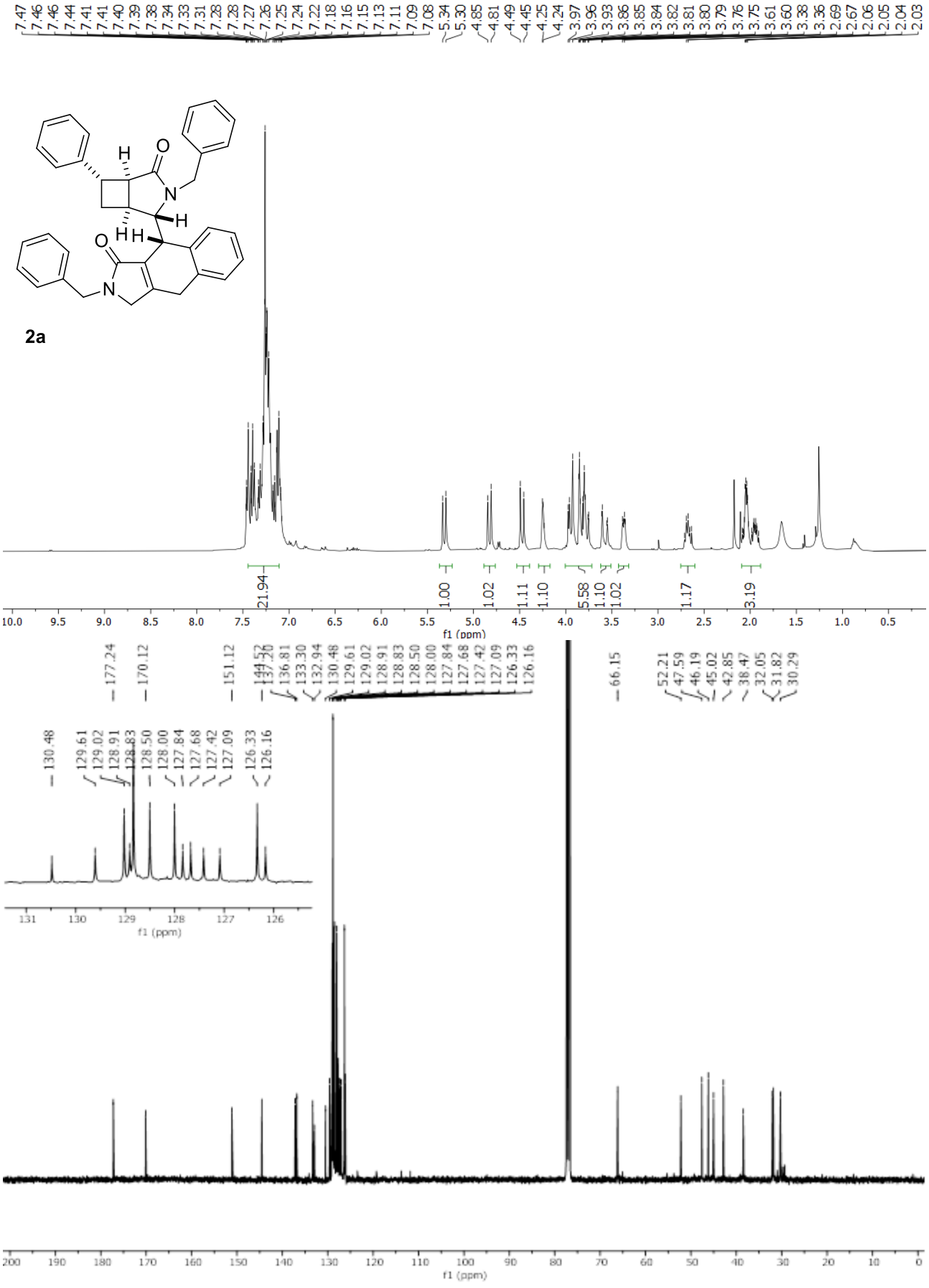

O
N
CN

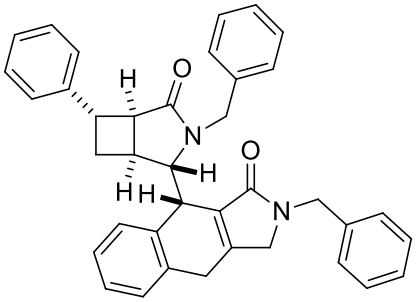
3j


5.22
0.86
0.95
1.99
2.00
3.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

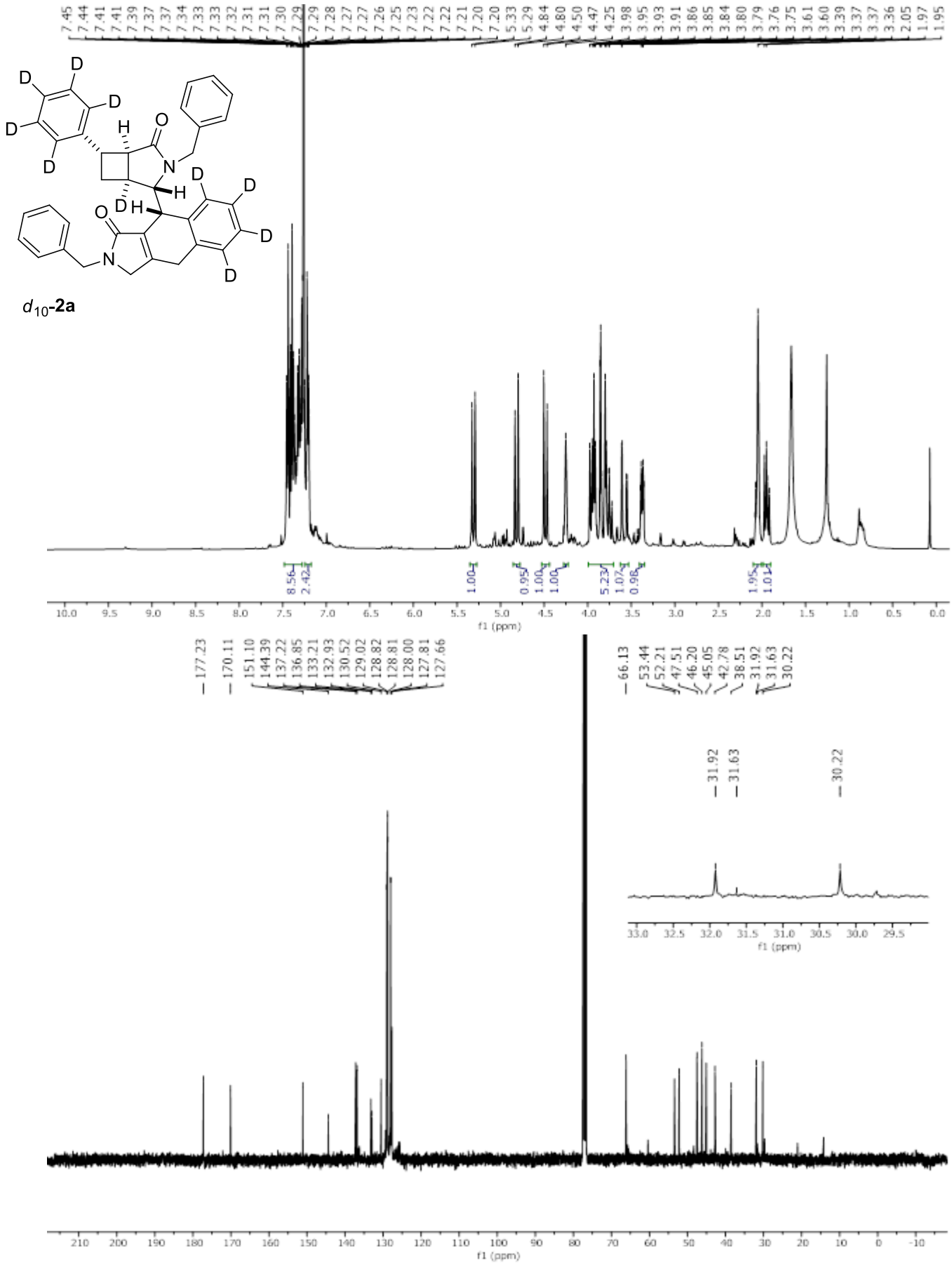

199.53
171.05
134.98
134.29
130.11
129.26
128.56
128.34
115.15
100.73
89.66
32.26
15.99
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

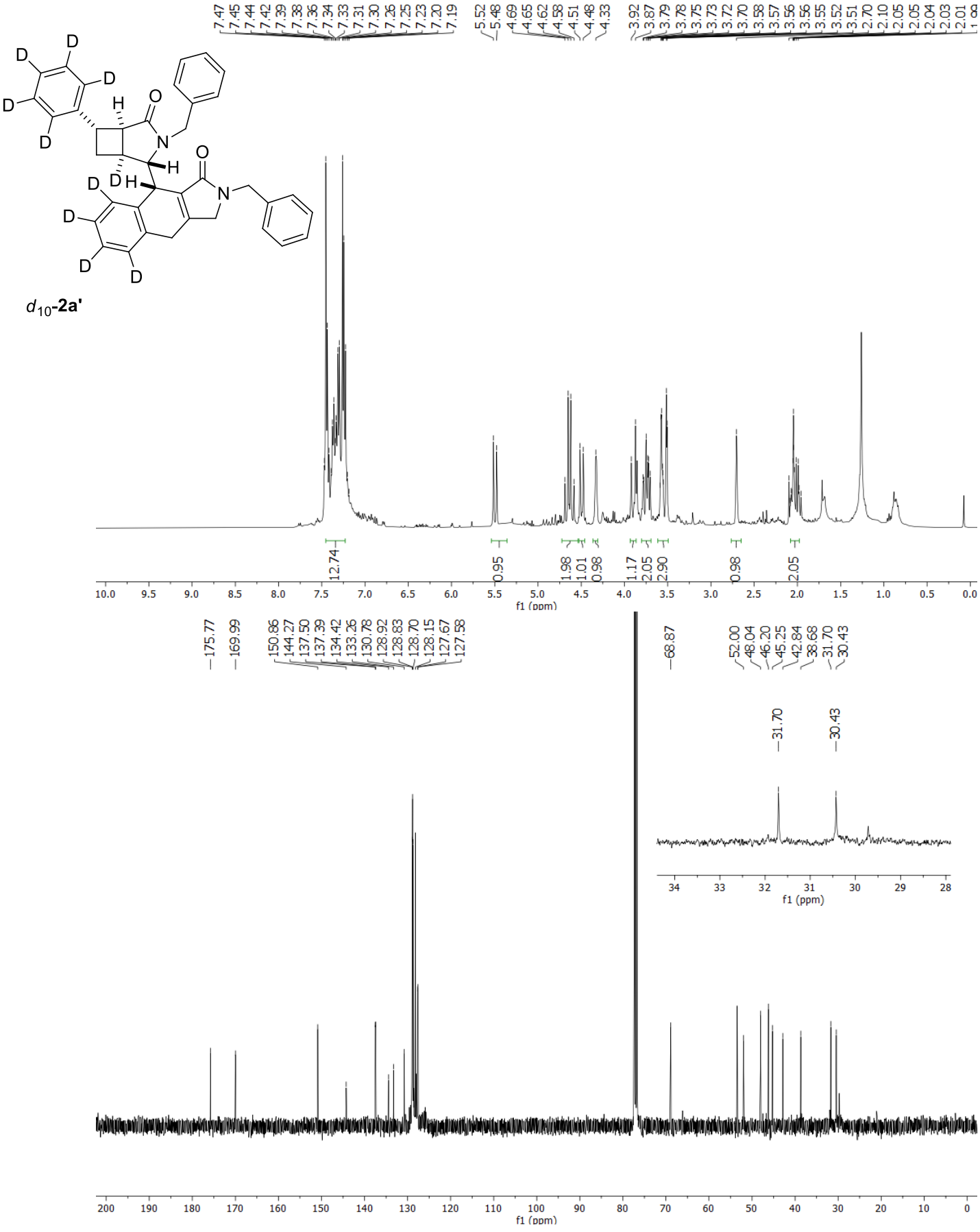

7.43
7.41
7.41
7.40
7.39
7.39
7.38
7.38
7.37
7.36
7.34
7.33
7.33
7.32
7.32
7.31
7.30
7.30
7.29
6.78
5.39
5.38
2.73
2.72
2.71
2.70
2.69
2.17
2.16
0.93
0.92
0.92
0.91
0.91
0.90
0.78
0.77
0.77
0.77
0.76
O
N
3k
6.78
1.00
2.09
1.03
3.50
4.59
f1 (ppm)
202.81
172.82
136.03
133.09
132.28
129.10
128.39
127.67
100.56
85.78
29.65
15.95
9.77
f1 (ppm)

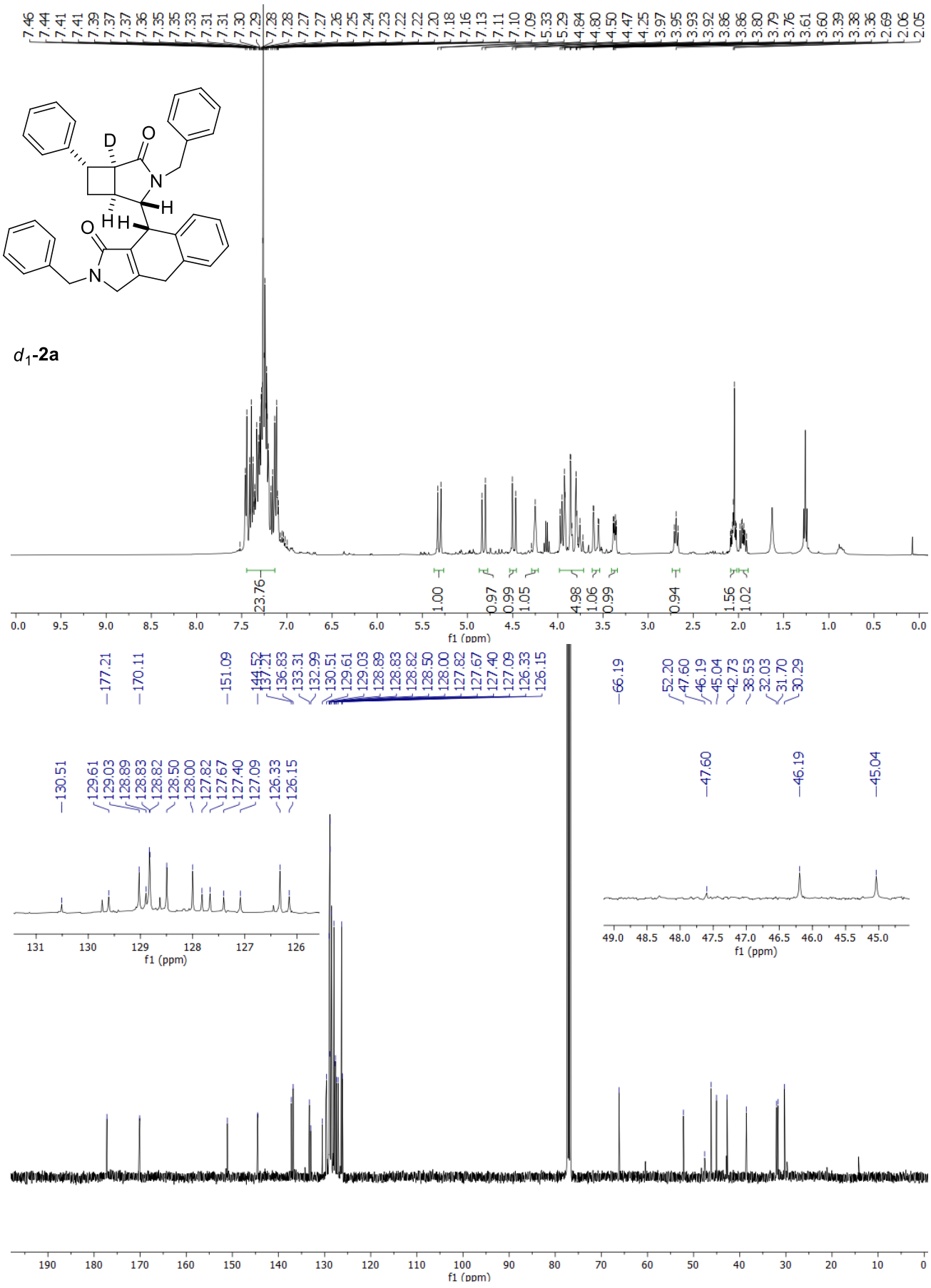

2a
f1 (ppm)

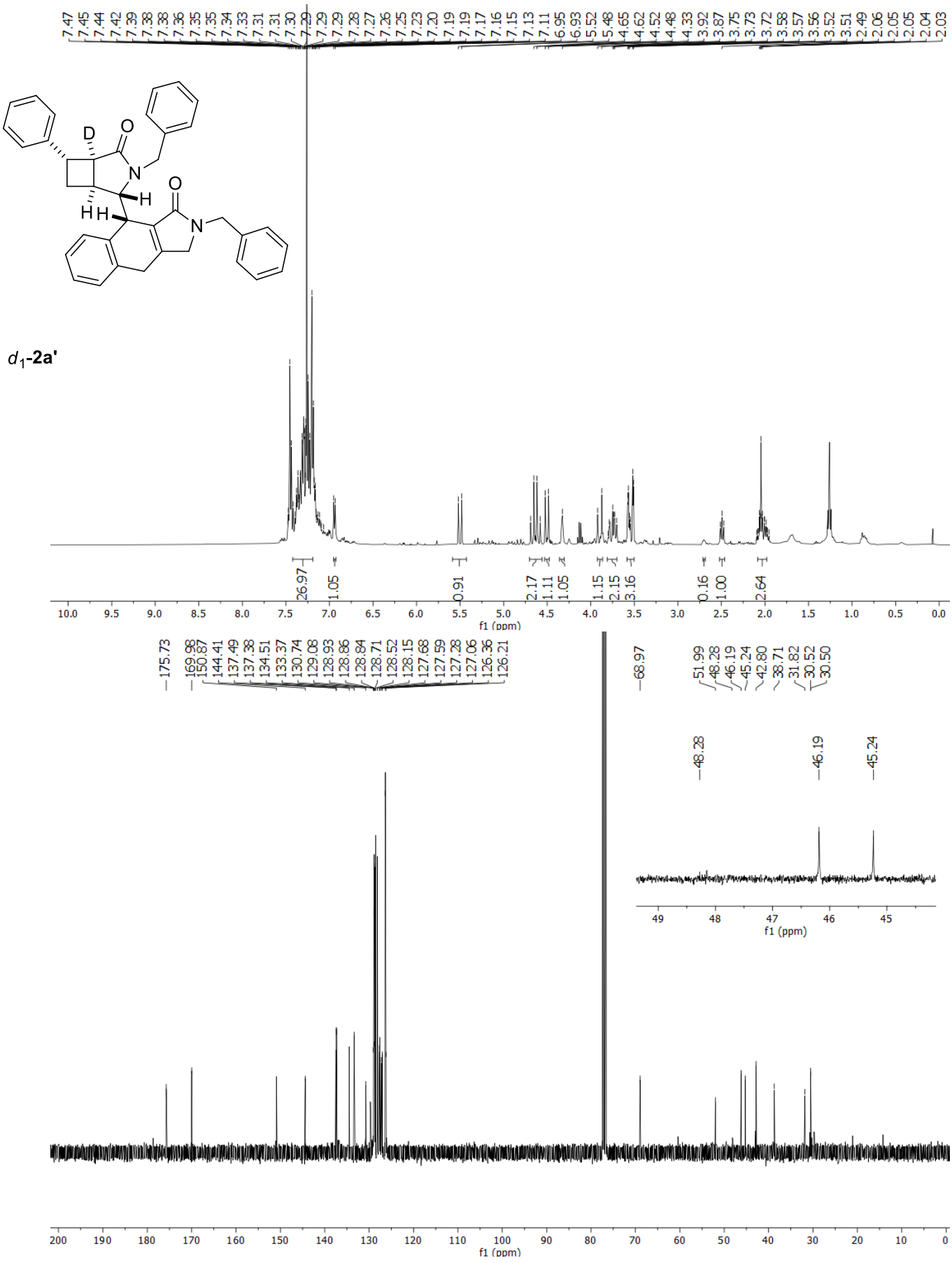


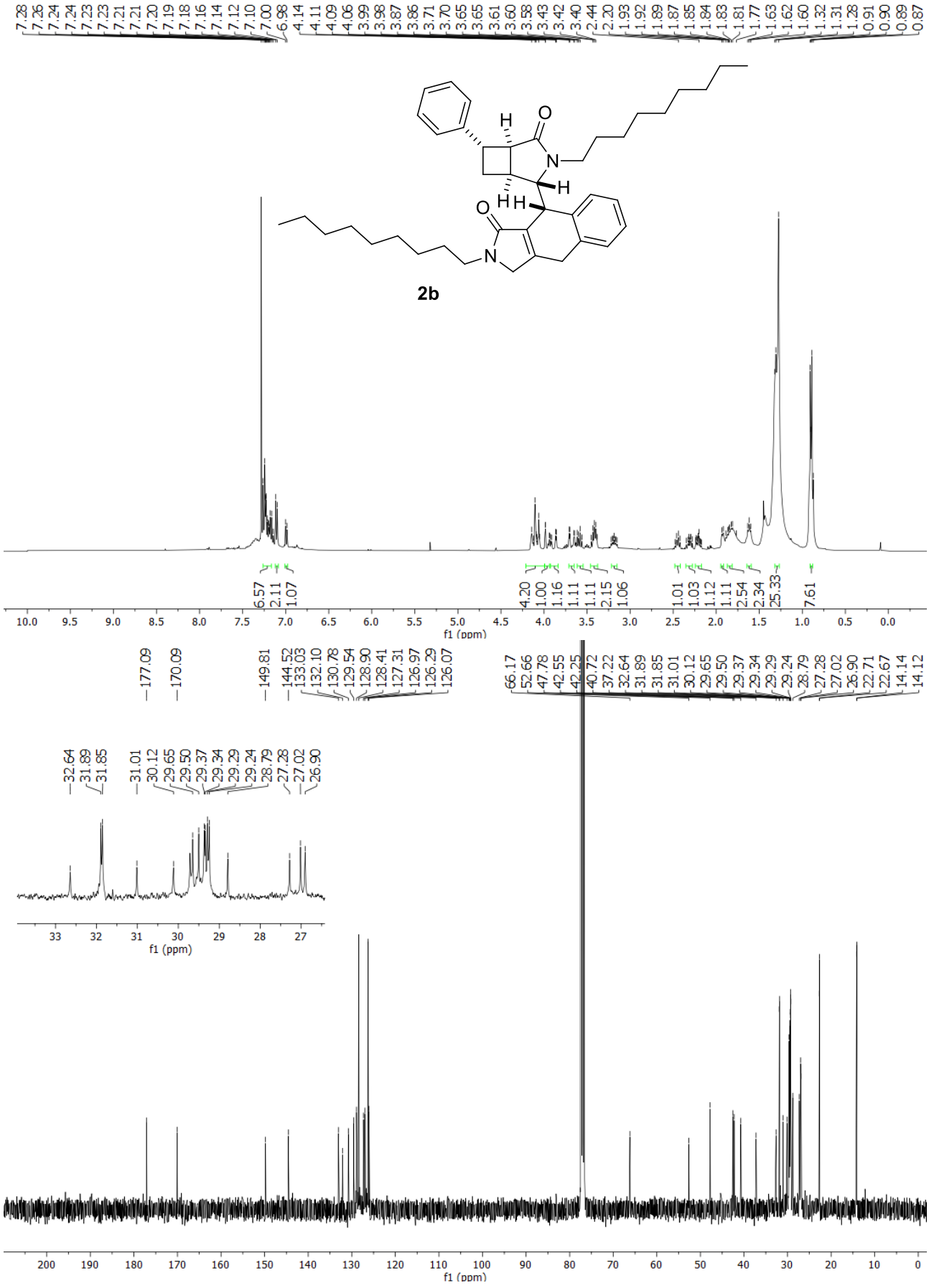
2a'

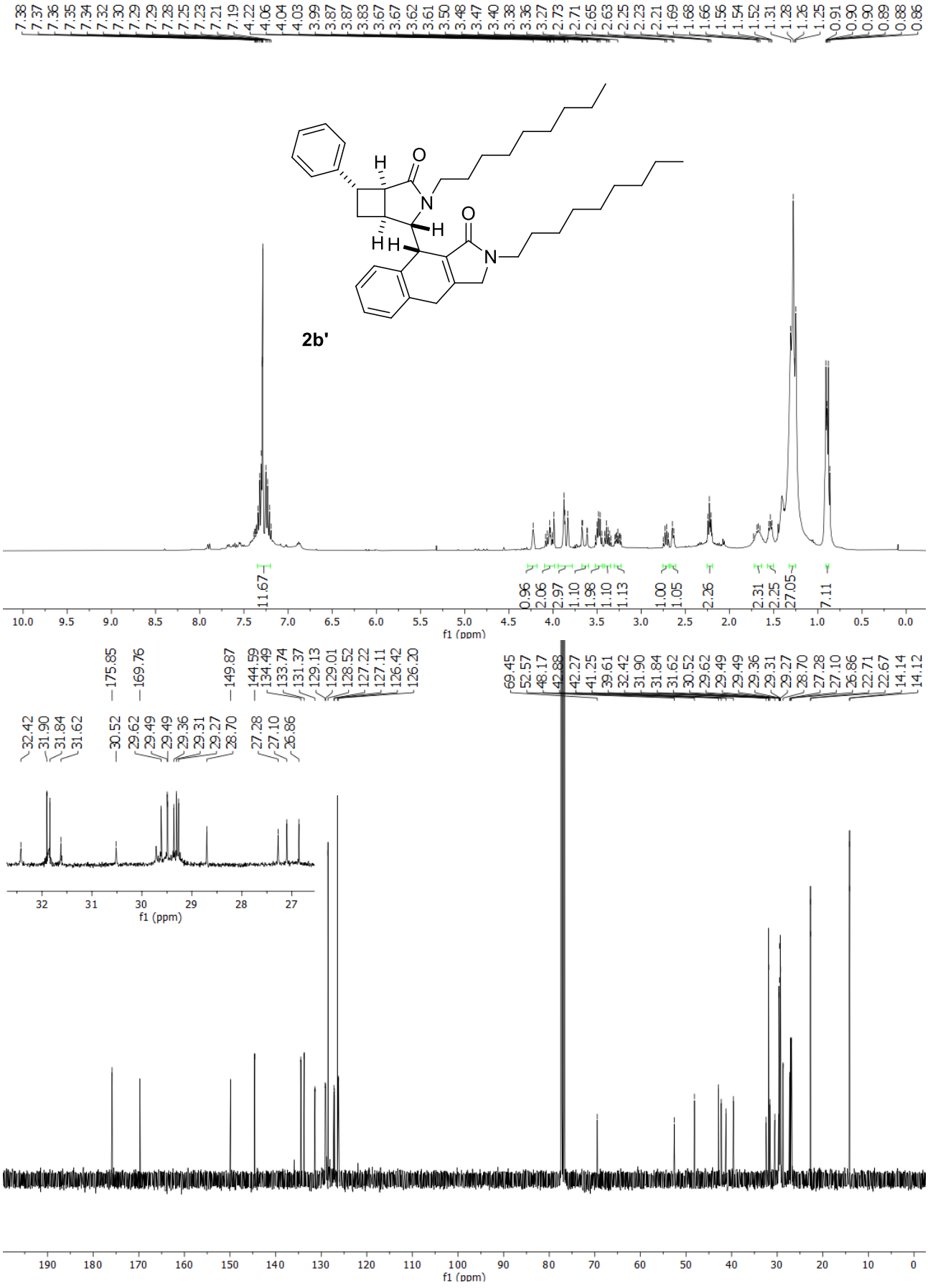

D
D
D
D
D
H
O
N
H
D
D
D
H
O
N
D
D
D
d_{10}-2a
7.45 7.44 7.41 7.41 7.39 7.37 7.37 7.34 7.33 7.33 7.32 7.31 7.31 7.30 7.29 7.29 7.28 7.27 7.27 7.26 7.25 7.23 7.22 7.22 7.21 7.20 5.33 5.29 4.84 4.80 4.50 4.47 4.25 3.98 3.95 3.93 3.91 3.86 3.85 3.84 3.80 3.79 3.76 3.75 3.61 3.60 3.39 3.37 3.37 3.36 2.05 1.97 1.95
8.56 2.42 1.00 0.95 1.00 1.00 5.23 1.07 0.98 1.95 1.01
f1 (ppm)
177.23 170.11 151.10 144.39 137.22 136.85 133.21 132.93 130.52 129.02 128.82 128.81 128.00 127.81 127.66
66.13 53.44 52.21 47.51 46.20 45.05 42.78 38.51 31.92 31.63 30.22
31.92 31.63 30.22
f1 (ppm)
f1 (ppm)

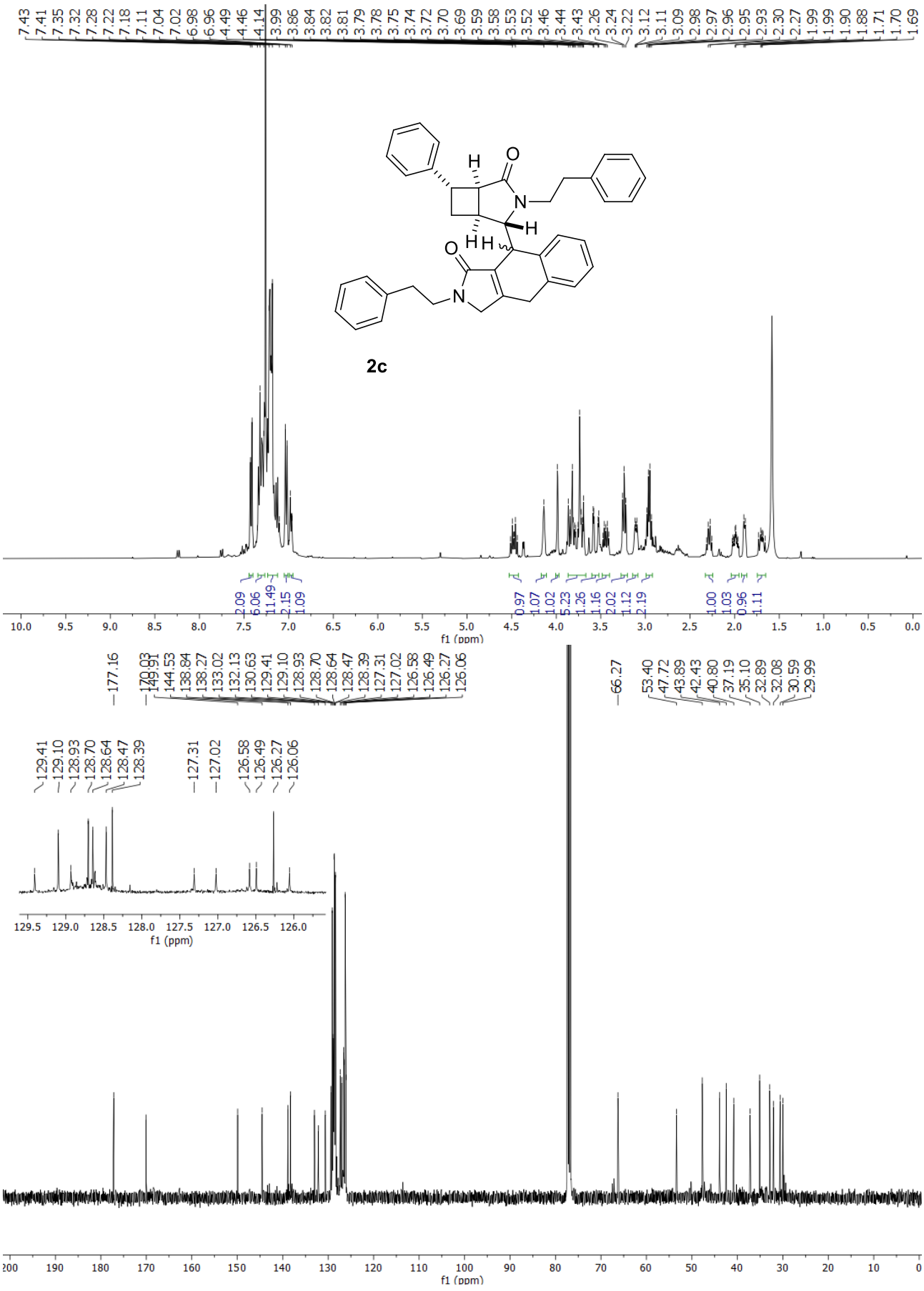

7.47 7.45 7.44 7.42 7.39 7.38 7.36 7.34 7.33 7.31 7.30 7.26 7.25 7.23 7.20 7.19
5.52 5.48
4.69 4.65 4.62 4.58 4.51 4.48 4.33
3.92 3.87 3.79 3.78 3.75 3.73 3.72 3.70 3.58 3.57 3.56 3.56 3.55 3.52 3.51
2.70 2.10 2.05 2.04 2.03 2.01
D
D
D
D
D
H
O
N
H
O
D
D
H
N
D
D
D
D
d_{10}-2a'
12.74
0.95
1.98
1.01
0.98
1.17
2.05
2.90
0.98
2.05
f1 (ppm)
175.77
169.99
150.86
144.27
137.50
137.39
134.42
133.26
130.78
128.92
128.83
128.70
128.15
127.67
127.58
68.87
52.00
48.04
46.20
45.25
42.84
38.68
31.70
30.43
f1 (ppm)
f1 (ppm)

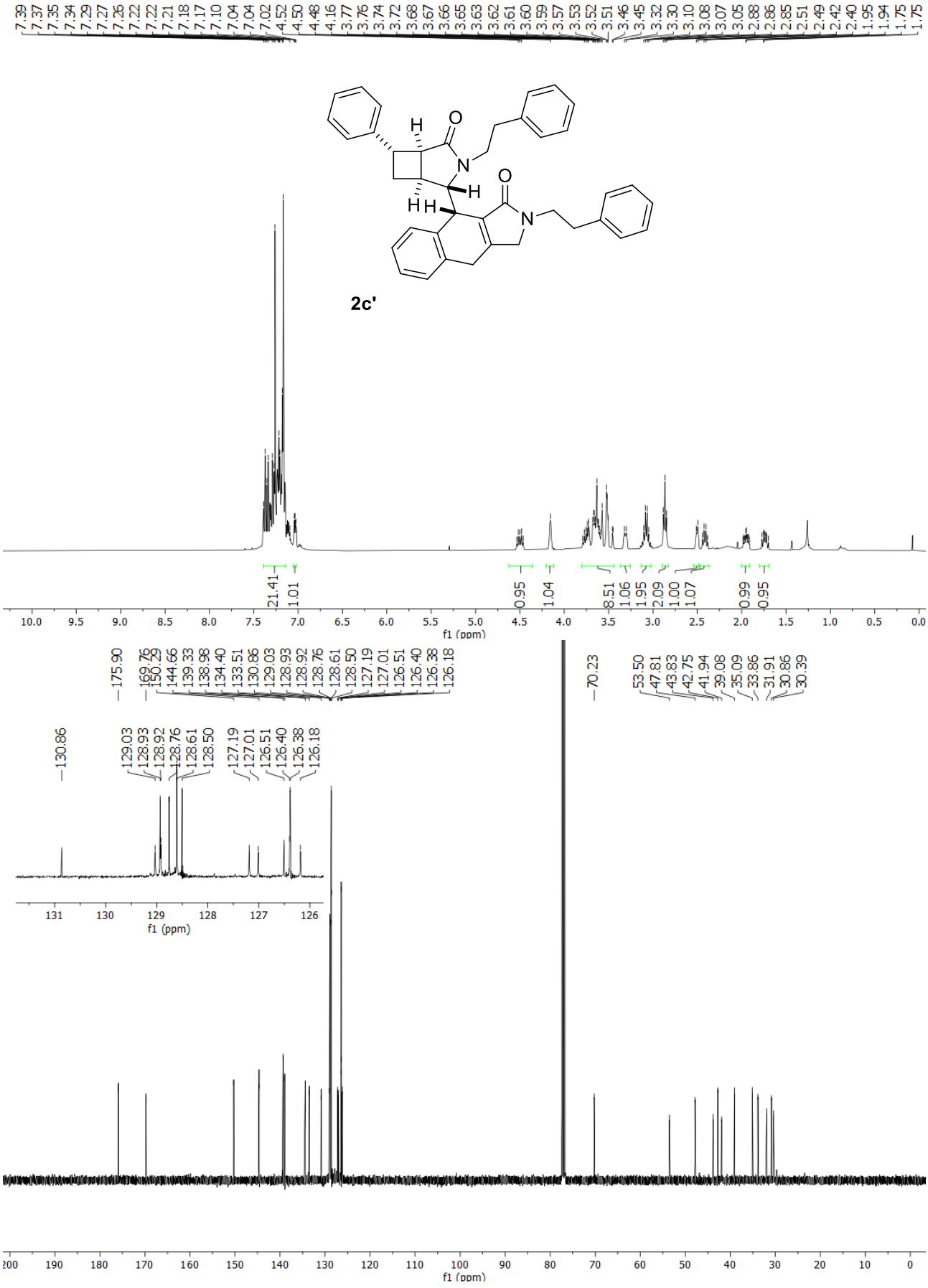

D
O
N
H
H
H
O
N
d_1-2a
f1 (ppm)

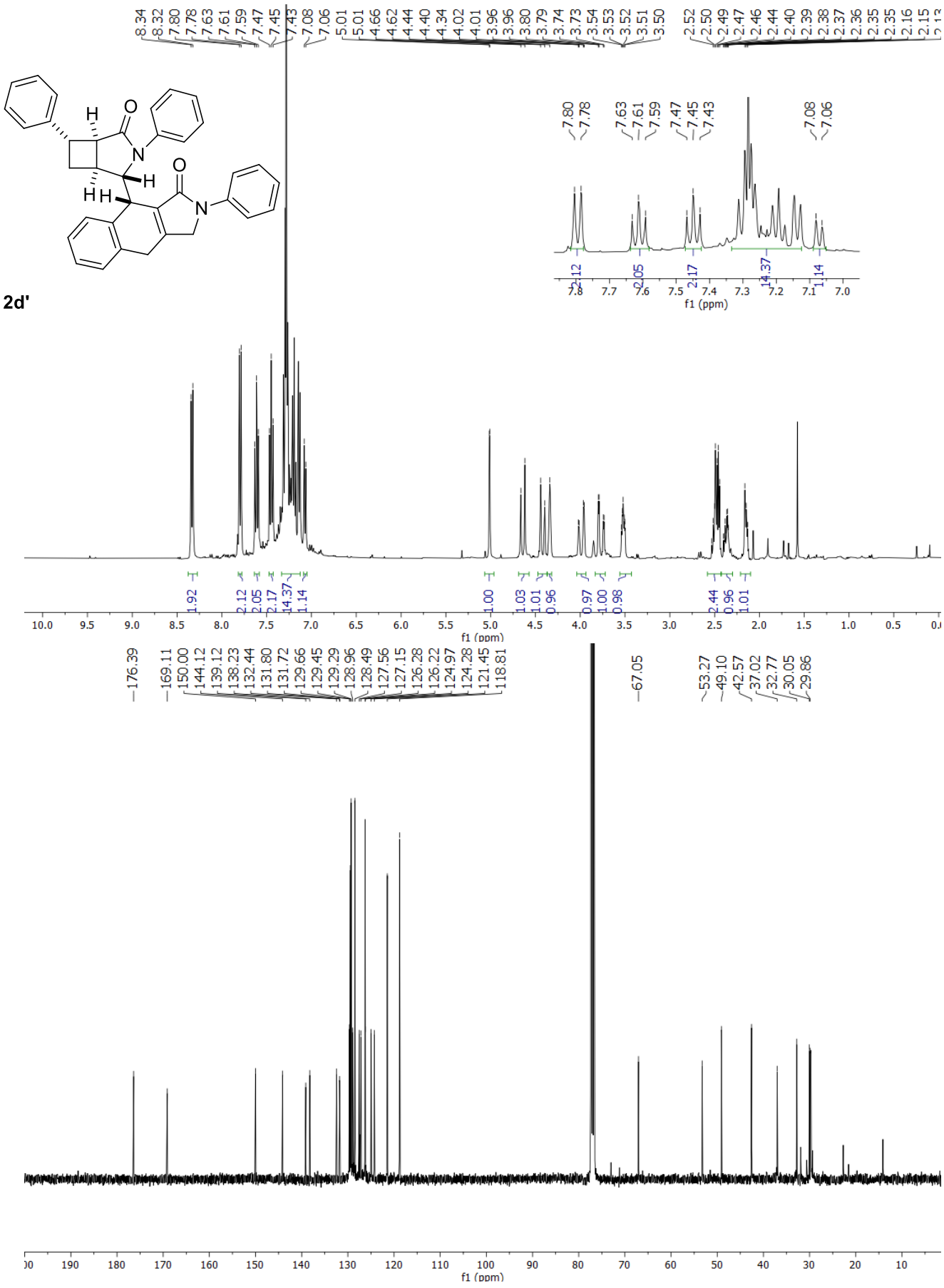

D
O
N
H
H
H
O
N
d_1-2a'
7.47 7.45 7.44 7.42 7.39 7.38 7.38 7.36 7.35 7.35 7.34 7.33 7.31 7.31 7.30 7.29 7.29 7.29 7.28 7.27 7.26 7.25 7.23 7.20 7.19 7.19 7.17 7.16 7.15 7.13 7.11 6.95 6.93 5.52 5.48 4.65 4.62 4.52 4.48 4.33 3.92 3.87 3.75 3.73 3.72 3.58 3.57 3.56 3.52 3.51 2.49 2.06 2.05 2.05 2.04 2.03
26.97 1.05 0.91 2.17 1.11 1.05 1.15 2.15 3.16 0.16 1.00 2.64
f1 (ppm)
175.73 169.98 150.87 144.41 137.49 137.38 134.51 133.37 130.74 129.08 128.93 128.86 128.84 128.71 128.52 128.15 127.68 127.59 127.28 127.06 126.36 126.21
68.97
51.99 48.28 46.19 45.24 42.80 38.71 31.82 30.52 30.50
48.28 46.19 45.24
f1 (ppm)

