Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Chiral Guanidine Catalyzed Cyclization Reactions of 1,3-Enynes for Lactone Synthesis: Switchable H-Bond Catalysis

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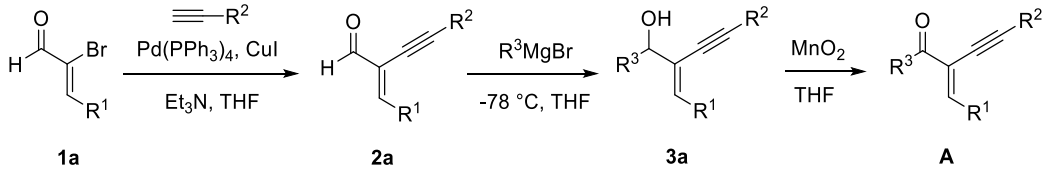
1. General Information

NMR characterization data were collected on bruker ASCENDTM operating at 400 MHz for ^{1}H NMR, 101 MHz for ^{13}C NMR (with complete proton decoupling), and 376 MHz for ^{19}F NMR (with complete proton decoupling). ^{1}H NMR and ^{13}C NMR: chemical shifts δ were recorded in ppm relative to tetramethylsilane and internally referenced to the residual solvent signal (for ^{1}H NMR: $CDCl_3$ = 7.26 ppm, $(CD_3)_2CO$ = 2.05 ppm; for ^{13}C NMR: $CDCl_3$ = 77.16 ppm, $(CD_3)_2CO$ = 30.92 ppm). Data were reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, td = triplet of doublets, dt = doublet of triplets, ddd = doublet of doublet of doublets, m = multiplet), coupling constants (Hz), integration. High performance liquid chromatography (HPLC) was performed on Alliance e2695 using Daicel Chiralcel IA, IC, AD-3 at 25 °C with UV detector at 254 nm, supercritical fluid chromatography (SFC) was performed on Acquity UPC^2 with Chiralcel IA-3, IC-3 at 35 °C at 254 nm, enantiomeric ratio (er) were determined in comparison with the authentic racemates by HPLC or SFC. High resolution mass spectra (HRMS) were performed on Thermo Q-Exactive Focus (FTMS+c ESI) and data were reported as (m/z). Infrared spectra (IR) were recorded on Bruker Tensor II spectrometer with Plantium ATR accessory and the peaks are reported as absorption maxima (ν, cm^{-1}). Optical rotations were measured on Rudolph Research Analytic Automatic Polarimeter, and reported as follows: $[\alpha]^{T}_{D}$ (*c*: g/100 mL, in CH_2Cl_2). Melting point ranges were determined on OptiMelt. X-ray crystallographic data were collected by a Bruker D8 Venture Photon II.

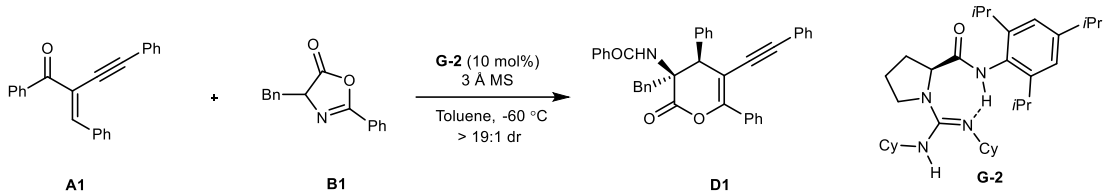
The experiments requiring chiral guanidines,[1] enynes[2] and azlactones[3] were synthesized according to known procedures and purified by recrystallization prior to use. All reactions were performed in sealed oven-dried glass tubes under an atmosphere of nitrogen unless otherwise noted. All of the starting materials were purchased from TCI, Aladdin, Adamas, Acros, Aldrich and other companies, and used without further purification. All the solvents including toluene, tetrahydrofuran, diethyl ether, dichloromethane, chloroform, 1,2-dichloroethane, ethyl acetate, acetonitrile and so on were pre-dried over appropriate desiccants, and distilled prior to use. Reactions were monitored using thin-layer chromatography (TLC) on GF254 silica gel. Visualization of the developed plates was performed under UV light (254 nm) or using iodine, cobalt thiocyanate or $KMnO_4$. The products were purified by flash column chromatography with silicycle 300-400 mesh silica gel.

2. Substrates synthesis

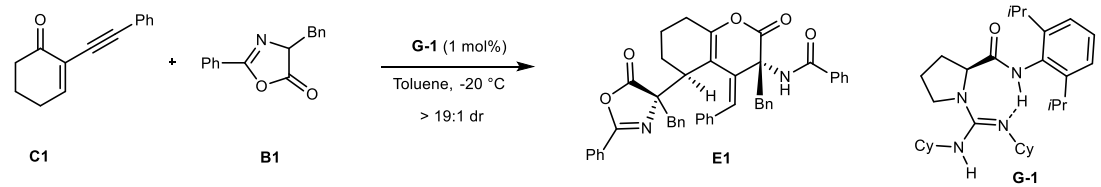


General procedure: **2a** was prepared from **1a** by following a procedure from the literature.[4] To a solution of **2a** (10 mmol) in dry THF (30 mL) cooled to –78 °C was added R^3MgBr (1 M in THF, 12.5 mmol) under nitrogen atmosphere. The reaction was stirred at the same temperature for 1 hour and then stirred overnight at room temperature. Next, quenched with saturated NH_4Cl. The resulting mixture was extracted with EtOAc. The organic layer was washed with brine, dried over anhydrous $MgSO_4$, filtered and concentrated under reduced pressure. The residue was dissolved in dry THF (80 mL). To this solution was added MnO_2 (20 equiv.), followed by stirring at room temperature for 12 h. The reaction mixture was filtered through a short pad of celite, which was rinsed with EtOAc. The combined organic layer was concentrated under reduced pressure, and the residue was purified by flash column chromatography.

3. Typical procedure for the preparation of δ-lactones

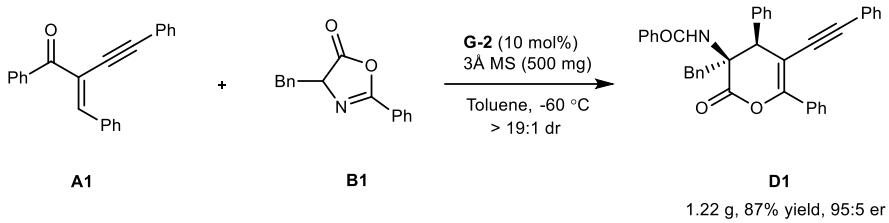


A dry reaction tube was charged with **G-2** (5.2 mg, 10 mol%), 3 Å MS (20 mg), enyne **A1** (30.8 mg, 0.1 mmol) and azlactone **B1** (25.1 mg, 0.1 mmol) under N_2 atmosphere. Then toluene (1.0 mL) was added at -60 ºC and the mixture was stirred for 12 h. The reaction mixture was purified by silica gel column chromatographic (ethyl acetate/acetone/petroleum ether 1/5/50) to afford the desired product **D1**. The white solid **D1** was obtained in 89% yield (49.8 mg). The enantiomeric ratio (er) and diastereoisomeric ratio (dr) were determined by UPC^2 with Daicel chiralcel IC-3 (95:5 er, >19:1 dr).

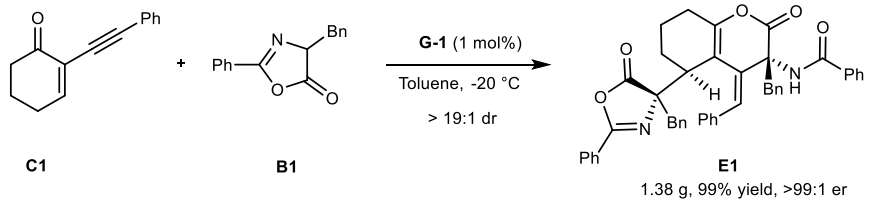


A dry reaction tube was charged with **G-1** (0.5 mg, 1 mol%), enyne **C1** (19.6 mg, 0.1 mmol) and azlactone **B1** (50.2 mg, 0.2 mmol) under N_2 atmosphere. Then toluene (1.0 mL) was added at -20 ºC and the mixture was stirred for 15 h. The reaction mixture was purified by silica gel column chromatographic (ethyl acetate/petroleum ether 1/6) to afford the desired product **E1**. The pale yellow solid **E1** was obtained in 99% yield (69.2 mg). The enantiomeric ratio (er) and diastereoisomeric ratio (dr) were determined by HPLC with Daicel chiralcel IC (>99:1 er, >19:1 dr).

4. Experimental procedure for the scale-up reaction



A dry 100 mL round-bottom flask was charged with **G-2** (130 mg, 10 mol%), 3 Å MS (500 mg), enyne **A1** (770 mg, 2.5 mmol) and azlactone **B1** (628 mg, 2.5 mmol) under N_2 atmosphere. Then toluene (25 mL) was added at -60 ºC and the mixture was stirred for 24 h. The reaction mixture was concentrated under reduced pressure and then was purified by silica gel column chromatographic (ethyl acetate/acetone/petroleum ether 1/5/50) to afford the desired product. The white solid **D1** was obtained. The enantiomeric ratio (er) and diastereoisomeric ratio (dr) were determined by UPC^2 with Daicel chiralcel IC-3.

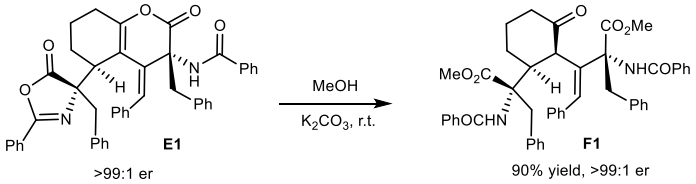


A dry 100 mL round-bottom flask was charged with **G-1** (9.6 mg, 1 mol%), enyne **C1** (392 mg, 2 mmol) and azlactone **B1** (1004 mg, 4 mmol) under N_2 atmosphere. Then toluene (20 mL) was added at -20 ºC and the mixture

was stirred for 36 h. The reaction mixture was concentrated under reduced pressure and then was purified by silica gel column chromatographic (ethyl acetate/petroleum ether 1/6) to afford the desired product. The pale yellow solid **E1** was obtained. The enantiomeric ratio (er) and diastereoisomeric ratio (dr) were determined by HPLC with Daicel chiralcel IC.

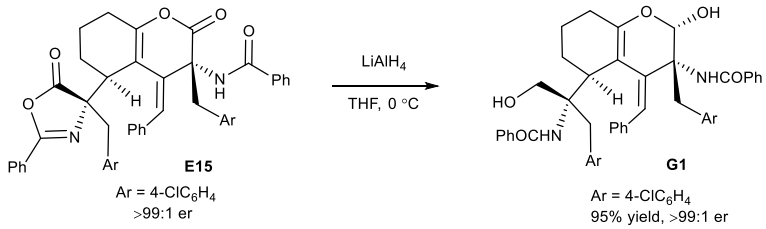
5. Experimental procedure for further transformations of the products

Procedure 1 The ring opening of the compound **E1**



Under N_2, 4 mL methanol was added to a mixture of **E1** (140 mg, 0.2 mmol) and K_2CO_3 (14.0 mg, 0.1 mmol). It become a clear solution after stirred at room temperature for 60 min. The reaction mixture was concentrated under reduced pressure and then was purified by silica gel column chromatographic (ethyl acetate/petroleum ether 1/3) to afford the desired product. The white solid **F1** was obtained. The enantiomeric ratio (er) and diastereoisomeric ratio (dr) were determined by UPC^2 with Daicel chiralcel AD-3.

Procedure 2 The reduction of the compound **E15**

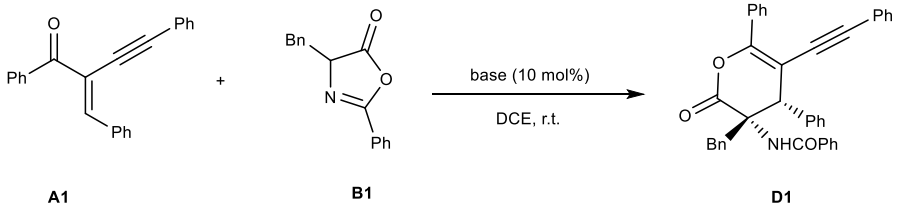


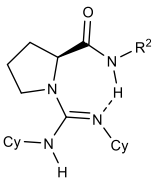
2 mL THF was added to a tube charged with **E15** (153.4 mg, 0.2 mmol). Then $LiAlH_4$ (45.6 mg, 1.2 mmol) was added under 0 ºC. The mixture was stirring at 0 ºC for 10 min. After the reaction was completed, saturated NH_4Cl solution was added, washing aqueous phase with EtOAc three times, separating and concentrating organic phase, the crude product was purified by silica gel column chromatographic (ethyl acetate/petroleum ether 1/3) to afford the desired product. The white solid **G1** was obtained. The enantiomeric ratio (er) and diastereoisomeric ratio (dr) were determined by UPC^2 with Daicel chiralcel IA-3.

6. Optimazition of the reaction conditions

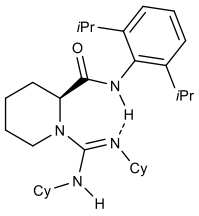
Evaluation of the reaction of acyclicenyne

Table S1 Evaluation of chiral guanidines

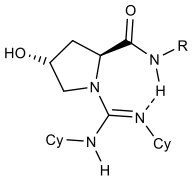




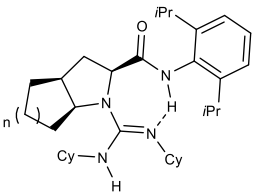
G-1 R^2 = 2,6-*i*$Pr_2C_6H_3$
G-2 R^2 = 2,4,6-*i*$Pr_3C_6H_2$
G-3 R^2 = 2,6-*i*Pr_2-4-(1-Ad)C_6H_2



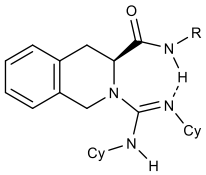
G-4



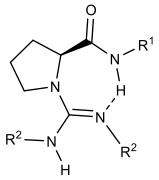
G-5 R = 2,6-*i*$Pr_2C_6H_3$



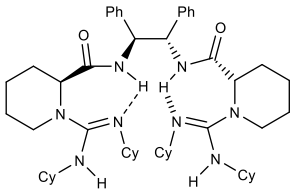
G-6 n = 1
G-7 n = 2



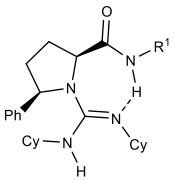
G-8 R = 2,6-*i*$Pr_2C_6H_3$



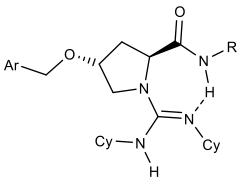
G-9 R^1 = $CHPh_2$, R^2 = Cy
G-10 R^1 = 2,6-*i*$Pr_2C_6H_3$, R^2 = *i*Pr
G-11 R^1 = 2,6-*i*$Pr_2C_6H_3$, R^2 = Ph
G-12 R^1 = 2,6-$Me_2C_6H_3$, R^2 = Cy



G-13



G-14 R^1 = 2,6-*i*$Pr_2C_6H_3$

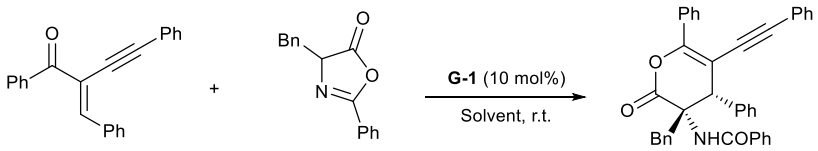


G-15 R = 2,4,6-*i*$Pr_3C_6H_2$, Ar = C_6H_5
G-16 R = 2,4,6-*i*$Pr_3C_6H_2$, Ar = 3, 5-$Br_2C_6H_3$

entry[a]	base	yield (%)[b]	er	dr
1	K_2CO_3	NR	-	-
2	**G-1**	79	71:29	>19:1
3	**G-2**	75	70:30	>19:1
4	**G-3**	75	71:29	>19:1
5	**G-4**	65	62:38	>19:1
6	**G-5**	50	54:46	>19:1
7	**G-6**	58	58:42	>19:1
8	**G-7**	69	59:41	>19:1
9	**G-8**	80	62:38	>19:1
10	**G-9**	50	53:47	>19:1
11	**G-10**	81	67:33	>19:1
12	**G-11**	68	68:32	>19:1
13	**G-12**	55	54:46	>19:1
14	**G-13**	38	59:41	>19:1
15	**G-14**	46	55:45	>19:1

[a]Unless otherwise noted, all reactions were carried out with base (10 mol%), **A1** (0.1 mmol), **B1** (0.1 mmol) in DCE (1.0 mL) at r.t. for 12 h. [b]Isolated yield. The er and dr were determined by UPC[2] analysis on a chiral stationary phase.

Table S2 Evaluation of solvents

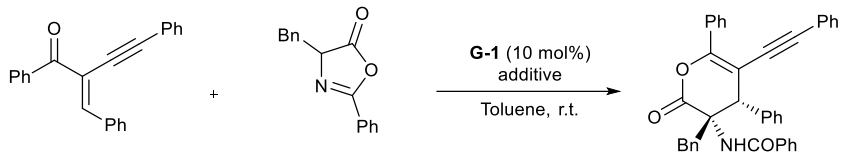


A1 **B1** **D1**

entry[a]	solvent	yield (%)[b]	er	dr
1	THF	49	50:50	>19:1
2	Toluene	68	73:27	>19:1
3	Et_2O	44	50:50	>19:1
4	DCE	79	71:29	>19:1
5	DCM	53	56:44	>19:1
6	EtOAc	49	52:48	>19:1

[a]Unless otherwise noted, all reactions were carried out with **G-1** (10 mol%), **A1** (0.1 mmol), **B1** (0.1 mmol) in solvent (1.0 mL) at r.t. for 12 h. [b]Isolated yield. The er and dr were determined by UPC[2] analysis on a chiral stationary phase.