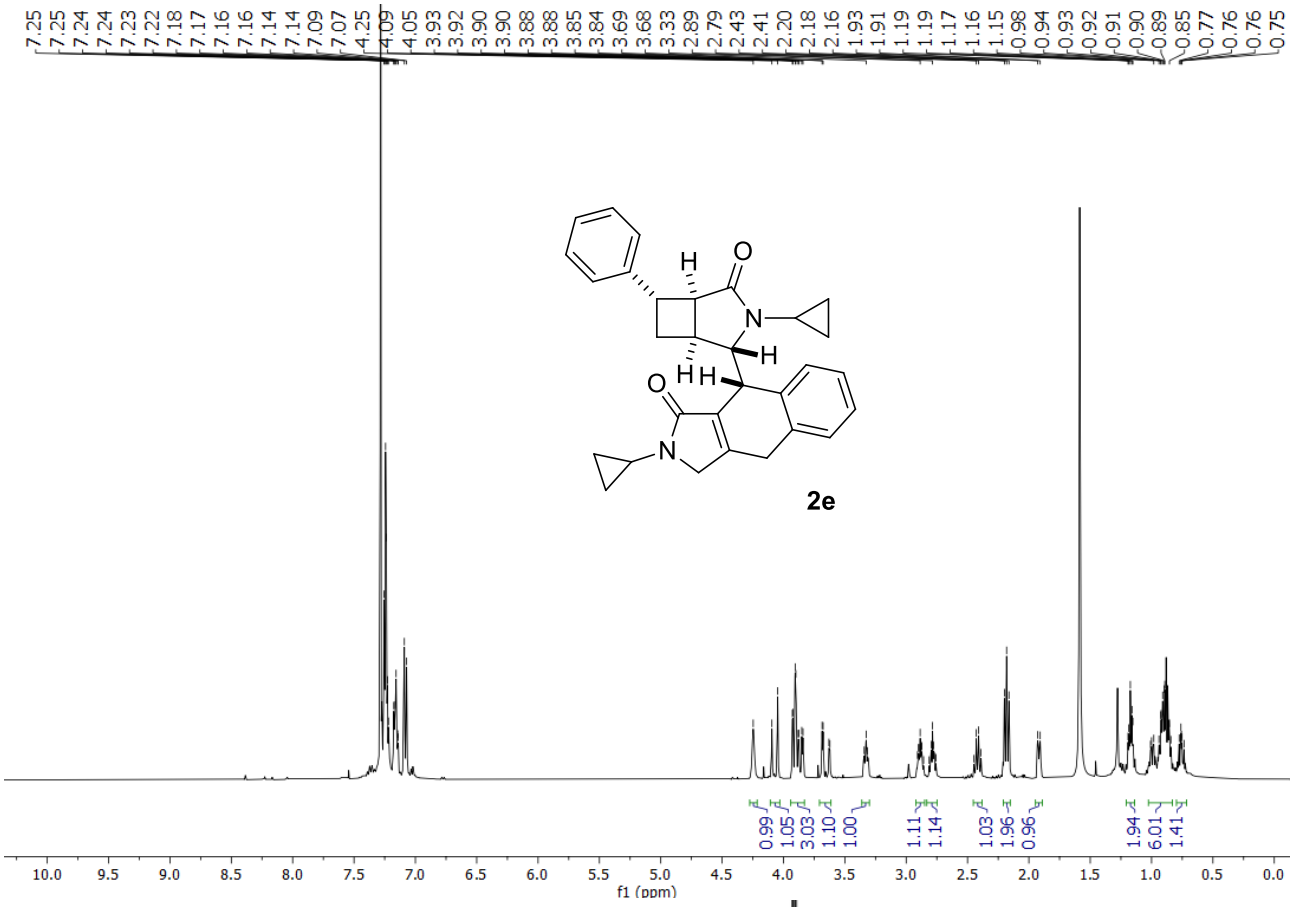

7.28 7.26 7.24 7.24 7.23 7.23 7.21 7.21 7.20 7.19 7.18 7.16 7.14 7.12 7.10 7.00 6.98 4.14 4.11 4.09 4.06 3.99 3.98 3.87 3.86 3.71 3.70 3.65 3.61 3.60 3.58 3.43 3.42 3.40 2.44 2.20 1.93 1.92 1.89 1.87 1.85 1.84 1.83 1.81 1.77 1.63 1.62 1.60 1.32 1.31 1.28 0.91 0.90 0.89 0.87
2b
6.57 2.11 1.07 4.20 1.00 1.16 1.11 1.11 2.15 1.06 1.01 1.03 1.12 1.11 2.54 2.34 25.33 7.61
f1 (ppm)
177.09 170.09 149.81 144.52 133.03 132.10 130.78 129.54 128.90 128.41 127.31 126.97 126.29 126.07 66.17 52.66 47.78 42.55 42.25 40.72 37.22 32.64 31.89 31.85 31.01 30.12 29.65 29.50 29.37 29.34 29.29 29.24 28.79 27.28 27.02 26.90 22.71 22.67 14.14 14.12
32.64 31.89 31.85 31.01 30.12 29.65 29.50 29.37 29.34 29.29 29.24 28.79 27.28 27.02 26.90
f1 (ppm)
f1 (ppm)


2b'
f1 (ppm)


7.43 7.41 7.35 7.32 7.28 7.22 7.18 7.11 7.04 7.02 6.98 6.96 6.49 6.46 4.14 3.99 3.86 3.84 3.82 3.81 3.79 3.78 3.75 3.74 3.72 3.70 3.69 3.59 3.58 3.53 3.52 3.46 3.44 3.43 3.26 3.24 3.22 3.12 3.11 3.09 2.98 2.97 2.96 2.95 2.93 2.30 2.27 1.99 1.99 1.90 1.88 1.71 1.70 1.69
2.09 6.06 11.49 2.15 1.09 0.97 1.07 1.02 5.23 1.26 1.16 2.02 1.12 2.19 1.00 1.03 0.96 1.11
f1 (ppm)
2c
177.16 170.83 149.91 144.53 138.84 138.27 133.02 132.13 130.63 129.41 129.10 128.93 128.70 128.64 128.47 128.39 127.31 127.02 126.58 126.49 126.27 126.06
66.27 53.40 47.72 43.89 42.43 40.80 37.19 35.10 32.89 32.08 30.59 29.99
129.41 129.10 128.93 128.70 128.64 128.47 128.39 127.31 127.02 126.58 126.49 126.27 126.06
f1 (ppm)

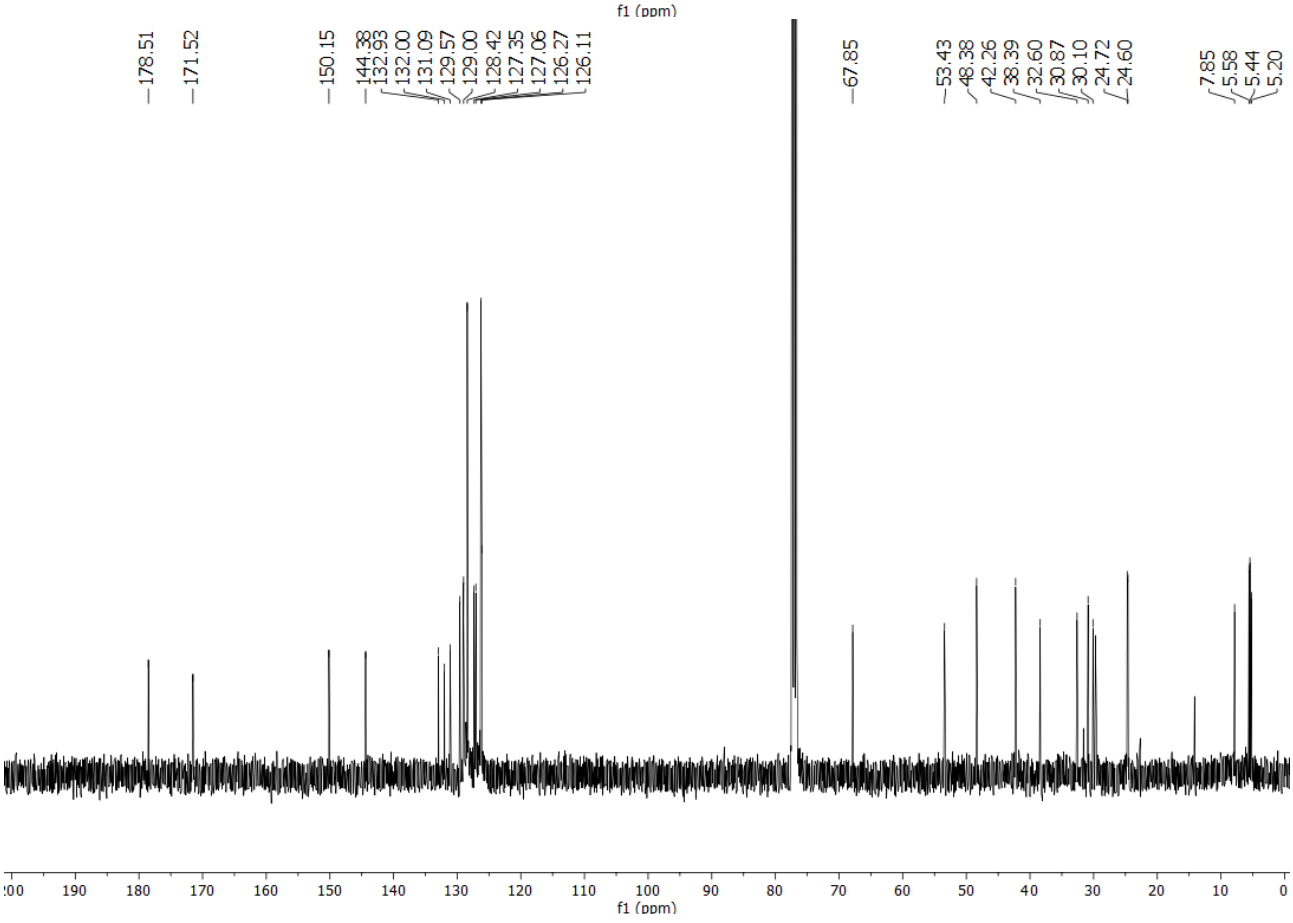

7.39 7.37 7.35 7.34 7.29 7.27 7.26 7.22 7.22 7.21 7.18 7.17 7.10 7.04 7.04 7.02 4.52 4.50 4.48 4.16 3.77 3.76 3.74 3.72 3.68 3.67 3.66 3.65 3.63 3.62 3.61 3.60 3.59 3.57 3.53 3.52 3.51 3.46 3.45 3.32 3.30 3.10 3.08 3.07 3.05 2.88 2.86 2.85 2.51 2.49 2.42 2.40 1.95 1.94 1.75 1.75
H
O
N
H
O
H H
N
2c'
21.41 1.01 0.95 1.04 8.51 1.06 1.95 2.09 1.00 1.07 0.99 0.95
f1 (ppm)
175.90 169.76 150.29 144.66 139.33 138.98 134.40 133.51 130.86 129.03 128.93 128.92 128.76 128.61 128.50 127.19 127.01 126.51 126.40 126.38 126.18
70.23
53.50 47.81 43.83 42.75 41.94 39.08 35.09 33.86 31.91 30.86 30.39
130.86 129.03 128.93 128.92 128.76 128.61 128.50 127.19 127.01 126.51 126.40 126.38 126.18
f1 (ppm)

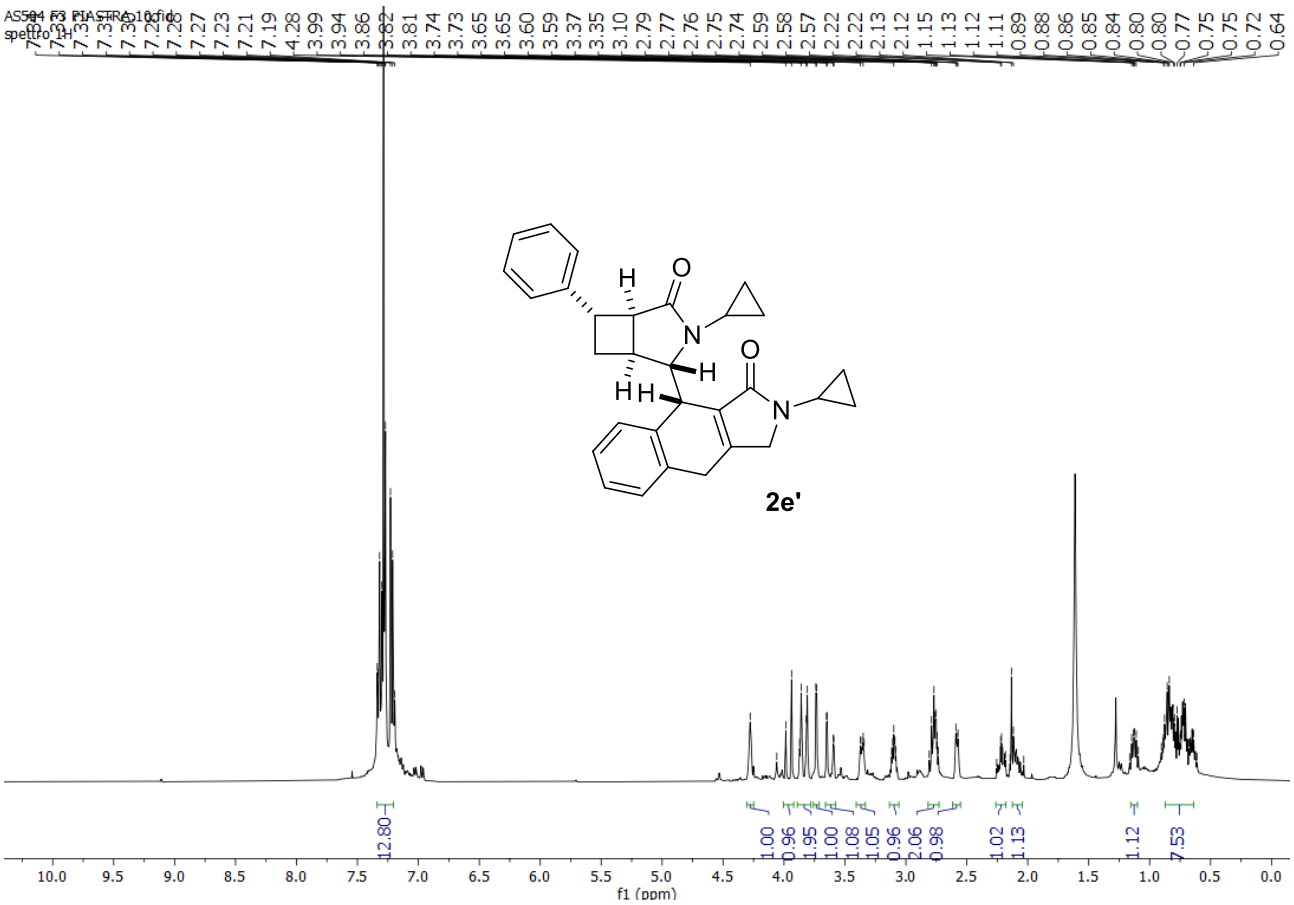

2d'
f1 (ppm)

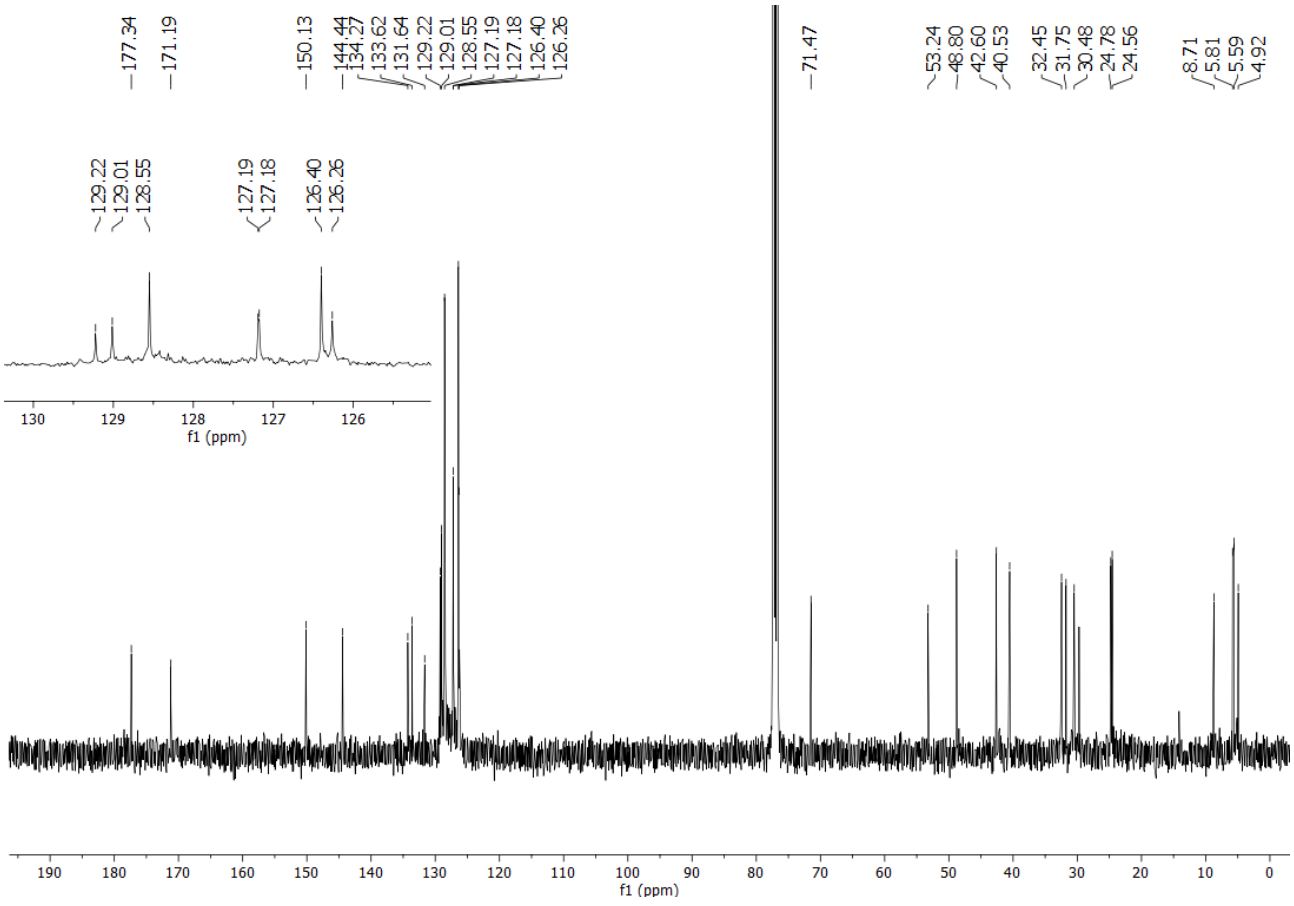

7.25 7.25 7.24 7.24 7.23 7.22 7.18 7.17 7.16 7.16 7.14 7.14 7.09 7.07 4.25 4.09 4.05 3.93 3.92 3.90 3.90 3.88 3.88 3.85 3.84 3.69 3.68 3.33 2.89 2.79 2.43 2.41 2.20 2.18 2.16 1.93 1.91 1.19 1.19 1.17 1.16 1.15 0.98 0.94 0.93 0.92 0.91 0.90 0.89 0.85 0.77 0.76 0.76 0.75
0.99 1.05 3.03 1.10 1.00 1.11 1.14 1.03 1.96 0.96 1.94 6.01 1.41
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

H
O
N
H
O
H H
N

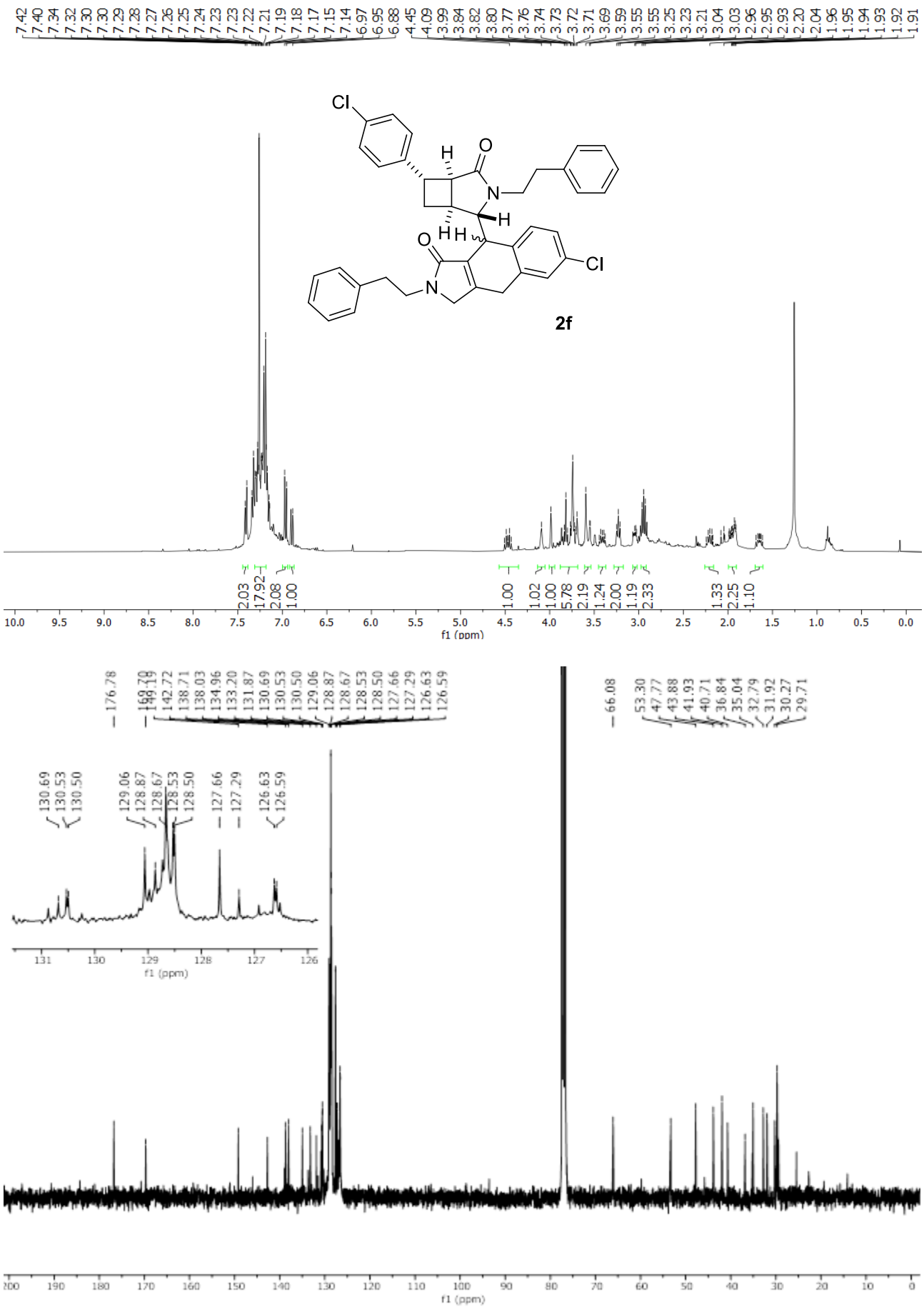
2e

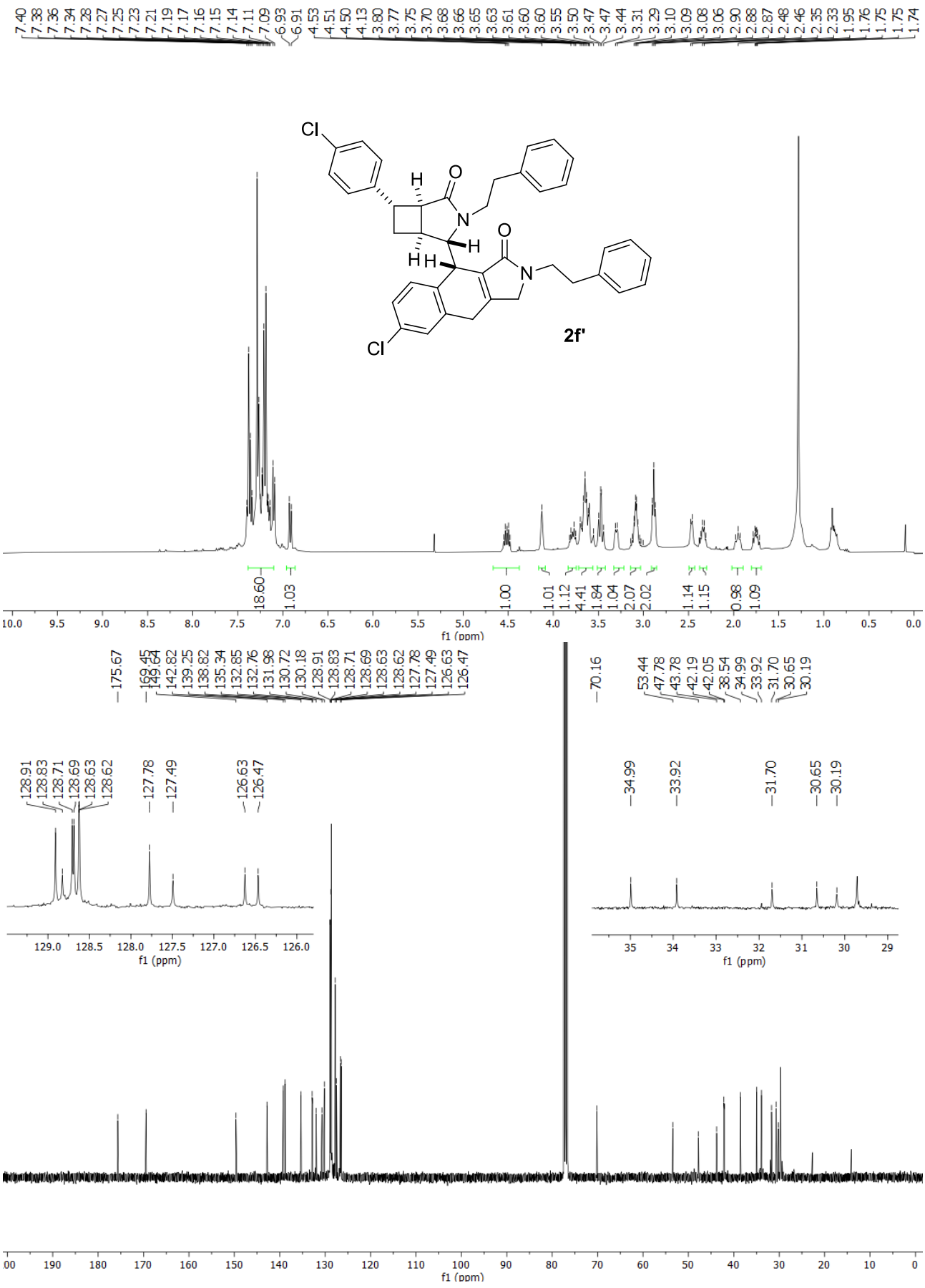

178.51 171.52 150.15 144.38 132.93 132.00 131.09 129.57 129.00 128.42 127.35 127.06 126.27 126.11 67.85 53.43 48.38 42.26 38.39 32.60 30.87 30.10 24.72 24.60 7.85 5.58 5.44 5.20
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

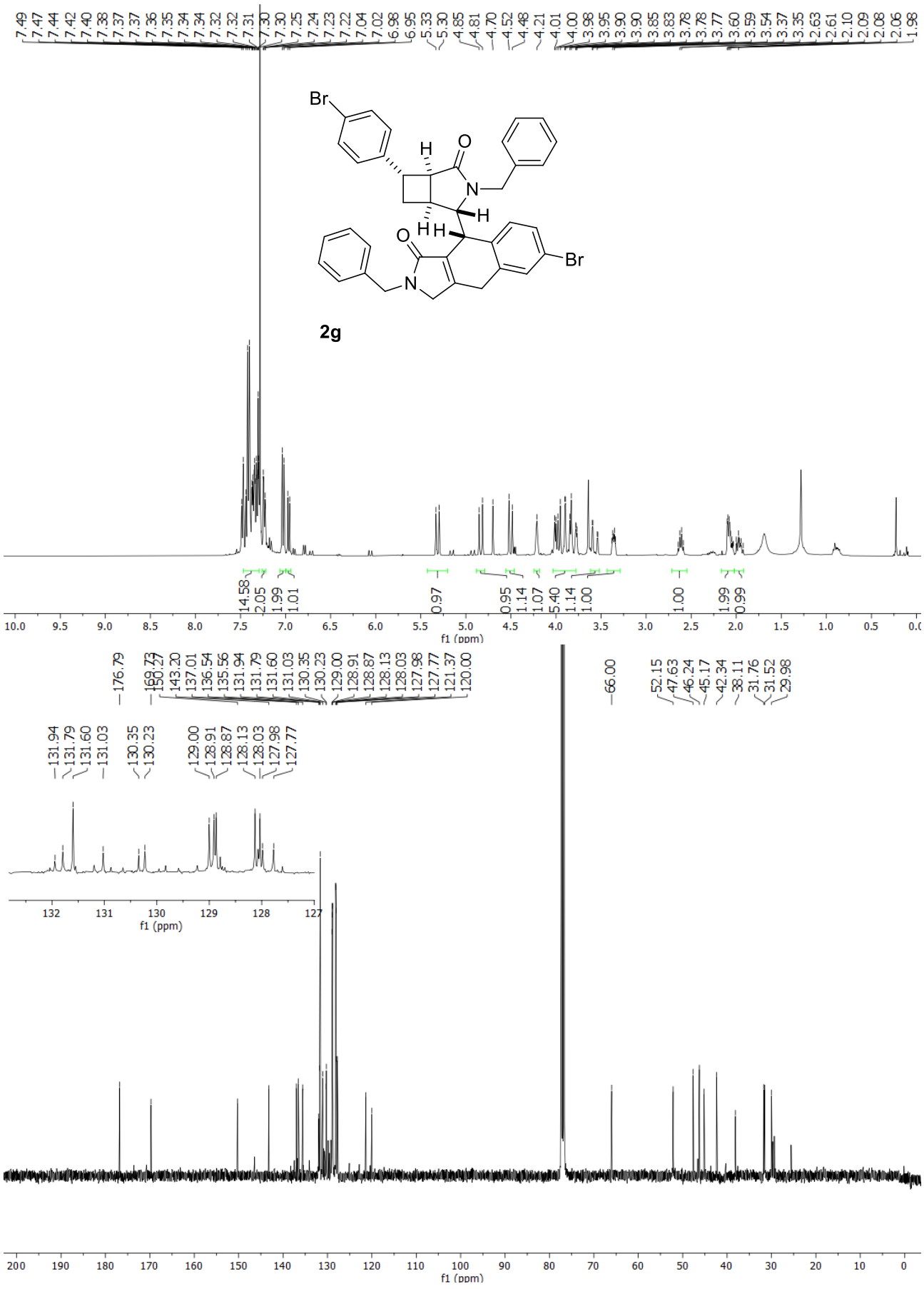


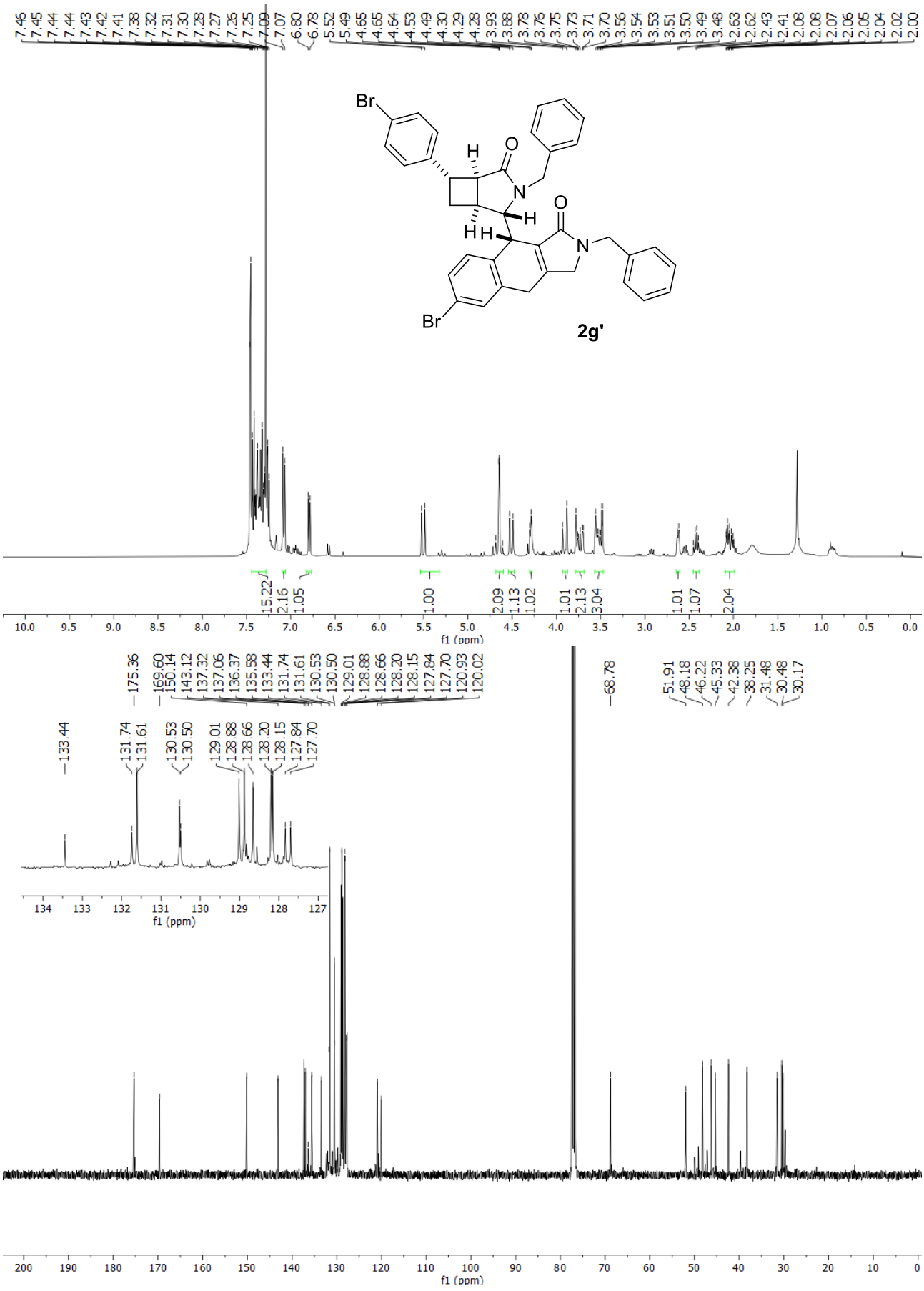


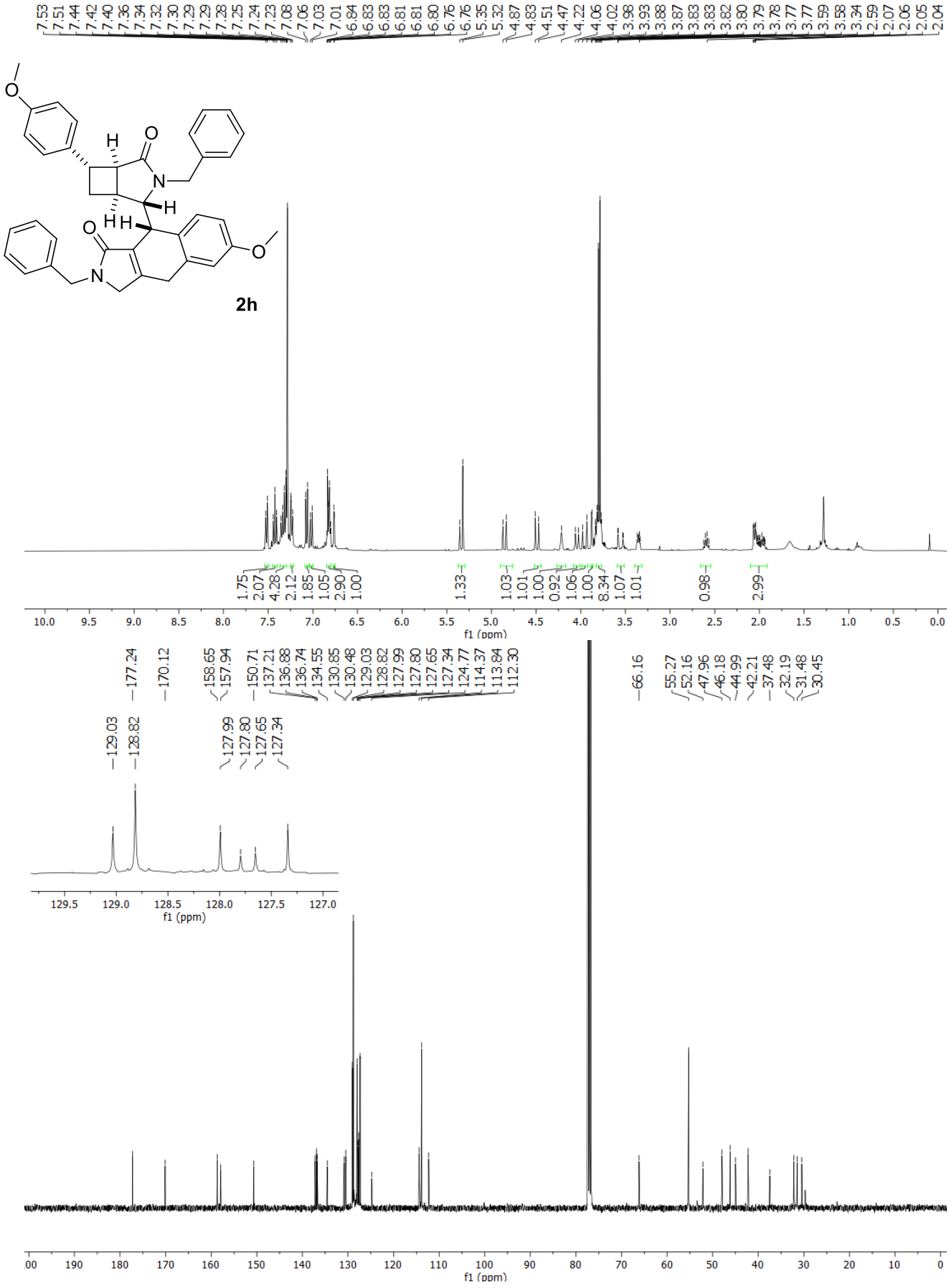
106

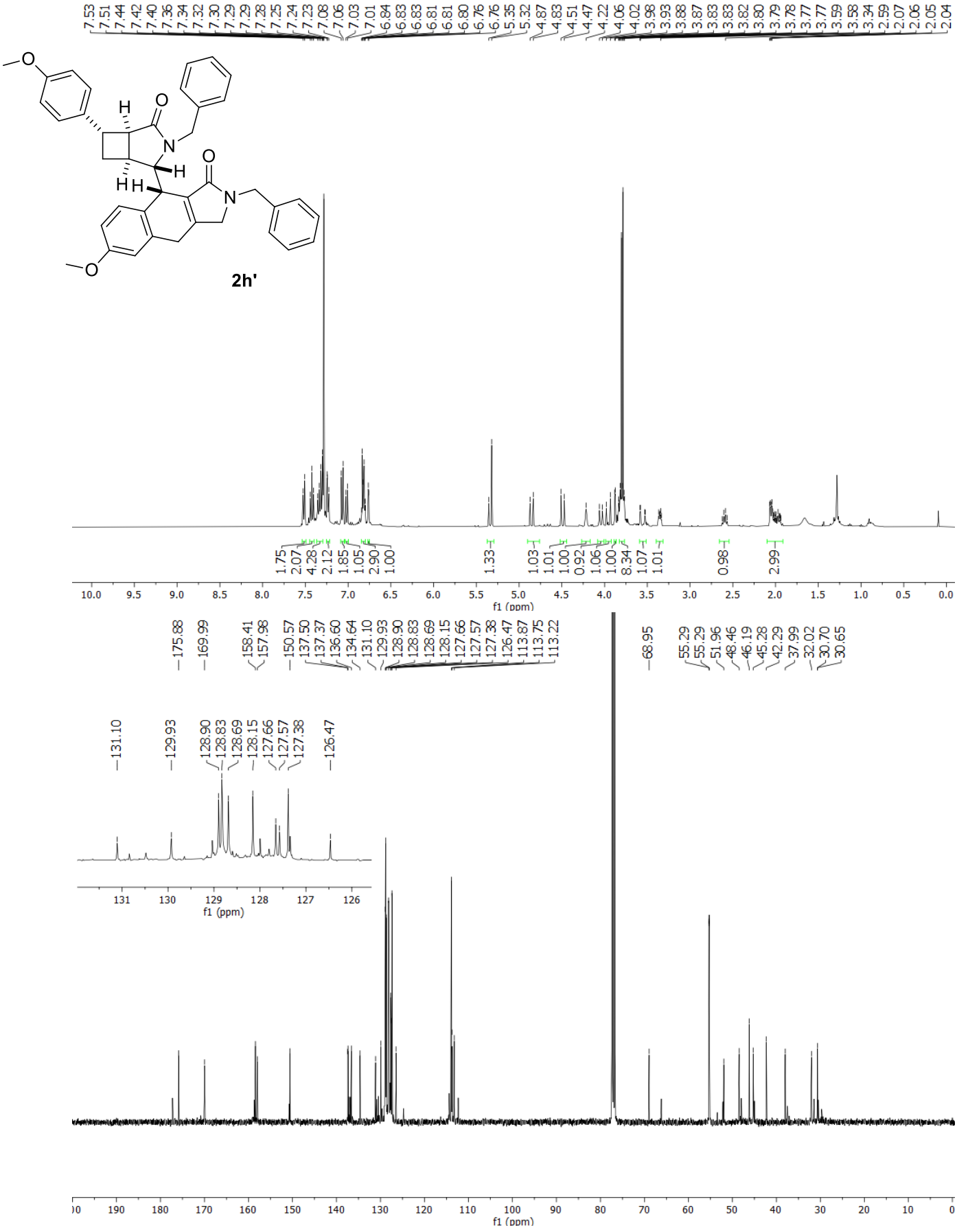

7.42 7.40 7.34 7.32 7.30 7.30 7.29 7.28 7.27 7.26 7.25 7.24 7.23 7.23 7.22 7.21 7.19 7.18 7.17 7.15 7.14 6.97 6.95 6.88 4.45 4.09 3.99 3.84 3.82 3.80 3.77 3.76 3.74 3.73 3.72 3.71 3.69 3.59 3.55 3.55 3.25 3.23 3.21 3.04 3.03 2.96 2.95 2.93 2.20 2.04 1.96 1.95 1.94 1.93 1.92 1.91
Cl
H
O
N
H
H H
O
N
Cl
2f
2.03 17.92 2.08 1.00 1.00 1.02 1.00 5.78 2.19 1.24 2.00 1.19 2.33 1.33 2.25 1.10
f1 (ppm)
176.78 169.70 169.19 142.72 138.71 138.03 134.96 133.20 131.87 130.69 130.53 130.50 129.06 128.87 128.67 128.53 128.50 127.66 127.29 126.63 126.59
66.08 53.30 47.77 43.88 41.93 40.71 36.84 35.04 32.79 31.92 30.27 29.71
f1 (ppm)

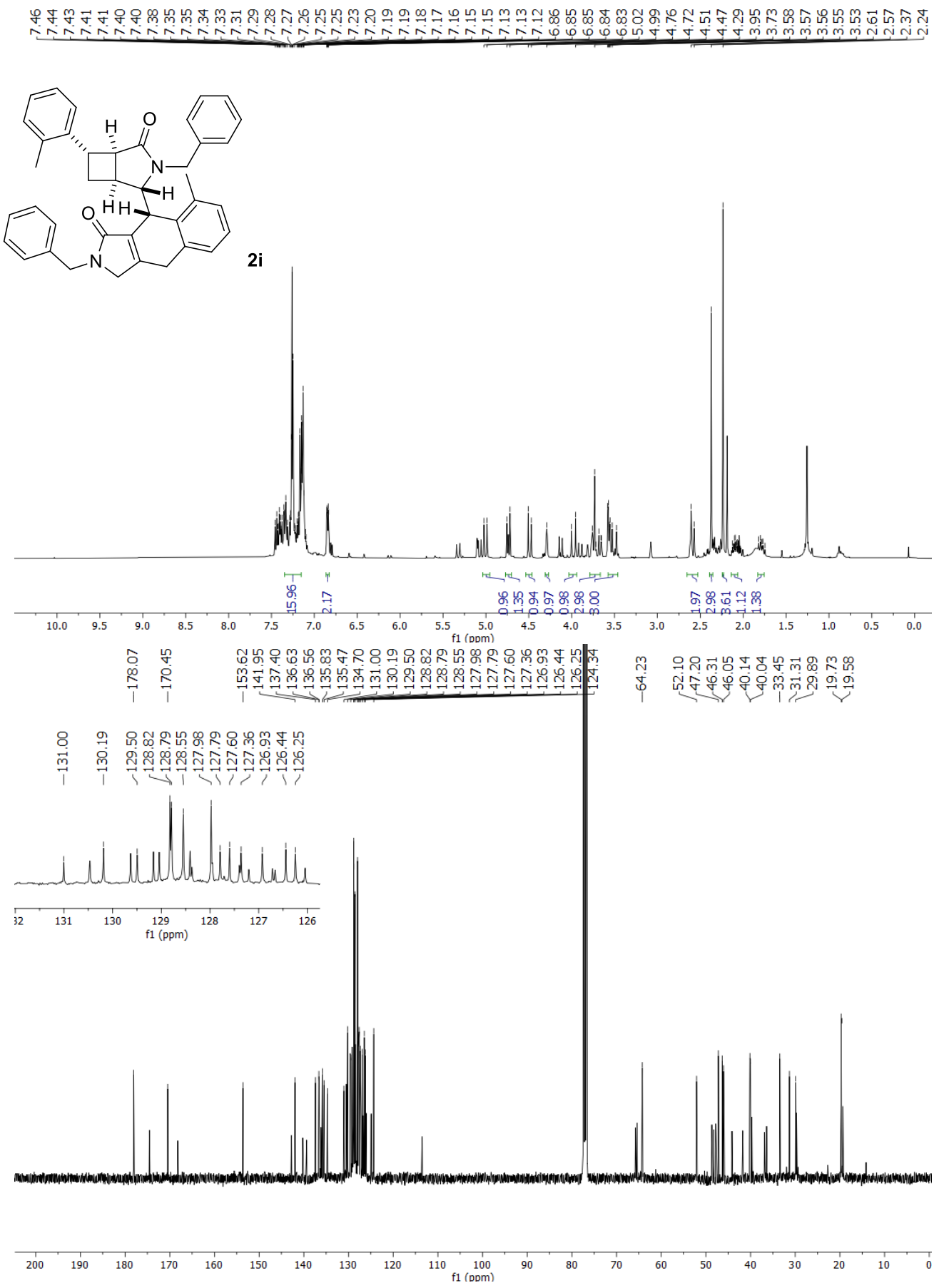

Cl
H
O
N
H
O
H H
N
Cl
2f'
f1 (ppm)
f1 (ppm)
f1 (ppm)

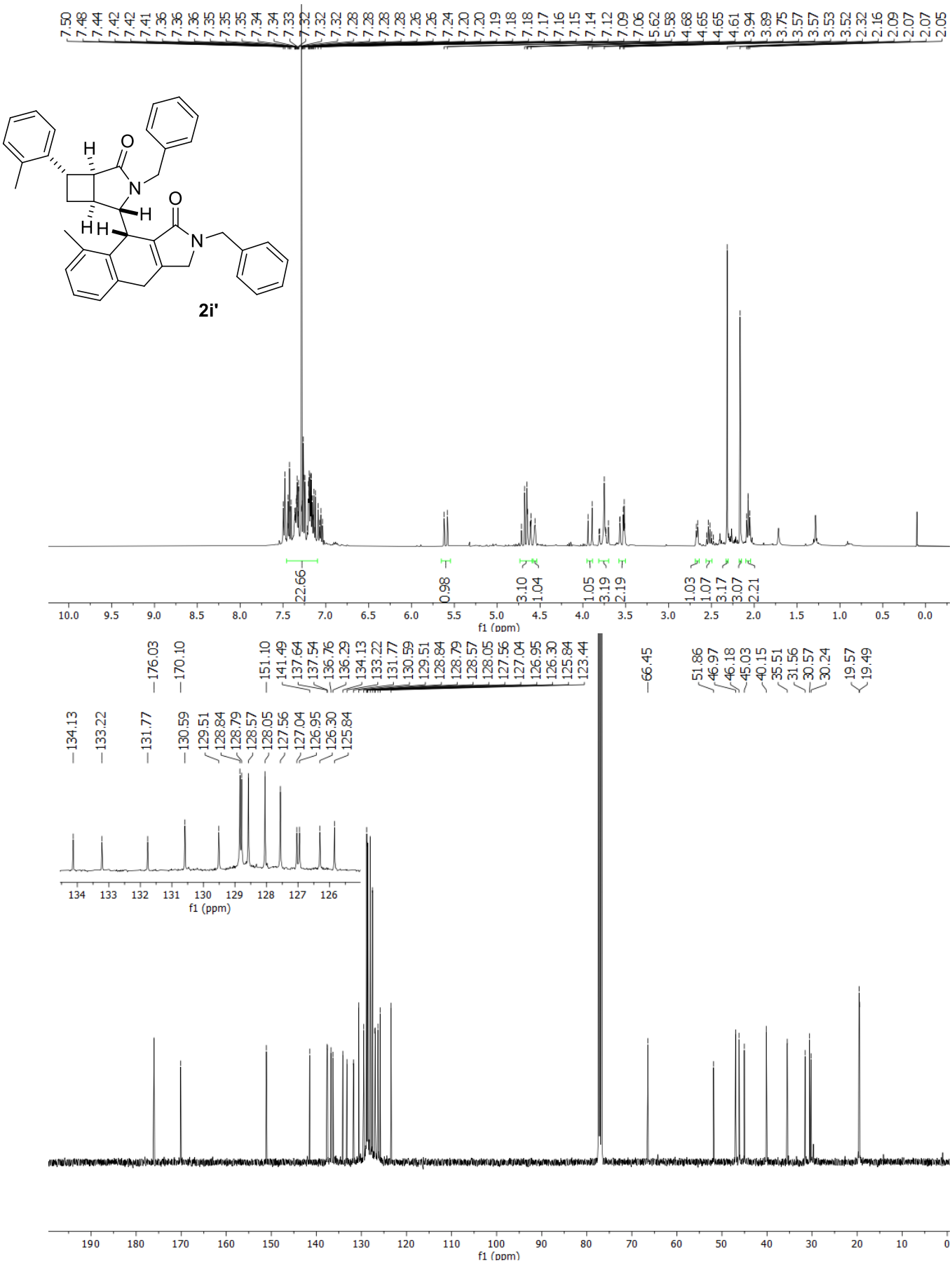

Br
H
O
N
H
H
H
O
N
Br
2g
f1 (ppm)
f1 (ppm)
f1 (ppm)


Br
H
O
N
O
H
H H
N
Br
2g'
f1 (ppm)

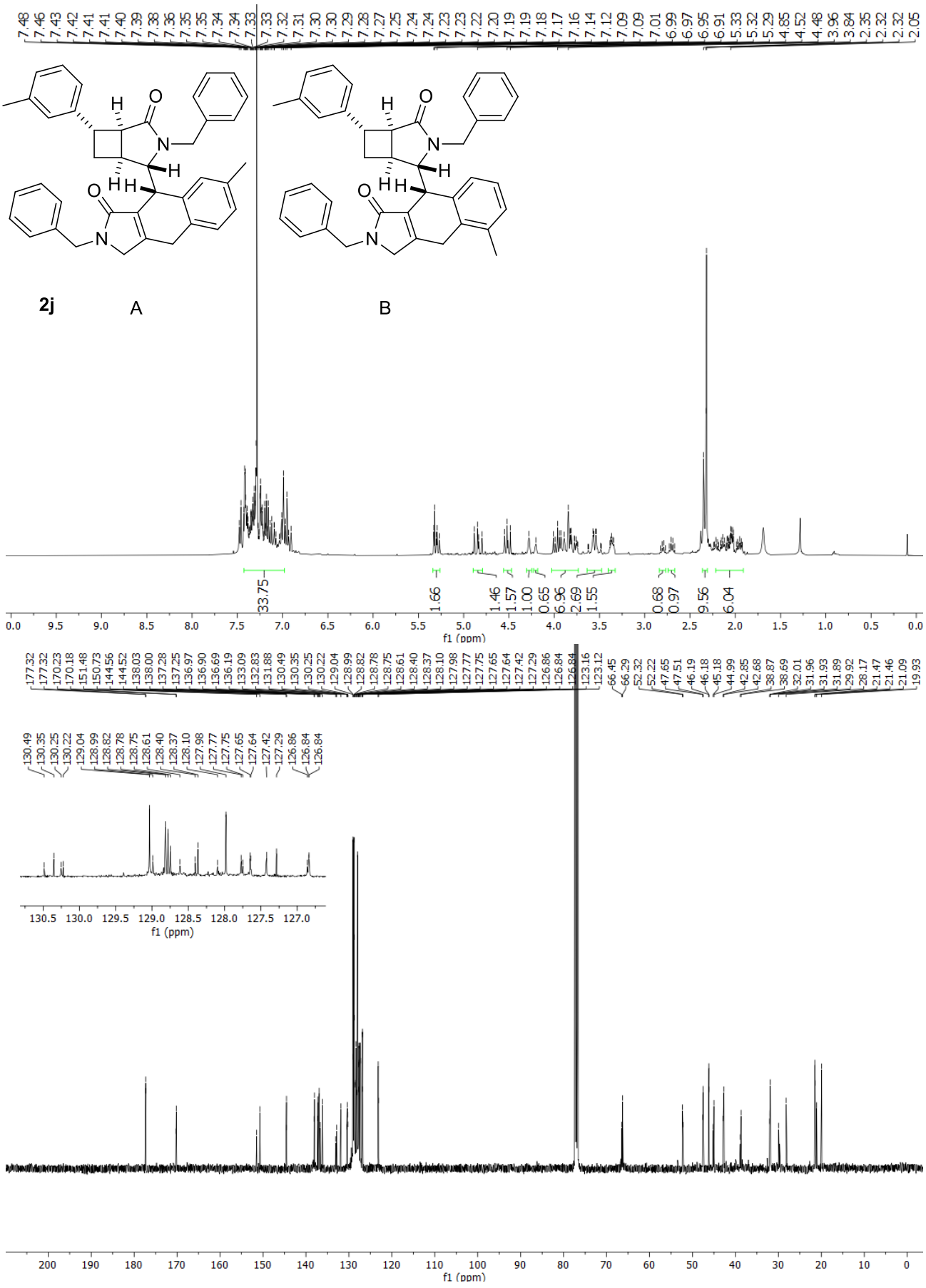

7.53 7.51 7.44 7.42 7.40 7.36 7.34 7.32 7.30 7.29 7.29 7.28 7.25 7.24 7.23 7.08 7.06 7.03 7.01 6.84 6.83 6.83 6.81 6.81 6.80 6.76 6.76 5.35 5.32 4.87 4.83 4.51 4.47 4.22 4.06 4.02 3.98 3.93 3.88 3.87 3.83 3.83 3.82 3.80 3.79 3.78 3.77 3.77 3.59 3.58 3.34 2.59 2.07 2.06 2.05 2.04
2h
1.75 2.07 4.28 2.12 1.85 1.05 2.90 1.00 1.33 1.03 1.01 1.00 0.92 1.06 1.00 8.34 1.07 1.01 0.98 2.99
f1 (ppm)
177.24 170.12 158.65 157.94 150.71 137.21 136.88 136.74 134.55 130.85 130.48 129.03 128.82 127.99 127.80 127.65 127.34 124.77 114.37 113.84 112.30 66.16 55.27 52.16 47.96 46.18 44.99 42.21 37.48 32.19 31.48 30.45
129.03 128.82 127.99 127.80 127.65 127.34
f1 (ppm)
f1 (ppm)

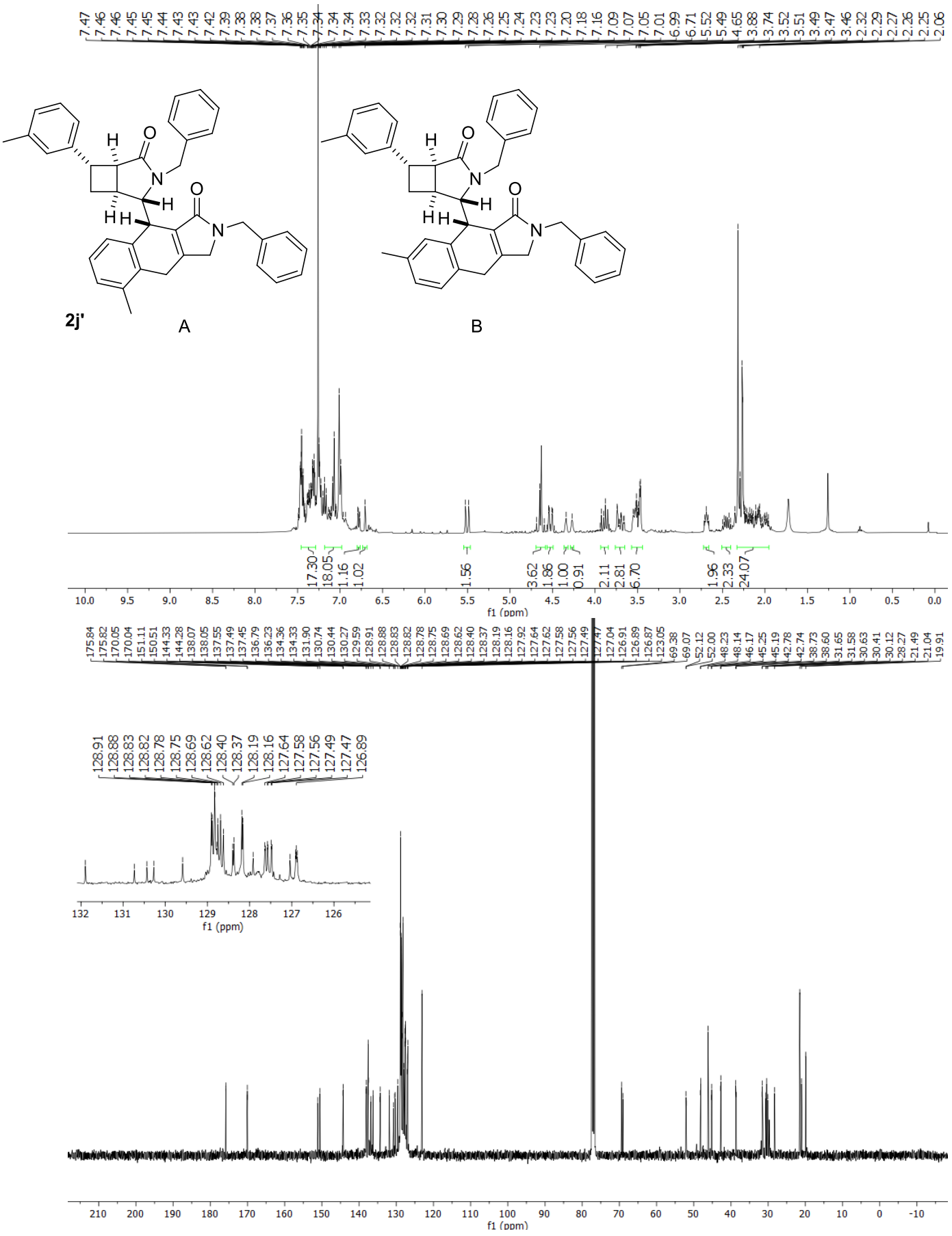

7.53 7.51 7.44 7.42 7.40 7.36 7.34 7.32 7.30 7.29 7.29 7.28 7.25 7.24 7.23 7.08 7.06 7.03 7.01 6.84 6.83 6.83 6.81 6.81 6.80 6.76 6.76 5.35 5.32 4.87 4.83 4.51 4.47 4.22 4.06 4.02 3.98 3.93 3.88 3.87 3.83 3.83 3.82 3.80 3.79 3.78 3.77 3.77 3.59 3.58 3.34 2.59 2.07 2.06 2.05 2.04
2h'
1.75 2.07 4.28 2.12 1.85 1.05 2.90 1.00 1.33 1.03 1.01 1.00 0.92 1.06 1.00 8.34 1.07 1.01 0.98 2.99
f1 (ppm)
175.88 169.99 158.41 157.98 150.57 137.50 137.37 136.60 134.64 131.10 129.93 128.90 128.83 128.69 128.15 127.66 127.57 127.38 126.47 113.87 113.75 113.22 68.95 55.29 55.29 51.96 48.46 46.19 45.28 42.29 37.99 32.02 30.70 30.65
131.10 129.93 128.90 128.83 128.69 128.15 127.66 127.57 127.38 126.47
f1 (ppm)
f1 (ppm)

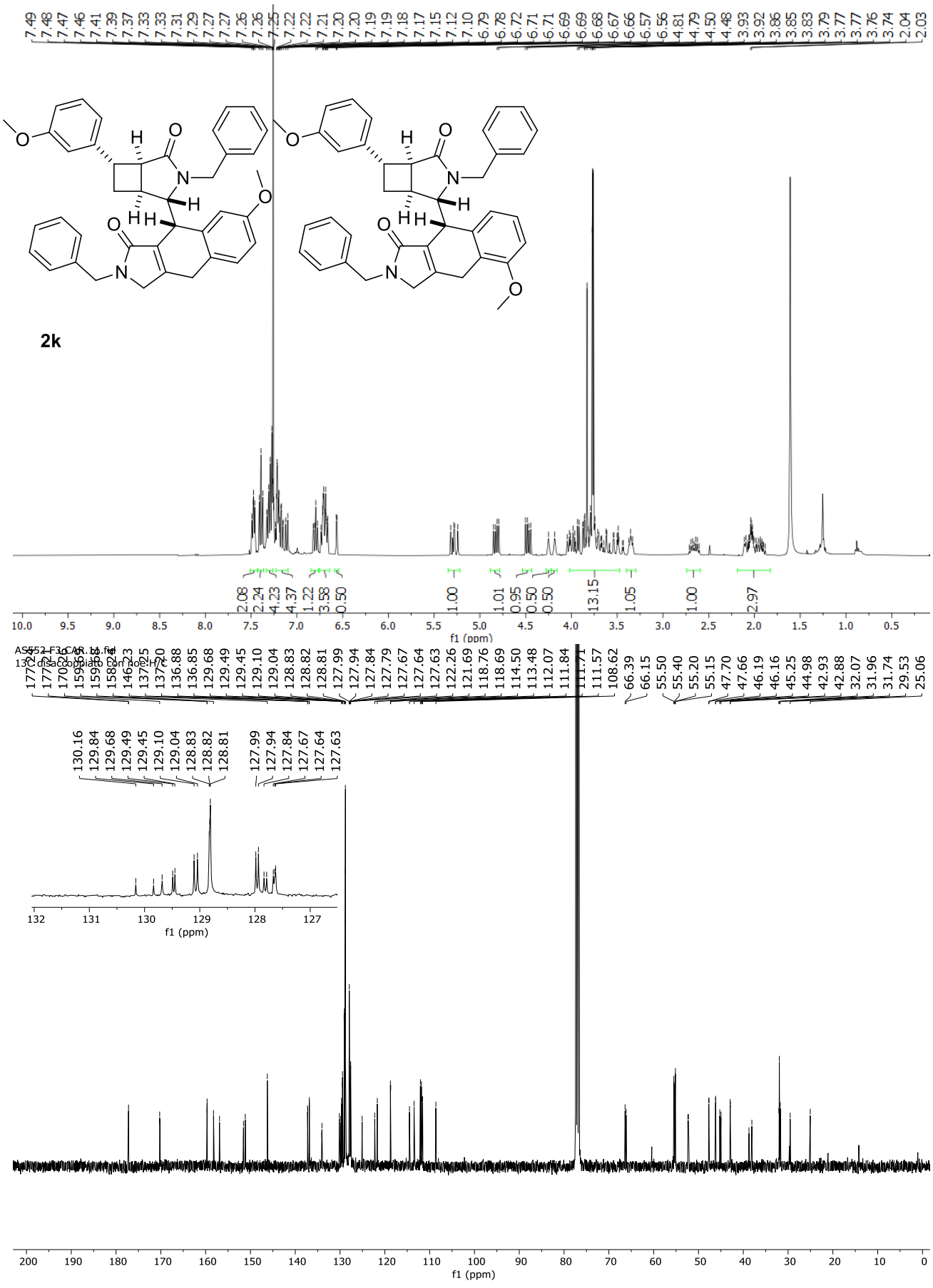

7.46 7.44 7.43 7.41 7.41 7.40 7.40 7.38 7.35 7.35 7.34 7.33 7.31 7.29 7.28 7.27 7.26 7.25 7.25 7.23 7.20 7.19 7.19 7.18 7.17 7.16 7.15 7.15 7.13 7.13 7.12 6.86 6.85 6.84 6.83 5.02 4.99 4.76 4.72 4.51 4.47 4.29 3.95 3.73 3.58 3.57 3.56 3.55 3.53 2.61 2.57 2.37 2.24
H
O
N
H
H
H
O
N
2i
15.96 2.17 0.96 1.35 0.94 0.97 0.98 2.98 3.00 1.97 2.98 3.61 1.12 1.38
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
178.07 170.45 153.62 141.95 137.40 136.63 136.56 135.83 135.47 134.70 131.00 130.19 129.50 128.82 128.79 128.55 127.98 127.79 127.60 127.36 126.93 126.44 126.25 124.34 64.23 52.10 47.20 46.31 46.05 40.14 40.04 33.45 31.31 29.89 19.73 19.58
131.00 130.19 129.50 128.82 128.79 128.55 127.98 127.79 127.60 127.36 126.93 126.44 126.25
32 131 130 129 128 127 126
f1 (ppm)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

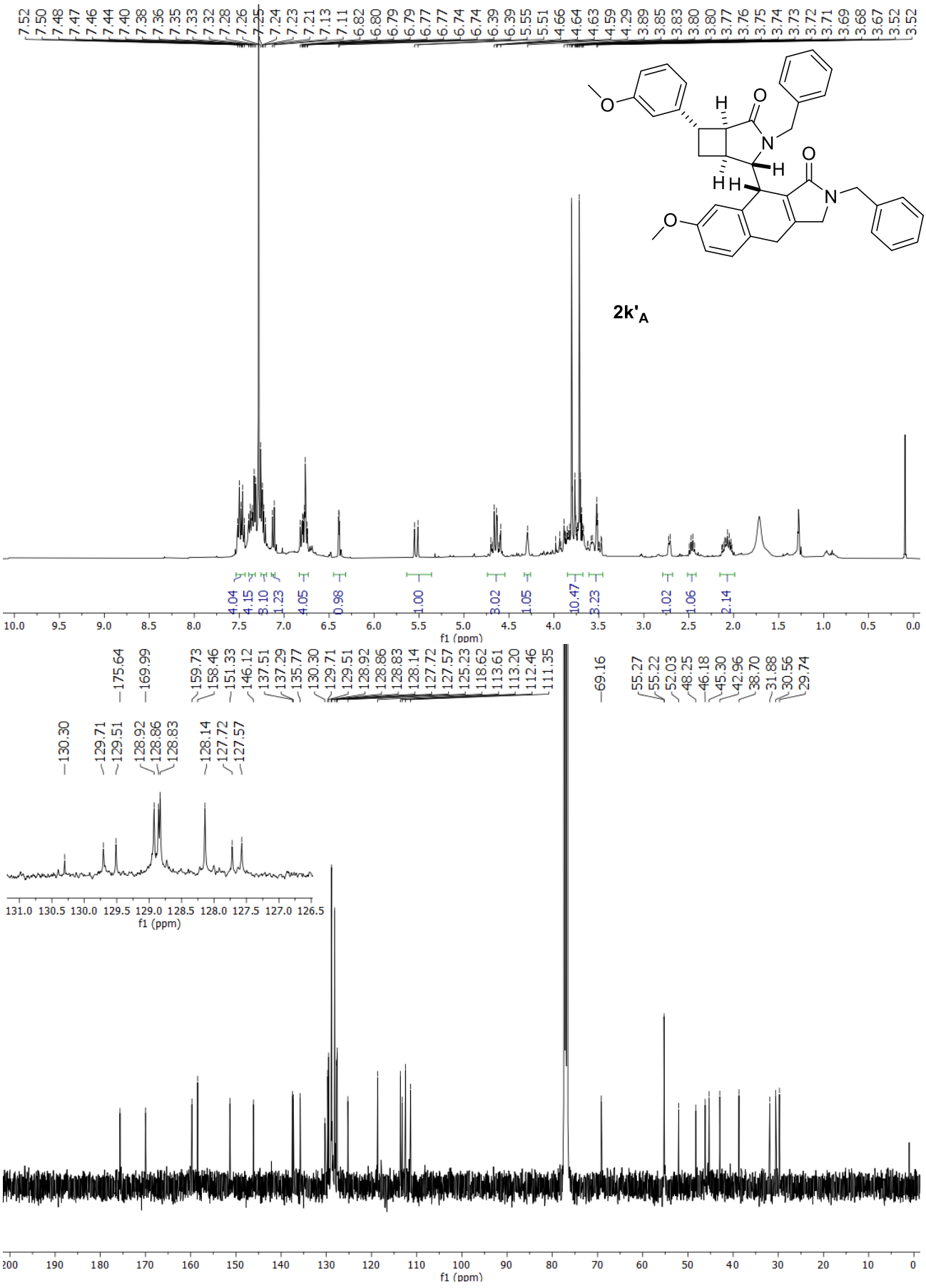

7.50 7.48 7.44 7.42 7.42 7.41 7.36 7.36 7.36 7.35 7.35 7.35 7.34 7.34 7.33 7.32 7.32 7.32 7.28 7.28 7.28 7.28 7.26 7.26 7.24 7.20 7.20 7.19 7.18 7.18 7.17 7.16 7.15 7.14 7.12 7.09 7.06 5.62 5.58 4.68 4.65 4.65 4.61 3.94 3.89 3.75 3.57 3.57 3.53 3.52 2.32 2.16 2.09 2.07 2.07 2.05
22.66 0.98 3.10 1.04 1.05 3.19 2.19 1.03 1.07 3.17 3.07 2.21
f1 (ppm)
176.03 170.10 151.10 141.49 137.64 137.54 136.76 136.29 134.13 133.22 131.77 130.59 129.51 128.84 128.79 128.57 128.05 127.56 127.04 126.95 126.30 125.84 123.44 66.45 51.86 46.97 46.18 45.03 40.15 35.51 31.56 30.57 30.24 19.57 19.49
f1 (ppm)

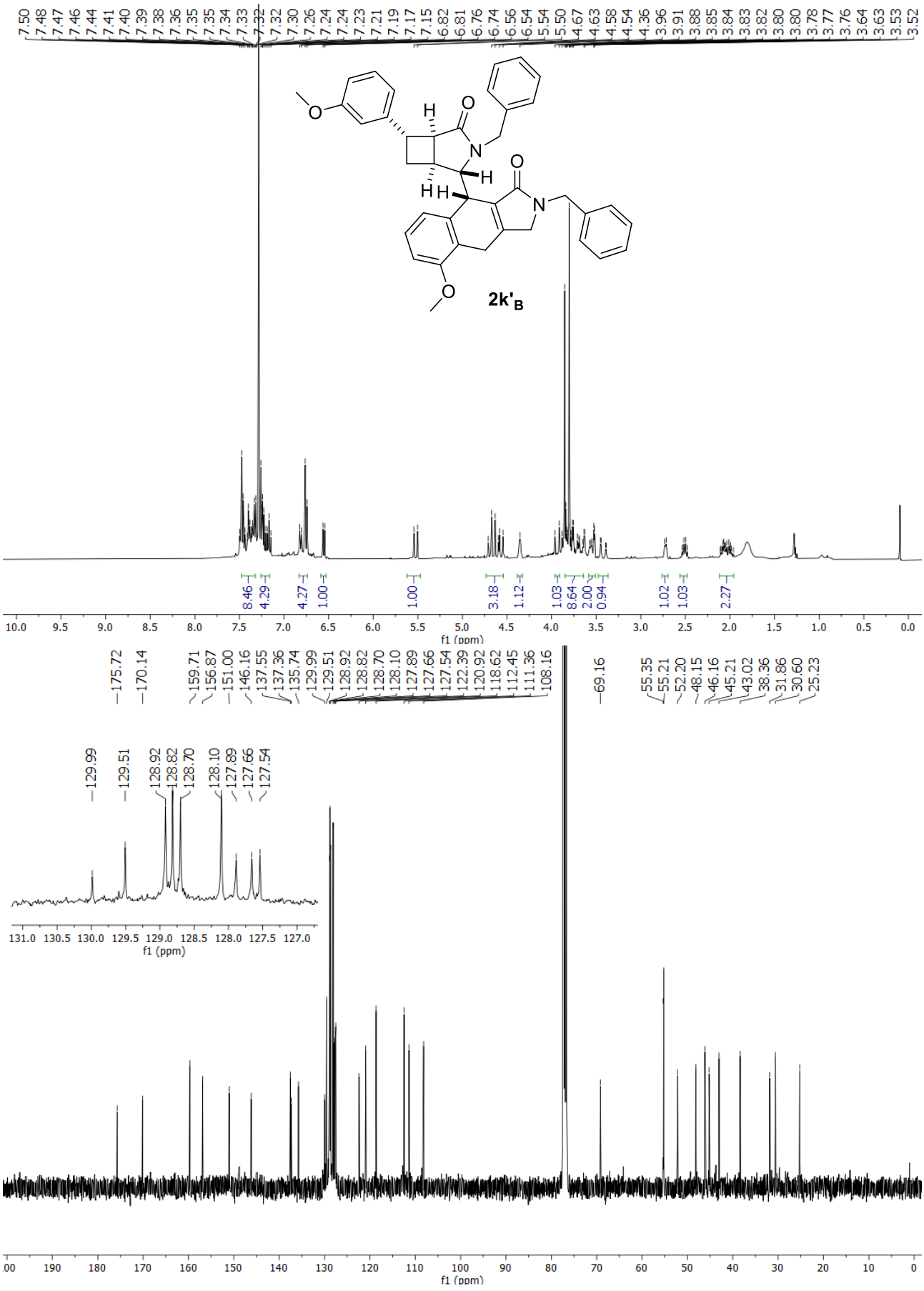
2i'

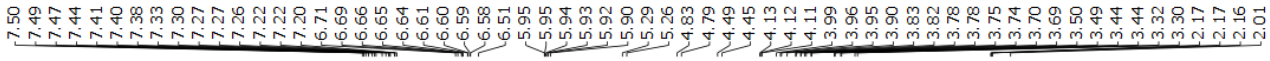

2j
A
B
f1 (ppm)

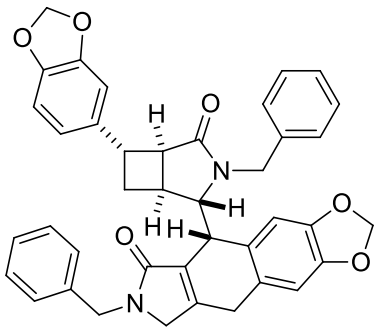

2j'
A
B
f1 (ppm)
f1 (ppm)


2k
f1 (ppm)

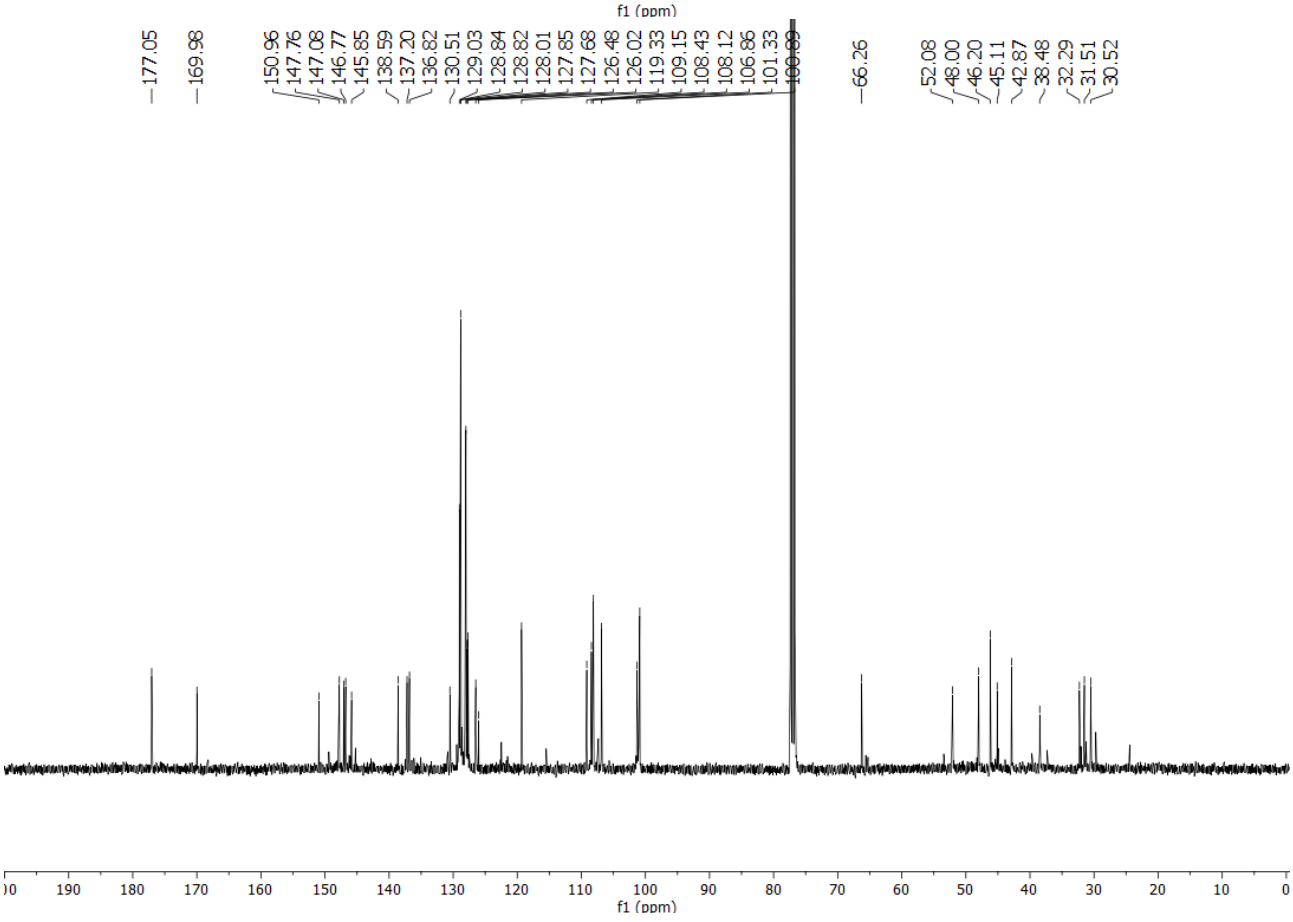

7.52 7.50 7.48 7.47 7.46 7.44 7.40 7.38 7.36 7.35 7.33 7.32 7.28 7.26 7.25 7.24 7.23 7.21 7.13 7.11 6.82 6.80 6.79 6.79 6.77 6.77 6.74 6.74 6.39 6.39 5.55 5.51 4.66 4.64 4.63 4.59 4.29 3.89 3.85 3.83 3.80 3.80 3.77 3.76 3.75 3.74 3.73 3.72 3.71 3.69 3.68 3.67 3.52 3.52
O
H
O
N
H
H H
O
N
O
2k'A
4.04 4.15 3.10 1.23 4.05 0.98 1.00 3.02 1.05 10.47 3.23 1.02 1.06 2.14
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
175.64 169.99 159.73 158.46 151.33 146.12 137.51 137.29 135.77 130.30 129.71 129.51 128.92 128.86 128.83 128.14 127.72 127.57 125.23 118.62 113.61 113.20 112.46 111.35 69.16 55.27 55.22 52.03 48.25 46.18 45.30 42.96 38.70 31.88 30.56 29.74
130.30 129.71 129.51 128.92 128.86 128.83 128.14 127.72 127.57
131.0 130.5 130.0 129.5 129.0 128.5 128.0 127.5 127.0 126.5
f1 (ppm)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

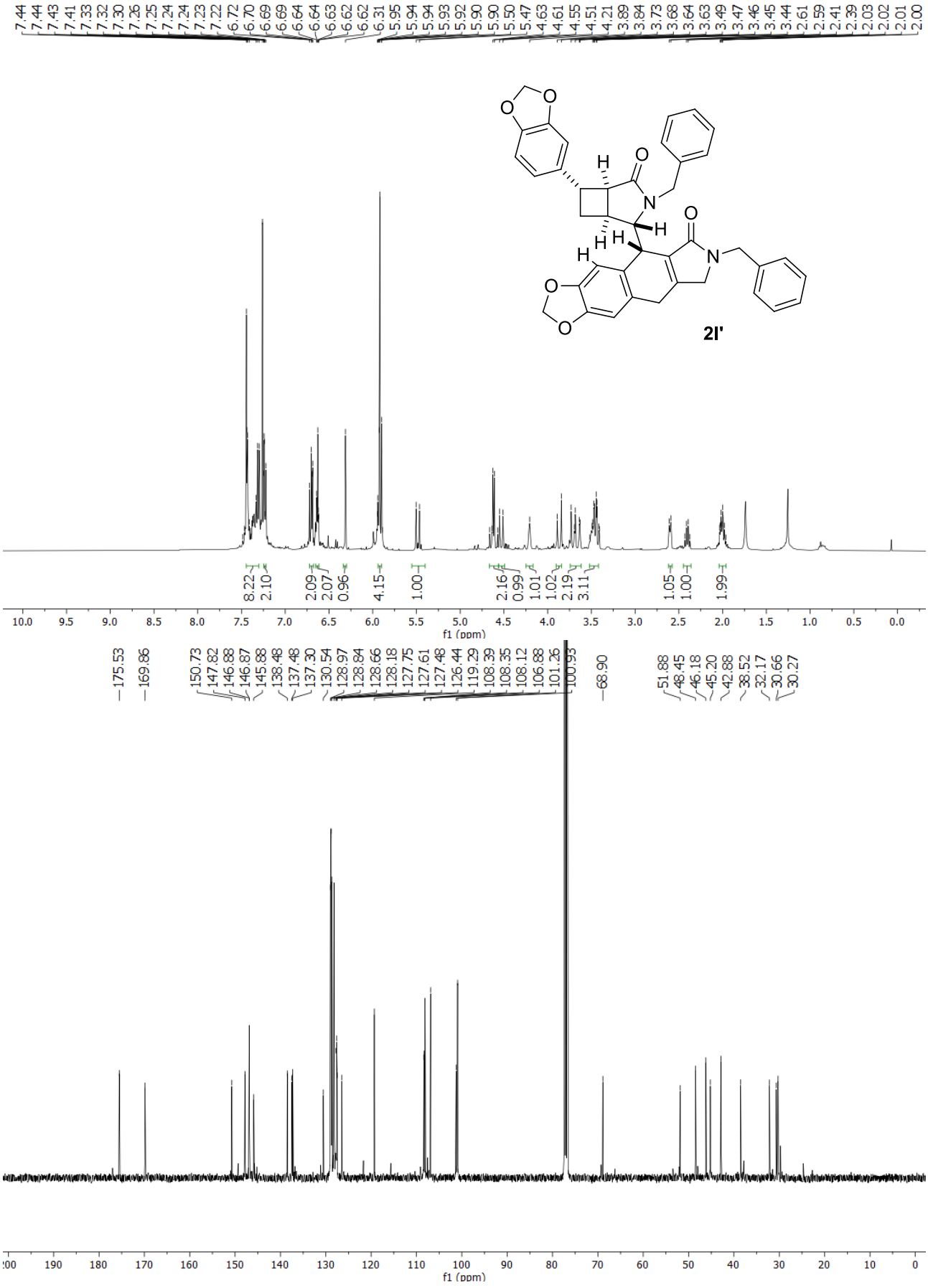

2k'B
f1 (ppm)