Table S3 Evaluation of additive

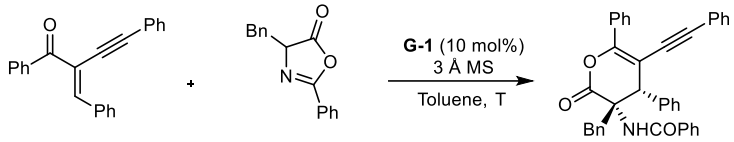


A1 B1 D1

entry[a]	additive	yield (%)[b]	er	dr
1	-	68	73:27	>19:1
2	3 Å MS	78	73:27	>19:1
3	4 Å MS	65	61:39	>19:1
4	5 Å MS	79	64:36	>19:1
5	Na_2SO_4	78	56:44	>19:1

[a]Unless otherwise noted, all reactions were carried out with **G-1** (10 mol%), **A1** (0.1 mmol), additive (20 mg), **B1** (0.1 mmol) in toluene (1.0 mL) at r.t. for 12 h. [b]Isolated yield. The er and dr were determined by UPC[2] analysis on a chiral stationary phase.

Table S4 Evaluation of temperature

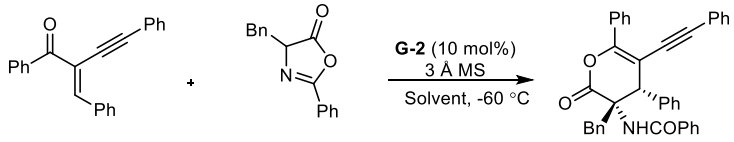


A1 B1 D1

entry[a]	T	yield (%)[b]	er	dr
1	r.t.	78	73:27	>19:1
2	0 °C	86	79:21	>19:1
3	-20 °C	82	86:14	>19:1
4	-40 °C	83	89:11	>19:1
5	-60 °C	84	92:8	>19:1
6	-78 °C	79	89:11	>19:1
7[c]	-60 °C	89	95:5	>19:1
8[d]	-60 °C	81	91:9	>19:1

[a]Unless otherwise noted, all reactions were carried out with **G-1** (10 mol%), **A1** (0.1 mmol), 3 Å MS (20 mg), **B1** (0.1 mmol) in toluene (1.0 mL) at T °C for 12 h. [b]Isolated yield. The er and dr were determined by UPC[2] analysis on a chiral stationary phase. [c]use **G-2**. [d]use **G-3**.

Table S5 Supplementary evaluation of benzene solvents

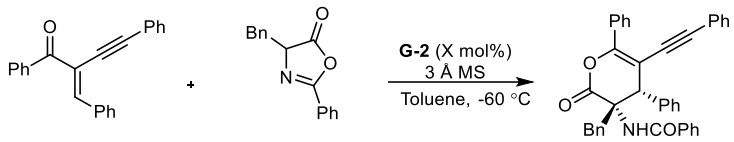


A1 B1 D1

entry[a]	solvent	yield (%)[b]	er	dr
1	Toluene	89	95:5	>19:1
2	Fluorobenzene	73	78:22	>19:1
3	Chlorobenzene	64	83:17	>19:1
4	Bromobenzene	88	82:18	>19:1
5	*o*-Xylene	63	84:16	>19:1
6	*m*-Xylene	72	87:13	>19:1
7	*p*-Xylene	54	78:22	>19:1
8	Trimethylbenzene	77	91:9	>19:1

[a]Unless otherwise noted, all reactions were carried out with **G-2** (10 mol%), **A1** (0.1 mmol), 3Å MS (20 mg), **B1** (0.1 mmol) in benzene solvent (1.0 mL) at -60 °C for 12 h. [b]Isolated yield. The er and dr were determined by UPC[2] analysis on a chiral stationary phase.

Table S6 Evaluation of the amount of guanidine



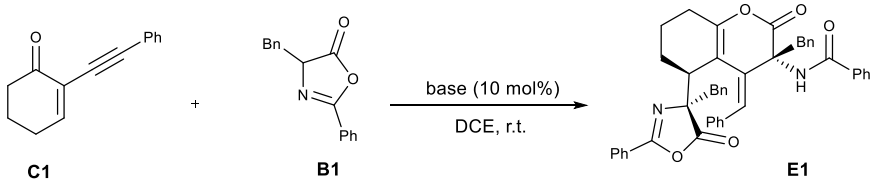
A1 B1 D1

entry[a]	X	yield (%)[b]	er	dr
1	10	89	95:5	>19:1
2	5	78	95:5	>19:1
3	2.5	Trace	-	-
4	1	NR	-	-

[a]Unless otherwise noted, all reactions were carried out with **G-2** (X mol%), **A1** (0.1 mmol), 3Å MS (20 mg), **B1** (0.1 mmol) in toluene (1.0 mL) at -60 °C for 12 h. [b]Isolated yield. The er and dr were determined by UPC^2 analysis on a chiral stationary phase.

Evaluation of the reaction of cyclicenyne

Table S7 Evaluation of chiral guanidines

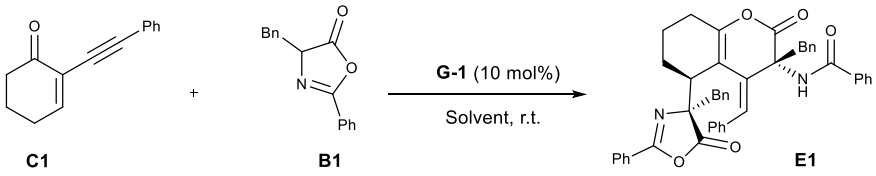


C1 B1 E1

entry[a]	base	yield (%)[b]	er	dr
1	K_2CO_3	NR	-	-
2	**G-1**	99	89:11	>19:1
3	**G-2**	99	87:13	>19:1
4	**G-3**	99	87:13	>19:1
5	**G-4**	77	75:25	>19:1
6	**G-5**	99	53:47	>19:1
7	**G-6**	94	88:12	>19:1
8	**G-7**	99	87:13	>19:1
9	**G-8**	80	79:21	>19:1

[a]Unless otherwise noted, all reactions were carried out with base (10 mol%), **C1** (0.1 mmol), **B1** (0.2 mmol) in DCE (1.0 mL) at r.t. for 15 h. [b]Isolated yield. The er and dr were determined by HPLC analysis on a chiral stationary phase.

Table S8 Evaluation of solvents

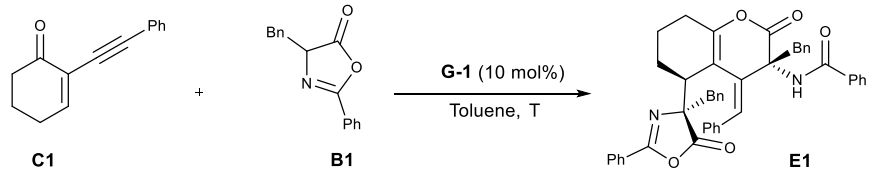


C1 B1 E1

entry[a]	solvent	yield (%)[b]	er	dr
1	THF	99	88:12	>19:1
2	Toluene	99	91:9	>19:1
3	Et_2O	99	89:11	>19:1
4	DCE	99	89:11	>19:1
5	DCM	99	87:13	>19:1
6	EtOAc	90	91:9	>19:1

[a]Unless otherwise noted, all reactions were carried out with **G-1** (10 mol%), **C1** (0.1 mmol), **B1** (0.2 mmol) in solvent (1.0 mL) at r.t. for 15 h. [b]Isolated yield. The er and dr were determined by HPLC analysis on a chiral stationary phase.

Table S9 Evaluation of temperature



C1 B1 E1

entry[a]	T	yield (%)[b]	er	dr
1	r.t.	99	91:9	>19:1
2	0 °C	99	95:5	>19:1
3	-20 °C	99	>99:1	>19:1
4	-40 °C	90	>99:1	>19:1
5	-60 °C	88	99:1	>19:1
6	-78 °C	82	98:2	>19:1

[a]Unless otherwise noted, all reactions were carried out with **G-1** (10 mol%), **C1** (0.1 mmol), **B1** (0.2 mmol) in toluene (1.0 mL) at T °C for 15 h. [b]Isolated yield. The er and dr were determined by HPLC analysis on a chiral stationary phase.

Table S10 Evaluation of the amount of guanidine

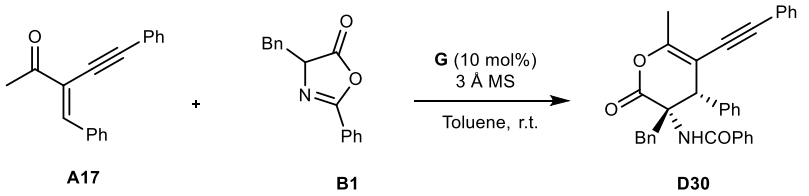
C1 B1 E1

entry[a]	X	yield (%)[b]	er	dr
1	10	99	>99:1	>19:1
2	5	99	>99:1	>19:1
3	2.5	99	>99:1	>19:1
4	1	99	>99:1	>19:1
5	0.5	trace	-	-
6[c]	0.5	76	>99:1	>19:1

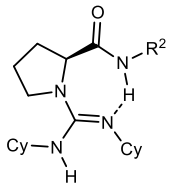
[a]Unless otherwise noted, all reactions were carried out with **G-1** (X mol%), **C1** (0.1 mmol), **B1** (0.2 mmol) in toluene (1.0 mL) at -20 °C for 15 h. [b]Isolated yield. The er and dr were determined by HPLC analysis on a chiral stationary phase. [c]**B1** (0.25 mmol).