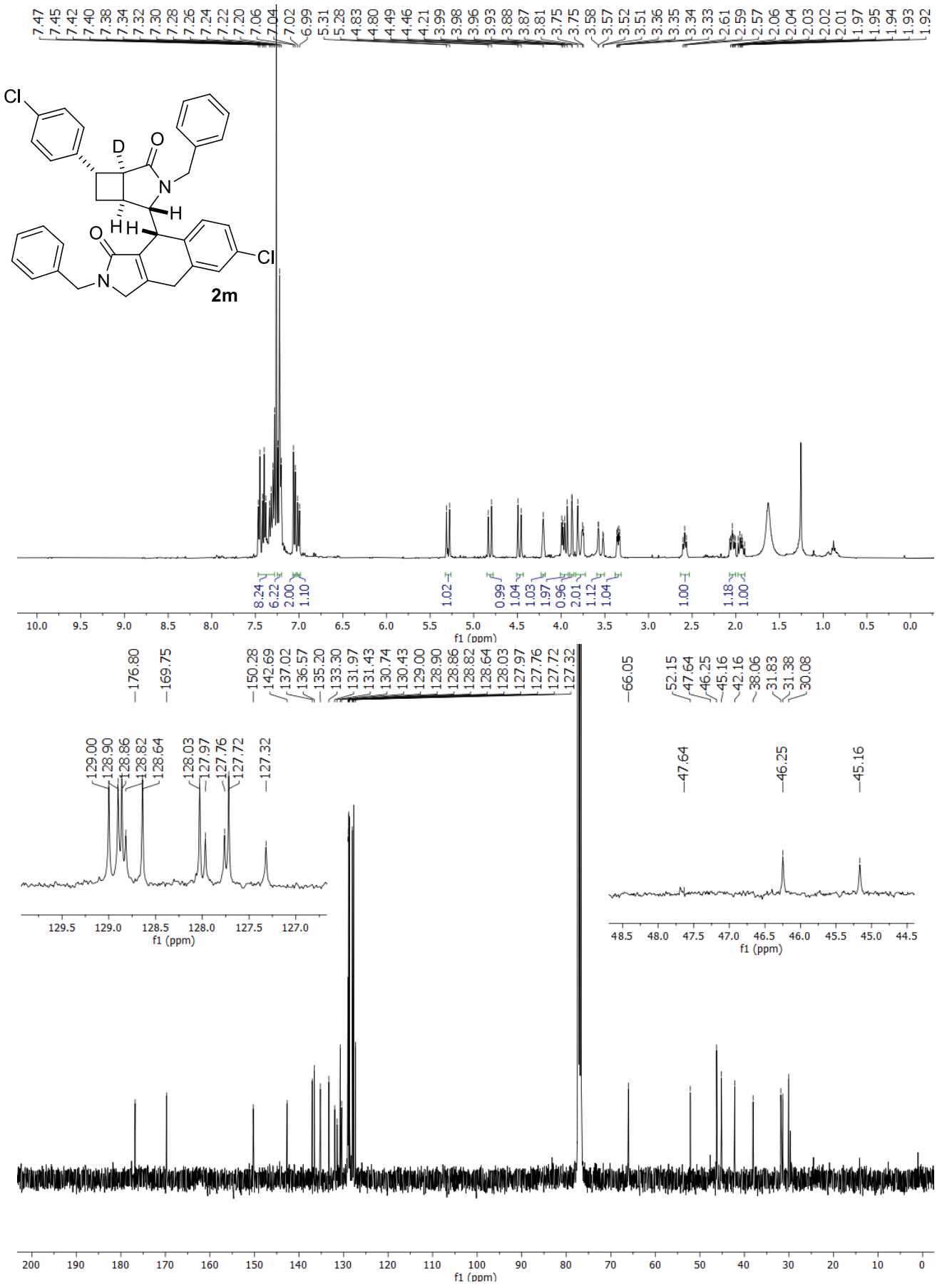


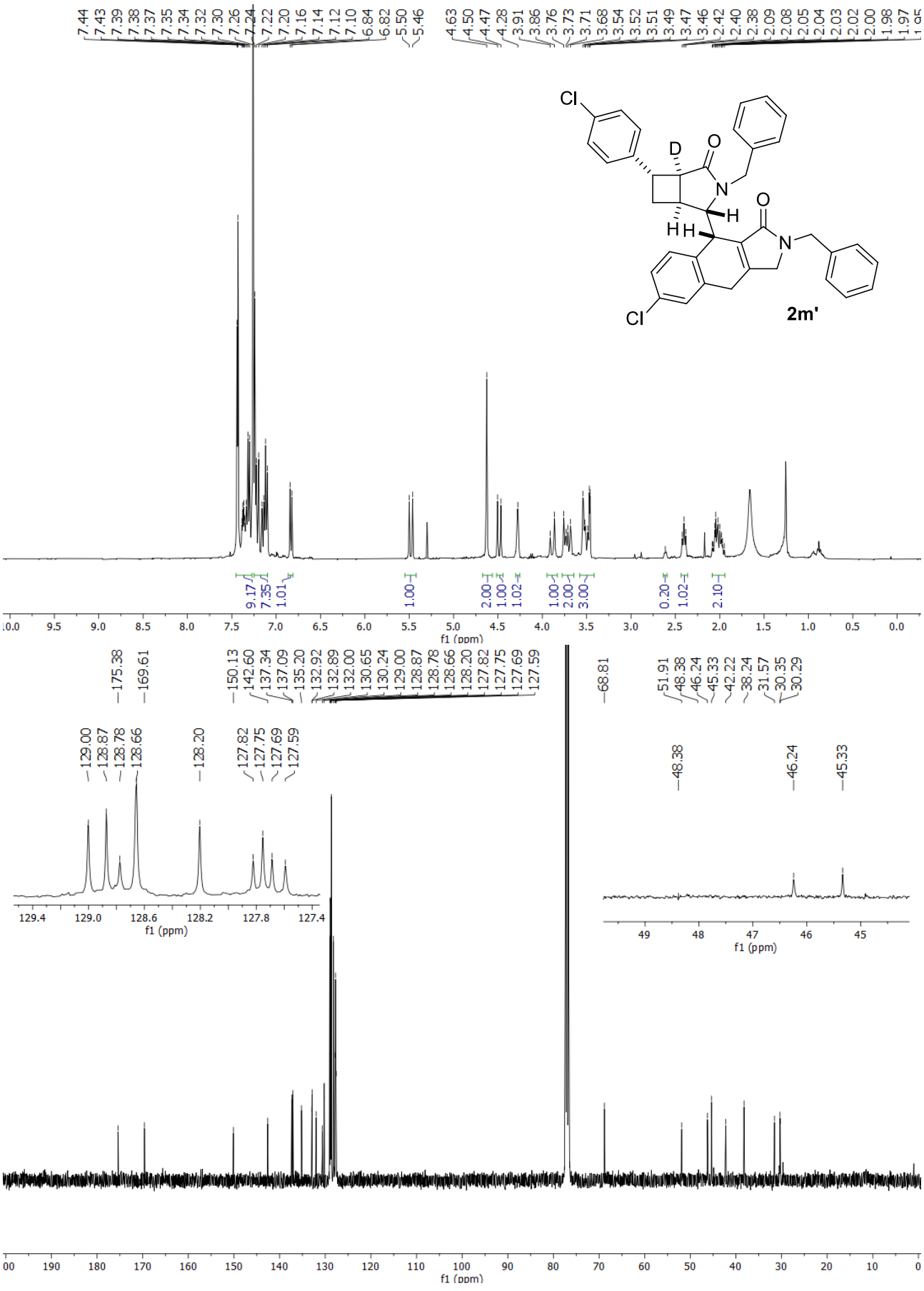


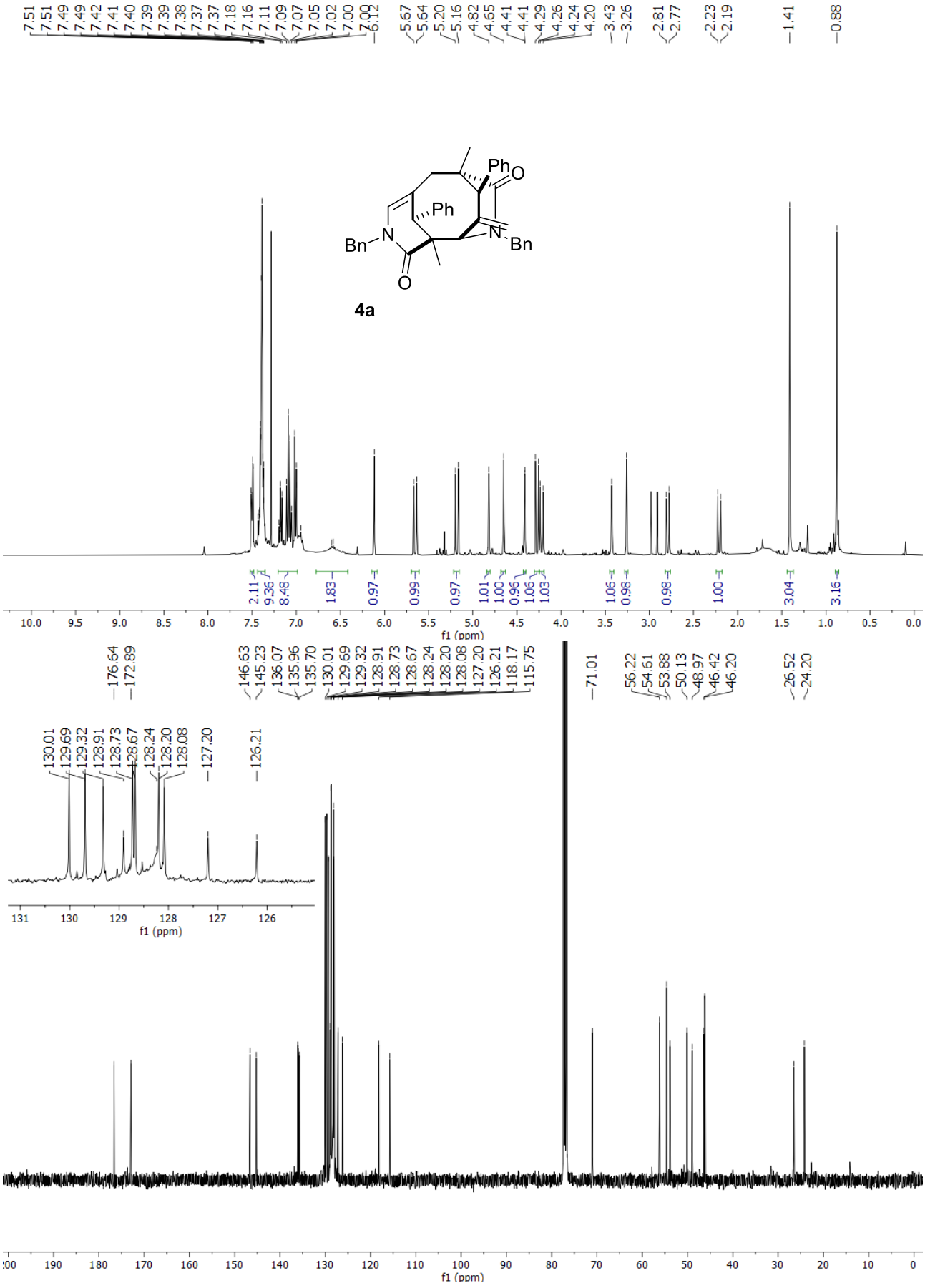
2l

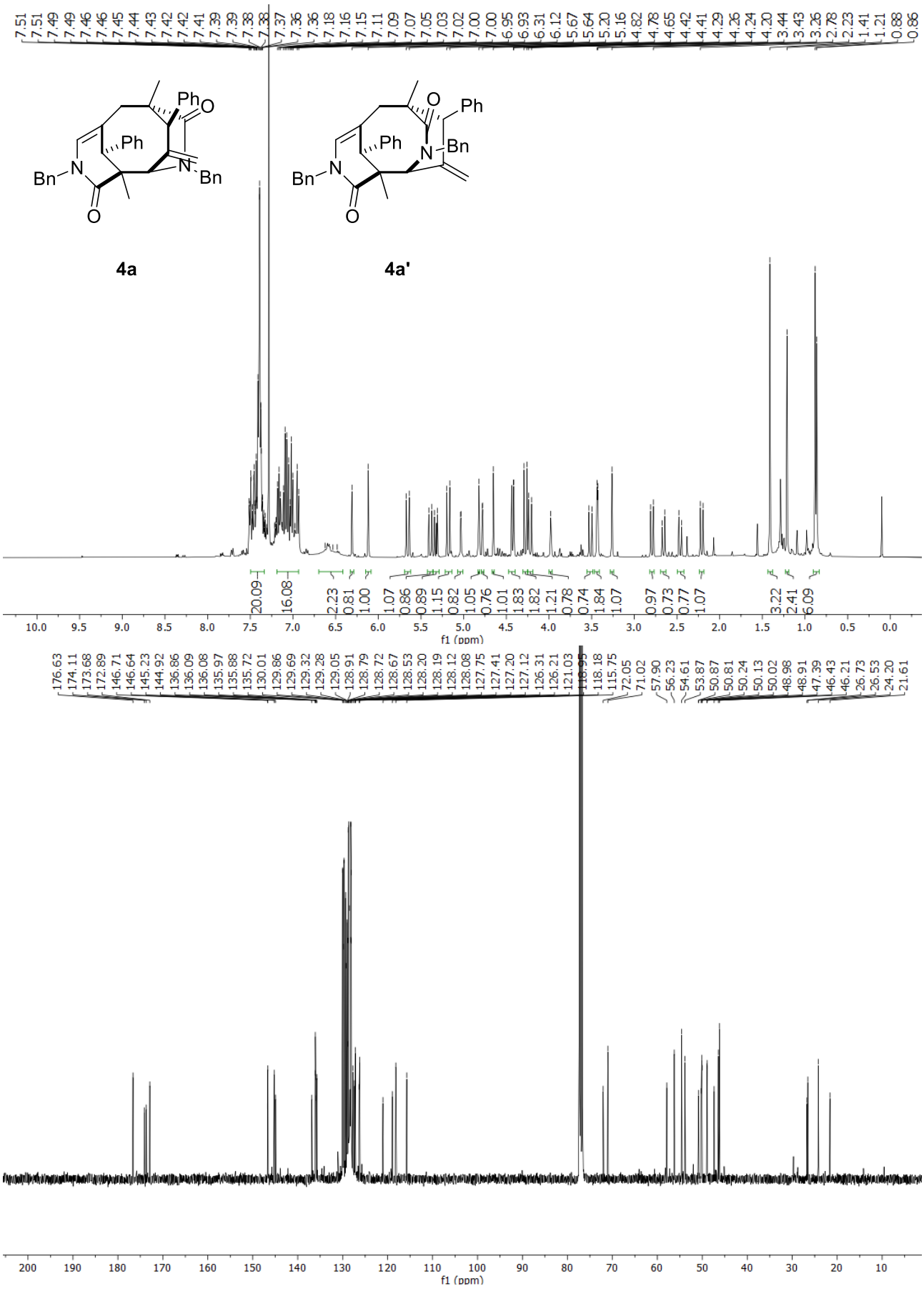


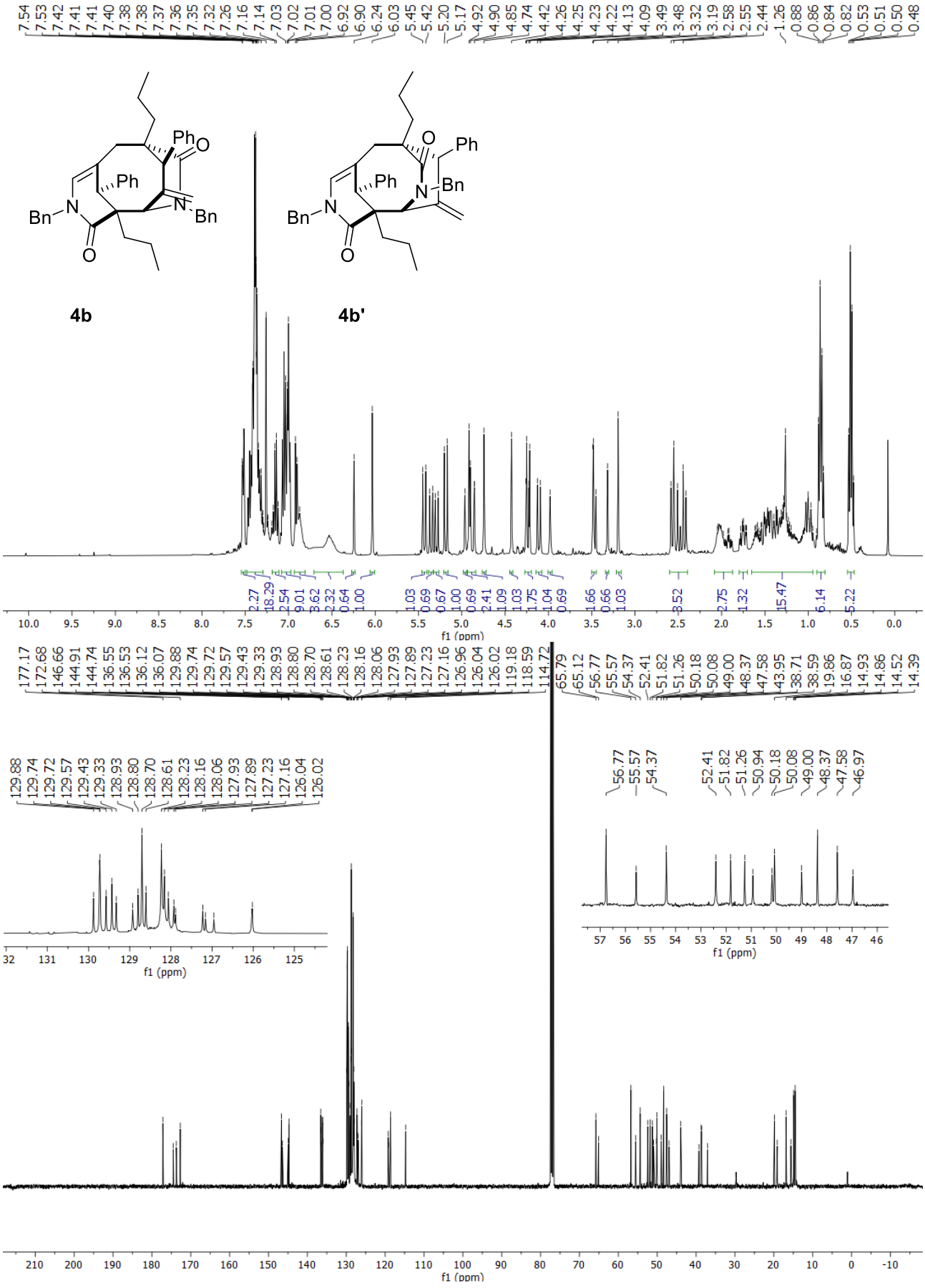

7.44 7.44 7.43 7.41 7.33 7.32 7.30 7.26 7.25 7.24 7.24 7.23 7.22 6.72 6.70 6.69 6.69 6.64 6.64 6.63 6.62 6.62 6.31 5.95 5.94 5.94 5.93 5.92 5.90 5.90 5.50 5.47 4.63 4.61 4.55 4.51 4.21 3.89 3.84 3.73 3.68 3.64 3.63 3.49 3.47 3.46 3.45 3.44 2.61 2.59 2.41 2.39 2.03 2.02 2.01 2.00
2I'
8.22 2.10 2.09 2.07 0.96 4.15 1.00 2.16 0.99 1.01 1.02 2.19 3.11 1.05 1.00 1.99
f1 (ppm)
175.53 169.86 150.73 147.82 146.88 146.87 145.88 138.48 137.48 137.30 130.54 128.97 128.84 128.66 128.18 127.75 127.61 127.48 126.44 119.29 108.39 108.35 108.12 106.88 101.26 100.93 68.90 51.88 48.45 46.18 45.20 42.88 38.52 32.17 30.66 30.27
f1 (ppm)

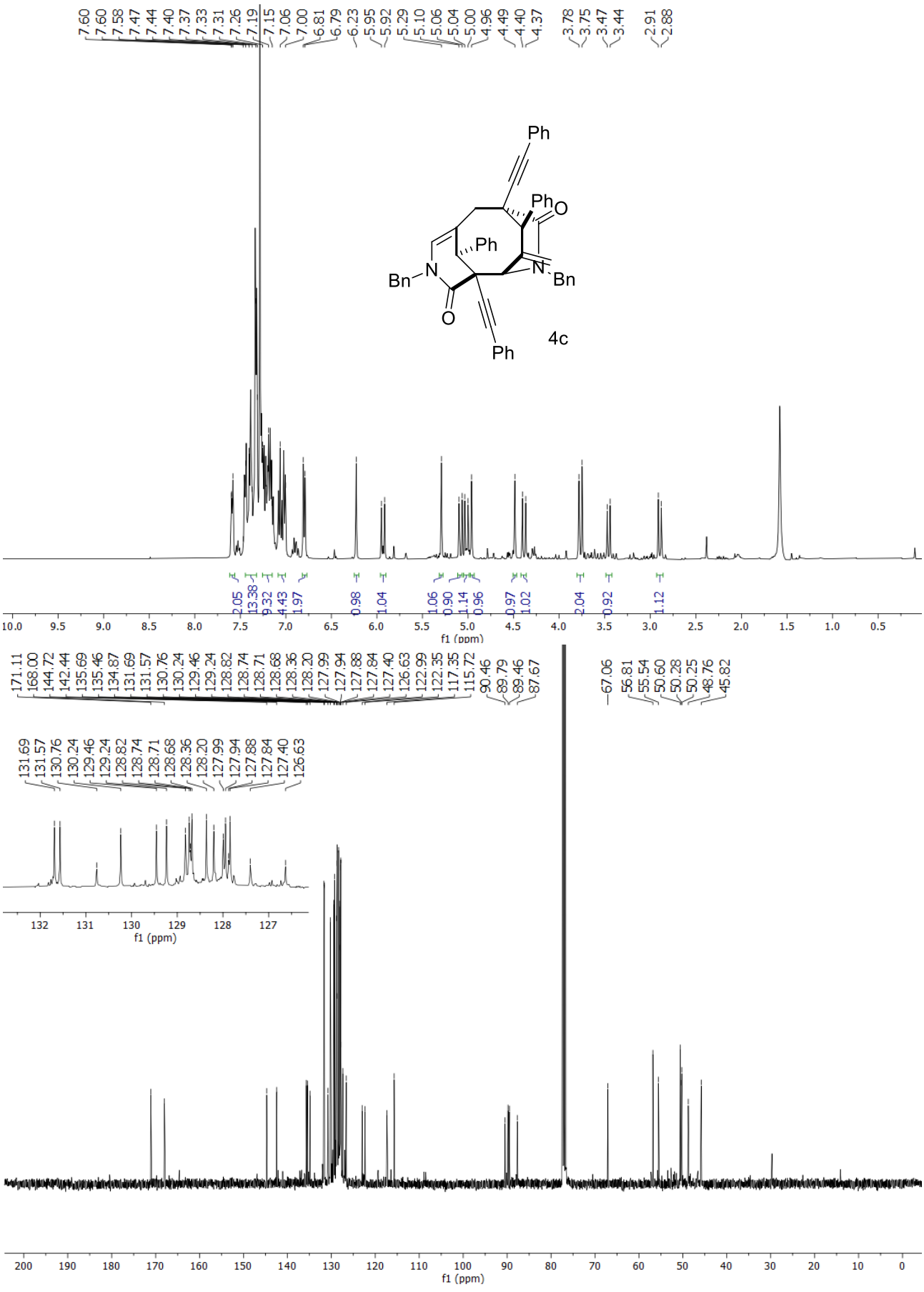

Cl
D
O
N
H
H
H
O
Cl
N
2m
f1 (ppm)
f1 (ppm)
f1 (ppm)
f1 (ppm)

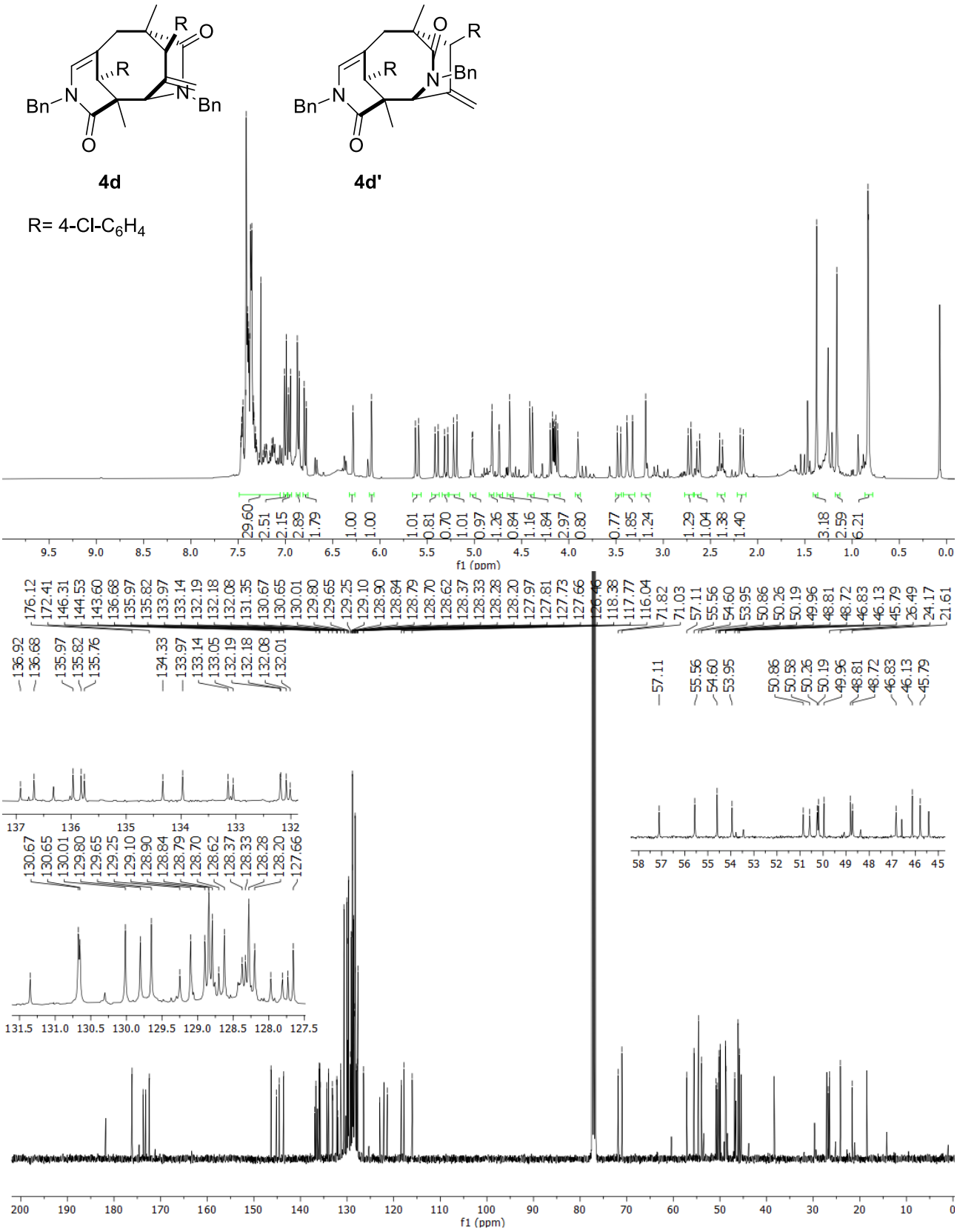

Cl
D
O
N
H
H
H
O
N
Cl
2m'
f1 (ppm)
f1 (ppm)
f1 (ppm)
f1 (ppm)

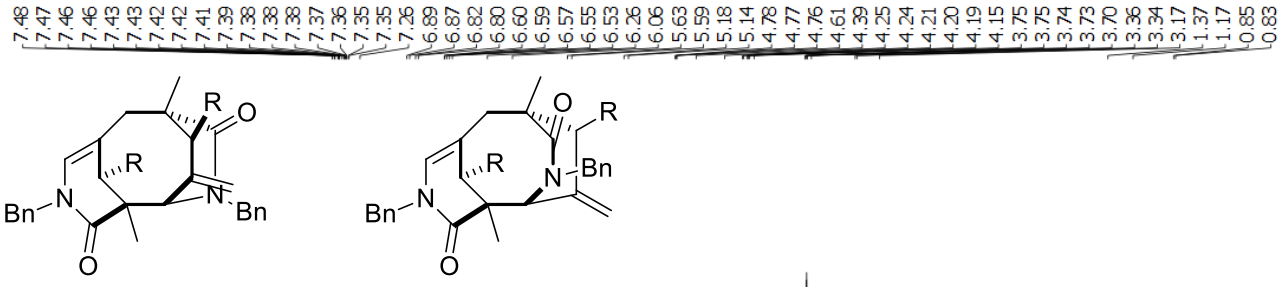

7.51 7.51 7.49 7.49 7.42 7.41 7.40 7.39 7.39 7.38 7.37 7.37 7.18 7.16 7.11 7.09 7.07 7.05 7.02 7.00 7.00 6.12
5.67 5.64 5.20 5.16 4.82 4.65 4.41 4.41 4.29 4.26 4.24 4.20
3.43 3.26
2.81 2.77
2.23 2.19
1.41
0.88
Ph
O
Ph
Bn
N
N
Bn
O
4a
2.11 9.36 8.48 1.83 0.97 0.99 0.97 1.01 1.00 0.96 1.06 1.03 1.06 0.98 0.98 1.00 3.04 3.16
f1 (ppm)
176.64 172.89
146.63 145.23 136.07 135.96 135.70 130.01 129.69 129.32 128.91 128.73 128.67 128.24 128.20 128.08 127.20 126.21 118.17 115.75
71.01
56.22 54.61 53.88 50.13 48.97 46.42 46.20
26.52 24.20
130.01 129.69 129.32 128.91 128.73 128.67 128.24 128.20 128.08 127.20 126.21
f1 (ppm)
f1 (ppm)


Ph
O
Ph
N
Bn
N
Bn
O
4a
O
Ph
Ph
N
Bn
Bn
N
O
4a'
f1 (ppm)
f1 (ppm)


4b
4b'
f1 (ppm)

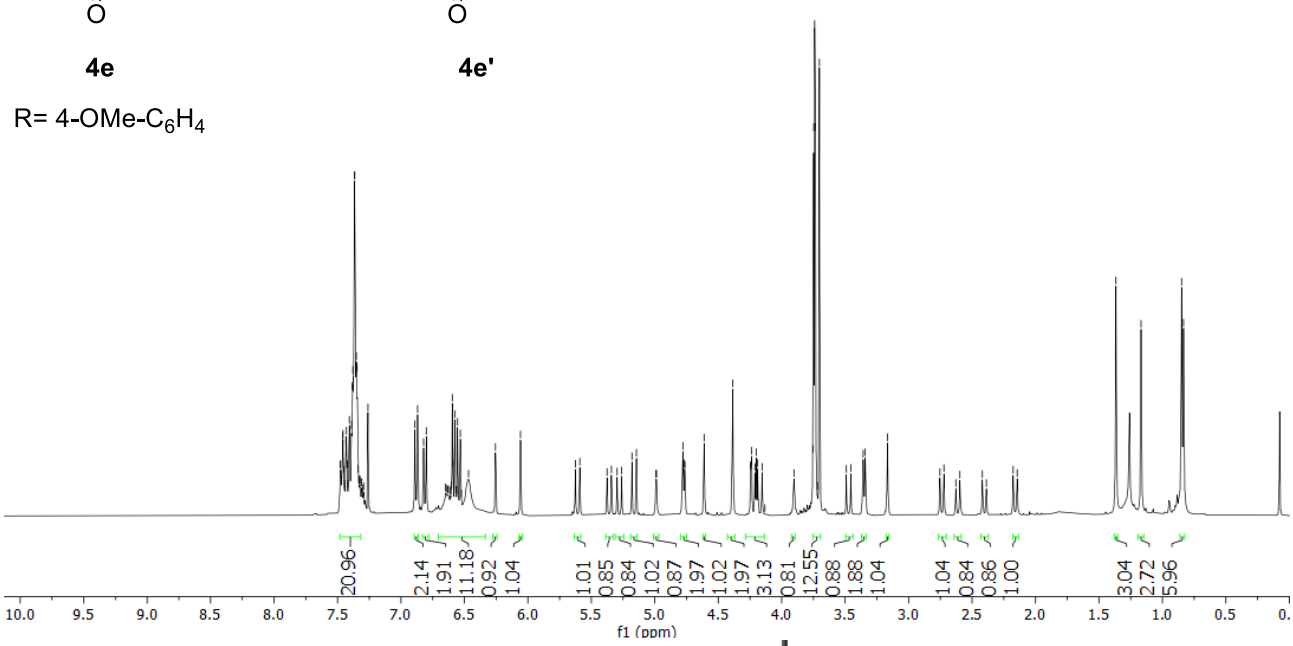

7.60
7.60
7.58
7.47
7.44
7.40
7.37
7.33
7.31
7.26
7.19
7.15
7.06
7.00
6.81
6.79
6.23
5.95
5.92
5.29
5.10
5.06
5.04
5.00
4.96
4.49
4.40
4.37
3.78
3.75
3.47
3.44
2.91
2.88
Ph
Ph
O
Ph
N
Bn
N
Bn
O
Ph
4c
2.05
13.38
9.32
4.43
1.97
0.98
1.04
1.06
0.90
1.14
0.96
0.97
1.02
2.04
0.92
1.12
f1 (ppm)
171.11
168.00
144.72
142.44
135.69
135.46
134.87
131.69
131.57
130.76
130.24
129.46
129.24
128.82
128.74
128.71
128.68
128.36
128.20
127.99
127.94
127.88
127.84
127.40
126.63
122.99
122.35
117.35
115.72
90.46
89.79
89.46
87.67
67.06
56.81
55.54
50.60
50.28
50.25
48.76
45.82
f1 (ppm)

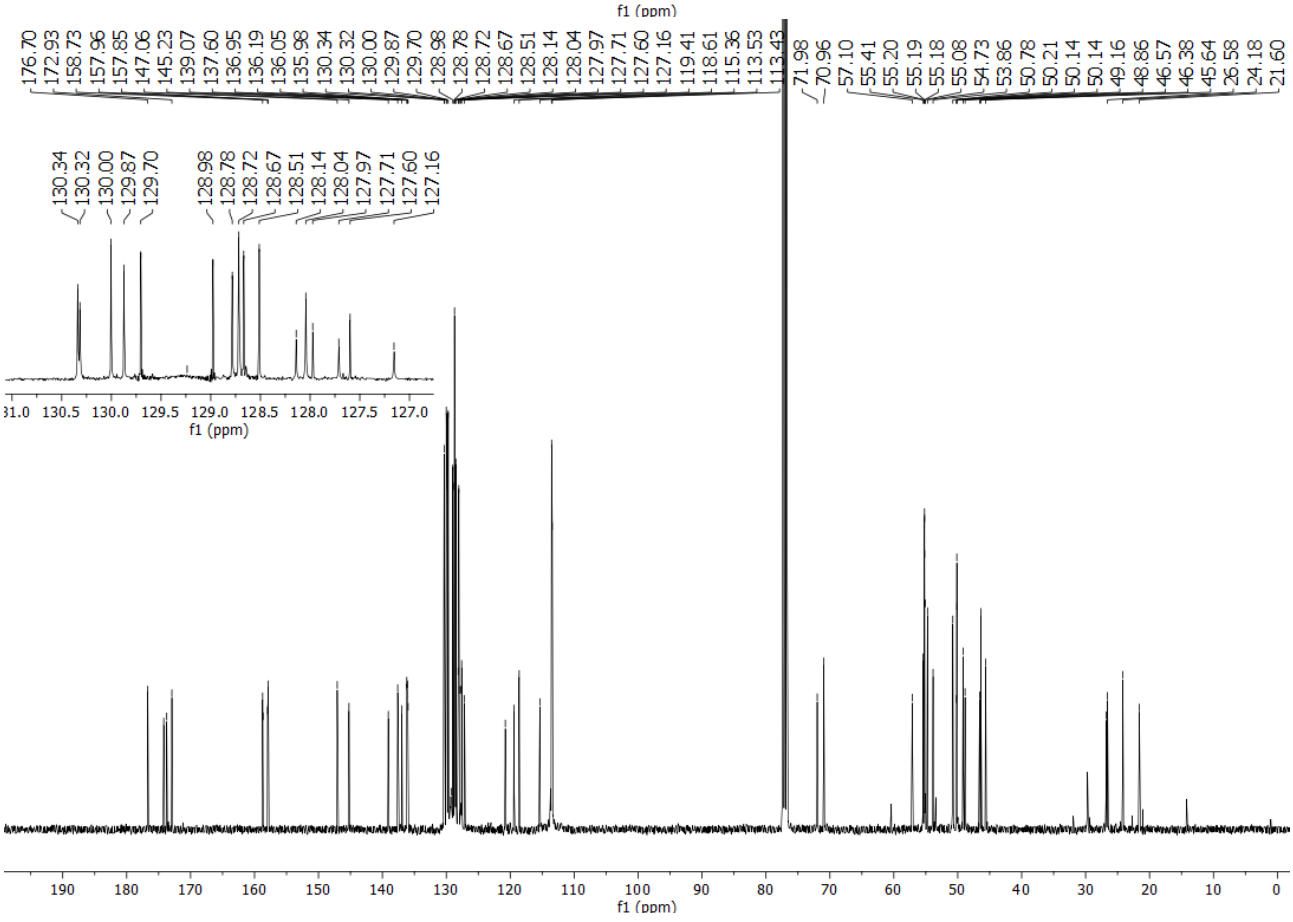

4d
4d'
R= 4-Cl-C6H4
f1 (ppm)
f1 (ppm)

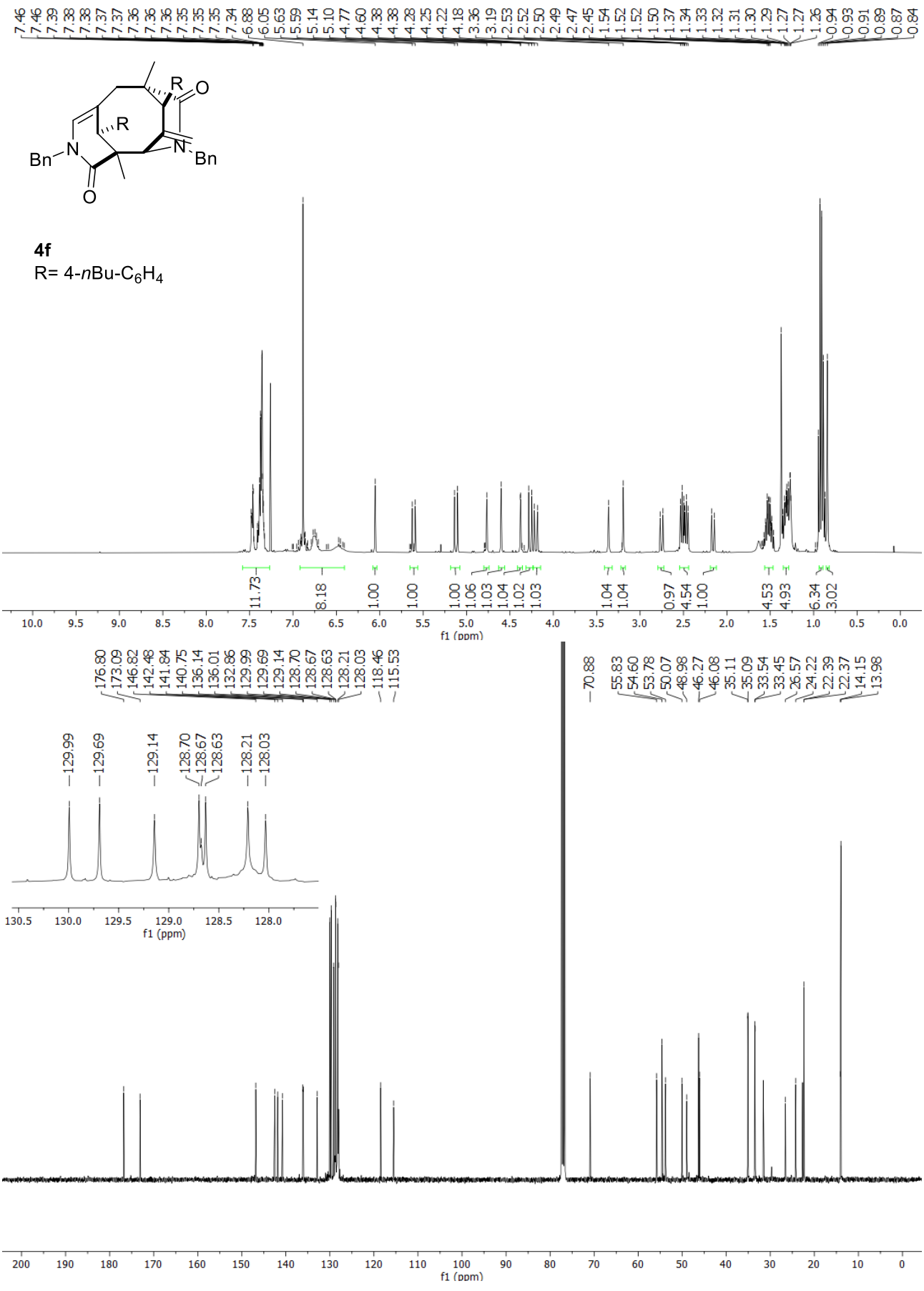


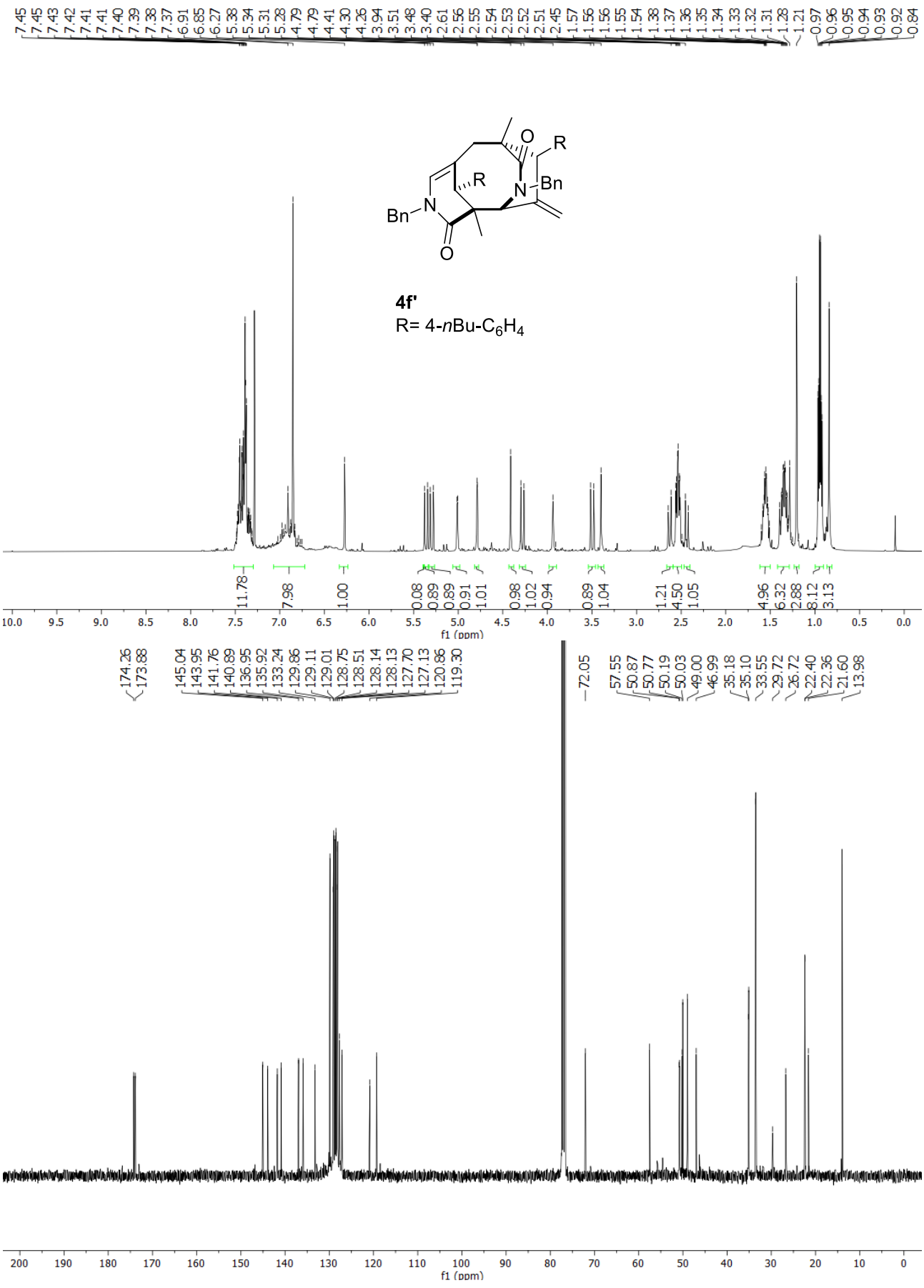
4e **4e'**

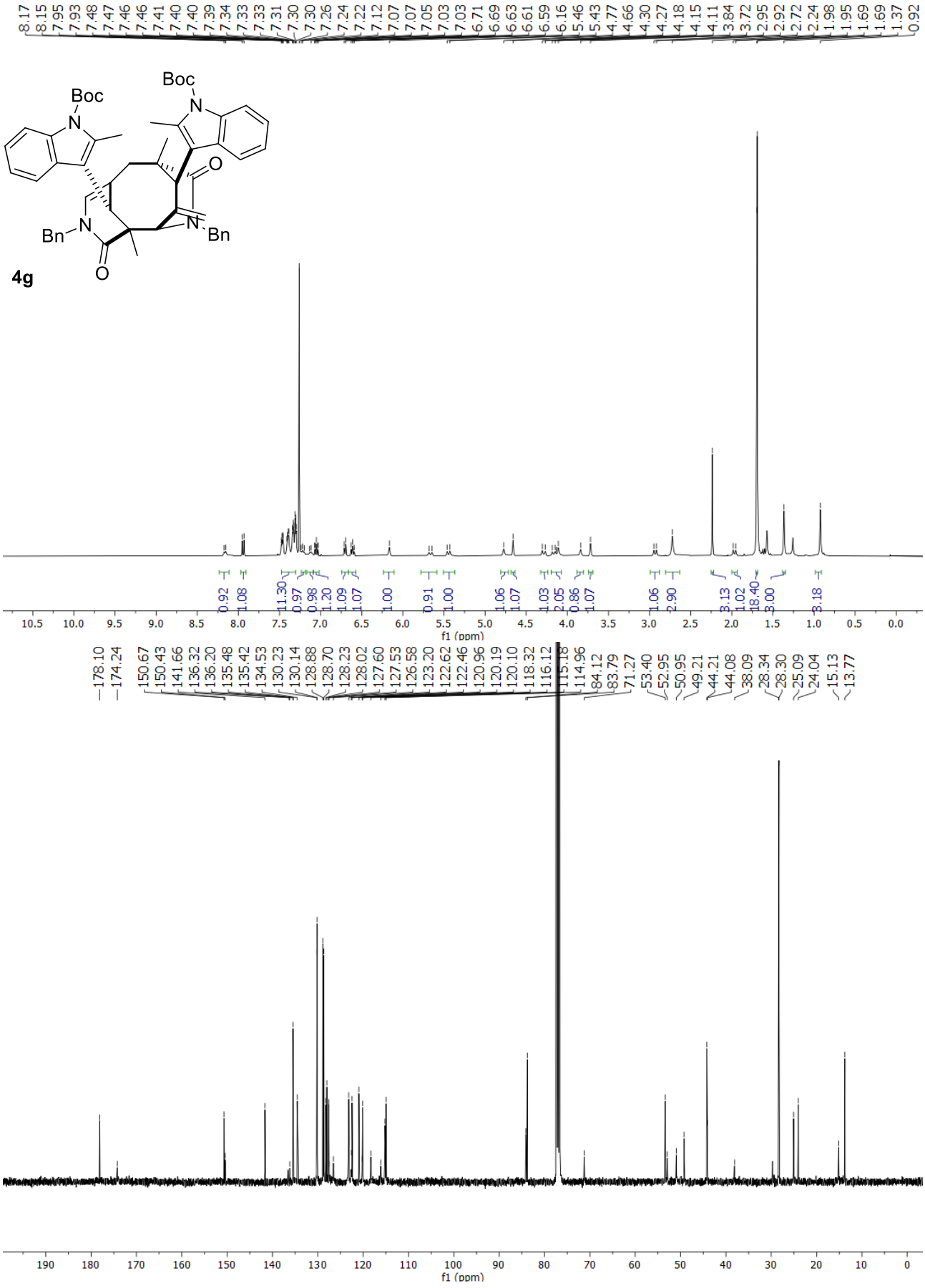
R= 4-OMe-C_6H_4

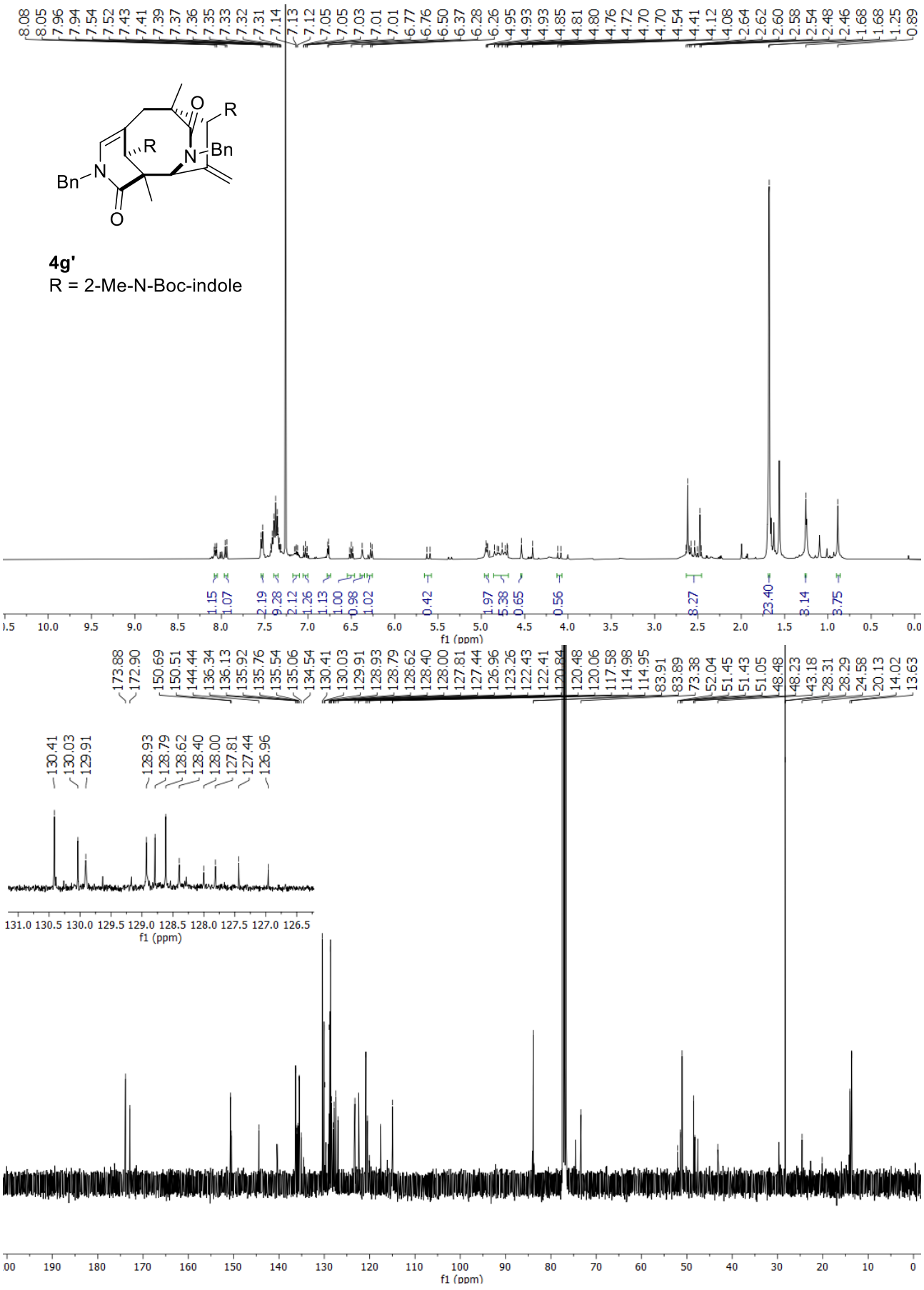


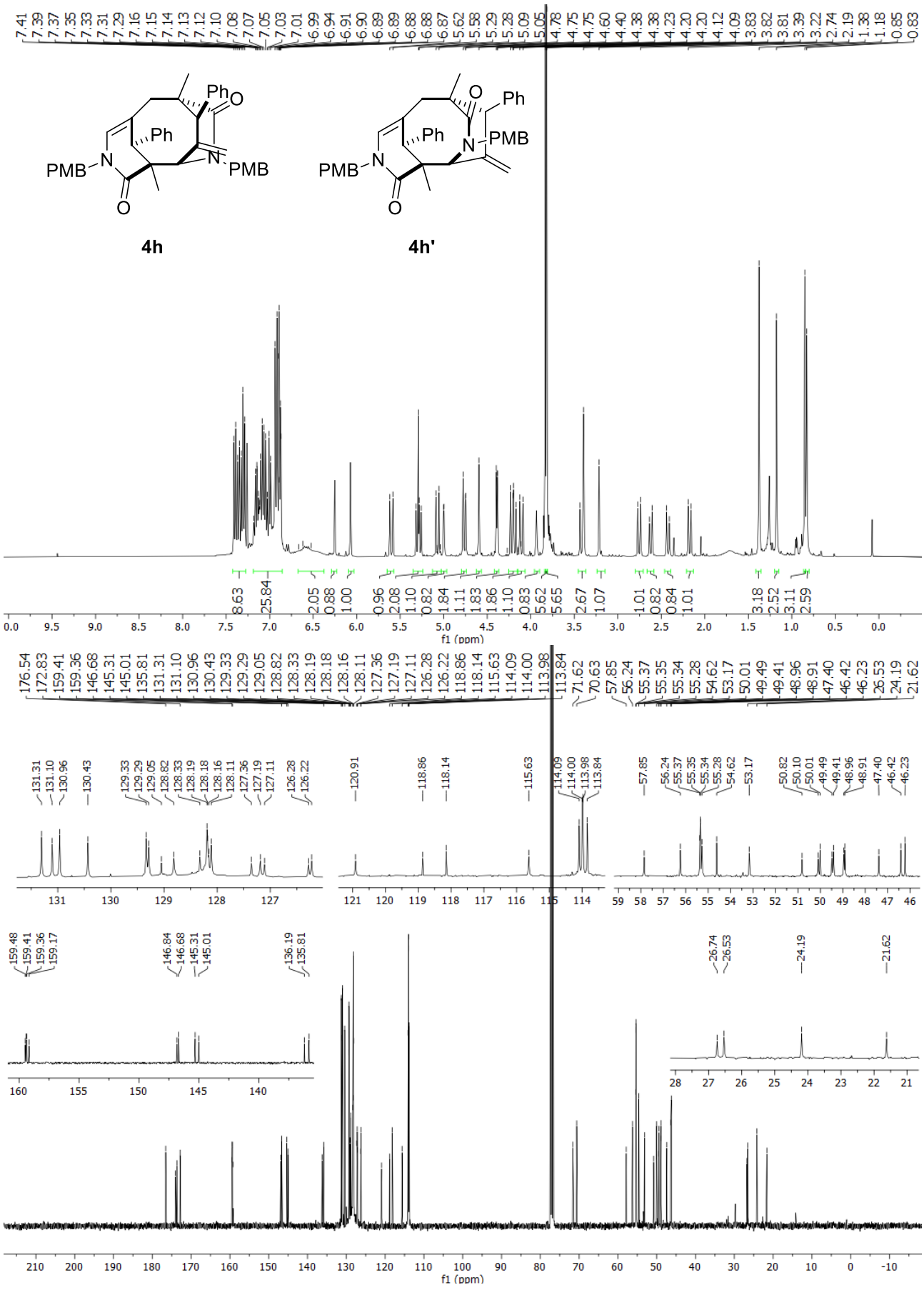


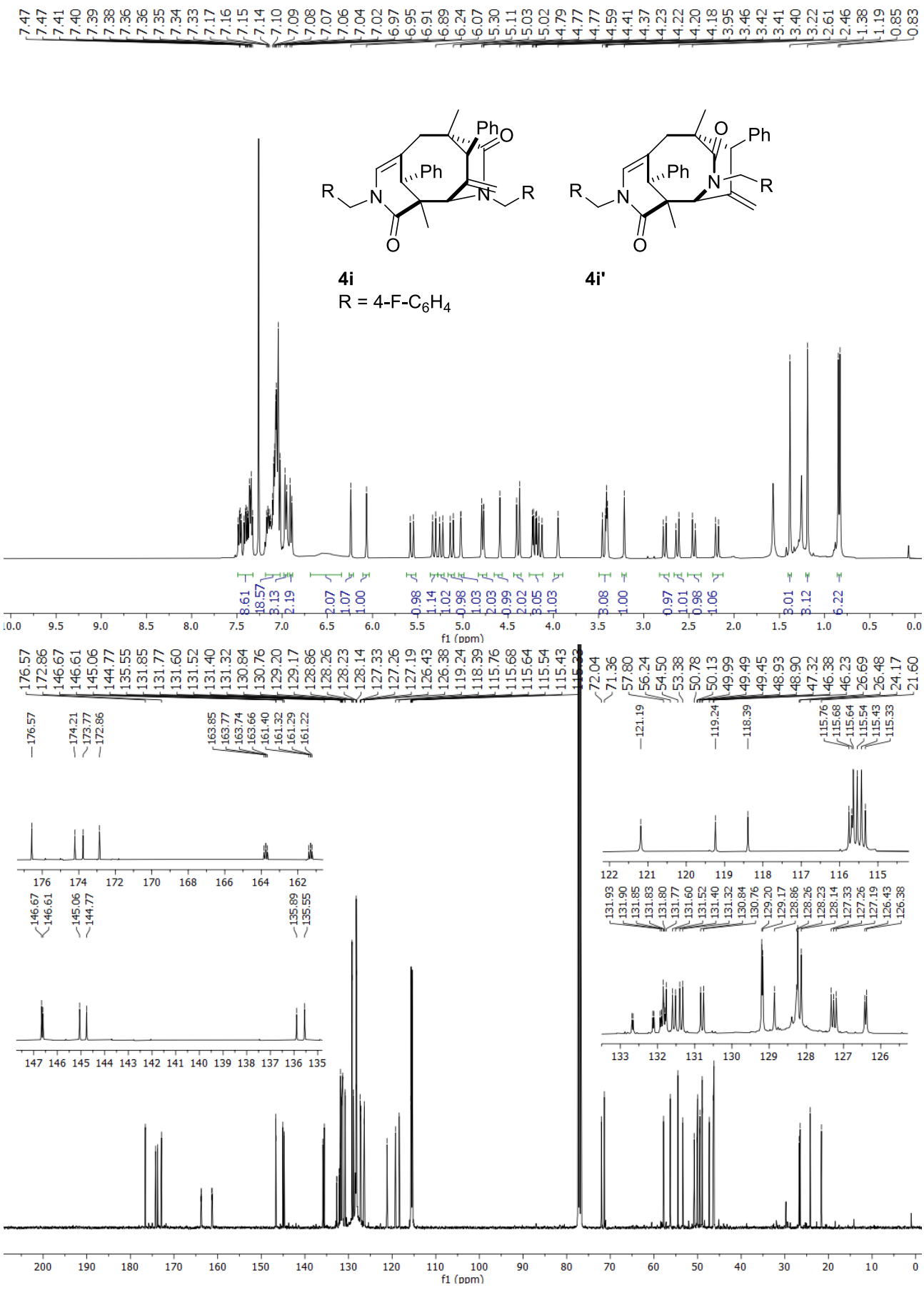

7.46 7.46 7.39 7.38 7.38 7.37 7.37 7.36 7.36 7.36 7.35 7.35 7.34 6.88 6.05 5.63 5.59 5.14 5.10 4.77 4.60 4.38 4.28 4.25 4.22 4.18 3.36 3.19 2.53 2.52 2.50 2.49 2.47 2.45 1.54 1.52 1.52 1.50 1.37 1.34 1.33 1.32 1.31 1.30 1.29 1.27 1.27 1.26 0.94 0.93 0.91 0.89 0.87 0.84
R
O
R
Bn
N
N
Bn
O
4f
R= 4-nBu-C6H4
11.73 8.18 1.00 1.00 1.00 1.06 1.03 1.04 1.02 1.03 1.04 1.04 0.97 4.54 1.00 4.53 4.93 6.34 3.02
f1 (ppm)
176.80 173.09 146.82 142.48 141.84 140.75 136.14 136.01 132.86 129.99 129.69 129.14 128.70 128.67 128.63 128.21 128.03 118.46 115.53
70.88 55.83 54.60 53.78 50.07 48.98 46.27 46.08 35.11 35.09 33.54 33.45 26.57 24.22 22.39 22.37 14.15 13.98
129.99 129.69 129.14 128.70 128.67 128.63 128.21 128.03
f1 (ppm)
f1 (ppm)

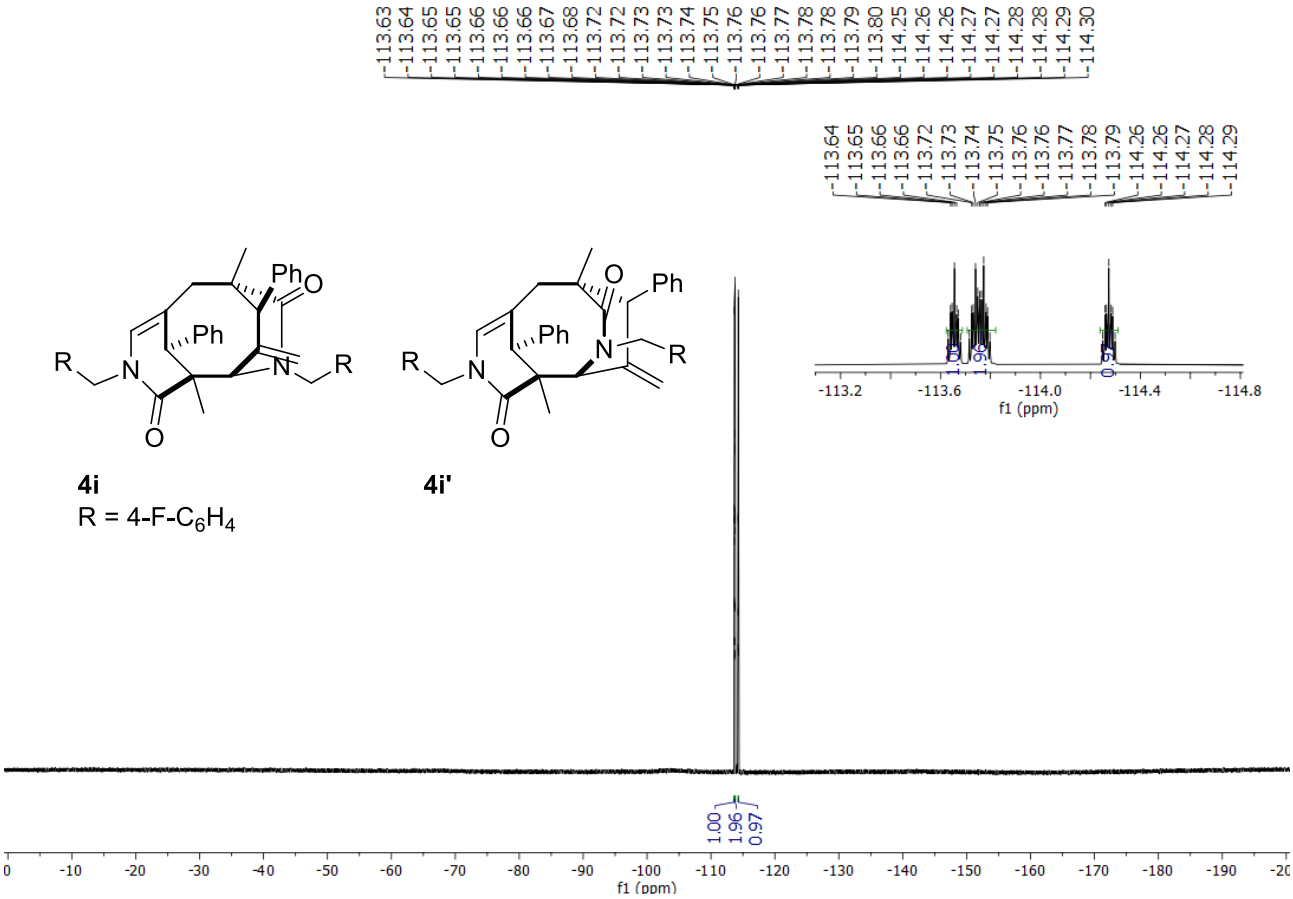

7.45 7.45 7.43 7.42 7.41 7.41 7.40 7.39 7.38 7.37 6.91 6.85 6.27 5.38 5.34 5.31 5.28 4.79 4.79 4.41 4.30 4.26 3.94 3.51 3.48 3.40 2.61 2.56 2.55 2.54 2.53 2.52 2.51 2.45 1.57 1.56 1.56 1.55 1.54 1.38 1.37 1.36 1.35 1.34 1.33 1.32 1.31 1.28 1.21 0.97 0.96 0.95 0.94 0.93 0.92 0.84
O
R
R
N
Bn
Bn
N
O
4f'
R= 4-nBu-C6H4
11.78 7.98 1.00 0.08 0.89 0.89 0.91 1.01 0.98 1.02 0.94 0.89 1.04 1.21 4.50 1.05 4.96 6.32 2.88 8.12 3.13
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
174.26 173.88 145.04 143.95 141.76 140.89 136.95 135.92 133.24 129.86 129.11 129.01 128.75 128.51 128.14 128.13 127.70 127.13 120.86 119.30 72.05 57.55 50.87 50.77 50.19 50.03 49.00 46.99 35.18 35.10 33.55 29.72 26.72 22.40 22.36 21.60 13.98
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Boc
N
Boc
N
O
N
Bn
N
Bn
O
4g
f1 (ppm)
f1 (ppm)


O
R
R
N
Bn
Bn
N
O
4g'
R = 2-Me-N-Boc-indole
f1 (ppm)


Ph
O
Ph
PMB
N
N
PMB
O
4h
O
Ph
Ph
N
PMB
PMB
N
O
4h'
f1 (ppm)
f1 (ppm)

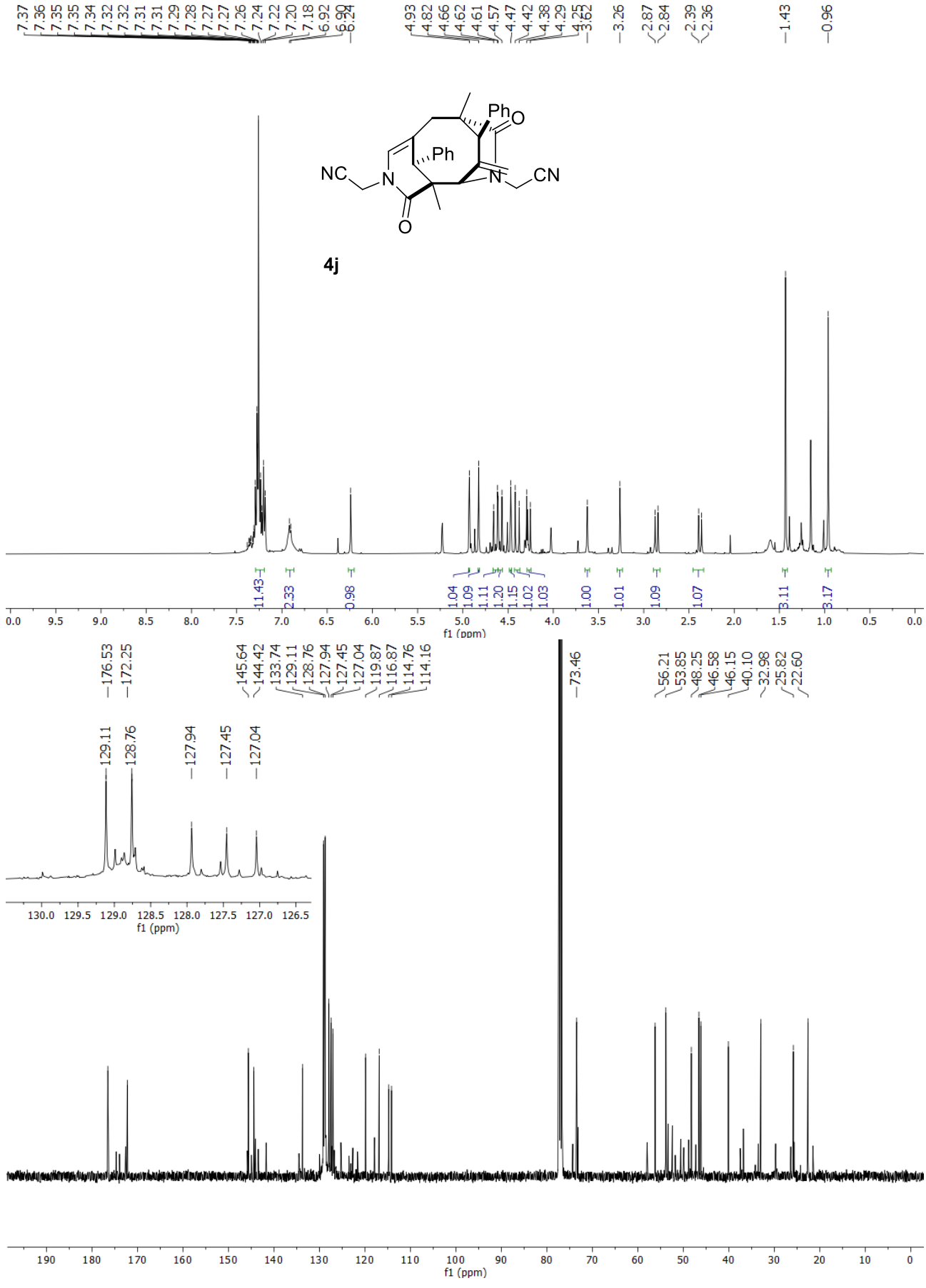

4i
R = 4-F-C6H4
4i'

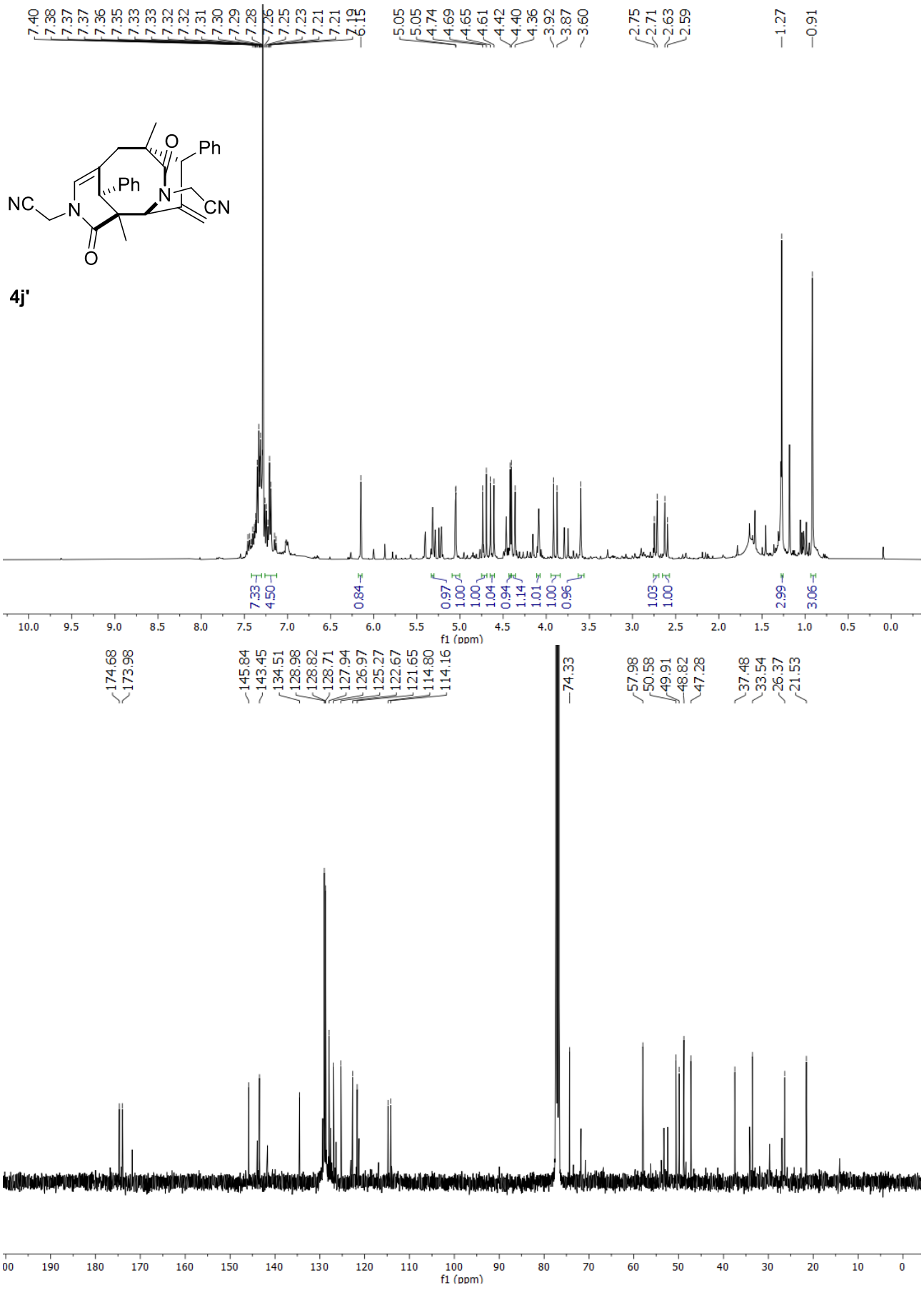


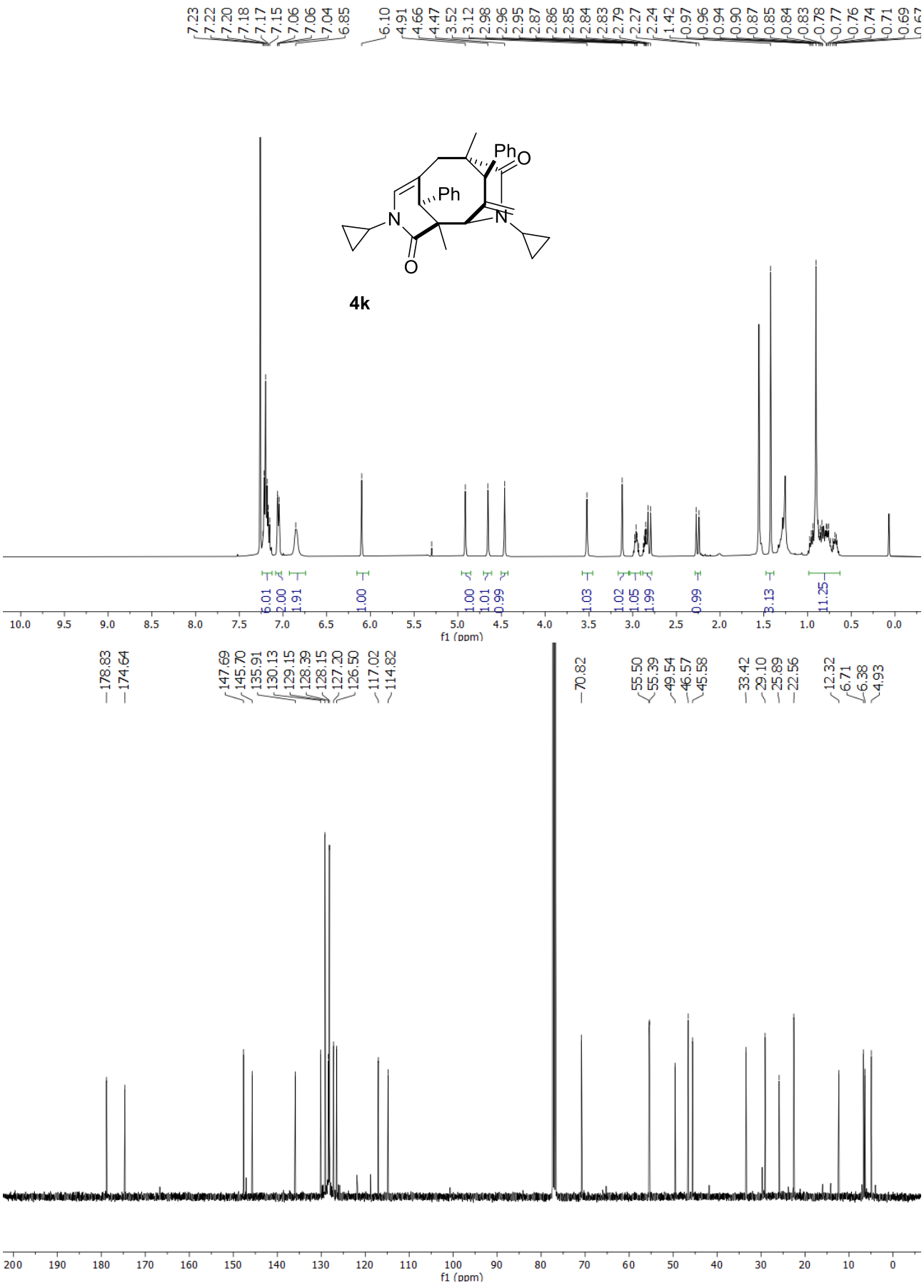
4i

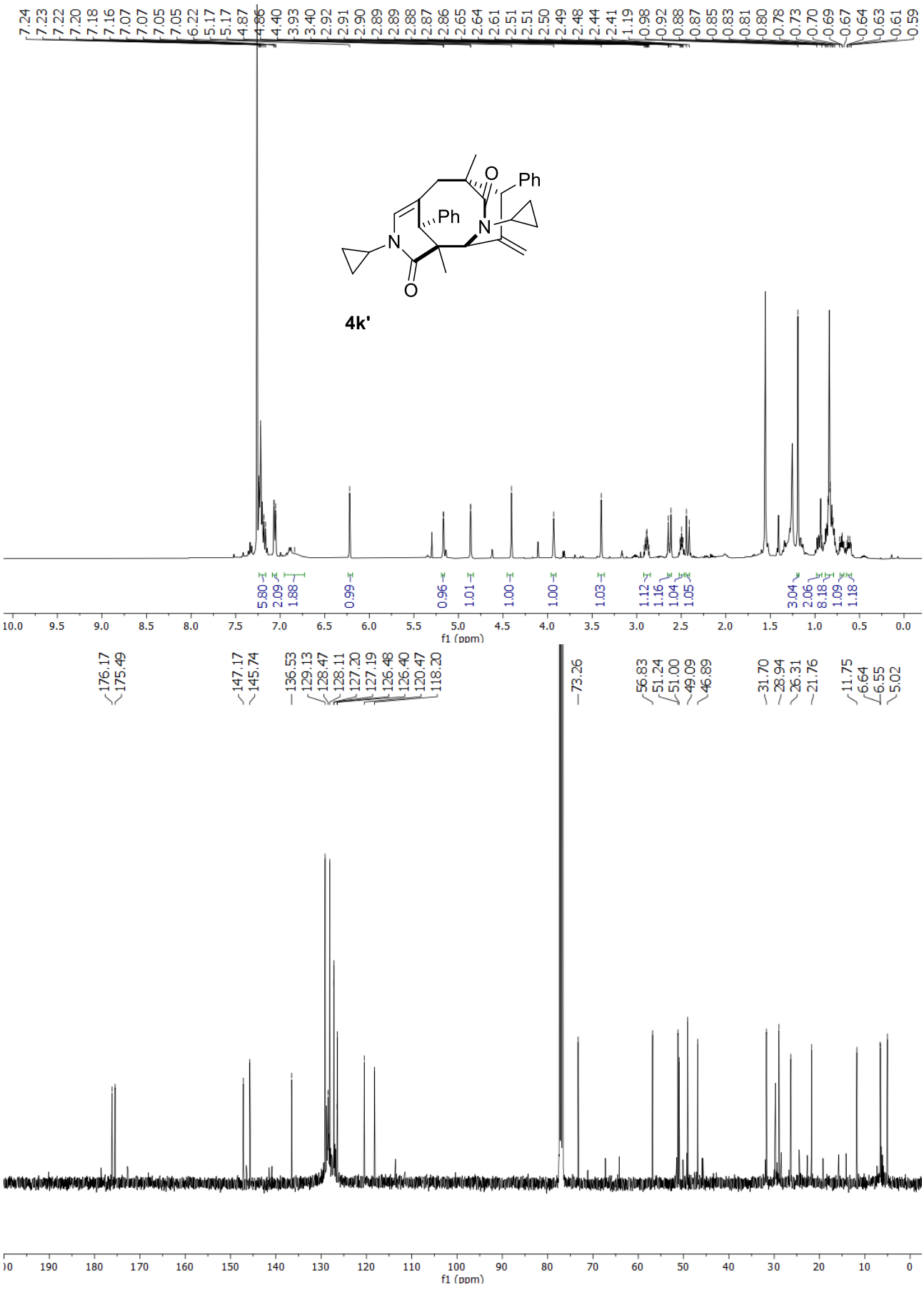
R = 4-F-C_6H_4

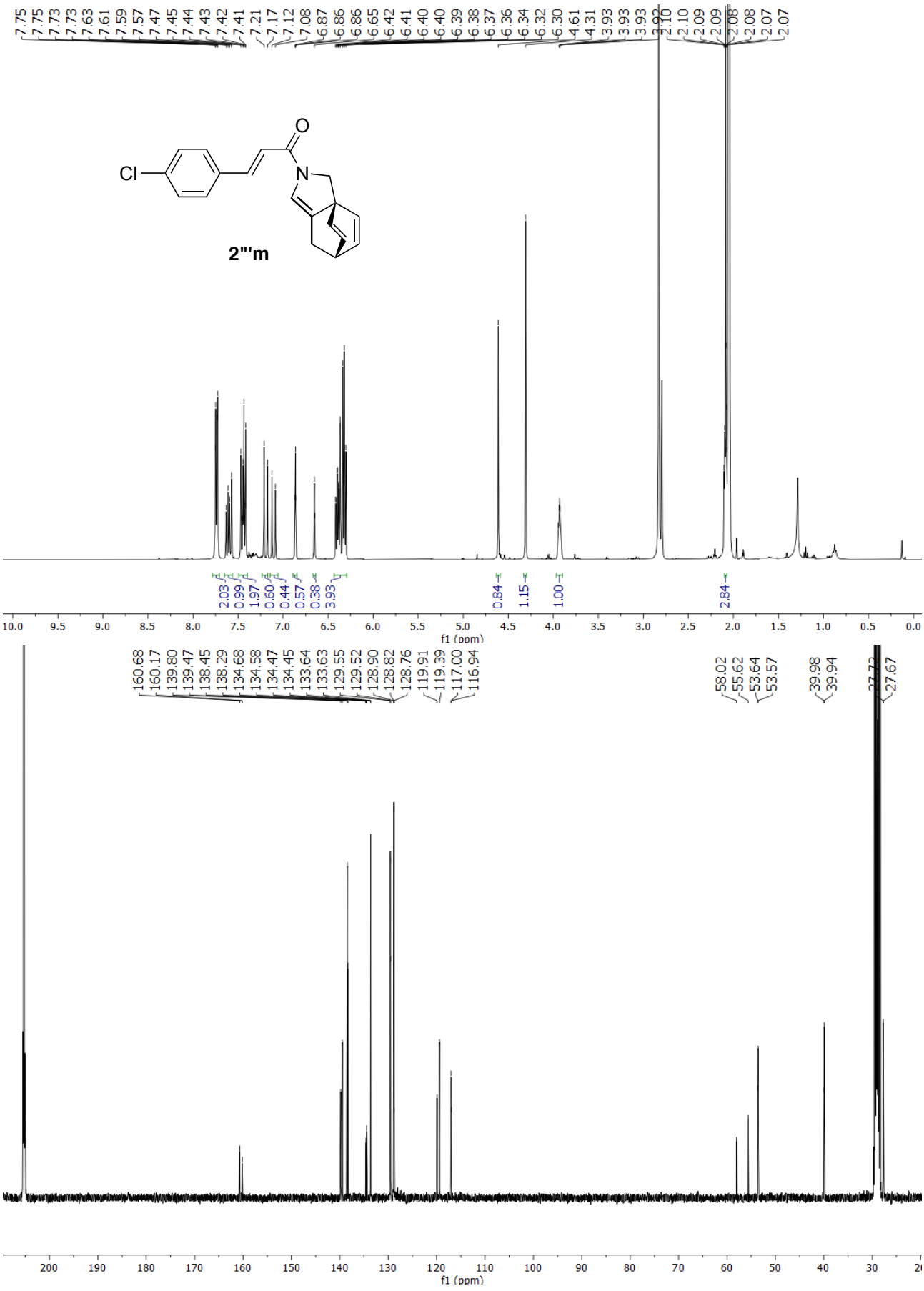
4i'


7.37 7.36 7.35 7.35 7.34 7.32 7.32 7.31 7.31 7.29 7.28 7.27 7.27 7.26 7.24 7.22 7.20 7.18 6.92 6.90 6.24
4.93 4.82 4.66 4.62 4.61 4.57 4.47 4.42 4.38 4.29 4.25 3.62 3.26 2.87 2.84 2.39 2.36 1.43 0.96
Ph
O
Ph
NC
N
N
CN
O
4j
11.43 2.33 0.98 1.04 1.09 1.11 1.20 1.15 1.02 1.03 1.00 1.01 1.09 1.07 3.11 3.17
f1 (ppm)
176.53 172.25 145.64 144.42 133.74 129.11 128.76 127.94 127.45 127.04 119.87 116.87 114.76 114.16 73.46 56.21 53.85 48.25 46.58 46.15 40.10 32.98 25.82 22.60
129.11 128.76 127.94 127.45 127.04
f1 (ppm)
f1 (ppm)


7.40
7.38
7.37
7.37
7.36
7.35
7.33
7.33
7.32
7.32
7.31
7.30
7.29
7.28
7.26
7.25
7.23
7.21
7.21
7.19
6.15
5.05
5.05
4.74
4.69
4.65
4.61
4.42
4.40
4.36
3.92
3.87
3.60
2.75
2.71
2.63
2.59
1.27
0.91
O
Ph
Ph
N
NC
N
CN
O
4j'
7.33
4.50
0.84
0.97
1.00
1.00
1.04
0.94
1.14
1.01
1.00
0.96
1.03
1.00
2.99
3.06
f1 (ppm)
174.68
173.98
145.84
143.45
134.51
128.98
128.82
128.71
127.94
126.97
125.27
122.67
121.65
114.80
114.16
74.33
57.98
50.58
49.91
48.82
47.28
37.48
33.54
26.37
21.53
f1 (ppm)


7.23 7.22 7.20 7.18 7.17 7.15 7.06 7.06 7.04 6.85
6.10 4.91 4.66 4.47 3.52 3.12 2.98 2.96 2.95 2.87 2.86 2.85 2.84 2.83 2.79 2.27 2.24 1.42 0.97 0.96 0.94 0.90 0.87 0.85 0.84 0.83 0.78 0.77 0.76 0.74 0.71 0.69
Ph
O
Ph
N
N
O
4k
6.01 2.00 1.91 1.00 1.00 1.01 0.99 1.03 1.02 1.05 1.99 0.99 3.13 11.25
f1 (ppm)
178.83 174.64 147.69 145.70 135.91 130.13 129.15 128.39 128.15 127.20 126.50 117.02 114.82 70.82 55.50 55.39 49.54 46.57 45.58 33.42 29.10 25.89 22.56 12.32 6.71 6.38 4.93
f1 (ppm)


7.24 7.23 7.22 7.20 7.18 7.16 7.07 7.07 7.05 7.05 6.22 5.17 5.17 4.87 4.86 4.40 3.93 3.40 2.92 2.91 2.90 2.89 2.89 2.88 2.87 2.86 2.65 2.64 2.61 2.51 2.51 2.50 2.49 2.48 2.44 2.41 1.19 0.98 0.92 0.88 0.87 0.85 0.83 0.81 0.80 0.78 0.73 0.70 0.69 0.67 0.64 0.63 0.61 0.59
O
Ph
Ph
N
N
O
4k'
5.80 2.09 1.88 0.99 0.96 1.01 1.00 1.00 1.03 1.12 1.16 1.04 1.05 3.04 2.06 8.18 1.09 1.18
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
176.17 175.49 147.17 145.74 136.53 129.13 128.47 128.11 127.20 127.19 126.48 126.40 120.47 118.20 73.26 56.83 51.24 51.00 49.09 46.89 31.70 28.94 26.31 21.76 11.75 6.64 6.55 5.02
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.75 7.75 7.73 7.73 7.63 7.61 7.59 7.57 7.47 7.45 7.44 7.43 7.42 7.41 7.21 7.17 7.12 7.08 6.87 6.86 6.86 6.65 6.42 6.41 6.40 6.40 6.39 6.38 6.37 6.36 6.34 6.32 6.30 4.61 4.31 3.93 3.93 3.93 3.92 2.10 2.10 2.09 2.09 2.08 2.08 2.07 2.07
Cl
O
N
2"'m
2.03 0.99 1.97 0.60 0.44 0.57 0.38 3.93 0.84 1.15 1.00 2.84
f1 (ppm)
160.68 160.17 139.80 139.47 138.45 138.29 134.68 134.58 134.47 134.45 133.64 133.63 129.55 129.52 128.90 128.82 128.76 119.91 119.39 117.00 116.94
58.02 55.62 53.64 53.57 39.98 39.94 27.72 27.67
f1 (ppm)