Evaluation of the reaction of acetyl substituted 1,3-enyne

Table S11 Evaluation of chiral guanidines



A17 B1 D30



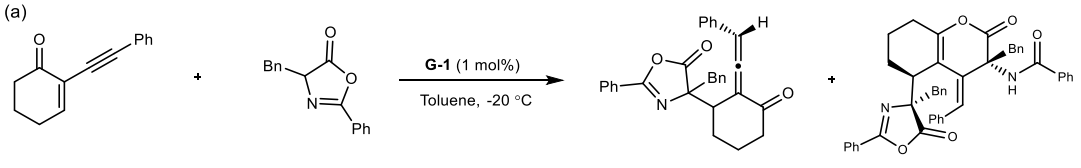
G-17 R^2 = 2,4,6-$Me_3C_6H_2$
G-18 R^2 = Bn
G-19 R^2 = Ts
G-20 R^2 = Ad
G-21 R^2 = CPh_3

entry[a]	G	yield (%)[b]	er	dr
1[c]	**G-2**	25	83:17	>19:1
2	**G-2**	73	74:26	>19:1
3	**G-1**	77	73:27	>19:1
4	**G-3**	64	70:30	>19:1
5	**G-17**	49	53:47	>19:1
6	**G-18**	48	0	>19:1
7	**G-19**	31	0	>19:1
8	**G-20**	64	0	>19:1
9	**G-9**	72	53:47	>19:1
10	**G-21**	65	59:41	>19:1

[a]Unless otherwise noted, all reactions were carried out with **G** (10 mol%), **A17** (0.1 mmol), **B1** (0.1 mmol) in toluene (1.0 mL) at r.t. for 12 h. [b]Isolated yield. The er and dr were determined by UPC^2 analysis on a chiral stationary phase. [c]at 0 °C.

7. Control experiments

(a)



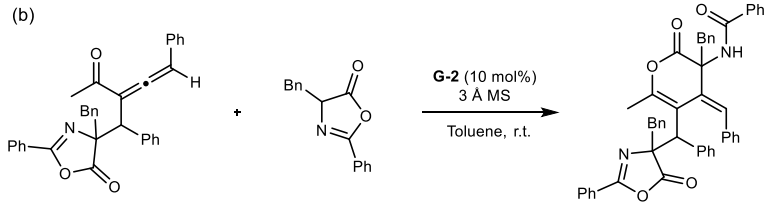
C1 0.1 mmol + **B1** X mmol → **Int1** Not Detected + **E1**

entry[a]	X	yield (%)[b]	er	dr
1	0.10	42	>99:1	>19:1
2	0.15	70	>99:1	>19:1
3	0.20	99	>99:1	>19:1
4	0.25	99	99:1	>19:1

[a]Unless otherwise noted, all reactions were carried out with **G-1** (1 mol%), **C1** (0.1 mmol), **B1** (X mmol) in toluene (1.0 mL) at -20 °C for 15 h. [b]Isolated yield. The er and dr were determined by HPLC analysis on a chiral stationary phase.

A dry reaction tube was charged with **G-1** (0.5 mg, 1 mol%), enyne **C1** (19.6 mg, 0.1 mmol) and azlactone **B1** (X mmol) under N_2 atmosphere. Then toluene (1.0 mL) was added at -20 °C and the mixture was stirred for 15 h. The generation of **Int1** was not monitored in the reaction.

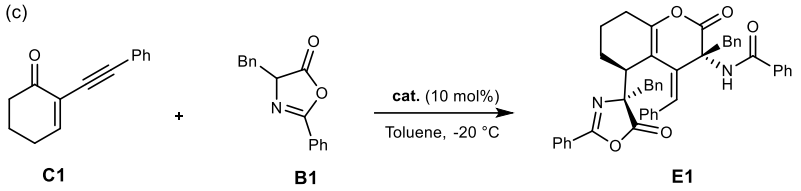
(b)



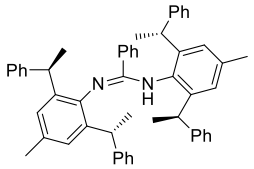
(±) **1a** 0.1 mmol + **B1** 0.1 mmol → **2a** Not Detected

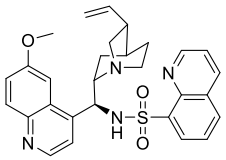
A dry reaction tube was charged with **G-2** (5.2 mg, 10 mol%), (±) **1a** (49.7 mg, 0.1 mmol), azlactone **B1** (25.1 mg, 0.1 mmol) and 3Å MS (20 mg) under N_2 atmosphere. Then toluene (1.0 mL) was added at r.t. and **B1** was consumed in 1.5 hours to form dimer byproduct, but the generation of **2a** was not monitored in the reaction.

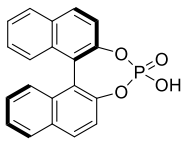
(c)

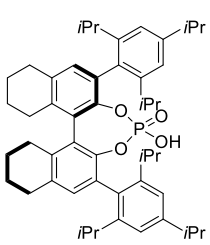


C1 + **B1** → **E1**


NR


NR


NR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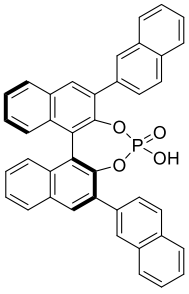
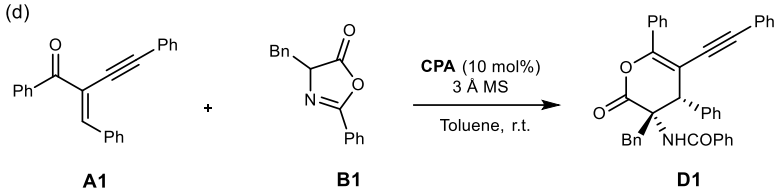
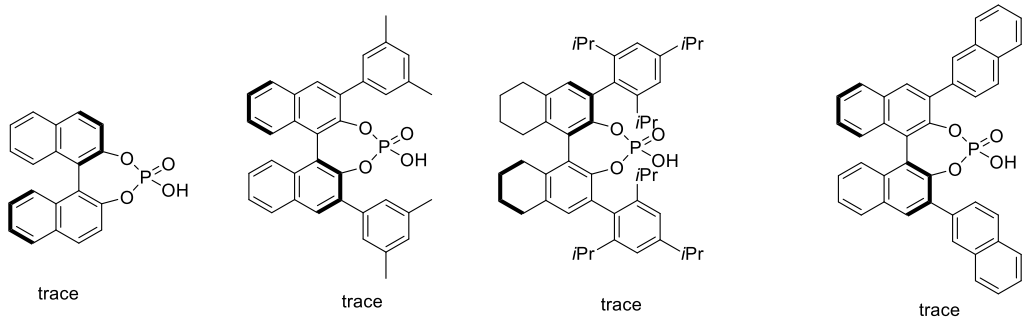

NR

A dry reaction tube was charged with **cat.** (10 mol%), enyne **C1** (19.6 mg, 0.1 mmol) and azlactone **B1** (50.2 mg, 0.2 mmol) under N_2 atmosphere. Then toluene (1.0 mL) was added at -20 °C and the mixture was stirred for 14 h. The generation of **E1** was not monitored with **C1** and **B1** maintaining in the system.

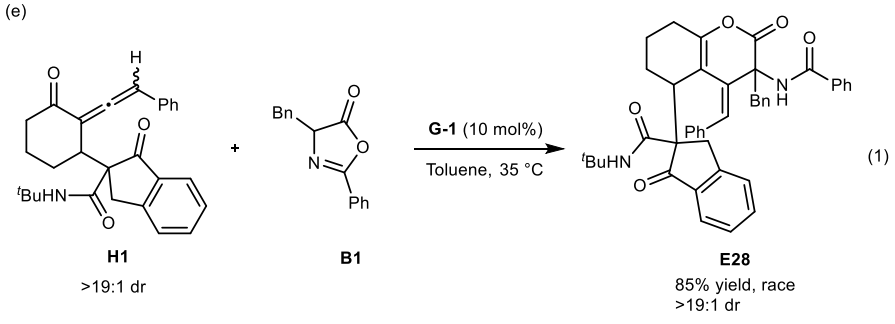
(d)

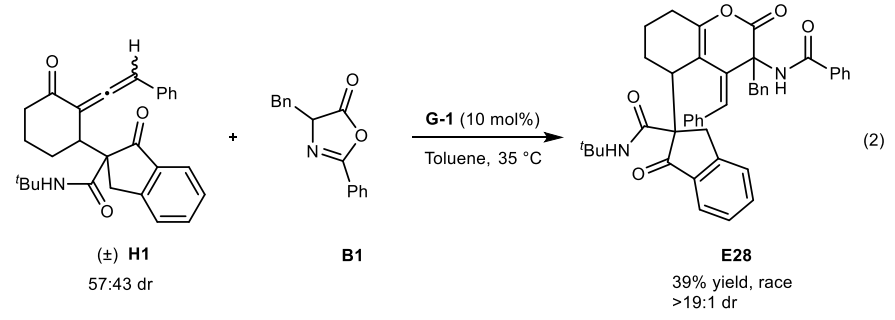


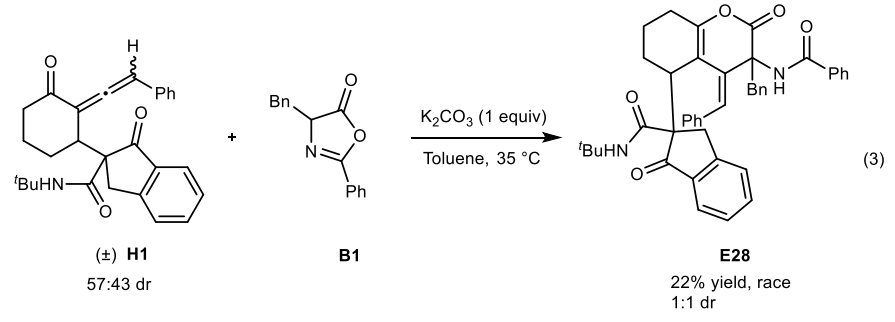


A dry reaction tube was charged with **CPA** (10 mol%), enyne **A1** (30.8 mg, 0.1 mmol), azlactone **B1** (25.1 mg, 0.1 mmol) and 3Å MS (20 mg) under N_2 atmosphere. Then toluene (1.0 mL) was added at r.t. and the mixture was stirred for 12 h. Only trace amounts of **D1** were obtained.

(e)

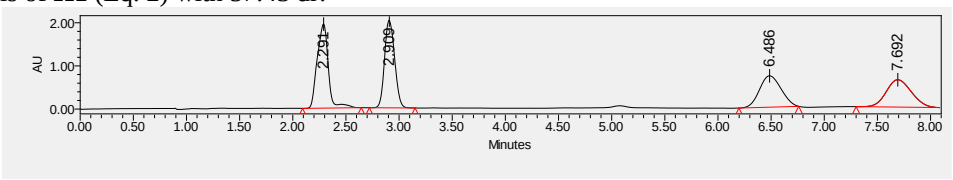






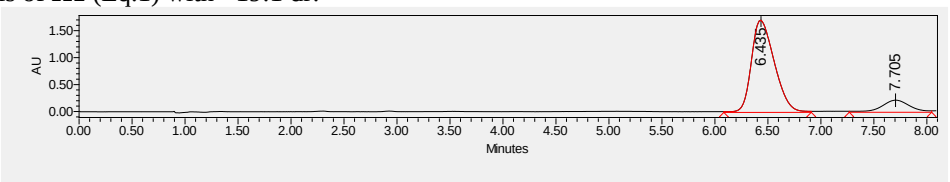
A dry reaction tube was charged with base, trisubstituted allenone **H1** (42.7 mg, 0.1 mmol) and azlactone **B1** (50.2 mg, 0.2 mmol) under N_2 atmosphere. Then toluene (1.0 mL) was added at 35 °C and the mixture was stirred for 12 h, the [4+2] reaction occurred as expected. The dr was determined by UPCC analysis on a chiral stationary phase.

The UPCC analysis of **H1** (Eq. 2) with 57:43 dr:



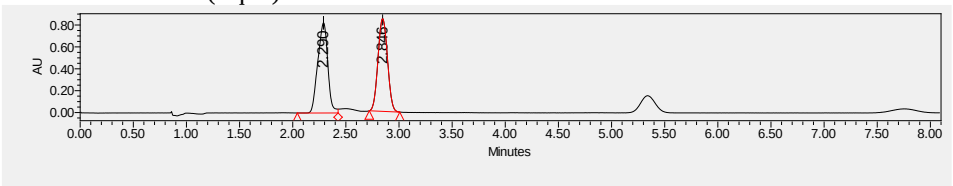
	Retention Time	Area	% Area
1	2.291	14051496	29.21
2	2.909	13352457	27.76
3	6.486	10292433	21.40
4	7.692	10402125	21.63

The UPCC analysis of **H1** (Eq.1) with >19:1 dr:

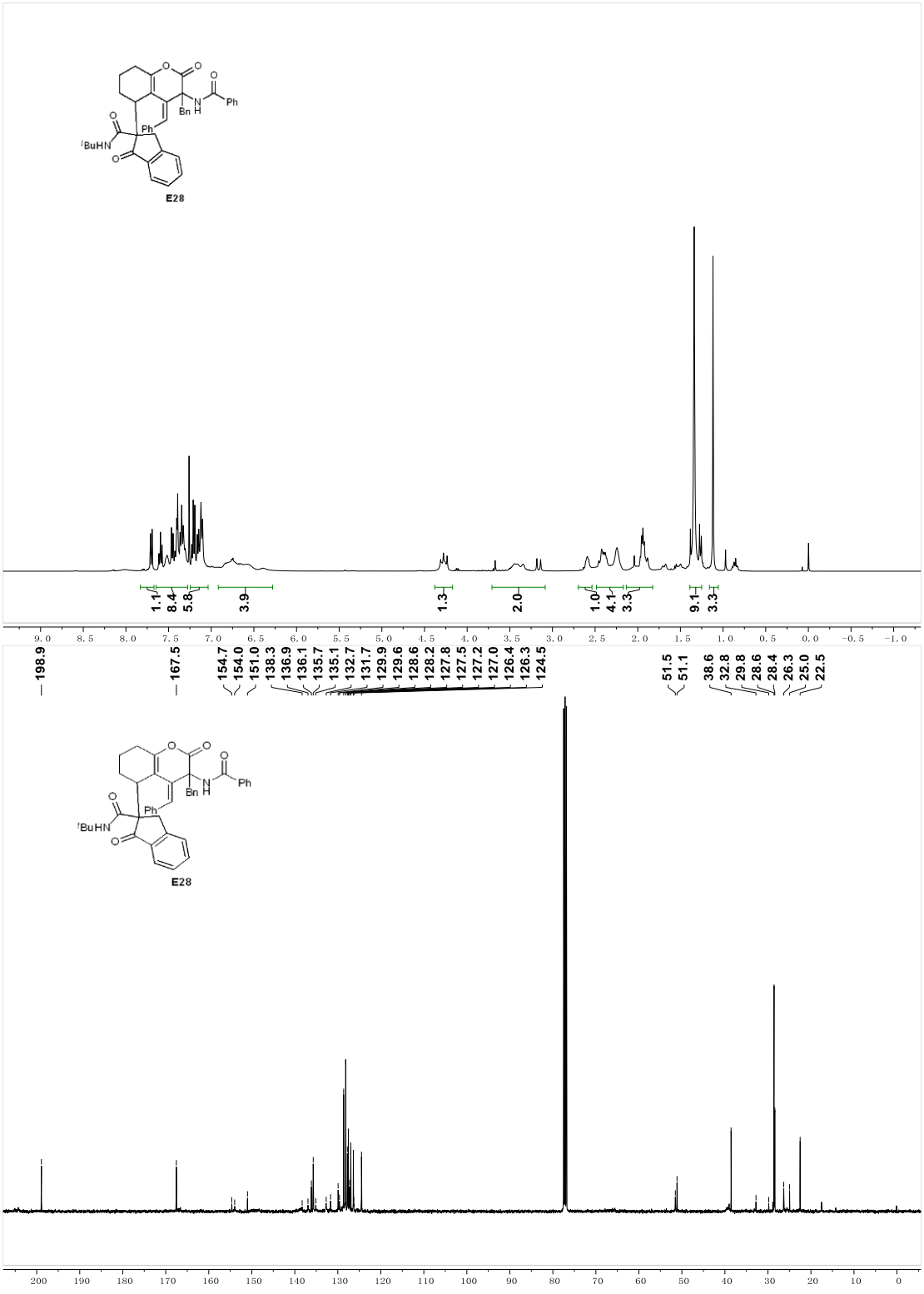


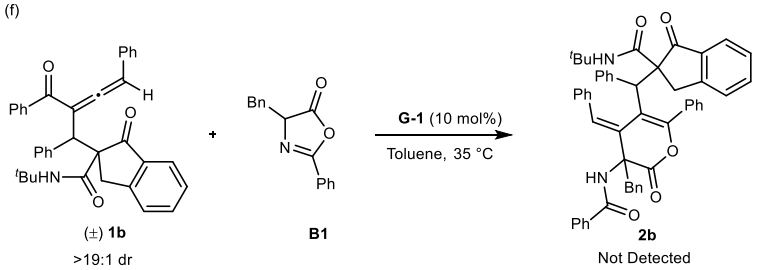
	Retention Time	Area	% Area
1	6.435	25759351	85.89
2	7.705	4230093	14.11

The UPCC analysis of recovered **H1** (Eq. 2) with >19:1 dr:

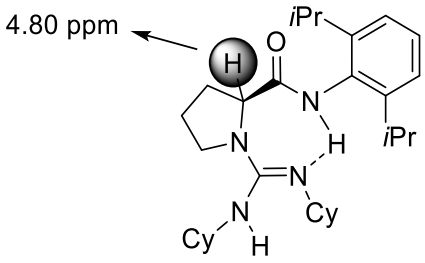


	Retention Time	Area	% Area
1	2.290	5390383	50.59
2	2.846	5265618	49.41

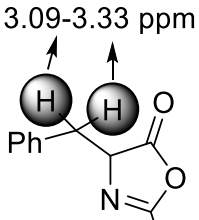




A dry reaction tube was charged with **G-1** (4.8 mg, 10 mol%), trisubstituted allenone (±) **1b** (53.9 mg, 0.1 mmol) and azlactone **B1** (50.2 mg, 0.2 mmol) under N_2 atmosphere. Then toluene (1.0 mL) was added at 35 °C and the mixture was stirred for 4 h, **B1** was consumed to form dimer byproduct, but the generation of **2b** was not monitored in the reaction.