XYZ Coordinates

^{1}1

28

scf done: -632.892887

C	-1.582367	0.288462	2.466943
C	-0.448461	-0.004206	1.737355
C	0.821456	0.175114	2.291581
C	0.911971	0.658699	3.597086
C	-0.224268	0.949959	4.330191
C	-1.475220	0.765556	3.766606
C	2.049339	-0.116901	1.570103
C	2.164421	-0.648918	0.351710
C	3.500026	-0.844452	-0.243708
O	4.484054	-0.262709	0.185311
N	3.597816	-1.692260	-1.326463
C	4.853305	-1.782691	-2.042360
C	2.580579	-2.561643	-1.736226
C	2.643444	-3.342875	-2.781965
C	2.655848	-4.148053	-3.798464
H	1.703061	-2.607449	-1.103839
H	2.972406	0.124096	2.093371
H	3.042387	-5.161366	-3.723710
H	2.283291	-3.845175	-4.773774
H	1.282754	-0.908689	-0.220028
H	1.893683	0.803890	4.036050
H	-0.132698	1.323205	5.343331
H	-2.368233	0.994539	4.336113
H	-2.560064	0.146135	2.021700
H	-0.550001	-0.372731	0.722869
H	4.684290	-1.604050	-3.106528
H	5.539470	-1.040404	-1.648681
H	5.288170	-2.778854	-1.927872

^{2}1^{-}

28

scf done: -632.985531

C	-1.560653	0.169759	2.446909
C	-0.395059	-0.136521	1.777560
C	0.878700	0.179892	2.320662
C	0.870135	0.831193	3.581151
C	-0.298610	1.131916	4.240712
C	-1.538180	0.806104	3.685686
C	2.104017	-0.121435	1.679779
C	2.278437	-0.779885	0.461369
C	3.561277	-0.991830	-0.097093
O	4.621339	-0.511869	0.345184
N	3.652904	-1.805460	-1.264819
C	4.825045	-1.724478	-2.097296
C	2.660264	-2.677182	-1.664845
C	2.611260	-3.330474	-2.802695
C	2.528025	-4.023626	-3.899577
H	1.877082	-2.854963	-0.933816
H	3.006797	0.187493	2.203111
H	2.990926	-5.003707	-4.004774
H	1.991817	-3.661251	-4.775173
H	1.405869	-1.108100	-0.089872
H	1.824902	1.092397	4.030259
H	-0.253605	1.629033	5.204781
H	-2.459222	1.043251	4.204808
H	-2.513432	-0.090685	1.995616

H	-0.455149	-0.629827	0.813051
H	4.572037	-1.352231	-3.097135
H	5.536793	-1.051050	-1.628675
H	5.286745	-2.710232	-2.218160

$^{2}1^{+}$

28

scf done: -632.675670

C	-1.567164	0.367757	2.429960
C	-0.433398	0.017454	1.730422
C	0.829529	0.144195	2.319642
C	0.915715	0.633346	3.625942
C	-0.222117	0.982398	4.326530
C	-1.464761	0.849434	3.729374
C	2.050431	-0.212288	1.639841
C	2.175074	-0.731215	0.405991
C	3.497580	-0.998459	-0.110239
O	4.547663	-0.648508	0.350199
N	3.566935	-1.763306	-1.366951
C	4.814839	-1.642512	-2.102877
C	2.608479	-2.612937	-1.721540
C	2.650534	-3.388357	-2.831543
C	2.635252	-4.150468	-3.859196
H	1.753914	-2.700288	-1.059313
H	2.969006	-0.047002	2.199061
H	3.068958	-5.148349	-3.830094
H	2.196982	-3.824457	-4.800620
H	1.310061	-0.916944	-0.215805
H	1.892720	0.734486	4.086146
H	-0.141287	1.358546	5.338938
H	-2.359937	1.121987	4.275674
H	-2.540585	0.266652	1.965723
H	-0.527215	-0.357191	0.717877
H	4.707342	-2.102550	-3.080290
H	5.066204	-0.588988	-2.202669
H	5.609704	-2.136207	-1.543480

^{1}Ir(III) ppy$_3$

61

scf done: -1540.113588

C	2.359371	-2.691904	-1.727104
C	2.038270	-1.592451	-0.933868
N	0.760093	-1.397980	-0.542583
C	-0.190193	-2.256263	-0.915605
C	0.069225	-3.360820	-1.696009
C	1.375257	-3.576960	-2.108528
C	2.984120	-0.586422	-0.461173
C	2.449079	0.459176	0.328619
C	3.353661	1.423116	0.786613
C	4.701015	1.372360	0.471534
C	5.204006	0.342577	-0.314559
C	4.343306	-0.632898	-0.775236
Ir	0.453509	0.379345	0.654465
C	-0.070334	1.373919	-1.028569
C	-1.461089	1.475863	-1.271689
C	-1.952882	2.156188	-2.386939
C	-1.088630	2.745254	-3.287176
C	0.280991	2.648645	-3.072605
C	0.774579	1.973523	-1.969030
C	-2.341497	0.853838	-0.287862
N	-1.708141	0.250715	0.741653
C	-2.414592	-0.346092	1.702415

C	-3.790963	-0.387025	1.698547
C	-4.459306	0.224564	0.648843
C	-3.733683	0.845222	-0.343838
C	0.383528	1.987085	1.882988
C	0.632480	1.724425	3.251203
C	0.646159	2.753170	4.194581
C	0.404871	4.057592	3.813835
C	0.142222	4.335128	2.477714
C	0.131112	3.318972	1.537167
C	0.876478	0.331534	3.612005
N	0.838132	-0.538100	2.578998
C	1.030683	-1.840063	2.794567
C	1.270456	-2.359401	4.047226
C	1.318620	-1.481994	5.119914
C	1.122410	-0.136406	4.901251
H	4.737816	-1.438303	-1.386121
H	5.369858	2.143506	0.840793
H	6.257846	0.303258	-0.563581
H	2.990541	2.243359	1.399362
H	3.382023	-2.848044	-2.044497
H	1.622585	-4.432314	-2.725655
H	-0.733591	-4.030528	-1.973581
H	-1.195108	-2.038113	-0.567474
H	-3.022069	2.230805	-2.556322
H	-1.475458	3.274846	-4.149799
H	0.969546	3.106998	-3.775506
H	1.850455	1.919761	-1.828227
H	-4.243641	1.326910	-1.167651
H	-5.541718	0.216701	0.606962
H	-4.321884	-0.883827	2.499363
H	-1.842067	-0.807020	2.501099
H	1.155884	0.558619	5.729992
H	1.507397	-1.848653	6.121682
H	1.417085	-3.423457	4.174895
H	0.984874	-2.480894	1.919738
H	0.847003	2.537299	5.238825
H	0.417762	4.852582	4.550052
H	-0.053730	5.357095	2.168812
H	-0.071404	3.569209	0.499581

^{3}Ir(III) ppy$_3$

61

scf done: -1540.020005

C	2.349290	-2.786579	-1.594677
C	2.031177	-1.631157	-0.885002
N	0.749108	-1.404853	-0.524709
C	-0.210193	-2.273584	-0.846601
C	0.047727	-3.428524	-1.548753
C	1.358026	-3.683842	-1.926109
C	2.984388	-0.605281	-0.469066
C	2.467004	0.481439	0.272104
C	3.374424	1.455773	0.689531
C	4.721130	1.379248	0.373626
C	5.210114	0.312511	-0.369960
C	4.341951	-0.676633	-0.785370
Ir	0.457185	0.423105	0.601022
C	-0.024499	1.436585	-1.022996
C	-1.477304	1.545354	-1.239922
C	-1.941541	2.291897	-2.359384
C	-1.053800	2.878991	-3.214422
C	0.345215	2.767183	-3.027174
C	0.825814	2.050673	-1.946488

C	-2.318932	0.896589	-0.326871
N	-1.671992	0.233453	0.721799
C	-2.393081	-0.375233	1.652139
C	-3.773322	-0.422287	1.642291
C	-4.455892	0.217531	0.579345
C	-3.739556	0.862302	-0.380264
C	0.354571	2.006209	1.863028
C	0.592342	1.724809	3.226898
C	0.554916	2.740132	4.183562
C	0.276137	4.040844	3.817330
C	0.027495	4.331805	2.482377
C	0.066168	3.331227	1.526349
C	0.868318	0.334072	3.575343
N	0.862122	-0.525764	2.536155
C	1.097944	-1.822366	2.736177
C	1.346170	-2.346188	3.985086
C	1.355539	-1.479091	5.066808
C	1.118259	-0.138051	4.861675
H	4.728320	-1.508772	-1.364337
H	5.398439	2.159303	0.706091
H	6.262226	0.254988	-0.622432
H	3.015602	2.304210	1.265545
H	3.373939	-2.978031	-1.884294
H	1.603697	-4.582425	-2.479175
H	-0.757185	-4.107966	-1.793864
H	-1.213095	-2.014365	-0.520862
H	-3.005493	2.399980	-2.537209
H	-1.429692	3.445820	-4.060049
H	1.023553	3.244410	-3.724065
H	1.898665	1.973579	-1.798218
H	-4.248280	1.354469	-1.200321
H	-5.537846	0.193334	0.531288
H	-4.302633	-0.939489	2.430692
H	-1.833926	-0.860032	2.448890
H	1.123718	0.548162	5.698047
H	1.547513	-1.850338	6.066180
H	1.527344	-3.405894	4.103193
H	1.079385	-2.455783	1.854873
H	0.742835	2.515256	5.227801
H	0.249553	4.823856	4.565646
H	-0.196841	5.350825	2.184685
H	-0.121126	3.586476	0.487224

^{2}Ir(II) ppy$_3^-$

61

scf done: -1540.186513

C	2.258279	-2.630761	-1.819384
C	1.992040	-1.546692	-0.982726
N	0.736959	-1.348121	-0.522673
C	-0.243032	-2.182635	-0.869952
C	-0.038876	-3.266901	-1.695646
C	1.243037	-3.489611	-2.177656
C	2.975732	-0.571089	-0.523756
C	2.492989	0.462640	0.319470
C	3.448111	1.375719	0.786287
C	4.782305	1.299893	0.424887
C	5.227394	0.289921	-0.421751
C	4.322237	-0.642300	-0.887711
Ir	0.500548	0.423433	0.695461
C	-0.035534	1.413401	-1.001547
C	-1.450188	1.432247	-1.249191
C	-1.940242	2.108105	-2.390782

C	-1.082057	2.741093	-3.269491
C	0.289913	2.720519	-3.044509
C	0.787466	2.052849	-1.916382
C	-2.286925	0.771326	-0.303804
N	-1.629449	0.217101	0.798815
C	-2.338773	-0.410669	1.736583
C	-3.702267	-0.578699	1.695351
C	-4.395035	-0.045600	0.571274
C	-3.689493	0.612414	-0.393912
C	0.453940	2.034045	1.903149
C	0.624518	1.779337	3.288377
C	0.618080	2.816096	4.225363
C	0.439996	4.124044	3.825119
C	0.262104	4.397911	2.472061
C	0.267905	3.375917	1.539760
C	0.823566	0.386682	3.668441
N	0.851941	-0.484333	2.635224
C	1.034266	-1.784963	2.865215
C	1.189651	-2.305241	4.130918
C	1.156144	-1.427754	5.205899
C	0.975229	-0.082813	4.973464
H	4.672407	-1.434523	-1.542162
H	5.487021	2.034816	0.802445
H	6.270584	0.231268	-0.709899
H	3.128212	2.180138	1.444004
H	3.262427	-2.793714	-2.188993
H	1.446819	-4.330141	-2.830442
H	-0.864373	-3.916324	-1.955227
H	-1.223662	-1.954996	-0.460892
H	-3.009401	2.144049	-2.581829
H	-1.485886	3.256943	-4.135719
H	0.968492	3.214205	-3.733018
H	1.863113	2.051403	-1.750255
H	-4.208076	1.018059	-1.256227
H	-5.469355	-0.161193	0.480191
H	-4.214848	-1.098340	2.493900
H	-1.763762	-0.808048	2.572107
H	0.946380	0.611951	5.802989
H	1.270531	-1.794934	6.218882
H	1.331803	-3.368884	4.268385
H	1.048112	-2.425065	1.987987
H	0.754768	2.601325	5.280619
H	0.436838	4.924508	4.555839
H	0.116538	5.423581	2.146472
H	0.129067	3.618335	0.489817

^{2}Ir(IV) ppy$_3^+$

61

scf done: -1539.922312

C	2.193279	-2.687244	-1.693690
C	1.913904	-1.579033	-0.900790
N	0.644945	-1.329617	-0.513470
C	-0.340773	-2.144947	-0.894640
C	-0.122550	-3.255371	-1.677454
C	1.173833	-3.527139	-2.083117
C	2.905239	-0.618039	-0.427534
C	2.435191	0.445749	0.363935
C	3.364223	1.373043	0.833378
C	4.708706	1.259326	0.519398
C	5.162122	0.209331	-0.265064
C	4.261549	-0.724626	-0.734052
Ir	0.427129	0.489223	0.716727

C	-0.069532	1.482279	-0.983500
C	-1.446347	1.478170	-1.290705
C	-1.925579	2.139672	-2.421861
C	-1.054888	2.807431	-3.257751
C	0.303283	2.812794	-2.968676
C	0.787872	2.154918	-1.849676
C	-2.319352	0.764632	-0.368302
N	-1.701853	0.224449	0.708188
C	-2.397755	-0.459220	1.622211
C	-3.754021	-0.650615	1.516873
C	-4.407526	-0.110014	0.418027
C	-3.692691	0.597744	-0.521794
C	0.383334	2.051267	1.909962
C	0.711328	1.795355	3.279274
C	0.768452	2.836893	4.190005
C	0.495082	4.133464	3.785064
C	0.149903	4.402942	2.461510
C	0.086714	3.380287	1.544006
C	0.962697	0.405413	3.647369
N	0.856206	-0.472534	2.629654
C	1.062986	-1.769278	2.839821
C	1.381934	-2.270563	4.085308
C	1.492567	-1.384631	5.142315
C	1.282205	-0.038594	4.923455
H	4.620873	-1.544928	-1.344876
H	5.408397	2.000470	0.890196
H	6.213453	0.121600	-0.510375
H	3.036058	2.210485	1.440129
H	3.209702	-2.885592	-2.005304
H	1.387345	-4.390354	-2.701310
H	-0.952423	-3.888392	-1.959864
H	-1.340304	-1.897637	-0.554637
H	-2.985179	2.139519	-2.651884
H	-1.430633	3.324374	-4.132340
H	0.991009	3.337662	-3.622816
H	1.853195	2.179512	-1.642893
H	-4.194619	1.019818	-1.381712
H	-5.475557	-0.243157	0.297662
H	-4.284074	-1.207343	2.277061
H	-1.832576	-0.859661	2.456324
H	1.364266	0.665821	5.740144
H	1.741854	-1.740954	6.133963
H	1.538251	-3.332565	4.215885
H	0.962327	-2.421729	1.979027
H	1.023819	2.652276	5.226574
H	0.545998	4.940532	4.505780
H	-0.065432	5.420661	2.158515
H	-0.174216	3.599194	0.514849

^{1}Ir(III) ppy$_2$bpy^{+}

61

scf done: -1556.639223

C	0.317735	1.999514	1.848537
C	0.554940	1.743238	3.213802
C	0.551876	2.773926	4.152467
C	0.307752	4.072863	3.753546
C	0.063011	4.341296	2.412895
C	0.066924	3.319322	1.476548
C	0.809881	0.352256	3.551913
N	0.792198	-0.497230	2.495096
C	1.004275	-1.804786	2.682073
C	1.237731	-2.341316	3.926477

C	1.260733	-1.489237	5.019828
C	1.047721	-0.142461	4.829330
Ir	0.406494	0.367781	0.660289
N	-1.755985	0.274215	0.716982
C	-2.364151	0.902482	-0.305283
C	-3.747268	0.952304	-0.387053
C	-4.505381	0.349494	0.596395
C	-3.868107	-0.291909	1.642511
C	-2.488916	-0.304688	1.665218
C	-1.468132	1.510188	-1.295850
N	-0.142853	1.366129	-1.068411
C	0.730375	1.900570	-1.927872
C	0.332825	2.604947	-3.043206
C	-1.018840	2.763291	-3.284063
C	-1.923163	2.208472	-2.402456
C	2.414992	0.437401	0.365843
C	2.952334	-0.601012	-0.426443
C	4.316009	-0.644756	-0.717297
C	5.168223	0.325899	-0.230814
C	4.656344	1.349236	0.554099
C	3.302730	1.399204	0.847628
C	2.013395	-1.604339	-0.925348
N	0.729838	-1.421131	-0.549020
C	-0.212390	-2.280623	-0.939614
C	0.063070	-3.374620	-1.728710
C	1.374633	-3.577437	-2.128059
C	2.350478	-2.691837	-1.725939
H	4.721109	-1.443942	-1.328312
H	5.319158	2.115934	0.941201
H	6.225924	0.286390	-0.461740
H	2.930098	2.213510	1.461440
H	3.377169	-2.840219	-2.032757
H	1.634165	-4.424927	-2.750690
H	-0.731704	-4.047253	-2.021010
H	-1.221734	-2.077121	-0.596849
H	-2.984670	2.321032	-2.572752
H	-1.367552	3.313850	-4.148162
H	1.079804	3.021226	-3.705106
H	1.778153	1.757303	-1.693582
H	-4.232706	1.457074	-1.210668
H	-5.586030	0.381431	0.544645
H	-4.424621	-0.775827	2.433468
H	-1.943547	-0.793245	2.465388
H	1.060630	0.538190	5.670282
H	1.443494	-1.876833	6.014390
H	1.399963	-3.405287	4.030294
H	0.979211	-2.425589	1.794525
H	0.742133	2.565015	5.199882
H	0.306789	4.874742	4.481883
H	-0.130838	5.360356	2.095304
H	-0.121122	3.567817	0.435511

^{3}Ir(III) ppy$_2$bpy$^+$

61

scf done: -1556.555704

C	0.372363	2.094261	1.887135
C	0.634810	1.853584	3.268423
C	0.678829	2.904164	4.167202
C	0.462226	4.200050	3.724005
C	0.191762	4.455378	2.380127
C	0.143673	3.420437	1.474209
C	0.848440	0.461794	3.631753

N	0.773815	-0.397016	2.589044
C	0.958579	-1.703429	2.779927
C	1.215586	-2.228118	4.028397
C	1.289250	-1.365992	5.108254
C	1.106232	-0.013203	4.908270
Ir	0.388985	0.504495	0.751297
N	-1.682962	0.164487	0.694495
C	-2.293839	0.739030	-0.410091
C	-3.690150	0.584436	-0.559308
C	-4.409995	-0.121845	0.354762
C	-3.760051	-0.695779	1.474088
C	-2.413311	-0.519082	1.593216
C	-1.454019	1.438254	-1.305694
N	-0.107990	1.480359	-0.992501
C	0.745821	2.148523	-1.782492
C	0.350285	2.808268	-2.913607
C	-1.014808	2.779256	-3.259861
C	-1.896163	2.105949	-2.468778
C	2.413297	0.417171	0.403883
C	2.871479	-0.621475	-0.424396
C	4.227963	-0.734463	-0.726348
C	5.138768	0.166687	-0.214087
C	4.696786	1.189089	0.610416
C	3.351271	1.309853	0.920044
C	1.872899	-1.557963	-0.935320
N	0.610698	-1.325441	-0.523264
C	-0.380368	-2.122027	-0.926940
C	-0.171609	-3.196607	-1.762096
C	1.119108	-3.449464	-2.195243
C	2.144599	-2.628213	-1.780461
H	4.580385	-1.536155	-1.365044
H	5.404181	1.902900	1.017996
H	6.190432	0.072071	-0.455288
H	3.034134	2.124971	1.561618
H	3.156860	-2.812886	-2.113116
H	1.324687	-4.284126	-2.854075
H	-1.004622	-3.817345	-2.062230
H	-1.373259	-1.886785	-0.559600
H	-2.947625	2.083221	-2.723751
H	-1.364814	3.292102	-4.147241
H	1.079763	3.333914	-3.513443
H	1.782617	2.147627	-1.464686
H	-4.185699	1.028786	-1.412794
H	-5.478591	-0.242084	0.226021
H	-4.303076	-1.257010	2.221221
H	-1.865162	-0.936175	2.431710
H	1.160947	0.677356	5.739123
H	1.489097	-1.746710	6.101784
H	1.354259	-3.294204	4.142284
H	0.887492	-2.334260	1.901754
H	0.881061	2.727899	5.217097
H	0.500553	5.019754	4.430940
H	0.019022	5.473256	2.051903
H	-0.070296	3.628750	0.431981

^{2}Ir(II) ppy$_2$bpy

61

C	0.349573	2.030860	1.861850
C	0.570175	1.788336	3.235059
C	0.561035	2.827518	4.165656
C	0.327310	4.124178	3.754502

C	0.096322	4.380962	2.407263
C	0.105464	3.352418	1.479939
C	0.809668	0.398862	3.588449
N	0.795901	-0.458325	2.537680
C	0.995276	-1.765022	2.739341
C	1.212033	-2.295143	3.990038
C	1.230610	-1.434389	5.077452
C	1.030603	-0.087666	4.873338
Ir	0.428073	0.401490	0.689077
N	-1.710707	0.242736	0.736305
C	-2.319452	0.841037	-0.346821
C	-3.730684	0.781405	-0.452436
C	-4.468585	0.148843	0.503419
C	-3.822766	-0.447830	1.605031
C	-2.452446	-0.364436	1.662419
C	-1.464754	1.468428	-1.283060
N	-0.101022	1.395411	-1.040605
C	0.751022	1.997304	-1.879644
C	0.355643	2.694693	-2.991952
C	-1.025887	2.779268	-3.264492
C	-1.911667	2.175850	-2.424258
C	2.437638	0.432445	0.368449
C	2.941301	-0.611231	-0.443206
C	4.300094	-0.689952	-0.751271
C	5.186391	0.249436	-0.263500
C	4.712184	1.276525	0.541816
C	3.364191	1.359732	0.851032
C	1.971021	-1.585786	-0.942001
N	0.699747	-1.383026	-0.536896
C	-0.270630	-2.208302	-0.928007
C	-0.037078	-3.291573	-1.746251
C	1.262217	-3.518135	-2.173203
C	2.267076	-2.665085	-1.771212
H	4.675338	-1.493337	-1.376490
H	5.401878	2.018613	0.931110
H	6.240003	0.182968	-0.507648
H	3.019563	2.175956	1.479890
H	3.283706	-2.831372	-2.102115
H	1.489444	-4.357908	-2.818807
H	-0.853269	-3.937469	-2.040617
H	-1.266897	-1.978083	-0.561366
H	-2.974624	2.241991	-2.619589
H	-1.382505	3.323174	-4.131157
H	1.094494	3.159561	-3.629939
H	1.801253	1.909883	-1.620900
H	-4.223648	1.238630	-1.301269
H	-5.547729	0.106009	0.413448
H	-4.373155	-0.955147	2.385240
H	-1.905052	-0.808469	2.490123
H	1.040186	0.599793	5.709129
H	1.399470	-1.815533	6.077125
H	1.363868	-3.359782	4.104265
H	0.971566	-2.391528	1.854977
H	0.736680	2.625401	5.217400
H	0.320974	4.932415	4.476072
H	-0.093158	5.398343	2.080278
H	-0.078671	3.584332	0.434161

^{2}Ir(IV)ppy$_2$bpy^{++}

61

scf done: -1556.426938

C	0.369987	2.056372	1.882142

C	0.675221	1.799995	3.262121
C	0.756981	2.838999	4.168115
C	0.538114	4.139888	3.741226
C	0.227337	4.414546	2.403114
C	0.142846	3.395724	1.491240
C	0.884521	0.405011	3.600911
N	0.771231	-0.441278	2.548634
C	0.938596	-1.752017	2.721234
C	1.219121	-2.292208	3.959324
C	1.336382	-1.444682	5.045490
C	1.168598	-0.086791	4.864476
Ir	0.369271	0.476581	0.737725
N	-1.773932	0.232015	0.693758
C	-2.363446	0.775368	-0.389656
C	-3.729806	0.658075	-0.576076
C	-4.484836	-0.022845	0.359348
C	-3.865289	-0.574135	1.465388
C	-2.501267	-0.424613	1.596489
C	-1.470028	1.468833	-1.325234
N	-0.154773	1.468122	-1.011179
C	0.719943	2.085489	-1.809325
C	0.328006	2.736434	-2.958949
C	-1.012061	2.746737	-3.292853
C	-1.916342	2.107291	-2.468477
C	2.389864	0.462281	0.419264
C	2.875277	-0.584780	-0.385093
C	4.235625	-0.671809	-0.675406
C	5.121296	0.262645	-0.178932
C	4.650379	1.295479	0.614934
C	3.300284	1.391515	0.913468
C	1.901595	-1.549128	-0.890213
N	0.626497	-1.324376	-0.510427
C	-0.346756	-2.145850	-0.912761
C	-0.106362	-3.237593	-1.714318
C	1.196875	-3.482641	-2.114354
C	2.202675	-2.636798	-1.701295
H	4.610500	-1.478471	-1.294346
H	5.337473	2.036867	1.006842
H	6.176119	0.187212	-0.411992
H	2.960006	2.217089	1.529647
H	3.223686	-2.816428	-2.008511
H	1.427275	-4.331487	-2.745980
H	-0.924568	-3.877662	-2.013823
H	-1.351318	-1.921069	-0.572677
H	-2.968504	2.109623	-2.714779
H	-1.355322	3.250977	-4.186764
H	1.070561	3.226260	-3.573209
H	1.757243	2.057556	-1.498880
H	-4.206480	1.091012	-1.444193
H	-5.553811	-0.121840	0.221980
H	-4.422940	-1.112602	2.218822
H	-1.965659	-0.839594	2.442341
H	1.255352	0.593998	5.700333
H	1.557024	-1.839255	6.028904
H	1.342188	-3.361609	4.057711
H	0.835591	-2.375204	1.841546
H	0.991404	2.653131	5.209042
H	0.606978	4.953367	4.452837
H	0.056025	5.438339	2.094554
H	-0.095844	3.624211	0.459361

^{1}3

31
scf done: -672.184525

C	-1.364584	0.522320	3.966428
C	-1.614161	0.062131	2.683543
C	-0.568553	-0.215376	1.821380
C	0.757324	-0.035839	2.224212
C	0.989170	0.402076	3.531726
C	-0.055112	0.686941	4.389851
C	1.917769	-0.296649	1.381277
C	2.021699	-0.351191	0.048821
C	3.400894	-0.574073	-0.494136
N	3.569829	-1.611967	-1.377158
C	2.622579	-2.631089	-1.531722
C	2.714486	-3.614845	-2.385661
C	2.767262	-4.619480	-3.204095
O	4.323111	0.162268	-0.192837
C	4.822122	-1.752801	-2.090897
H	1.784032	-2.595383	-0.844924
H	2.844158	-0.432839	1.936380
H	3.254984	-5.553265	-2.935963
H	2.327849	-4.572885	-4.197224
C	0.937604	-0.072963	-0.947341
H	2.013685	0.523981	3.868408
H	0.152637	1.033811	5.395399
H	-2.186971	0.740681	4.637386
H	-2.634645	-0.089015	2.351088
H	-0.790644	-0.602229	0.835880
H	4.635003	-1.798126	-3.165925
H	5.452600	-0.899008	-1.863630
H	5.330362	-2.672328	-1.791071
H	1.362018	0.209516	-1.912373
H	0.285542	-0.932278	-1.127372
H	0.302183	0.745907	-0.604566

^{1}1iso
28
scf done: -632.893681

C	-1.450346	0.863260	3.779423
C	-1.577198	0.238172	2.545928
C	-0.454964	-0.099172	1.817803
C	0.823443	0.181677	2.307473
C	0.933472	0.811082	3.547882
C	-0.191113	1.149144	4.278803
C	2.039590	-0.152411	1.585724
C	2.136799	-0.766415	0.404041
C	3.460417	-1.002555	-0.197350
N	3.507927	-1.833480	-1.296771
C	4.721120	-1.930717	-1.986996
C	4.928723	-2.646785	-3.059122
C	5.185838	-3.335608	-4.127961
O	4.473900	-0.476567	0.237951
C	2.382779	-2.591453	-1.809699
H	5.516316	-1.334770	-1.553916
H	2.970021	0.130621	2.073540
H	5.049668	-2.920990	-5.123722
H	5.547105	-4.359716	-4.078043
H	1.248146	-1.066554	-0.135297
H	1.921551	1.033809	3.937277
H	-0.083923	1.636545	5.240628
H	-2.334429	1.126090	4.348220
H	-2.561374	0.013867	2.151652
H	-0.572229	-0.586588	0.856640

H	2.753840	-3.533438	-2.213941
H	1.678871	-2.829122	-1.018080
H	1.865485	-2.056489	-2.610760

^{1}3iso

31

scf done: -672.185157

C	0.008192	0.860339	4.399941
C	-1.313707	0.700693	4.015263
C	-1.602080	0.194797	2.757982
C	-0.582979	-0.134483	1.882492
C	0.755915	0.035581	2.246516
C	1.026079	0.522921	3.529354
C	1.893866	-0.278338	1.392166
C	1.967372	-0.438418	0.065384
C	3.335575	-0.693829	-0.486004
O	4.281379	0.017779	-0.196088
N	3.467705	-1.738776	-1.369560
C	2.481881	-2.785766	-1.537463
C	4.668875	-1.861028	-2.078722
C	4.958974	-2.831740	-2.901869
C	5.291658	-3.768216	-3.735909
H	5.369729	-1.054040	-1.896847
H	2.835813	-0.364232	1.930519
H	5.059628	-3.700693	-4.795749
H	5.816702	-4.663711	-3.413480
C	0.855774	-0.251044	-0.921457
H	2.060235	0.640565	3.836551
H	0.246343	1.244049	5.385132
H	-2.115850	0.959472	4.696297
H	-2.632792	0.049442	2.455924
H	-0.837664	-0.551664	0.917836
H	2.977344	-3.756516	-1.471266
H	1.738353	-2.732485	-0.747461
H	1.987482	-2.718689	-2.510301
H	1.251013	-0.115643	-1.929426
H	0.165828	-1.098313	-0.960278
H	0.266557	0.633194	-0.669970

^{3}1alpha

28

scf done: -632.810997

C	-1.089063	-0.057483	3.890534
C	-0.889866	-0.807273	2.735273
C	0.144495	-0.508822	1.877394
C	1.025784	0.563574	2.149614
C	0.805586	1.309195	3.331368
C	-0.232113	1.001429	4.179601
C	2.090171	0.885648	1.289935
C	2.368403	0.191623	0.049229
C	3.288930	-0.932745	0.023406
N	3.419186	-1.622829	-1.163409
C	2.466058	-1.628143	-2.195334
C	1.172079	-1.535763	-2.046391
C	-0.109941	-1.389474	-1.926442
O	3.976002	-1.228624	0.995885
C	4.496017	-2.588606	-1.268090
H	2.885117	-1.746665	-3.192439
H	2.747317	1.705830	1.577715
H	-0.569004	-0.403770	-1.901492
H	-0.777937	-2.241395	-1.838367
H	1.976075	0.576907	-0.887940

H	1.473377	2.134223	3.557744
H	-0.382870	1.586917	5.079392
H	-1.904954	-0.297192	4.561861
H	-1.553392	-1.634133	2.508719
H	0.297473	-1.098408	0.978068
H	4.714891	-2.757052	-2.322310
H	5.383762	-2.206905	-0.768419
H	4.226138	-3.544854	-0.810878

^{3}1alpha iso

28

scf done: -632.813467

C	-0.110915	1.110744	4.249048
C	-0.978813	0.037032	4.067660
C	-0.858248	-0.761508	2.934414
C	0.111965	-0.497893	1.994508
C	1.004392	0.587246	2.157636
C	0.862028	1.385003	3.316415
C	2.005005	0.868487	1.211344
C	2.201325	0.100967	-0.001561
C	3.070131	-1.063582	0.008643
O	3.715309	-1.365897	1.008259
N	3.150643	-1.806427	-1.153622
C	2.347822	-1.544508	-2.333550
C	4.089303	-2.839662	-1.196960
C	4.318711	-3.623978	-2.216641
C	4.588767	-4.425706	-3.199651
H	4.650856	-2.950885	-0.276155
H	2.672352	1.707662	1.403105
H	5.341652	-4.185343	-3.946237
H	4.073378	-5.374905	-3.324381
H	1.738517	0.437981	-0.924004
H	1.538687	2.221457	3.458048
H	-0.201341	1.734527	5.130898
H	-1.743166	-0.175765	4.805365
H	-1.532277	-1.598267	2.790898
H	0.202227	-1.123951	1.111550
H	2.300435	-2.454399	-2.929634
H	1.329800	-1.277672	-2.057814
H	2.777492	-0.752057	-2.951263

^{3}3alpha

31

scf done: -672.109699

C	-0.210275	0.932474	4.180119
C	-1.197482	0.045645	3.757027
C	-1.062775	-0.596980	2.529998
C	0.034141	-0.361165	1.732615
C	1.046919	0.539069	2.139143
C	0.889929	1.177282	3.392677
C	2.173878	0.800671	1.344285
C	2.410853	0.242786	0.015547
C	3.308478	-0.907282	-0.055265
O	4.017777	-1.198938	0.903733
N	3.427727	-1.608956	-1.240331
C	4.553789	-2.517808	-1.360493
C	2.380061	-1.821952	-2.152309
C	1.105568	-1.878023	-1.877957
C	-0.174178	-1.892239	-1.671571
H	2.707825	-1.982587	-3.177738
H	2.917481	1.498148	1.730678
H	-0.769823	-0.982701	-1.708839

H	-0.707004	-2.812108	-1.447195
C	1.965929	1.059148	-1.143636
H	1.658529	1.868500	3.723490
H	-0.309255	1.433095	5.136639
H	-2.063276	-0.144461	4.379903
H	-1.826909	-1.291489	2.199315
H	0.138553	-0.872097	0.780049
H	4.716139	-2.732824	-2.416837
H	5.447212	-2.057103	-0.944593
H	4.374029	-3.461005	-0.836108
H	2.420308	0.755580	-2.085299
H	0.875989	1.014189	-1.261590
H	2.207724	2.110654	-0.958117

^{3}3alpha iso

31

scf done: -672.106340

C	0.864496	1.158064	3.380421
C	-0.219358	0.805137	4.149657
C	-1.128094	-0.146612	3.694048
C	-0.932982	-0.744154	2.452631
C	0.148406	-0.399886	1.674157
C	1.083566	0.567144	2.113443
C	2.191077	0.937717	1.333316
C	2.455315	0.414172	-0.002670
C	1.937194	1.197235	-1.156377
C	3.435991	-0.670271	-0.112038
N	3.355153	-1.538069	-1.178063
C	4.400173	-2.429216	-1.459839
C	5.578726	-2.552257	-0.908208
C	6.779959	-2.800679	-0.485900
O	4.331061	-0.774965	0.717794
C	2.146917	-1.731970	-1.964246
H	4.165909	-3.095735	-2.285763
H	2.872298	1.688541	1.733419
H	6.972871	-3.519491	0.306135
H	7.645778	-2.279624	-0.886117
H	1.571718	1.900458	3.736112
H	-0.366634	1.271389	5.117252
H	-1.981217	-0.421275	4.302816
H	-1.636808	-1.487415	2.095633
H	0.295796	-0.875660	0.709032
H	1.927471	-2.798658	-2.029966
H	1.299242	-1.252237	-1.482610
H	2.250385	-1.336037	-2.977375
H	2.369454	0.900046	-2.111251
H	0.844965	1.120237	-1.231609
H	2.154560	2.258976	-1.000471

^{3}1beta

28

scf done: -632.824276

C	4.785145	-1.531073	-2.721532
N	3.641705	-1.563803	-1.824400
C	2.725027	-2.577723	-2.016200
C	2.796563	-3.438744	-3.068182
C	2.222106	-4.503392	-3.637788
C	3.591144	-0.642264	-0.787096
O	4.555985	0.064274	-0.543932
C	2.330470	-0.536031	-0.037948
H	4.433704	-1.531358	-3.754890
H	1.958504	-2.695735	-1.256519

H	1.332727	-4.970216	-3.212842
H	2.613611	-4.948896	-4.546715
H	5.362962	-0.634548	-2.523000
H	5.414019	-2.411406	-2.571833
C	2.294903	0.141330	1.112780
H	1.429189	-0.968476	-0.453383
C	1.138025	0.396469	1.953144
H	3.234069	0.562239	1.466005
C	1.304344	1.181399	3.094944
C	0.235170	1.471762	3.922772
C	-1.022789	0.976754	3.624191
C	-1.204009	0.188776	2.494969
C	-0.137250	-0.099344	1.668791
H	2.291238	1.568934	3.325629
H	0.384424	2.085770	4.802870
H	-1.863622	1.201148	4.269806
H	-2.186778	-0.203205	2.260852
H	-0.295158	-0.718553	0.793108

^{3}1beta iso

28

scf done: -632.825848

C	1.288635	1.361102	2.967527
C	0.244105	1.633929	3.831808
C	-0.971569	0.991298	3.670274
C	-1.135500	0.074761	2.639802
C	-0.093009	-0.197523	1.778421
C	1.141021	0.442124	1.927347
C	2.271965	0.196572	1.051116
C	2.329753	-0.652507	0.019342
C	3.562220	-0.767319	-0.765556
O	4.557344	-0.094741	-0.540328
N	3.556614	-1.691507	-1.804472
C	2.405072	-2.533151	-2.102573
C	4.692801	-1.808156	-2.574525
C	4.823850	-2.673959	-3.618415
C	5.662822	-3.095293	-4.567672
H	2.669203	-3.188283	-2.930903
H	5.494996	-1.138076	-2.277509
H	6.665299	-2.678448	-4.672185
H	5.386141	-3.869191	-5.276503
H	2.138495	-3.153713	-1.247315
H	1.543492	-1.935132	-2.400133
H	1.471570	-1.255969	-0.243509
H	3.170175	0.772014	1.265345
H	2.242209	1.863916	3.091251
H	0.379192	2.350725	4.633085
H	-1.792851	1.202233	4.344959
H	-2.086104	-0.429183	2.510257
H	-0.238939	-0.914799	0.978657

^{3}3beta

31

scf done: -672.115521

C	-0.243716	-0.198654	1.735884
C	1.080835	0.211734	1.909130
C	1.408434	0.881847	3.091764
C	0.450456	1.165254	4.045654
C	-0.861824	0.764496	3.849713
C	-1.200454	0.074336	2.697105
C	2.153641	-0.031086	0.953238
C	2.102573	-0.288393	-0.359685

C	3.426085	-0.417022	-1.044136
O	4.311074	0.405096	-0.893153
N	3.598164	-1.495683	-1.891722
C	2.801283	-2.624031	-1.840584
C	2.955367	-3.672548	-2.692204
C	2.508736	-4.891303	-3.014465
C	4.753961	-1.522590	-2.771339
H	4.441077	-1.851570	-3.763728
H	2.068822	-2.649214	-1.037257
H	1.687767	-5.362938	-2.473481
H	2.942316	-5.463324	-3.828478
H	5.180849	-0.526290	-2.826419
H	5.508243	-2.219170	-2.397997
C	0.870544	-0.311241	-1.213117
H	3.150835	0.044229	1.382337
H	2.437256	1.187672	3.252306
H	0.728993	1.695363	4.948952
H	-1.615820	0.978649	4.597908
H	-2.220128	-0.260481	2.545656
H	-0.528579	-0.761631	0.857203
H	0.307484	-1.245225	-1.138622
H	0.194682	0.495784	-0.923353
H	1.123675	-0.175583	-2.265625

^{3}3beta iso

31

scf done: -672.115877

C	-1.189355	0.123247	2.735221
C	-0.246629	-0.172678	1.767050
C	1.084239	0.225723	1.919743
C	1.431650	0.909717	3.088907
C	0.487636	1.216118	4.049517
C	-0.830687	0.825527	3.874422
C	2.144363	-0.044531	0.957821
C	2.078674	-0.330141	-0.349034
C	0.837627	-0.358133	-1.188154
C	3.394465	-0.485953	-1.039801
N	3.537020	-1.562398	-1.900026
C	2.642947	-2.707286	-1.896086
O	4.300761	0.312901	-0.886894
C	4.632894	-1.603691	-2.740200
C	4.895824	-2.656375	-3.559769
C	5.734838	-3.123434	-4.490987
H	3.239062	-3.621393	-1.901299
H	5.261665	-0.718105	-2.703315
H	6.596859	-2.545439	-4.826102
H	5.596112	-4.095331	-4.953747
H	2.033081	-2.703043	-0.997014
H	1.997360	-2.711989	-2.777610
H	3.146773	0.030683	1.374314
H	2.465242	1.207279	3.233598
H	0.781824	1.756136	4.941903
H	-1.573818	1.057446	4.628132
H	-2.214044	-0.203095	2.599979
H	-0.547828	-0.744617	0.899786
H	0.264182	-1.282849	-1.085053
H	0.174927	0.463631	-0.909659
H	1.079207	-0.247993	-2.246505

^{1}3l

21

scf done: -441.231182

H	0.679952	-0.874702	1.838343
C	1.504429	-1.024885	1.150047
C	1.646230	-0.257689	0.077604
C	0.721773	0.856611	-0.275432
C	2.873652	-0.352404	-0.773512
O	3.568355	0.638940	-0.917887
N	3.201219	-1.553864	-1.345289
C	4.465768	-1.682039	-2.042024
C	2.329009	-2.649581	-1.407826
C	2.619706	-3.800283	-1.952340
C	2.849610	-4.961295	-2.483075
H	1.346276	-2.487256	-0.981847
H	2.208424	-1.813961	1.389738
H	3.259195	-5.785091	-1.904127
H	2.646088	-5.163508	-3.531571
H	4.299924	-1.819238	-3.113290
H	5.051558	-0.783646	-1.877495
H	5.005796	-2.551932	-1.663300
H	1.259076	1.807137	-0.294712
H	0.296332	0.712752	-1.272671
H	-0.095373	0.926877	0.442275

^{3}3l alpha

21

scf done: -441.134853

H	0.687180	0.160574	1.737715
C	1.643703	0.549243	1.399972
C	2.178525	0.181710	0.105712
C	1.886570	1.060300	-1.058596
C	3.129428	-0.928299	0.060089
N	3.227096	-1.652974	-1.111754
C	2.116123	-1.897899	-1.938559
C	0.868390	-1.891356	-1.554121
C	-0.378112	-1.833258	-1.202256
O	3.857826	-1.179434	1.014202
C	4.343522	-2.568565	-1.252709
H	2.363846	-2.124077	-2.973310
H	2.158133	1.248103	2.052294
H	-0.934185	-0.898543	-1.223806
H	-0.920479	-2.713013	-0.867732
H	4.463766	-2.813082	-2.308356
H	5.254630	-2.099311	-0.887662
H	4.183373	-3.496435	-0.695406
H	2.452047	0.784104	-1.948296
H	0.820378	1.050135	-1.311759
H	2.128872	2.096916	-0.801013