G-1



B1

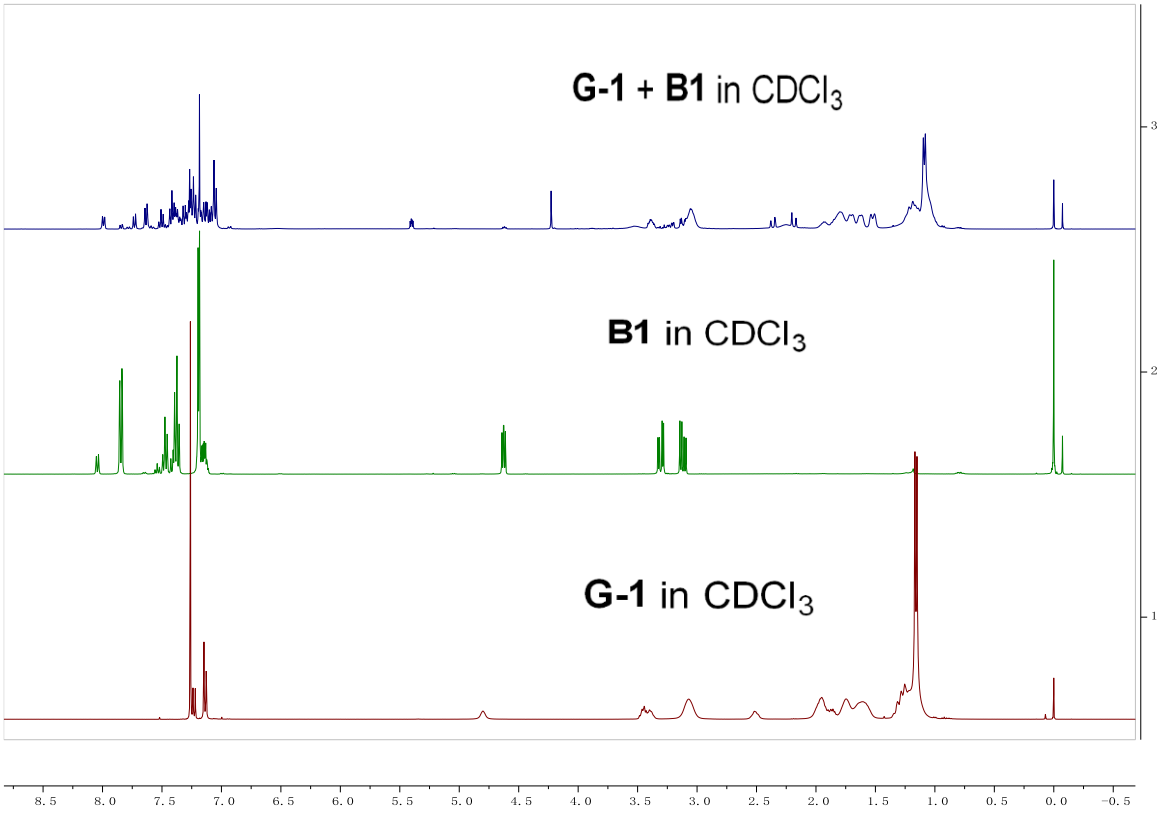
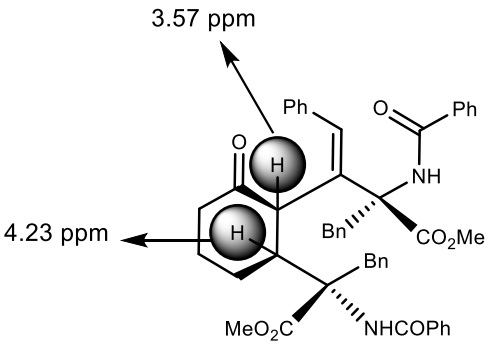


Figure S1 1H NMR of **G-1**, **B1**, **G-1** + **B1**



F1

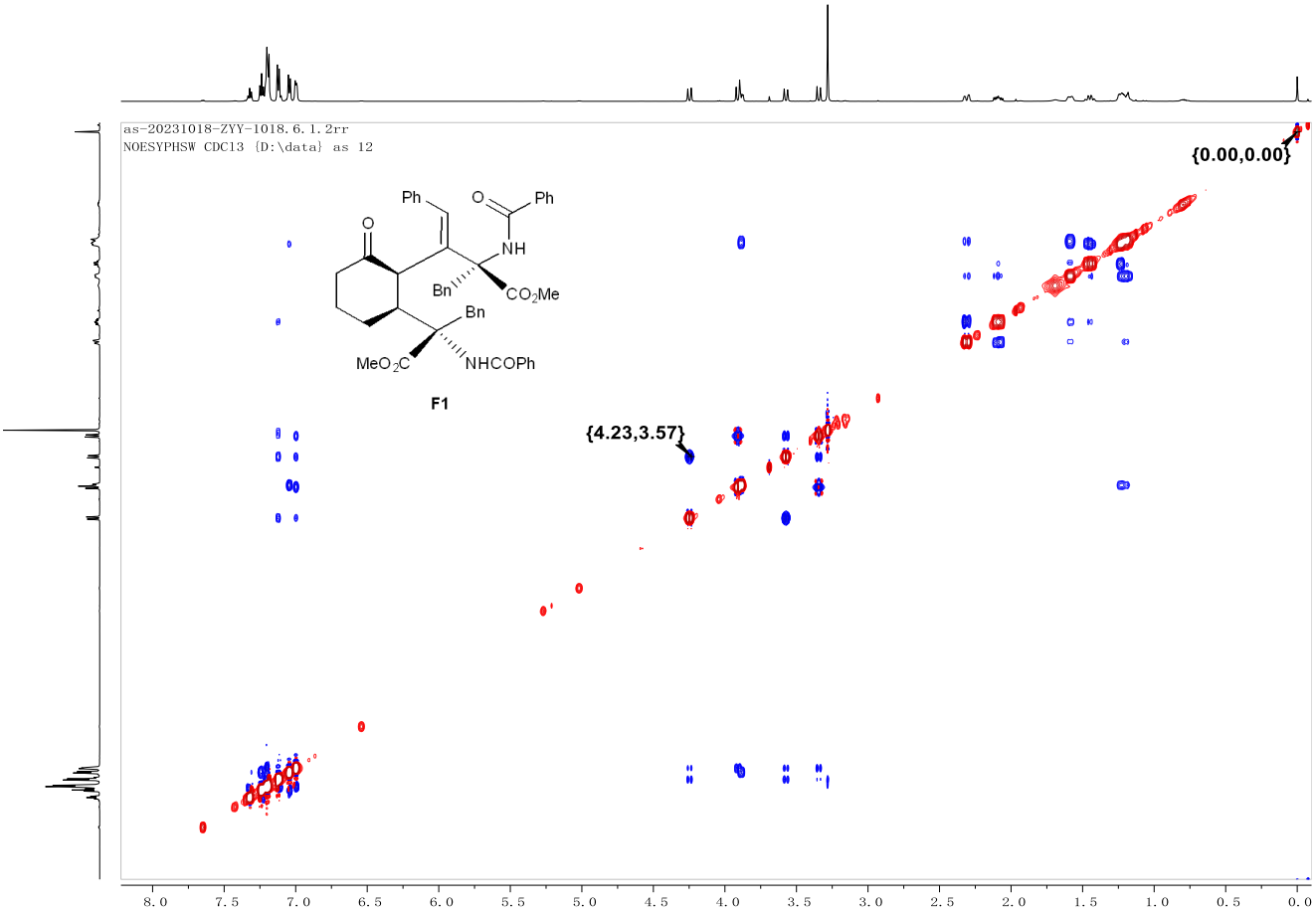
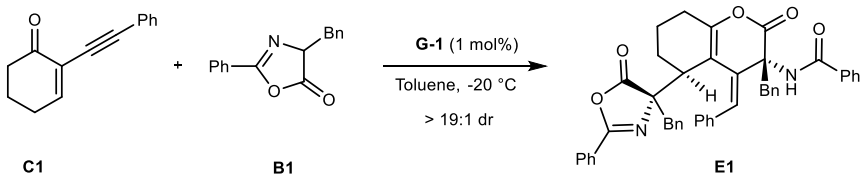


Figure S2. The NOESY of **F1**

8. Computational details

8.1 Computational methods

All DFT calculations were performed with the Gaussian 09 software package.[5] The geometry optimizations were carried out with the B3LYP functional[6] including the D3 version of Grimme's dispersion correction with the combination of Becke–Johnson damping (B3LYP-D3).[7] The 6-31G(d) basis set[8] for the C, H O and N atoms. All structures were analyzed by harmonic vibrational frequencies at the same level to characterize each stationary point as a minimum (no imaginary frequency) or a transition state (one imaginary frequency) and to obtain the thermodynamic corrections to Gibbs free energy. To have more accurate relative energies, the single point energies were calculated using the B3LYP-D3 functional with 6-311G(d) basis set and the IEF-PCM model[9] for considering the solvation effect (toluene). The three-dimensional geometry structures displayed in this work were generated with CYLview.[10] The non-covalent interaction analysis for transition state was performed using Multiwfn 3.8(dev) Program[11] with IGMH method[12].



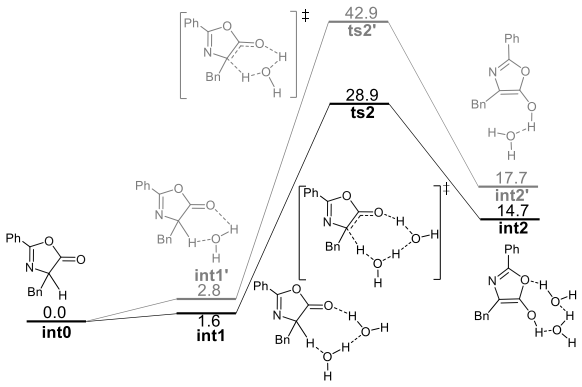


Figure S3. Energy profile of enolization of azlactone via DFT calculations. The relative Gibbs free energy (ΔG) is given in kcal/mol.

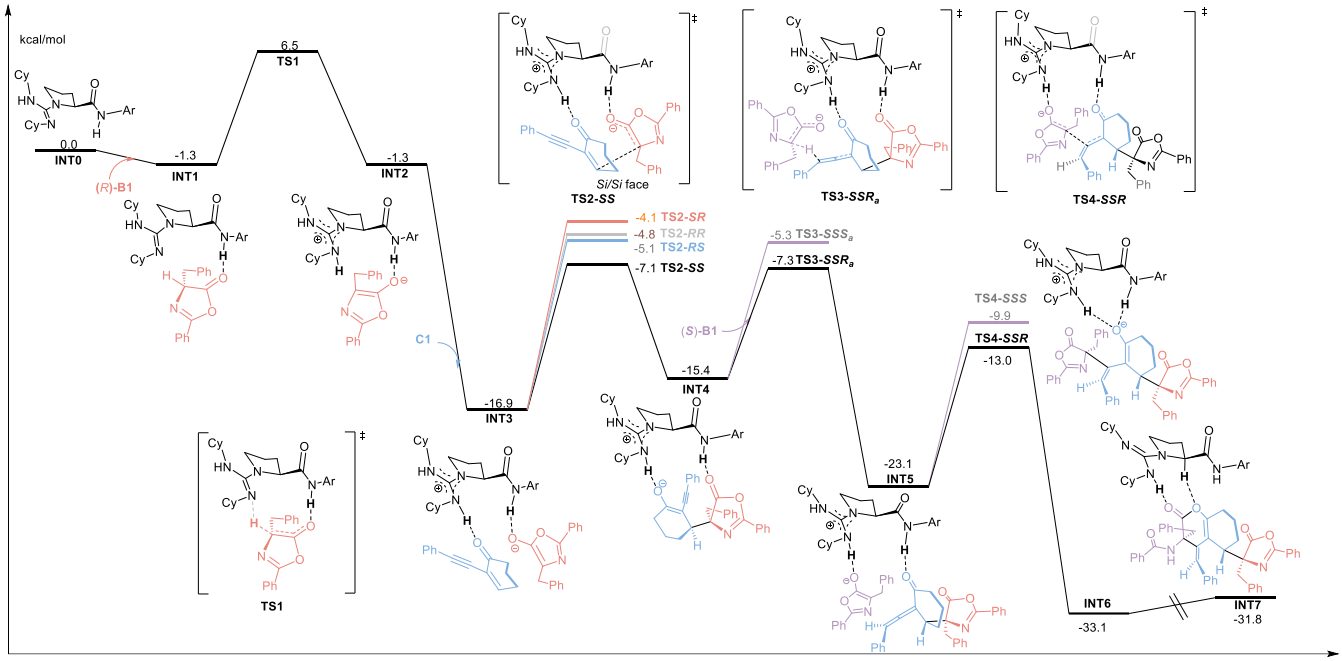


Figure S4. The Gibbs free energy profile of the reaction of azlactone **B1** with cyclic 1,3-enyne **C1** catalyzed by **G-1**.

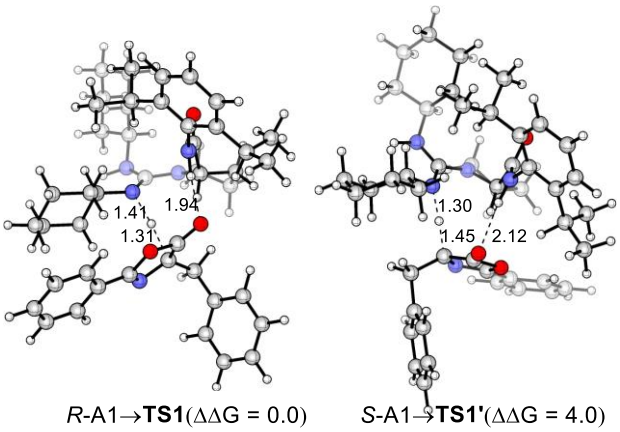


Figure S5. DFT-Calculated relative Gibbs free energies (in kcal/mol), selective bond distances (Å) of the transition states (**TS1**) in proton transfer step.

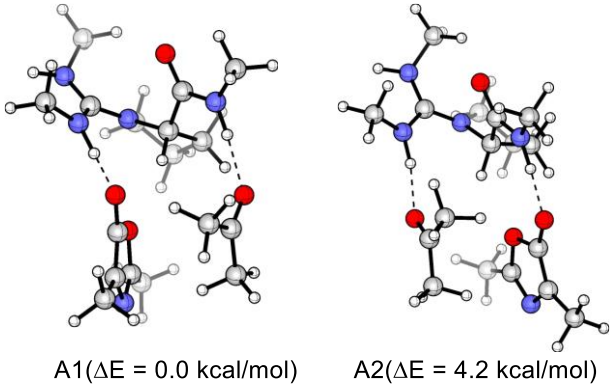


Figure S6. DFT-Calculated relative energies of selected model complexes.

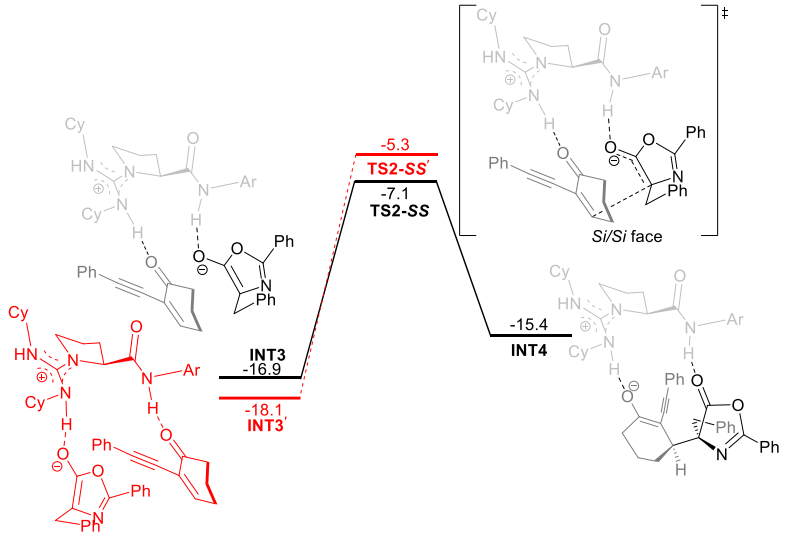


Figure S7. DFT-Calculated relative Gibbs free energies (in kcal/mol) of the transition states (**TS2-*SS*** and **TS2-*SS*′**).