^{3}3l beta

21

scf done: -441.161699

H	0.997819	-0.707085	1.552151
C	1.756521	-0.847851	0.790279
C	1.691608	-0.197312	-0.364062
C	0.610308	0.769103	-0.709839
C	2.818945	-0.260270	-1.343055
N	3.255763	-1.490352	-1.788258
C	4.467779	-1.547256	-2.589697
O	3.346931	0.773022	-1.713169
C	2.550177	-2.671352	-1.624292
C	3.008438	-3.863556	-2.088362
C	2.725064	-5.167536	-2.195644
H	4.228661	-1.791670	-3.626978

H	1.590560	-2.583352	-1.123340
H	1.799237	-5.586169	-1.799542
H	3.401924	-5.863995	-2.679801
H	4.964198	-0.583388	-2.548880
H	5.123915	-2.324697	-2.194747
H	2.569352	-1.525122	1.026796
H	0.114634	0.487275	-1.642887
H	-0.138142	0.813508	0.080815
H	1.024182	1.768269	-0.861250

Reagent 1

28

scf done: -632.892887

C	-1.582367	0.288462	2.466943
C	-0.448461	-0.004206	1.737355
C	0.821456	0.175114	2.291581
C	0.911971	0.658699	3.597086
C	-0.224268	0.949959	4.330191
C	-1.475220	0.765556	3.766606
C	2.049339	-0.116901	1.570103
C	2.164421	-0.648918	0.351710
C	3.500026	-0.844452	-0.243708
O	4.484054	-0.262709	0.185311
N	3.597816	-1.692260	-1.326463
C	4.853305	-1.782691	-2.042360
C	2.580579	-2.561643	-1.736226
C	2.643444	-3.342875	-2.781965
C	2.655848	-4.148053	-3.798464
H	1.703061	-2.607449	-1.103839
H	2.972406	0.124096	2.093371
H	3.042387	-5.161366	-3.723710
H	2.283291	-3.845175	-4.773774
H	1.282754	-0.908689	-0.220028
H	1.893683	0.803890	4.036050
H	-0.132698	1.323205	5.343331
H	-2.368233	0.994539	4.336113
H	-2.560064	0.146135	2.021700
H	-0.550001	-0.372731	0.722869
H	4.684290	-1.604050	-3.106528
H	5.539470	-1.040404	-1.648681
H	5.288170	-2.778854	-1.927872

^{3}I alpha

28

scf done: -632.810997

C	-1.089063	-0.057483	3.890534
C	-0.889866	-0.807273	2.735273
C	0.144495	-0.508822	1.877394
C	1.025784	0.563574	2.149614
C	0.805586	1.309195	3.331368
C	-0.232113	1.001429	4.179601
C	2.090171	0.885648	1.289935
C	2.368403	0.191623	0.049229
C	3.288930	-0.932745	0.023406
N	3.419186	-1.622829	-1.163409
C	2.466058	-1.628143	-2.195334
C	1.172079	-1.535763	-2.046391
C	-0.109941	-1.389474	-1.926442
O	3.976002	-1.228624	0.995885
C	4.496017	-2.588606	-1.268090
H	2.885117	-1.746665	-3.192439
H	2.747317	1.705830	1.577715

H	-0.569004	-0.403770	-1.901492
H	-0.777937	-2.241395	-1.838367
H	1.976075	0.576907	-0.887940
H	1.473377	2.134223	3.557744
H	-0.382870	1.586917	5.079392
H	-1.904954	-0.297192	4.561861
H	-1.553392	-1.634133	2.508719
H	0.297473	-1.098408	0.978068
H	4.714891	-2.757052	-2.322310
H	5.383762	-2.206905	-0.768419
H	4.226138	-3.544854	-0.810878

TS 5-endo

28

scf done: -632.798579

C	-0.048713	0.164084	-0.103667
C	0.136635	-0.119706	1.230194
C	1.355920	0.190281	1.876592
C	2.368635	0.802455	1.100459
C	2.171293	1.082552	-0.231517
C	0.962878	0.765807	-0.846398
C	1.571252	-0.078613	3.239807
C	0.591318	-0.676192	4.131379
C	0.400124	-2.137956	4.208200
N	0.135265	-2.554131	5.489076
C	-0.187859	-3.935088	5.765941
C	0.454470	-1.667171	6.516705
C	1.095247	-0.539020	6.291229
C	1.783390	0.564616	6.533917
H	0.089298	-1.933568	7.503700
H	2.532506	0.208349	3.665297
H	1.399018	1.545577	6.267490
H	2.798207	0.526353	6.919888
H	-0.296426	-0.098682	4.393188
H	3.310835	1.050169	1.579142
H	2.961687	1.553106	-0.805203
H	0.810735	0.987631	-1.895999
H	-0.991397	-0.082751	-0.578969
H	-0.655994	-0.589936	1.802038
H	-0.677484	-3.999228	6.736733
H	-0.863381	-4.312283	5.000444
H	0.706551	-4.563857	5.779816
O	0.463920	-2.905650	3.265050

^{3}I beta

28

scf done: -632.824276

C	4.785145	-1.531073	-2.721532
N	3.641705	-1.563803	-1.824400
C	2.725027	-2.577723	-2.016200
C	2.796563	-3.438744	-3.068182
C	2.222106	-4.503392	-3.637788
C	3.591144	-0.642264	-0.787096
O	4.555985	0.064274	-0.543932
C	2.330470	-0.536031	-0.037948
H	4.433704	-1.531358	-3.754890
H	1.958504	-2.695735	-1.256519
H	1.332727	-4.970216	-3.212842
H	2.613611	-4.948896	-4.546715
H	5.362962	-0.634548	-2.523000
H	5.414019	-2.411406	-2.571833
C	2.294903	0.141330	1.112780

H	1.429189	-0.968476	-0.453383
C	1.138025	0.396469	1.953144
H	3.234069	0.562239	1.466005
C	1.304344	1.181399	3.094944
C	0.235170	1.471762	3.922772
C	-1.022789	0.976754	3.624191
C	-1.204009	0.188776	2.494969
C	-0.137250	-0.099344	1.668791
H	2.291238	1.568934	3.325629
H	0.384424	2.085770	4.802870
H	-1.863622	1.201148	4.269806
H	-2.186778	-0.203205	2.260852
H	-0.295158	-0.718553	0.793108

TS rot

28

scf done: -632.811238

C	-0.257463	0.480569	0.069696
C	-0.192793	-0.070499	1.352125
C	1.043697	-0.517358	1.818605
C	2.178934	-0.424534	1.033465
C	2.097280	0.122539	-0.235594
C	0.874718	0.575672	-0.713371
C	-1.352566	-0.196153	2.219808
C	-2.617126	0.116348	1.934091
C	-3.677841	-0.065577	2.943651
O	-3.443534	-0.439023	4.083687
N	-4.950370	0.216483	2.526381
C	-5.285205	0.630987	1.213114
C	-5.677267	-0.247044	0.256404
C	-6.099414	-0.326145	-1.012914
C	-6.067624	0.105629	3.445016
H	-6.761606	-0.669342	3.109436
H	-5.293547	1.707933	1.021617
H	-6.233754	0.566327	-1.625247
H	-6.324969	-1.276671	-1.485750
H	-5.686798	-0.150341	4.430717
H	-6.607158	1.054520	3.497449
H	-2.897040	0.508646	0.962680
H	-1.158591	-0.595143	3.213726
H	1.105622	-0.943712	2.814565
H	3.129476	-0.779179	1.414113
H	2.983678	0.198601	-0.854150
H	0.807718	1.006661	-1.705453
H	-1.203668	0.841455	-0.317481

I rot

28

scf done: -632.823198

C	-0.516881	0.482410	0.017253
C	-0.413978	-0.162057	1.253208
C	0.825583	-0.682213	1.628098
C	1.932600	-0.544411	0.810846
C	1.817032	0.106583	-0.406204
C	0.586965	0.615097	-0.801007
C	-1.544200	-0.321325	2.151694
C	-2.728941	0.289822	2.054790
C	-3.784161	0.053291	3.048466
O	-3.556043	-0.297035	4.194805
N	-5.089094	0.291153	2.645523
C	-5.510171	0.327892	1.329945
C	-4.775133	-0.085263	0.259637

C	-4.755869	-0.182284	-1.071355
C	-6.102347	0.309276	3.688407
H	-6.337297	-0.702156	4.026335
H	-6.528475	0.692160	1.198683
H	-5.601060	0.136595	-1.682226
H	-3.903767	-0.595424	-1.602361
H	-5.746992	0.882684	4.541755
H	-7.005567	0.768843	3.292275
H	-2.923514	1.015433	1.273853
H	-1.400693	-1.011694	2.980462
H	0.913127	-1.196067	2.579890
H	2.887810	-0.949945	1.122871
H	2.680560	0.211281	-1.052243
H	0.489360	1.112314	-1.759037
H	-1.476061	0.866690	-0.313978

TS (I rot-II)

28

scf done: -632.821239

C	-0.581258	0.737305	0.090260
C	-0.556669	-0.141115	1.179865
C	0.596410	-0.905235	1.383068
C	1.687776	-0.786967	0.543323
C	1.649771	0.094339	-0.525455
C	0.508632	0.853656	-0.748349
C	-1.671636	-0.291445	2.089703
C	-2.809787	0.435554	2.083669
C	-3.833242	0.268663	3.137829
O	-3.574068	0.102908	4.316085
N	-5.137975	0.333525	2.694494
C	-5.423529	0.166961	1.352715
C	-4.435071	-0.127300	0.463228
C	-4.117458	-0.353173	-0.813055
C	-6.204377	0.346303	3.676268
H	-6.321669	-0.634697	4.141710
H	-6.472499	0.264223	1.080836
H	-4.865537	-0.347338	-1.605779
H	-3.094822	-0.570496	-1.109910
H	-5.981946	1.072268	4.456137
H	-7.134587	0.619908	3.182797
H	-2.905763	1.319360	1.460120
H	-1.586067	-1.089619	2.824247
H	0.626291	-1.595943	2.219643
H	2.572353	-1.387070	0.721882
H	2.502440	0.186125	-1.187641
H	0.469166	1.537059	-1.588635
H	-1.472084	1.323881	-0.108670

II

28

scf done: -632.883367

C	-0.499319	0.870351	0.101233
C	-0.715893	-0.194076	1.008923
C	0.356301	-1.097975	1.210774
C	1.557107	-0.940557	0.560659
C	1.746401	0.119038	-0.322552
C	0.707630	1.017166	-0.544691
C	-1.921503	-0.387006	1.701528
C	-3.128337	0.466877	1.592666
C	-3.828382	0.659520	2.931919
O	-3.330725	1.033370	3.970627
N	-5.146676	0.332401	2.745140

C	-5.385370	-0.112777	1.455597
C	-4.220759	-0.094162	0.695766
C	-4.041390	-0.494976	-0.592375
C	-6.151050	0.409940	3.774638
H	-6.596832	-0.570866	3.949557
H	-6.377374	-0.429282	1.167295
H	-4.866746	-0.881297	-1.177976
H	-3.066314	-0.444627	-1.061696
H	-5.676724	0.756536	4.690377
H	-6.939336	1.109350	3.490845
H	-2.861129	1.472017	1.245083
H	-1.998228	-1.259355	2.346027
H	0.211925	-1.924708	1.898863
H	2.360167	-1.647011	0.737329
H	2.693483	0.241958	-0.834114
H	0.846921	1.841372	-1.234971
H	-1.295063	1.580426	-0.096084

II_1

56

scf done: -1265.789684

C	-4.684947	-2.960284	-3.967379
C	-4.171105	-3.380894	-2.597222
C	-3.977845	-2.060767	-1.868265
C	-4.261053	-1.056287	-2.787146
N	-4.681135	-1.589256	-3.994225
C	-5.063663	-4.345580	-1.912976
C	-4.638645	-5.433233	-1.134152
C	-5.603189	-6.262790	-0.510388
C	-5.230859	-7.337571	0.261358
C	-3.883730	-7.634960	0.450272
C	-2.916588	-6.834119	-0.148510
C	-3.274887	-5.754415	-0.924824
C	-3.586720	-1.930919	-0.571005
C	-5.060235	-0.803170	-5.139825
O	-5.017970	-3.686391	-4.878909
H	-3.184212	-3.830493	-2.774200
H	-4.215007	0.015535	-2.653911
H	-6.132741	-4.159308	-1.981919
H	-6.653954	-6.032226	-0.654862
H	-5.991217	-7.955167	0.725760
H	-3.591260	-8.481684	1.059665
H	-1.866237	-7.059541	-0.001717
H	-2.497734	-5.141761	-1.371848
H	-3.395944	-2.801540	0.045375
H	-3.450468	-0.952729	-0.123822
H	-4.196356	-0.274737	-5.550458
H	-5.458587	-1.473640	-5.898886
H	-5.824505	-0.075327	-4.863728
C	-0.466612	-1.032730	-1.272716
C	-0.204485	0.251371	-0.646675
C	-0.517421	-1.307013	-2.578161
C	0.173189	1.389049	-1.364425
C	-0.805369	-2.683239	-3.015557
O	-0.686206	-3.636063	-2.258455
N	-1.212834	-2.873370	-4.320461
C	-1.337579	-4.222978	-4.836792
C	-1.599344	-1.836977	-5.179015
C	-1.966016	-1.997641	-6.422983
C	-2.373431	-2.103643	-7.649484
C	-0.339364	0.355315	0.738464
C	-0.109216	1.553963	1.389036

C	0.264447	2.672187	0.663146
C	0.405539	2.584504	-0.715592
H	-1.633398	-0.843937	-4.746560
H	-0.667455	-1.856388	-0.590860
H	-3.420625	-2.276079	-7.888288
H	-1.690466	-2.031477	-8.491752
H	-0.336897	-0.535333	-3.315168
H	-0.630203	-0.524351	1.304104
H	-0.218935	1.614981	2.465191
H	0.448836	3.613004	1.168389
H	0.701365	3.457258	-1.285779
H	0.293343	1.335355	-2.440512
H	-0.715480	-4.337873	-5.727072
H	-1.019030	-4.925400	-4.072985
H	-2.374926	-4.430010	-5.114878

TS (II_1-IV)

56

scf done: -1265.766306

C	0.194877	0.054051	0.110214
C	0.105525	-0.067816	1.496679
C	1.290207	-0.154479	2.226194
C	2.518227	-0.105678	1.590808
C	2.590287	0.023064	0.212316
C	1.421609	0.101608	-0.527139
C	-1.232088	-0.122961	2.110546
C	-1.462928	0.157073	3.451889
C	-2.826793	0.372266	3.908036
N	-3.104279	0.252416	5.259543
C	-2.198066	-0.218420	6.214772
C	-2.477772	-0.415072	7.476650
C	-2.699983	-0.633006	8.735513
O	-3.732471	0.628725	3.117684
C	-4.464085	0.462430	5.712138
C	-1.731024	-2.146734	1.862445
N	-1.609584	-2.831127	3.066512
C	-2.821007	-3.134073	3.641356
C	-3.904666	-2.583758	2.731254
C	-3.134579	-2.193848	1.489382
C	-5.067685	-3.477781	2.543467
C	-6.396212	-3.035500	2.441925
C	-6.758205	-1.666607	2.488211
C	-8.076862	-1.282132	2.393238
C	-9.085144	-2.229365	2.246729
C	-8.753761	-3.580563	2.191637
C	-7.441078	-3.978162	2.283624
O	-2.972062	-3.712383	4.692217
C	-0.348181	-3.085246	3.709624
C	-3.631882	-1.967745	0.277149
H	-4.228280	-1.653925	3.220882
H	-0.952714	-2.316988	1.123605
H	-4.873804	-4.543641	2.457391
H	-7.184460	-5.031823	2.242536
H	-9.533888	-4.324206	2.075188
H	-10.120151	-1.917616	2.174114
H	-8.329880	-0.228663	2.430367
H	-5.988688	-0.906986	2.592372
H	-4.694676	-2.045287	0.079323
H	-2.985012	-1.701593	-0.551745
H	0.047958	-2.173603	4.167518
H	-0.495471	-3.832507	4.486707
H	0.375323	-3.451688	2.979582

H	-1.199323	-0.447671	5.865677
H	-2.041903	0.152138	1.438790
H	-3.054145	-1.595110	9.097275
H	-2.546327	0.137037	9.487419
H	-0.639291	0.174160	4.152364
H	-0.720057	0.119829	-0.471432
H	1.465199	0.202603	-1.605248
H	3.553873	0.061246	-0.281822
H	3.427159	-0.168828	2.177754
H	1.260673	-0.256995	3.305471
H	-4.463381	1.102256	6.596475
H	-5.037230	0.929364	4.918071
H	-4.928586	-0.492246	5.980307

IV

56

scf done: -1265.788179

C	-6.413418	-1.082847	3.623793
C	-6.075164	-2.420748	3.941528
C	-7.055111	-3.198156	4.604857
C	-8.285808	-2.674827	4.924001
C	-8.595812	-1.356528	4.600058
C	-7.649252	-0.570798	3.950013
C	-4.826448	-2.983313	3.633160
C	-3.733656	-2.267325	2.940836
C	-2.787221	-1.467484	3.795428
C	-1.492141	-1.397444	3.037941
N	-1.534593	-2.620322	2.250516
C	-2.771834	-3.170725	2.175719
C	-1.412529	-0.130560	2.146746
C	-1.637688	1.099601	2.939713
C	-2.855900	1.869561	2.803166
O	-3.866364	1.412095	2.276802
C	-3.000736	-0.980098	5.003086
O	-3.063782	-4.196655	1.596336
C	-0.369258	-3.222205	1.653513
C	-0.098273	-0.016489	1.408175
C	-0.087494	0.118104	0.025976
C	1.107648	0.235826	-0.665443
C	2.310374	0.225827	0.021129
C	2.310009	0.101923	1.402246
C	1.114716	-0.013603	2.089983
N	-2.858333	3.130384	3.362204
C	-4.124813	3.823556	3.487440
C	-1.692356	3.890775	3.555204
C	-0.625452	3.833529	2.803007
C	0.452084	3.742368	2.088772
H	-0.633843	-1.416821	3.720435
H	-4.151605	-1.580682	2.185474
H	-4.637424	-4.008201	3.940508
H	-6.815367	-4.225928	4.858439
H	-9.017936	-3.292938	5.431131
H	-9.565626	-0.945355	4.853488
H	-7.884319	0.457390	3.698233
H	-5.686817	-0.447831	3.126754
H	-0.046202	-2.696127	0.751579
H	0.457035	-3.216587	2.368010
H	-0.610913	-4.251408	1.392129
H	-1.732714	4.579331	4.396242
H	-2.220400	-0.212780	1.411483
H	0.631395	4.395558	1.239636
H	1.216420	2.998275	2.304558

H	-0.901329	1.385469	3.683099
H	-1.028996	0.121085	-0.514214
H	1.097936	0.333138	-1.744756
H	3.246718	0.315493	-0.516872
H	3.246939	0.096668	1.947161
H	1.130877	-0.104616	3.171886
H	-4.029856	4.591539	4.255132
H	-4.419754	4.303009	2.549494
H	-4.903093	3.119249	3.774613
H	-2.219272	-0.452315	5.539874
H	-3.959458	-1.090329	5.497425

TS (IV-V)

56

scf done: -1265.772199

C	-0.024348	0.006176	0.016445
C	-0.016887	-0.023478	1.432032
C	1.243475	-0.088318	2.074807
C	2.407308	-0.125277	1.339451
C	2.373396	-0.098474	-0.051145
C	1.145715	-0.031700	-0.705040
C	-1.227964	0.020530	2.140810
C	-1.339863	-0.007418	3.615624
C	-1.247464	1.311383	4.335512
C	-1.997180	1.144160	5.627015
N	-2.986892	0.136594	5.262509
C	-2.675502	-0.537114	4.126918
C	-1.116579	0.678202	6.821254
C	0.098955	1.541609	6.974803
C	1.377686	1.035554	6.451895
O	1.490765	0.224979	5.545429
C	-0.731413	2.438754	3.883336
O	-3.343305	-1.408263	3.607797
C	-4.226653	-0.061147	5.971247
C	-1.933673	0.585535	8.088482
C	-2.672401	1.665541	8.557715
C	-3.426718	1.558076	9.712560
C	-3.447381	0.367541	10.423231
C	-2.704648	-0.710556	9.971684
C	-1.954135	-0.598991	8.811814
N	2.457159	1.538914	7.125644
C	3.800750	1.188811	6.725870
C	2.194520	2.055784	8.393026
C	0.985703	2.071335	8.910786
C	0.094558	2.356082	9.863416
H	-2.499520	2.079725	5.900519
H	-0.571158	-0.670846	4.044435
H	-2.149867	0.100536	1.571112
H	-0.980520	0.058771	-0.494775
H	1.110720	-0.009216	-1.788285
H	3.294664	-0.127298	-0.620758
H	3.361557	-0.172626	1.852507
H	1.294299	-0.096289	3.159074
H	-4.081307	-0.558819	6.933146
H	-4.708093	0.902916	6.153989
H	-4.878163	-0.674458	5.350495
H	3.051501	2.452393	8.927790
H	-0.767962	-0.331641	6.575856
H	-0.169974	1.633463	10.631945
H	-0.510787	3.258065	9.826694
H	-0.045030	2.616908	6.879062
H	-1.380565	-1.448855	8.455002

H	-2.712882	-1.645328	10.520341
H	-4.040648	0.282207	11.325958
H	-4.000266	2.408869	10.061956
H	-2.658248	2.608398	8.018618
H	4.501313	1.892224	7.173233
H	4.065832	0.175512	7.041125
H	3.884239	1.244924	5.642187
H	-0.778322	3.353170	4.464816
H	-0.243166	2.487326	2.916274

IV

56

scf done: -1265.856785

C	0.307742	-0.472933	0.830338
C	-0.098062	-0.439101	2.161991
C	0.877409	-0.328335	3.147075
C	2.220173	-0.240519	2.817583
C	2.609618	-0.266370	1.489152
C	1.648739	-0.386316	0.497775
C	-1.549452	-0.508186	2.568173
C	-2.143513	-1.918743	2.387835
C	-1.371394	-2.880938	3.278540
N	-0.916886	-3.895318	2.477923
C	-1.332074	-3.727252	1.169307
C	-2.090868	-2.569688	1.023996
C	-2.696654	-2.151317	-0.124677
C	-2.413987	0.603565	1.937476
C	-3.790862	0.670436	2.547806
C	-3.731346	1.696689	3.652350
C	-2.609125	2.607257	3.171439
N	-1.892180	1.936330	2.238186
C	-4.990723	2.410941	3.957056
C	-5.947821	1.991318	4.894214
C	-5.810339	0.810450	5.662638
C	-6.777942	0.438763	6.568959
C	-7.917421	1.216226	6.749257
C	-8.078472	2.380161	6.002144
C	-7.118735	2.762036	5.094836
C	-4.868224	0.025347	2.138096
C	-0.818563	2.564831	1.506873
O	-2.397343	3.738667	3.557265
O	-1.171723	-2.773884	4.468906
C	-0.124749	-5.003281	2.947052
H	-2.464890	0.475543	0.850586
H	-3.345636	1.210402	4.562099
H	-5.198541	3.312998	3.387890
H	-7.245379	3.669765	4.513665
H	-8.964811	2.989579	6.136183
H	-8.674469	0.916829	7.464053
H	-6.649819	-0.470503	7.145106
H	-4.935407	0.183101	5.530359
H	0.167455	2.263610	1.868028
H	-0.890963	2.303913	0.449277
H	-0.916559	3.644021	1.617348
H	-1.085825	-4.467939	0.422277
H	-1.582731	-0.334508	3.652140
H	-2.595502	-2.729710	-1.035580
H	-3.294033	-1.251097	-0.177926
H	-3.175152	-1.893905	2.756256
H	0.572781	-0.309122	4.188735
H	2.962862	-0.148974	3.601632
H	3.658425	-0.195178	1.225858

H	1.944483	-0.407826	-0.544726
H	-0.429953	-0.554301	0.039493
H	-0.645498	-5.947590	2.778621
H	0.835861	-5.033450	2.430023
H	0.046098	-4.873340	4.013717
H	-4.840134	-0.666357	1.303118
H	-5.825999	0.170244	2.625698

TS (V_1,7)

56

scf done: -1265.815407

C	0.005499	-0.084647	0.017663
C	0.004580	0.015088	1.402005
C	1.236866	0.095537	2.053470
C	2.425507	0.089961	1.349882
C	2.411355	-0.001985	-0.034075
C	1.199361	-0.091872	-0.692080
C	-1.235562	0.001353	2.273129
C	-2.511725	-0.620964	1.651495
C	-3.285021	0.169928	0.588061
N	-4.517380	0.459272	1.109390
C	-4.656130	0.045383	2.443189
C	-3.566626	-0.878985	2.702654
O	-2.939431	0.459671	-0.536035
C	-5.460731	1.348098	0.486182
C	-3.510139	-1.777699	3.684120
C	-1.418456	1.356159	3.032196
C	-2.464930	2.308507	2.507666
C	-3.570753	2.330672	3.456441
C	-3.006230	1.784651	4.729300
N	-1.827773	1.182091	4.414145
C	-4.527766	3.444771	3.445096
C	-5.856336	3.438368	3.895348
C	-6.482078	2.317865	4.495757
C	-7.794339	2.375225	4.905732
C	-8.542086	3.538127	4.742666
C	-7.948109	4.657128	4.164848
C	-6.637894	4.612802	3.752095
C	-2.322726	3.030103	1.391825
C	-1.028304	0.480911	5.377328
O	-3.516358	1.810179	5.834414
H	-0.438271	1.849103	3.018263
H	-4.283660	1.186701	3.114265
H	-4.149906	4.388196	3.053889
H	-6.178073	5.486654	3.301256
H	-8.520457	5.569162	4.039331
H	-9.574672	3.573591	5.068357
H	-8.247262	1.505256	5.367889
H	-5.907846	1.415029	4.664160
H	-1.075993	-0.604988	5.240828
H	0.016105	0.795791	5.306428
H	-1.402330	0.715214	6.372627
H	-5.668208	-0.164929	2.784590
H	-0.987557	-0.710573	3.070030
H	-4.323198	-1.887445	4.392743
H	-2.652431	-2.430231	3.804606
H	-2.196064	-1.562892	1.189984
H	1.264831	0.147212	3.138640
H	3.367352	0.147963	1.883281
H	3.340779	-0.008948	-0.591449
H	1.173365	-0.168853	-1.773199
H	-0.933724	-0.143142	-0.516721

H	-6.449345	0.887566	0.443359
H	-5.534656	2.280376	1.058583
H	-5.119092	1.571262	-0.522322
H	-1.427251	2.951209	0.785712
H	-3.095565	3.706959	1.046128

V_1,7

56

scf done: -1265.857617

C	-5.996004	-2.091569	5.740615
C	-5.102133	-1.583000	4.766732
C	-4.347453	-2.465484	3.977492
C	-3.360068	-2.072269	2.989544
C	-3.534555	-2.270413	1.544818
N	-2.371713	-1.868517	0.952238
C	-2.088204	-2.057715	-0.441495
O	-4.505833	-2.731250	0.968123
C	-2.074442	-1.584772	3.228209
C	-1.519781	-1.373074	4.457472
C	-1.374651	-1.419782	1.899346
C	-0.788342	-0.033849	1.539387
C	0.537635	0.175603	2.239342
C	1.672767	-0.411817	1.689237
C	2.912170	-0.283098	2.291620
H	-0.538679	-0.125541	0.473560
C	-1.718237	1.197630	1.651721
C	-1.158402	2.302798	0.796270
C	-1.775027	2.143205	-0.565528
N	-2.999449	1.428531	-0.274919
C	-3.084959	0.988636	1.001925
H	-1.864010	1.485386	2.695408
C	3.040213	0.445824	3.462358
C	1.919814	1.036550	4.021738
C	0.681069	0.901571	3.415518
C	-6.727392	-1.248337	6.542436
C	-6.605650	0.132706	6.406842
C	-5.741773	0.655358	5.449182
C	-5.000496	-0.175969	4.639821
O	-4.081913	0.537248	1.529523
C	-4.043621	1.290656	-1.250276
C	-0.346345	3.281367	1.151886
H	-0.519488	-2.112271	1.861103
H	-1.141167	1.570449	-1.258114
H	-4.510993	-3.532876	4.119645
H	-6.089169	-3.167572	5.847718
H	-7.402175	-1.660845	7.283870
H	-7.183204	0.795429	7.040311
H	-5.653383	1.730082	5.336103
H	-4.348882	0.236217	3.875623
H	-2.072467	-1.114070	-0.997052
H	-1.117575	-2.546403	-0.569936
H	-2.864650	-2.690760	-0.869020
H	-1.987283	3.107148	-1.038398
H	-0.043170	4.040721	0.439195
H	0.045292	3.363015	2.158968
H	1.579142	-0.978405	0.766429
H	3.781248	-0.748086	1.840748
H	4.009177	0.555480	3.934944
H	2.006930	1.609677	4.937456
H	-0.180882	1.368469	3.878918
H	-4.490513	2.258208	-1.496364

H	-3.643394	0.853869	-2.169416
H	-4.815499	0.634281	-0.850210
H	-0.491961	-1.060821	4.581983
H	-2.106191	-1.553760	5.351159

V_1,7 rot)

56

scf done: -1265.858463

C	-0.112668	0.621534	0.193651
C	0.224226	-0.463206	1.040025
C	1.592136	-0.820124	1.128383
C	2.551349	-0.143971	0.413451
C	2.193656	0.914210	-0.418748
C	0.856765	1.288426	-0.519167
C	-0.736291	-1.177641	1.771864
C	-2.163876	-0.911518	1.740997
C	-2.792523	0.285493	2.322445
N	-4.137142	0.144368	2.133570
C	-4.496953	-1.080230	1.450700
C	-3.164539	-1.763269	1.279801
O	-2.243602	1.223105	2.876361
C	-5.106765	1.089441	2.612463
C	-2.985650	-3.036911	0.813711
C	-5.331256	-0.772197	0.185661
C	-4.615510	0.103593	-0.866064
C	-3.792705	-0.485520	-1.985935
C	-4.551138	-0.300381	-3.272112
N	-5.608125	0.617156	-2.922076
C	-5.700224	0.884008	-1.605357
C	-2.566769	-0.979268	-1.943467
C	-6.508698	1.125370	-3.918190
O	-6.528611	1.602251	-1.075962
C	-6.108020	-1.960277	-0.331226
C	-7.407063	-2.140021	0.139371
C	-8.179491	-3.215126	-0.265110
C	-7.665243	-4.137112	-1.161008
C	-6.376803	-3.973183	-1.640334
C	-5.604539	-2.898930	-1.227669
H	-6.099074	-0.091959	0.573794
H	-4.014651	0.830270	-0.303850
H	-5.146230	-1.683726	2.103434
H	-4.972431	-1.242832	-3.649828
H	-0.385209	-1.982576	2.415321
H	1.870475	-1.646288	1.774785
H	3.591559	-0.437028	0.497197
H	2.951846	1.446409	-0.980583
H	0.576022	2.116169	-1.160373
H	-1.149560	0.932312	0.115891
H	-5.536282	1.686874	1.801647
H	-5.920035	0.569884	3.126193
H	-4.612608	1.760916	3.313016
H	-3.918089	0.113571	-4.064251
H	-2.070477	-1.298459	-2.854195
H	-2.014367	-1.094779	-1.020257
H	-7.818527	-1.415586	0.836739
H	-9.187632	-3.327832	0.116577
H	-8.266365	-4.978374	-1.485599
H	-5.963365	-4.689266	-2.341273
H	-4.595485	-2.797427	-1.607338
H	-5.965237	1.702604	-4.670701
H	-7.025814	0.304085	-4.422124
H	-7.242947	1.767463	-3.435674

H	-3.821550	-3.671316	0.550131
H	-1.986380	-3.447880	0.720782

TS (V_1,5)

56

scf done: -1265.818083

C	-0.002576	-0.033418	0.019108
C	-0.004790	0.004249	1.405937
C	1.224047	0.036583	2.063358
C	2.413249	0.011318	1.361567
C	2.400908	-0.041511	-0.024725
C	1.190031	-0.058222	-0.691144
C	-1.251756	0.035951	2.257998
C	-1.362935	-1.127390	3.231517
C	-0.789489	-2.456042	3.076076
C	-0.657479	-3.044010	4.455844
N	-0.927373	-1.934776	5.336899
C	-1.311328	-0.809558	4.688323
C	-0.459088	-3.113038	1.960729
C	-0.898574	-2.082563	6.763263
O	-1.605590	0.257134	5.202497
C	-2.595847	0.263550	1.489714
N	-3.573139	0.851098	2.394296
C	-4.352930	-0.096815	2.986019
C	-3.915792	-1.402701	2.395318
C	-3.234507	-1.052955	1.164763
C	-4.630970	-2.662742	2.584693
C	-4.717502	-3.385382	3.780867
C	-4.210725	-2.909792	5.017536
C	-4.317108	-3.667221	6.161686
C	-4.919507	-4.921800	6.131612
C	-5.436008	-5.406501	4.931704
C	-5.345207	-4.657858	3.784237
O	-5.188479	0.091182	3.847377
C	-3.476101	2.202839	2.872131
C	-3.122895	-1.774544	0.047504
H	-1.152837	0.917481	2.904778
H	-2.686719	-1.423310	3.098470
H	-2.435703	0.918920	0.631015
H	0.342090	-3.456416	4.631508
H	-5.126480	-3.081761	1.711021
H	-5.749203	-5.035676	2.850627
H	-5.913727	-6.379040	4.903502
H	-4.996622	-5.511139	7.037260
H	-3.940484	-3.274383	7.099621
H	-3.775554	-1.917525	5.072899
H	-2.688380	2.312159	3.625752
H	-3.269053	2.876610	2.039241
H	-4.425318	2.482592	3.326743
H	-1.382438	-3.852495	4.625567
H	-0.067370	-4.122736	2.012813
H	-0.556484	-2.667205	0.979861
H	1.243044	0.080465	3.149260
H	3.355434	0.036819	1.896826
H	3.331395	-0.062724	-0.579625
H	1.164646	-0.091256	-1.774096
H	-0.933011	-0.046566	-0.535438
H	-1.575770	-2.883116	7.077996
H	0.107850	-2.328576	7.112082
H	-1.215183	-1.146088	7.219525
H	-2.577548	-1.413376	-0.815278
H	-3.598139	-2.744469	-0.040199

VI

56

scf done: -1265.861571

C	-0.229916	1.211859	-0.508882
C	0.037624	0.195979	0.439864
C	1.388711	0.007627	0.820100
C	2.396866	0.771377	0.280691
C	2.107778	1.758436	-0.657561
C	0.787764	1.970421	-1.042130
C	-0.961670	-0.614179	1.002609
C	-2.402377	-0.528138	0.680967
C	-3.170821	0.482782	1.541413
N	-4.351778	-0.074884	1.879454
C	-4.589189	-1.391048	1.309036
C	-3.205835	-1.786823	0.851675
O	-2.785364	1.591194	1.851899
C	-5.342964	0.607106	2.671429
C	-2.746778	-3.015651	0.693261
C	-5.685026	-1.319718	0.205596
C	-5.189690	-0.603225	-1.006411
C	-4.504478	-1.081794	-2.126350
C	-4.156649	0.097588	-2.993257
N	-4.711154	1.218571	-2.286379
C	-5.357806	0.853314	-1.144274
C	-4.157137	-2.358692	-2.457949
C	-4.641666	2.557495	-2.792592
O	-5.963153	1.606042	-0.395380
C	-6.390547	-2.623434	-0.107939
C	-7.376614	-2.605405	-1.093809
C	-8.085829	-3.743948	-1.421834
C	-7.826705	-4.938531	-0.765295
C	-6.862754	-4.969601	0.224381
C	-6.154459	-3.821509	0.552459
H	-6.452673	-0.658224	0.632594
H	-2.524334	-0.165708	-0.351912
H	-4.952220	-2.052245	2.103478
H	-4.589528	0.009885	-3.997051
H	-0.667213	-1.332346	1.763391
H	1.617132	-0.761869	1.550659
H	3.422517	0.602963	0.588900
H	2.903295	2.359500	-1.081437
H	0.555208	2.743449	-1.765810
H	-1.253002	1.409689	-0.810110
H	-6.112406	1.063335	2.043519
H	-5.809585	-0.099237	3.361069
H	-4.849799	1.391822	3.242869
H	-3.070869	0.199635	-3.116950
H	-3.603498	-2.558251	-3.368310
H	-4.431107	-3.205020	-1.841509
H	-7.585099	-1.674556	-1.613089
H	-8.847025	-3.699859	-2.192149
H	-8.377502	-5.835551	-1.022461
H	-6.653364	-5.892901	0.752135
H	-5.414627	-3.883374	1.340391
H	-3.601567	2.874352	-2.910622
H	-5.137533	2.636505	-3.764501
H	-5.137554	3.221475	-2.086475
H	-3.361968	-3.892095	0.856759
H	-1.722536	-3.189288	0.381326

TS (VI-VII)

56

scf done: -1265.817817

C	-0.028165	0.040801	-0.023481
C	-0.034928	0.006025	1.352015
C	1.210471	-0.053789	2.058939
C	2.395040	-0.257036	1.298344
C	2.368732	-0.212087	-0.074585
C	1.158138	-0.062943	-0.750896
C	-1.284006	0.348879	2.104321
C	-1.212830	1.852908	2.528951
C	-2.098637	2.698656	1.632781
N	-1.286491	3.623751	1.039604
C	0.037682	3.455933	1.456545
C	0.146418	2.461563	2.360187
O	-3.293611	2.572417	1.455320
C	-1.736691	4.639736	0.125458
C	1.307327	1.836201	2.886641
C	-1.602727	-0.574125	3.297675
C	-2.931453	-0.253836	3.925543
C	-3.954287	-1.079315	3.187733
C	-3.125270	-2.296140	2.786674
N	-1.816830	-1.949773	2.858663
C	-5.198248	-1.409762	3.915238
C	-6.338994	-0.593382	3.963289
C	-7.472845	-1.015007	4.699111
C	-8.606787	-0.240893	4.770464
C	-8.663736	0.986106	4.114835
C	-7.562062	1.425209	3.387386
C	-6.419951	0.659931	3.309121
C	-3.137621	0.502138	4.988584
C	-0.744738	-2.873354	2.590726
O	-3.563439	-3.379633	2.459463
H	-0.795589	-0.537302	4.040460
H	-4.192422	-0.562424	2.243049
H	-5.215922	-2.344263	4.469397
H	-7.430850	-1.971692	5.210026
H	-9.460555	-0.588801	5.340761
H	-9.557719	1.595401	4.172047
H	-7.599656	2.381774	2.878511
H	-5.569644	1.029405	2.744819
H	-0.201565	-2.618515	1.677427
H	-0.037870	-2.878451	3.424343
H	-1.172611	-3.868648	2.481379
H	0.808393	4.095221	1.048319
H	-2.133175	0.252965	1.417030
H	2.273494	2.233055	2.588250
H	1.268157	1.502575	3.919382
H	-1.584865	1.956348	3.553600
H	-0.972124	0.159359	-0.548781
H	1.134252	-0.043659	-1.833678
H	3.289713	-0.323450	-0.635889
H	3.332582	-0.410212	1.821363
H	1.201909	-0.473461	3.061238
H	-1.578032	5.637158	0.540743
H	-1.206141	4.567145	-0.825718
H	-2.801180	4.492843	-0.047989
H	-2.318234	0.995145	5.500484
H	-4.133172	0.645025	5.393951

VII

56

scf done: -1265.855952

C	0.350066	-1.565827	1.329431
C	-0.107786	-0.154146	1.556650
C	0.485931	0.886415	0.908227
C	1.554638	0.706601	0.015154
C	2.051432	-0.594146	-0.216862
C	1.502230	-1.670326	0.392701
C	-1.263006	0.080073	2.494706
C	-1.244326	-0.933819	3.593202
C	-0.405232	-1.971613	3.655118
C	-0.625265	-2.734337	4.911640
N	-1.676176	-1.999601	5.558388
C	-2.042718	-0.898137	4.843379
C	0.638993	-2.284996	2.658100
C	-2.182807	-2.338910	6.855738
O	-2.856920	-0.061759	5.197884
C	-2.601098	0.186345	1.695443
N	-3.697728	0.723355	2.477151
C	-4.654037	-0.176280	2.790872
C	-4.231310	-1.528648	2.188439
C	-3.175870	-1.114689	1.206478
C	-5.344750	-2.351441	1.677640
C	-6.116013	-3.228238	2.457558
C	-5.914563	-3.410584	3.847120
C	-6.690822	-4.291393	4.566168
C	-7.696675	-5.023576	3.943539
C	-7.920065	-4.857092	2.579478
C	-7.151577	-3.979767	1.851273
O	-5.659815	0.032274	3.434731
C	-3.694914	2.073930	2.966498
C	-2.876564	-1.701492	0.060995
H	-1.131677	1.074613	2.943270
H	-3.742462	-2.049850	3.027494
H	-2.392684	0.860999	0.855084
H	0.280327	-2.770441	5.531781
H	-5.609878	-2.236145	0.629875
H	-7.327415	-3.851900	0.787853
H	-8.704213	-5.421318	2.087563
H	-8.303423	-5.714483	4.516591
H	-6.518008	-4.410572	5.629884
H	-5.149334	-2.837079	4.360178
H	-2.998239	2.194006	3.800302
H	-3.417476	2.760930	2.163348
H	-4.696421	2.317821	3.317130
H	-0.916163	-3.773869	4.711431
H	1.614795	-1.965766	3.047168
H	0.719717	-3.364061	2.490975
H	0.121029	1.893636	1.097397
H	2.003512	1.560619	-0.476493
H	2.891511	-0.728634	-0.889910
H	1.898726	-2.665859	0.215398
H	-0.500936	-2.123586	0.897851
H	-2.598299	-3.350124	6.861791
H	-1.398433	-2.284271	7.616445
H	-2.970650	-1.632421	7.113499
H	-2.142925	-1.273749	-0.614827
H	-3.353211	-2.625596	-0.245951

TS (VII-VIII)

56

scf done: -1265.811466

C	0.009709	-0.150647	0.013240
C	-0.013476	0.006114	1.419623
C	1.237151	0.094962	2.079066
C	2.420681	0.029541	1.382886
C	2.415571	-0.125378	-0.000740
C	1.201241	-0.213635	-0.673911
C	-1.195534	0.085018	2.172912
C	-2.569166	0.039227	1.628274
C	-3.095852	1.450874	1.301110
N	-4.377474	1.534884	1.720312
C	-4.912238	0.309733	2.268540
C	-3.653779	-0.506042	2.551094
C	-5.959988	-0.382161	1.311307
C	-5.490669	-0.420182	-0.102298
C	-4.837512	-1.446508	-0.647826
C	-4.525084	-2.701596	0.061582
C	-5.007167	-2.645101	1.507262
C	-6.104468	-1.764548	1.851130
C	-4.500865	-1.142352	-2.063309
N	-5.059578	0.169252	-2.252674
C	-5.685584	0.625518	-1.130877
C	-4.899180	-3.854202	2.266995
C	-5.747157	-4.120879	3.311760
C	-6.787841	-3.245039	3.629110
C	-6.931617	-2.059197	2.904362
O	-6.298163	1.676144	-1.029989
C	-5.033565	0.848738	-3.514705
C	-5.150244	2.750904	1.701507
O	-2.458826	2.327865	0.755660
C	-3.399430	-0.906650	3.848102
H	-6.892260	0.186096	1.390730
H	-2.577163	-0.492169	0.667884
H	-5.442885	0.523639	3.203824
H	-4.937497	-1.869435	-2.760199
H	-1.095316	0.280569	3.237194
H	1.244359	0.217580	3.157453
H	3.362500	0.101548	1.915036
H	3.348893	-0.173479	-0.548870
H	1.190669	-0.328142	-1.751888
H	-0.923203	-0.206349	-0.536633
H	-6.064397	2.621413	1.122442
H	-5.401997	3.050213	2.722863
H	-4.551174	3.531594	1.235851
H	-3.415266	-1.149154	-2.231758
H	-5.003840	-3.543410	-0.455771
H	-3.450159	-2.917805	0.026954
H	-7.692370	-1.338192	3.190970
H	-7.464354	-3.472132	4.443734
H	-5.627439	-5.037906	3.877952
H	-4.124366	-4.564896	1.995834
H	-4.087084	-1.776289	1.993285
H	-4.006233	1.020100	-3.846620
H	-5.553709	0.272588	-4.285484
H	-5.531420	1.810527	-3.399820
H	-4.211207	-0.995161	4.561693
H	-2.433446	-1.299254	4.141758

VIII

56

scf done: -1265.874469

C	0.414597	0.665111	0.451687
C	0.244604	0.163528	1.833474
C	1.443629	-0.104271	2.348159
C	2.507893	0.249809	1.372594
N	1.760636	0.726956	0.239310
C	-1.040660	-0.007550	2.557374
C	-0.863049	-0.920046	3.750310
C	0.390820	-1.201525	4.294897
C	1.664190	-0.668840	3.693916
C	0.474512	-2.015789	5.420183
C	-0.654732	-2.553393	6.004899
C	-1.900233	-2.288414	5.456113
C	-1.994014	-1.479498	4.340812
C	-1.661677	1.333828	3.027573
N	-2.085250	2.193125	1.944718
C	-1.294308	3.267871	1.740652
C	-0.163742	3.212968	2.774213
C	-0.715799	2.238054	3.845403
C	0.282713	4.539150	3.245025
C	1.279360	5.316677	2.632581
C	1.621355	6.577100	3.180671
C	2.594377	7.365428	2.612717
C	3.271502	6.937985	1.473695
C	2.952812	5.705617	0.912000
C	1.979670	4.908686	1.471906
O	-1.437317	4.113641	0.880984
C	-3.207079	1.863303	1.108397
C	-1.458795	2.920094	4.928326
C	2.379738	1.140434	-0.986183
O	-0.451886	0.963190	-0.353171
H	-1.778580	-0.457377	1.879166
H	0.663037	2.710590	2.253490
H	-2.542410	1.075504	3.629814
H	3.134424	-0.612179	1.109430
H	-0.229844	4.961741	4.106733
H	1.094943	6.913551	4.068293
H	2.834027	8.325725	3.055184
H	4.037040	7.560692	1.026560
H	3.471284	5.368824	0.021185
H	1.737046	3.960767	1.003751
H	-2.974896	1.026838	0.444935
H	-4.069790	1.603255	1.726614
H	-3.451645	2.731135	0.497975
H	3.179414	1.025617	1.766937
H	2.417162	-1.464213	3.652569
H	2.103780	0.093788	4.351998
H	-2.968276	-1.278355	3.904261
H	-2.794889	-2.715042	5.894218
H	-0.564953	-3.186383	6.879811
H	1.454317	-2.232065	5.835547
H	0.102096	1.652890	4.270800
H	3.097170	1.946334	-0.808527
H	2.906192	0.311541	-1.468434
H	1.603513	1.501965	-1.659390
H	-2.420409	3.376759	4.717358
H	-1.033340	3.057742	5.912787

Product 2

56

scf done: -1265.958130

C	0.070622	0.014075	0.243919
C	0.093768	-0.205033	1.707882
C	1.220713	-0.839132	2.030168
C	2.071065	-1.014843	0.823981
N	1.275690	-0.425931	-0.219511
C	-0.965398	0.161931	2.684093
C	-0.857197	-0.689673	3.927945
C	0.318400	-1.359958	4.269054
C	1.538359	-1.331454	3.386025
C	0.362904	-2.092824	5.450702
C	-0.731223	-2.170247	6.289799
C	-1.903149	-1.512785	5.947825
C	-1.956937	-0.782331	4.776787
C	-0.921843	1.658343	3.087778
N	-1.188662	2.549163	1.974093
C	-0.105177	3.216602	1.504977
C	1.057239	2.946581	2.428739
C	0.428590	2.150266	3.583344
C	1.377041	4.099588	3.424789
C	1.230717	5.519927	2.984163
C	0.040657	6.227615	3.104406
C	-0.061772	7.530274	2.641695
C	1.024555	8.148203	2.046431
C	2.218114	7.453932	1.919665
C	2.316363	6.156040	2.387381
O	-0.086268	3.918181	0.509338
C	-2.474019	2.597364	1.327215
C	0.408900	3.441129	4.423215
C	1.652804	-0.464004	-1.602196
O	-0.835807	0.459064	-0.440960
H	-1.950868	-0.001681	2.227834
H	1.899372	2.539295	1.864584
H	-1.693687	1.806386	3.855697
H	2.279363	-2.073375	0.619285
H	2.404188	3.944412	3.767259
H	-0.825353	5.762060	3.562594
H	-0.998874	8.064869	2.748780
H	0.943883	9.167224	1.686312
H	3.077087	7.928519	1.458858
H	3.254242	5.616474	2.291185
H	-2.585101	1.785005	0.603638
H	-3.262045	2.524563	2.079387
H	-2.569111	3.547308	0.802237
H	3.041776	-0.512457	0.929526
H	1.979830	-2.332986	3.329894
H	2.322058	-0.709357	3.840507
H	-2.876343	-0.273541	4.500869
H	-2.773807	-1.574710	6.589916
H	-0.675210	-2.750540	7.203337
H	1.278830	-2.617599	5.705825
H	1.046938	1.365227	4.013789
H	2.610943	0.037497	-1.759648
H	1.737660	-1.492732	-1.965515
H	0.886861	0.049859	-2.181160
H	-0.584660	3.894965	4.424442
H	0.753259	3.368121	5.454124

Reagent 3

31

scf done: -672.184525

C	-1.364584	0.522320	3.966428
C	-1.614161	0.062131	2.683543
C	-0.568553	-0.215376	1.821380
C	0.757324	-0.035839	2.224212
C	0.989170	0.402076	3.531726
C	-0.055112	0.686941	4.389851
C	1.917769	-0.296649	1.381277
C	2.021699	-0.351191	0.048821
C	3.400894	-0.574073	-0.494136
N	3.569829	-1.611967	-1.377158
C	2.622579	-2.631089	-1.531722
C	2.714486	-3.614845	-2.385661
C	2.767262	-4.619480	-3.204095
O	4.323111	0.162268	-0.192837
C	4.822122	-1.752801	-2.090897
H	1.784032	-2.595383	-0.844924
H	2.844158	-0.432839	1.936380
H	3.254984	-5.553265	-2.935963
H	2.327849	-4.572885	-4.197224
C	0.937604	-0.072963	-0.947341
H	2.013685	0.523981	3.868408
H	0.152637	1.033811	5.395399
H	-2.186971	0.740681	4.637386
H	-2.634645	-0.089015	2.351088
H	-0.790644	-0.602229	0.835880
H	4.635003	-1.798126	-3.165925
H	5.452600	-0.899008	-1.863630
H	5.330362	-2.672328	-1.791071
H	1.362018	0.209516	-1.912373
H	0.285542	-0.932278	-1.127372
H	0.302183	0.745907	-0.604566

I beta Me

31

scf done: -672.115521

C	-0.243716	-0.198654	1.735884
C	1.080835	0.211734	1.909130
C	1.408434	0.881847	3.091764
C	0.450456	1.165254	4.045654
C	-0.861824	0.764496	3.849713
C	-1.200454	0.074336	2.697105
C	2.153641	-0.031086	0.953238
C	2.102573	-0.288393	-0.359685
C	3.426085	-0.417022	-1.044136
O	4.311074	0.405096	-0.893153
N	3.598164	-1.495683	-1.891722
C	2.801283	-2.624031	-1.840584
C	2.955367	-3.672548	-2.692204
C	2.508736	-4.891303	-3.014465
C	4.753961	-1.522590	-2.771339
H	4.441077	-1.851570	-3.763728
H	2.068822	-2.649214	-1.037257
H	1.687767	-5.362938	-2.473481
H	2.942316	-5.463324	-3.828478
H	5.180849	-0.526290	-2.826419
H	5.508243	-2.219170	-2.397997
C	0.870544	-0.311241	-1.213117
H	3.150835	0.044229	1.382337

H	2.437256	1.187672	3.252306
H	0.728993	1.695363	4.948952
H	-1.615820	0.978649	4.597908
H	-2.220128	-0.260481	2.545656
H	-0.528579	-0.761631	0.857203
H	0.307484	-1.245225	-1.138622
H	0.194682	0.495784	-0.923353
H	1.123675	-0.175583	-2.265625

TS rot Me

31

scf done: -672.101595

C	0.015558	-0.198704	-0.233948
C	-0.043603	-0.159710	1.149535
C	1.117841	-0.133721	1.900281
C	2.370221	-0.144941	1.281607
C	2.409570	-0.151967	-0.115575
C	1.249864	-0.190401	-0.865490
C	3.636222	-0.112228	2.004449
C	3.928534	-0.553475	3.234246
C	5.353440	-0.366881	3.657511
O	6.282524	-0.552624	2.889309
C	2.990442	-1.292690	4.136242
N	5.576934	0.019423	4.952295
C	4.574425	0.591147	5.776498
C	4.397087	1.934832	5.862966
C	3.678544	2.875306	6.489537
C	6.949476	0.253837	5.374200
H	7.007054	0.151038	6.457279
H	4.000460	-0.085472	6.412323
H	2.926399	2.613432	7.234840
H	3.808281	3.932879	6.283287
H	7.604297	-0.476641	4.904314
H	7.286690	1.257762	5.097299
H	4.466181	0.306340	1.439554
H	3.374670	-0.133236	-0.611809
H	1.308096	-0.206303	-1.947506
H	-0.896441	-0.222086	-0.818703
H	-1.004689	-0.142297	1.650391
H	1.046445	-0.070658	2.978069
H	2.378103	-0.631704	4.755274
H	2.306632	-1.906961	3.547302
H	3.537472	-1.952884	4.812006

I rot Me

31

scf done: -672.114528

C	-1.191995	0.031080	2.664983
C	-0.207109	-0.236535	1.730893
C	1.101508	0.211662	1.924486
C	1.390159	0.910876	3.099256
C	0.403552	1.190036	4.025257
C	-0.894477	0.753437	3.809337
C	2.186950	-0.050135	0.988428
C	2.129393	-0.241669	-0.336256
C	0.917455	-0.071634	-1.204058
C	3.435554	-0.461071	-1.025614
N	3.525577	-1.517187	-1.913979
C	4.696492	-1.552650	-2.776002
O	4.387396	0.281529	-0.864587
C	2.710027	-2.637039	-1.878496

C	1.868115	-2.947563	-0.856530
C	0.940351	-3.795919	-0.410397
H	4.517279	-2.262593	-3.581019
H	2.820738	-3.293121	-2.741139
H	0.643998	-4.679650	-0.976616
H	0.448591	-3.647539	0.547048
H	4.878073	-0.566157	-3.197110
H	5.585232	-1.861113	-2.221559
H	3.177132	-0.078723	1.439049
H	2.408456	1.242581	3.275486
H	0.648681	1.744409	4.923781
H	-1.668825	0.963685	4.537673
H	-2.199260	-0.334028	2.500779
H	-0.450577	-0.827777	0.856228
H	0.288565	-0.962892	-1.252599
H	0.299250	0.746371	-0.829756
H	1.211126	0.167801	-2.227890

TS 5-exo

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scf done: -672.113852

C	0.299542	0.560234	-0.174231
C	0.112687	0.692872	1.189786
C	0.989367	0.085903	2.097212
C	2.071878	-0.631933	1.572291
C	2.252522	-0.769387	0.210278
C	1.362069	-0.176834	-0.672703
C	0.867618	0.170569	3.541530
C	-0.239077	0.320849	4.306748
C	-0.031381	0.513934	5.779962
N	-0.427651	-0.514459	6.598562
C	-0.329265	-0.321338	8.033067
O	0.429113	1.544595	6.236429
C	-0.813994	-1.740116	6.075720
C	-0.807094	-1.950970	4.735363
C	-1.005456	-2.763188	3.697390
H	0.714426	-0.270342	8.347853
H	-1.107484	-2.483377	6.814229
H	-1.359570	-3.788072	3.806588
H	-0.810023	-2.420066	2.682392
H	-0.818810	0.608817	8.318215
H	-0.814824	-1.154263	8.535958
C	-1.624696	0.654308	3.840788
H	1.794656	-0.024524	4.079173
H	2.774415	-1.092467	2.259760
H	3.094867	-1.338292	-0.166052
H	1.502387	-0.278520	-1.742285
H	-0.389068	1.046178	-0.855934
H	-0.705181	1.302649	1.549493
H	-2.361822	0.407544	4.606919
H	-1.713231	1.725844	3.635534
H	-1.888737	0.111808	2.932065

III 5-exo

31

scf done: -672.174709

C	-4.275794	-0.026673	0.655410
C	-3.201752	0.712721	1.451288
C	-3.818317	0.785035	2.856553
N	-5.050939	0.194049	2.796680
C	-5.326887	-0.283662	1.526127
C	-1.980342	-0.143670	1.551703

C	-0.712847	-0.077247	0.945093
C	-0.274538	0.910778	0.028725
C	0.993993	0.871961	-0.506934
C	1.886079	-0.137976	-0.165940
C	1.482673	-1.125259	0.728621
C	0.219637	-1.098395	1.268410
O	-3.316612	1.285855	3.838675
C	-5.953586	0.093184	3.915280
C	-4.166283	-0.352353	-0.662651
H	-6.180165	-0.952261	4.131508
H	-6.265220	-0.781858	1.328864
H	-4.962883	-0.871917	-1.181099
H	-3.274176	-0.104967	-1.226742
H	-5.474573	0.543566	4.782207
H	-6.885931	0.620192	3.704911
C	-3.059273	2.151221	0.966319
H	-2.137621	-1.021780	2.177756
H	-0.087509	-1.873003	1.963709
H	2.165942	-1.921446	1.001652
H	2.881439	-0.157687	-0.593192
H	1.296340	1.642822	-1.206822
H	-0.938109	1.709713	-0.267408
H	-4.004959	2.677404	1.121102
H	-2.279976	2.676149	1.521940
H	-2.838601	2.197106	-0.099353

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scf done: -672.111140

C	0.163493	-0.162936	-0.097539
C	0.020750	-0.197863	1.278047
C	1.121083	0.004893	2.112901
C	2.369569	0.209976	1.524601
C	2.510283	0.256764	0.150274
C	1.405160	0.073699	-0.665995
C	1.032259	-0.053512	3.569371
C	0.024253	0.388538	4.363796
C	0.154553	0.190275	5.818720
N	0.655343	-1.027016	6.263983
C	0.827524	-1.143629	7.705325
O	-0.181198	1.039695	6.629697
C	0.718929	-2.208607	5.529583
C	0.717121	-2.326572	4.172006
C	0.691529	-3.248990	3.203621
H	-0.135146	-1.179748	8.219538
H	0.769848	-3.098405	6.155749
H	0.623542	-4.314630	3.426670
H	0.742500	-2.975696	2.153116
H	1.385970	-2.051584	7.920376
H	1.381836	-0.286499	8.081934
C	-1.215999	1.079903	3.914214
H	1.971362	-0.305194	4.056355
H	3.236962	0.340282	2.163533
H	3.486926	0.428401	-0.286929
H	1.513159	0.102175	-1.743799
H	-0.700087	-0.329964	-0.730518
H	-0.949010	-0.417169	1.709694
H	-1.508915	1.818607	4.661517
H	-1.078061	1.582691	2.956973
H	-2.055162	0.383788	3.805527

III

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scf done: -672.181624

C	1.849081	6.453203	7.451668
C	1.008516	6.667526	8.661652
C	1.221750	5.625593	9.732659
C	2.286631	4.755606	9.610320
N	3.158237	4.743251	8.539233
C	2.967242	5.535322	7.423072
C	1.233116	8.071470	9.203054
C	0.199293	8.993662	9.255412
C	0.418749	10.270699	9.750813
C	1.678087	10.636339	10.192769
C	2.719266	9.720338	10.137241
C	2.497398	8.447747	9.644081
C	0.360527	5.580174	10.802864
C	4.273833	3.819307	8.521958
O	3.729144	5.447917	6.463600
C	1.613985	7.305989	6.267938
H	-0.045454	6.621989	8.347465
H	2.486197	4.016545	10.376752
H	0.480802	4.846120	11.590638
H	-0.460143	6.282893	10.886254
H	2.293674	8.167991	6.264298
H	0.595681	7.700001	6.266702
H	1.796746	6.763113	5.339787
H	-0.788229	8.706324	8.906774
H	3.312061	7.729486	9.602491
H	1.851364	11.633840	10.579218
H	3.708360	10.001467	10.480245
H	-0.398984	10.981081	9.790270
H	4.353195	3.344613	9.497071
H	4.136563	3.049941	7.759187
H	5.201855	4.348245	8.304715

III_3

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scf done: -1344.378840

C	2.236489	8.422345	9.486869
C	1.026150	7.866201	9.085959
C	-0.067555	8.696619	8.899323
C	0.040678	10.063184	9.114037
C	1.247419	10.609021	9.514931
C	2.347712	9.783607	9.700926
C	0.932692	6.370401	8.829300
C	1.812182	5.998511	7.683574
C	2.933642	5.089255	7.804217
N	3.150635	4.519859	9.046445
C	2.302891	4.734022	10.114863
C	1.210360	5.580048	10.085609
C	1.597032	6.680272	6.390090
C	0.385937	5.731894	11.175087
C	4.273218	3.613178	9.181554
O	3.677666	4.819397	6.866172
H	-0.107693	6.171656	8.521751
H	2.554935	4.201728	11.025259
H	0.567095	5.187025	12.095774
H	-0.456530	6.412713	11.144152
H	2.093120	7.659039	6.379158
H	0.532465	6.866187	6.222243
H	2.001428	6.098804	5.562857

H	-1.013153	8.268238	8.580573
H	3.098423	7.776006	9.631257
H	1.334229	11.676357	9.680942
H	3.296136	10.205310	10.013293
H	-0.822501	10.701652	8.965723
H	4.375145	3.331414	10.227995
H	4.125772	2.713185	8.579652
H	5.194394	4.093141	8.851661
C	-0.189625	2.798910	7.989835
N	-1.023798	1.710878	8.280591
C	-1.931872	1.269409	7.242197
C	-1.062502	1.120597	9.520052
O	-1.946601	0.344579	9.834739
C	-0.012254	3.295435	6.794523
C	0.166826	3.822802	5.623637
C	0.059548	1.450895	10.453467
C	1.440919	1.110016	9.985407
C	-0.298070	1.963810	11.637174
C	0.497875	2.421811	12.767130
C	-0.185283	3.052760	13.812629
C	0.483345	3.576467	14.901918
C	1.863889	3.480199	14.978411
C	2.558845	2.842656	13.963240
C	1.888887	2.315318	12.873553
H	0.289871	3.271614	8.845628
H	-1.368108	2.102982	11.781686
H	-0.483519	4.605022	5.240277
H	0.982666	3.511871	4.975570
H	-1.265161	3.140253	13.751291
H	-0.073835	4.064974	15.692605
H	2.394953	3.893547	15.827554
H	3.637267	2.751260	14.020019
H	2.463166	1.814879	12.107029
H	-1.368282	0.934860	6.368384
H	-2.530989	0.449823	7.626282
H	-2.586947	2.088638	6.937585
H	1.426442	0.705246	8.973250
H	2.105817	1.978797	9.980485
H	1.894605	0.354685	10.631551

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scf done: -1344.339170

C	0.031183	-0.041598	0.001440
C	0.022468	-0.020761	1.403502
C	1.255930	0.017748	2.067568
C	2.441200	-0.009745	1.360060
C	2.430930	-0.076083	-0.026206
C	1.218757	-0.084724	-0.702687
C	-1.246859	-0.005241	2.092659
C	-1.672170	-0.590857	3.300214
C	-0.768684	-1.388473	4.200635
N	0.086002	-2.349992	3.705677
C	0.125609	-2.784802	2.383323
C	0.979672	-3.638676	1.886035
C	1.791271	-4.478790	1.319586
C	-2.573548	0.314502	4.120584
O	-0.813448	-1.187781	5.405030
C	1.000191	-3.012151	4.614256
C	-3.263005	-1.956979	2.757908
C	-2.868762	-3.348507	2.767526
C	-2.648620	-4.027410	1.434483

C	-2.490322	-3.039443	0.324071
C	-3.264804	-1.812539	0.339285
N	-3.788790	-1.448062	1.566223
C	-3.759639	-5.004412	1.076506
C	-5.098895	-4.626562	1.112873
C	-6.090527	-5.518324	0.745015
C	-5.759496	-6.799709	0.331217
C	-4.430412	-7.183639	0.290749
C	-3.437622	-6.289320	0.660459
C	-2.715237	-4.025173	3.912580
C	-4.734088	-0.349826	1.583152
O	-3.493583	-1.147144	-0.665221
C	-1.720272	-3.421202	-0.873530
H	-0.626426	-2.364467	1.728708
H	-1.726326	-4.617343	1.495319
H	-2.013996	0.573997	1.579019
H	-3.825877	-1.645242	3.629580
H	-3.123775	-0.221103	4.894561
H	-3.282871	0.835344	3.478347
H	-1.968024	1.072140	4.622726
H	-2.885586	-3.558229	4.876776
H	-2.412850	-5.066890	3.908807
H	-0.675899	-3.624901	-0.604054
H	-1.746667	-2.642084	-1.632981
H	-2.109027	-4.349571	-1.309523
H	-0.919378	-0.055118	-0.526130
H	1.278716	0.077370	3.150392
H	-2.395508	-6.592463	0.629708
H	1.201487	-0.122889	-1.785747
H	3.363414	-0.105042	-0.577320
H	3.384508	0.026020	1.893030
H	-5.371874	-3.627064	1.436891
H	-6.537395	-7.497178	0.043724
H	-7.129254	-5.211255	0.781138
H	-4.161861	-8.184429	-0.027296
H	-5.207235	-0.303960	2.562102
H	-4.261163	0.612429	1.367247
H	-5.499866	-0.517932	0.825836
H	2.025703	-2.891390	4.254451
H	0.903017	-2.576203	5.602238
H	0.774081	-4.081192	4.661099
H	1.592415	-5.547602	1.297601
H	2.713715	-4.150410	0.846146

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C	0.477817	0.450254	7.703368
C	1.258861	1.479075	7.109251
C	1.544945	1.355409	5.722067
C	1.083568	0.281261	4.981312
C	0.315683	-0.717316	5.589242
C	0.020644	-0.621344	6.951815
C	1.732412	2.625889	7.801113
C	1.606331	2.886318	9.273709
C	0.189597	2.694168	9.862337
N	-0.930813	3.147303	9.181260
C	-0.953635	3.752892	7.920335
H	0.016798	3.897643	7.430411
C	2.114800	4.344641	9.721925
C	1.058193	5.350605	10.125081

C	0.527397	6.302366	9.073893
C	1.266042	6.209790	7.774735
C	2.627472	5.681474	7.704453
N	3.057191	4.947804	8.799187
C	0.496581	7.749849	9.535702
C	-0.692784	8.479242	9.517888
C	-0.711350	9.821583	9.897885
C	0.465512	10.448525	10.295125
C	1.660414	9.727565	10.311549
C	1.675803	8.389313	9.934510
C	0.622332	5.395291	11.386035
C	4.419899	4.470281	8.768292
O	3.359761	5.876653	6.742415
C	0.703828	6.873192	6.577975
C	2.527483	1.877112	9.989018
C	-2.211451	3.058252	9.855634
O	0.069636	2.180573	10.957295
H	-0.526093	6.024887	8.863062
C	-2.035211	4.173512	7.298709
H	2.338498	3.319398	7.205730
H	2.678620	4.143966	10.648342
H	2.471974	2.002354	11.080219
H	3.567136	2.025044	9.659586
H	2.248437	0.839096	9.757228
H	0.986560	4.692358	12.141943
H	-0.128151	6.129290	11.699989
H	0.778967	7.975327	6.662691
H	-0.371781	6.643076	6.466443
H	1.249766	6.579659	5.670594
H	2.143037	2.136948	5.240997
H	0.228321	0.490077	8.767917
H	-1.619247	7.986605	9.199335
H	1.320553	0.216331	3.915309
H	-0.049497	-1.565902	5.003991
H	-0.577624	-1.399014	7.435798
H	2.613938	7.822658	9.952259
H	0.455101	11.501034	10.592518
H	2.589242	10.215713	10.621200
H	-1.652645	10.378833	9.882379
H	4.757593	4.249016	9.792522
H	4.542809	3.559098	8.150799
H	5.065753	5.242312	8.328621
H	-2.933785	2.511771	9.227981
H	-2.076866	2.539079	10.810114
H	-2.612779	4.071915	10.036084
C	-3.066826	4.621009	6.632159
H	-3.431351	5.651133	6.749573
H	-3.619144	3.988118	5.924668

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scf done: -1344.352364

C	-0.001682	-0.101691	0.095384
C	-0.003324	-0.087902	1.482927
C	1.215718	-0.109332	2.154118
C	2.406141	-0.141133	1.450428
C	2.397530	-0.150617	0.063372
C	1.190249	-0.130068	-0.612891
C	-1.315603	-0.062327	2.247443
C	-1.513739	-1.319985	3.043964
C	-1.121177	-1.363821	4.456675
N	-0.919966	-0.153851	5.086507

C	-1.145665	1.055944	4.454959
C	-1.412622	1.175761	3.103177
C	-1.383776	-2.607494	2.305778
C	-1.719534	2.379986	2.522587
C	-0.565735	-0.177219	6.493085
O	-1.000901	-2.415074	5.073579
C	-3.666222	-1.355097	3.345410
C	-4.263768	-0.205429	3.646804
C	-5.019936	0.800156	3.972707
N	-4.634614	2.143808	4.232652
C	-5.066434	3.047874	3.179036
C	-3.960529	2.663717	5.304524
O	-3.621862	3.840597	5.295491
C	-3.636941	1.856699	6.524666
C	-2.584465	2.490484	7.378615
C	-4.298187	0.744239	6.867129
C	-4.093757	-0.115905	8.032600
C	-3.834960	0.350629	9.321033
C	-3.629841	-0.536363	10.364104
C	-3.672368	-1.902735	10.141252
C	-3.946166	-2.382109	8.869063
C	-4.169754	-1.496782	7.831997
H	-2.113643	-0.019784	1.492919
H	-6.103966	0.648669	3.976123
H	-1.100028	1.932915	5.088552
H	-3.726885	-1.711925	2.320567
H	-3.572341	-2.123715	4.110454
H	-1.787729	3.288009	3.111052
H	-1.894345	2.452288	1.454960
H	-0.328448	-2.870546	2.174509
H	-1.827964	-2.530969	1.309985
H	-1.855136	-3.429859	2.844484
H	-0.948778	-0.089174	-0.435979
H	1.234787	-0.098364	3.239695
H	3.330917	-0.174369	-0.486716
H	3.347973	-0.158017	1.986826
H	1.172620	-0.136589	-1.696591
H	-0.127442	0.781042	6.764757
H	-1.444881	-0.360747	7.119970
H	0.157877	-0.968656	6.675910
H	-6.098577	2.814353	2.906924
H	-5.003720	4.075302	3.525461
H	-4.437470	2.927611	2.291362
H	-2.125649	1.766656	8.050498
H	-1.806801	2.956546	6.773343
H	-3.007994	3.291029	7.991335
H	-5.049733	0.365916	6.185538
H	-4.394928	-1.869804	6.836489
H	-3.991910	-3.449441	8.687218
H	-3.504504	-2.593727	10.958839
H	-3.438815	-0.155170	11.360502
H	-3.820520	1.415896	9.516668

IX

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scf done: -1344.392635

C	3.138030	7.396945	8.823581
C	1.760612	7.534150	8.977403
C	1.264492	8.759177	9.405104
C	2.113039	9.823909	9.664982
C	3.479290	9.677843	9.498539
C	3.988206	8.458851	9.077440

C	0.806110	6.398075	8.680041
C	0.661406	6.092578	7.172211
C	1.769217	5.193030	6.639454
N	2.302384	4.274810	7.506897
C	1.977836	4.219792	8.848977
C	1.194614	5.174707	9.477650
C	-0.684418	5.368844	6.900669
C	-1.010423	4.212308	7.728168
C	-1.992617	3.936447	8.550102
N	-2.259579	2.794021	9.330787
C	-1.408502	1.748945	9.614964
C	-0.253516	1.430603	8.733020
C	-0.414731	1.456580	7.405745
C	0.627602	7.375639	6.353924
C	0.827383	5.061109	10.790598
C	3.297513	3.355607	6.976652
O	2.142219	5.244095	5.480723
C	-3.435371	2.880554	10.188073
O	-1.618144	1.043150	10.589491
C	0.957962	0.956784	9.465643
H	-0.186568	6.721606	9.019734
H	-2.751987	4.707813	8.701730
H	2.380306	3.374154	9.391484
H	-1.479723	6.121621	7.037561
H	-0.700697	5.101954	5.835961
H	1.135139	4.211751	11.390006
H	0.221872	5.823718	11.266709
H	1.593789	7.881177	6.350103
H	-0.114257	8.059135	6.774956
H	0.353950	7.162047	5.320737
H	0.192709	8.879851	9.531634
H	3.558123	6.448368	8.503928
H	4.146631	10.507667	9.699198
H	5.057142	8.332925	8.948892
H	1.702817	10.769992	9.999170
H	3.548525	2.629889	7.747206
H	2.903792	2.835194	6.102392
H	4.201912	3.892700	6.685004
H	-4.162952	3.542828	9.724069
H	-3.878299	1.894963	10.309917
H	-3.182769	3.265586	11.179581
H	1.855728	1.041742	8.853302
H	1.100942	1.527543	10.385756
H	0.858586	-0.090963	9.762389
C	0.534262	1.107512	6.351921
H	-1.365272	1.825727	7.029469
C	0.492562	1.854094	5.172163
C	1.375596	1.607238	4.138173
C	2.305731	0.584948	4.251923
C	2.337379	-0.187267	5.402070
C	1.463408	0.070529	6.443973
H	-0.245951	2.645282	5.079430
H	1.334940	2.209861	3.238346
H	2.995188	0.382400	3.440929
H	3.045932	-1.002891	5.487691
H	1.482963	-0.560795	7.323732

TS (IX-X)

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scf done: -1344.382835

C	-0.237564	0.043439	-0.069918
C	-0.216732	0.007176	1.324581

C	0.995197	0.252933	1.973430
C	2.135397	0.569231	1.259360
C	2.091844	0.635891	-0.124636
C	0.903323	0.364460	-0.783700
C	-1.387248	-0.336484	2.144691
C	-2.676239	-0.546388	1.753682
C	-3.646223	-1.340045	2.556392
C	-3.268826	0.134025	0.583917
O	-3.905581	-0.462576	-0.272613
N	-3.137679	1.497226	0.546058
C	-3.715546	2.167982	-0.605994
C	-2.515327	2.281985	1.532960
C	-1.741805	1.903693	2.527704
C	-0.952789	2.702812	3.467752
C	-1.242937	2.626490	4.988363
C	-2.733364	2.929214	5.264749
C	-3.624514	1.725742	5.063941
C	-3.084723	0.476196	5.322757
N	-1.742425	0.273137	5.586537
C	-0.791310	1.252424	5.462974
C	-3.007847	3.517072	6.632558
C	-2.824669	2.781462	7.800882
C	-3.083604	3.342615	9.038742
C	-3.541399	4.648267	9.133622
C	-3.735456	5.386547	7.979587
C	-3.467900	4.822433	6.741381
C	-0.348171	3.681494	5.631797
O	0.381792	1.004036	5.683265
C	-1.288422	-1.045419	5.997676
C	-4.938158	1.892488	4.721673
H	-1.118127	-0.765945	3.109616
H	-3.700059	-0.413836	5.328199
H	-3.027264	3.691851	4.532118
H	-2.717182	3.347148	1.402802
H	-4.463488	-0.716548	2.937230
H	-3.157964	-1.829851	3.399540
H	-4.106610	-2.110410	1.931129
H	-1.070238	3.762571	3.185761
H	0.113043	2.473954	3.333756
H	-5.612181	1.047805	4.637364
H	-5.344525	2.881624	4.544392
H	-0.354143	3.614310	6.720119
H	-0.699200	4.677955	5.351192
H	0.680749	3.568232	5.291596
H	1.030910	0.198300	3.058804
H	-1.144579	-0.204864	-0.610484
H	-3.617290	5.407220	5.838590
H	3.064107	0.760076	1.784662
H	2.984514	0.880348	-0.688159
H	0.866784	0.386751	-1.866667
H	-2.473777	1.755305	7.748703
H	-3.746999	5.085182	10.103765
H	-2.929657	2.755187	9.936640
H	-4.096055	6.407033	8.039294
H	-0.927956	-1.026049	7.027274
H	-2.119191	-1.743665	5.924481
H	-0.470378	-1.383719	5.360548
H	-3.588669	3.241808	-0.492933
H	-3.216567	1.846667	-1.522950
H	-4.777218	1.938300	-0.698830

X

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scf done: -1344.459590

C	1.305157	2.781451	8.191578
C	1.289972	1.805033	7.020251
H	2.318240	3.209987	8.193773
C	0.297677	3.875501	8.003817
C	1.137118	2.058189	9.484632
C	0.162146	1.031400	6.768666
C	0.146538	0.134594	5.715815
C	1.259467	0.000434	4.898104
C	2.385991	0.766405	5.142311
C	2.400058	1.662784	6.200896
C	2.229147	1.167912	9.924406
C	-0.063310	2.163118	10.284383
N	-1.038717	3.020391	9.813652
C	-2.222988	3.199301	10.626936
C	-0.796967	3.893601	8.760881
C	0.560115	4.947336	7.002733
C	1.458207	6.146967	7.451465
C	2.895991	5.655532	7.553235
C	1.379598	7.169671	6.323175
O	3.600463	5.519905	6.568662
N	3.368558	5.313313	8.797437
C	4.697096	4.728562	8.867719
C	0.927650	6.748269	8.774603
C	1.286753	8.203748	8.990004
C	2.583427	8.613187	9.291849
C	1.342030	5.938702	9.981702
C	0.536618	5.872421	11.087592
C	2.577979	5.318968	9.935687
H	2.980820	4.787133	10.789578
O	-0.237710	1.534061	11.326486
C	2.876182	9.951905	9.485813
C	1.877480	10.908794	9.389483
C	0.583888	10.514279	9.096129
C	0.295823	9.173140	8.897416
H	-0.166228	6.710559	8.704844
H	-1.565619	4.647151	8.621892
H	2.057230	0.786797	10.929008
H	3.190420	1.695729	9.895584
H	2.334370	0.311975	9.246315
H	-0.390753	5.395423	6.695444
H	1.015357	4.526350	6.097548
H	0.838573	5.322299	11.972009
H	-0.428303	6.366805	11.103741
H	2.091791	7.984442	6.460543
H	0.374744	7.598360	6.288245
H	1.586615	6.696932	5.363233
H	3.285159	2.262719	6.394202
H	-0.712036	1.133414	7.405022
H	-0.720626	8.869318	8.665690
H	3.259167	0.668429	4.507810
H	1.246140	-0.700944	4.072154
H	-0.737829	-0.464071	5.530516
H	3.377499	7.879237	9.383876
H	2.108098	11.956013	9.546277
H	3.892100	10.249822	9.718798
H	-0.207217	11.251610	9.022043
H	5.000251	4.665131	9.909920
H	4.705523	3.726086	8.428459
H	5.408160	5.344945	8.321336

H	-2.950653	3.784666	10.068893
H	-2.660137	2.234601	10.880422
H	-1.983999	3.720912	11.559020

Product 4

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scf done: -1344.511102

C	14.089658	10.644016	8.456556
C	14.474037	10.389522	7.142001
C	15.817763	10.171331	6.876795
C	16.762168	10.213736	7.892628
C	16.370713	10.481107	9.191933
C	15.028249	10.697210	9.470003
C	13.459427	10.356865	6.016417
C	12.892421	11.772442	5.702329
C	11.715608	12.081424	6.618378
N	10.853123	11.068260	6.906289
C	10.960311	9.699085	6.401817
C	12.410826	9.298539	6.329095
C	9.723120	11.407656	7.753818
H	10.068108	11.850092	8.689862
O	11.523776	13.204976	7.056814
C	12.401145	11.938262	4.218097
C	11.082386	11.310738	3.966670
C	10.993337	9.817605	3.851671
C	10.170406	9.355062	5.069102
C	8.803895	10.055171	5.077758
N	8.769478	11.313707	4.534816
C	9.962923	11.977194	4.233256
C	13.981824	12.825119	5.873406
C	12.781647	8.054784	6.599726
C	9.916002	7.856961	5.039415
C	10.516648	9.299199	2.509451
C	11.095434	8.134757	2.010391
C	10.697300	7.592771	0.801201
C	9.706061	8.212064	0.057785
C	9.130442	9.378120	0.532803
C	9.533299	9.917994	1.744155
C	7.533453	12.066147	4.492765
H	7.279836	12.323704	3.461917
O	7.811057	9.519183	5.529708
H	10.485195	9.074844	7.164365
H	9.155691	10.505552	7.973376
H	9.060377	12.131248	7.269619
H	9.940677	13.053501	4.385642
H	11.993739	9.393471	3.981053
H	14.005294	10.040285	5.117888
H	12.327428	13.014485	4.037595
H	13.187046	11.544273	3.564270
H	7.635597	12.990511	5.067867
H	6.736879	11.464153	4.920441
H	16.130338	9.967653	5.856912
H	11.877493	7.646198	2.584151
H	9.081810	10.843155	2.082396
H	13.041147	10.802926	8.693703
H	10.852391	7.307760	4.936752
H	9.279230	7.595109	4.193957
H	9.414552	7.528975	5.950487
H	13.609703	13.807222	5.585543
H	14.829028	12.574475	5.228552
H	14.345129	12.892379	6.898068
H	11.167823	6.687147	0.435986

H	14.711196	10.903298	10.485865
H	17.806840	10.037094	7.663322
H	12.069157	7.290467	6.885370
H	13.825456	7.760658	6.564376
H	9.390891	7.793878	-0.890999
H	8.362505	9.879205	-0.045367
H	17.105451	10.517724	9.987599

Comprehensive Table in Atomic Unit

Part I. Substrate activations and photocatalysts

M06/Def2-TZVP, CPCM = dmf	H (Hartrees)	S (cal/K*mol)
Reagent **1**	-632.667649	125.921
^{3}**1** alpha	-632.589801	126.412
^{3}**1** beta	-632.601477	126.235
1 iso	-632.668363	126.351
^{3}**1**iso alpha	-632.591991	128.063
^{3}**1**iso beta	-632.602878	125.832
Reagent **3**	-671.930842	128.888
^{3}**3** alpha	-671.859936	130.165
^{3}**3** beta	-671.864472	133.721
3 iso	-671.931735	128.662
^{3}**3**iso alpha	-671.857104	134.505
^{3}**3**iso beta	-671.864605	130.497
Reagent **3l**	-441.059570	106.502
^{3}**3l** alpha	-440.967842	107.892
^{3}**3l** beta	-440.992467	107.672
^{1}Ir(III)ppy$_2$bpy $^{+}$	-1556.158575	188.462
^{3}Ir(III)ppy$_2$bpy $^{+}$	-1556.078310	193.662
^{2}Ir(II)ppy$_2$bpy	-1556.273358	192.329
^{2}Ir(IV)ppy$_2$bpy $^{++}$	-1555.946098	190.783
^{1}Ir(III)ppy$_3$	-1539.635775	191.664
^{3}Ir(III)ppy$_3$	-1539.545823	196.190
^{2}Ir(II)ppy$_3$ $^{-}$	-1539.713463	194.086
^{2}Ir(IV)ppy$_3$ $^{+}$	-1539.443413	192.542
^{2}**1** $^{-}$	-632.763854	123.841
^{2}**1** $^{+}$	-632.451506	126.899

Part II. Cascades of 1 and 3

M06 def2-TZVP CPCM =dmf	H (Hartrees)	S (kcal/K*mol)	imaginary frequency (cm-1)
Reagent **1**	-632.667649	125.921	
Iα	-632.589801	126.412	
TS$_{5\text{-}endo}$	-632.578219	121.362	-578.5805
Iβ	-632.601477	126.235	
TS $_{rot}$	-632.589881	125.073	-139.6421
I $_{rot}$	-632.600386	123.607	
TS (Irot-II)	-632.599432	120.319	-251.6237
II	-632.658893	119.200	
II_1	-1265.337079	195.744	
TS (II_1-IV)	-1265.314034	190.510	-574.8447
IV	-1265.333908	191.041	
TS (IV-V)	-1265.318438	184.344	-605.2125
V	-1265.399105	184.441	
TS (V_1,7)	-1265.361893	174.282	-1775.2805
V 1,7	-1265.399388	182.461	
V 1,7$_{rot}$	-1265.400327	183.102	
TS (V-1,5)	-1265.364662	177.478	-1606.7717
VI	-1265.403408	181.825	
TS (VI-VII)	-1265.361129	181.694	-641.4471
VII	-1265.396496	188.583	
TS (VII-VIII)	-1265.356803	174.606	-1778.0965
VIII	-1265.415290	179.656	
Product **2**	-1265.492364	173.032	
Reagent **3**	-671.930842	128.888	
Iβ_{Me}	-671.864472	133.721	
TS $_{rot\ Me}$	-671.851669	129.917	-98.6443
I $_{rot\ Me}$	-671.864117	131.336	
TS$_{5\text{-}exo}$	-671.861066	126.986	-248.9556
III$_{5\text{-}exo}$	-671.922333	125.249	
TS (I rot Me -III)	-671.864195	125.924	-248.4242
III	-671.928127	123.684	
III_3	-1343.869944	210.651	
TS (III_3-IX$_{iso}$**)**	-1343.829719	196.671	-580.3611
IX$_{iso}$	-1343.858348	199.352	
TS (III_3-IX)	-1343.842782	196.236	-550.1971
IX	-1343.874503	191.154	
TS (IX-X)	-1343.870492	191.857	-464.5808
X	-1343.943827	191.055	
Product **4**	-1343.988870	177.144	

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