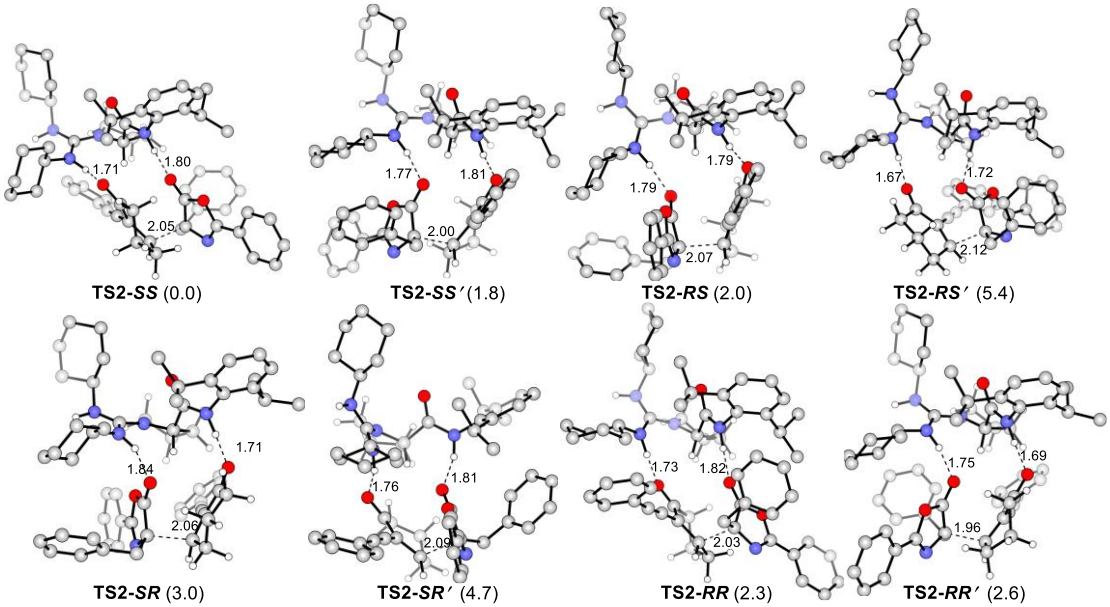


Figure S8. DFT-Calculated relative Gibbs free energies (in kcal/mol), selective bond distances (Å) of the transition states in the Michael-Addition step of **C1** and **B1** catalyzed by **G-1**.

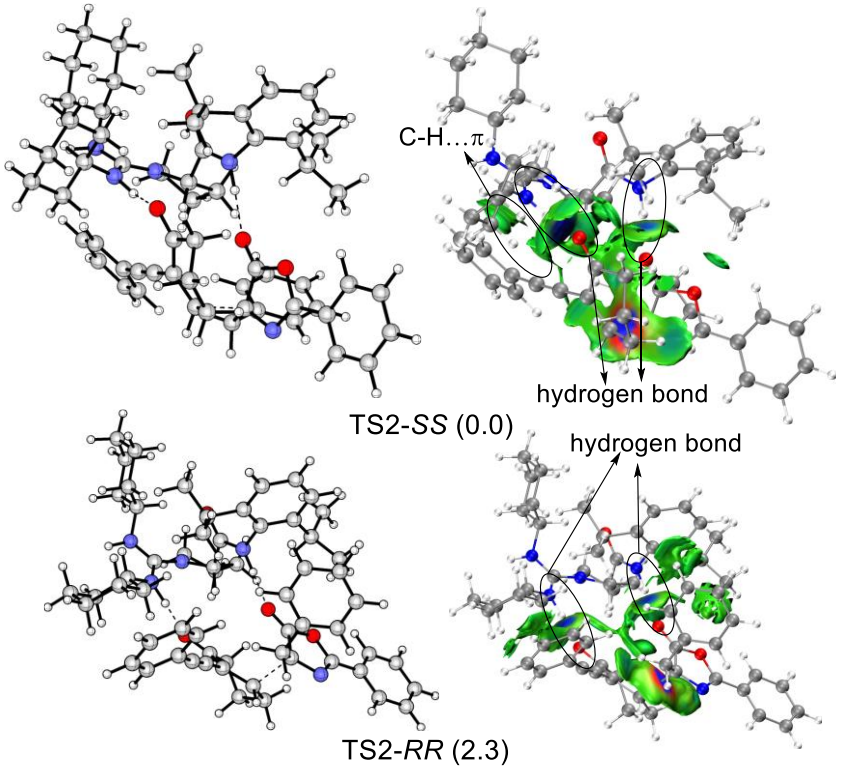


Figure S9. Optimized geometries and non-covalent interaction analysis of **TS2-*SS*** and **TS2-*RR***.

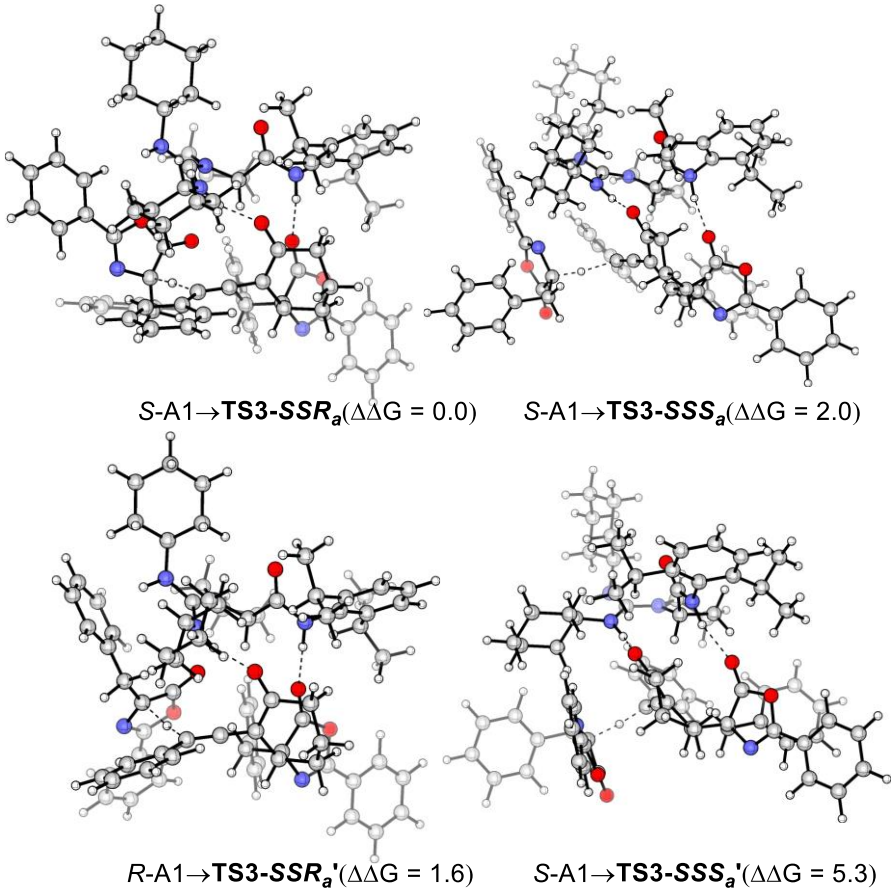


Figure S10. DFT-Calculated relative Gibbs free energies (in kcal/mol), selective bond distances (Å) of the transition states (**TS3**) in proton transfer step.

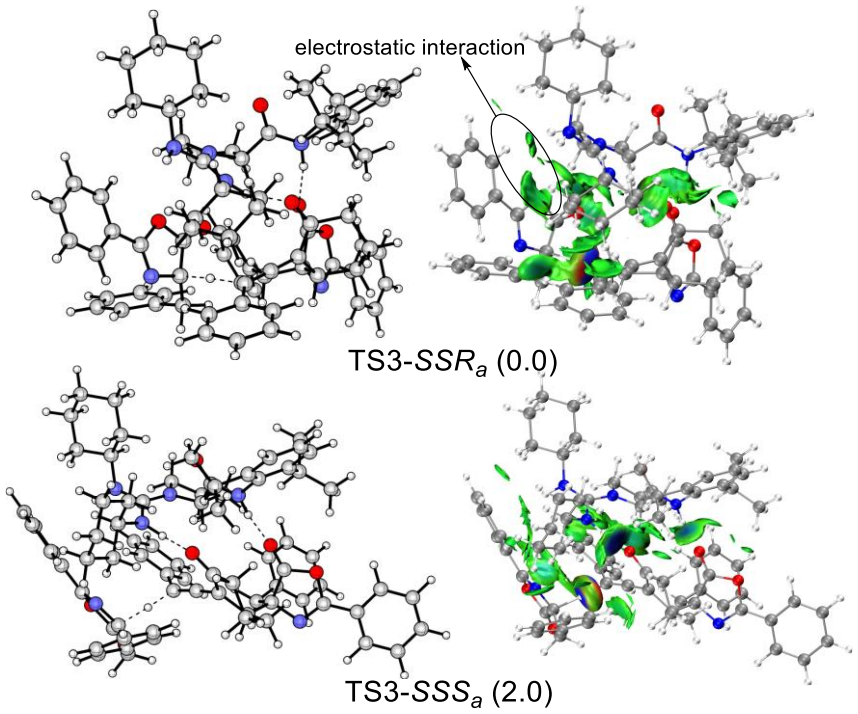
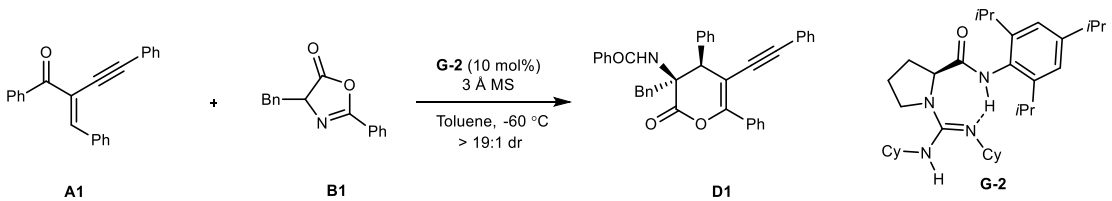


Figure S11. Optimized geometries and non-covalent interaction analysis of **TS3-*SSR*$_a$** and **TS3-*SSS*$_a$**.

To understand the origin of enantioselectivity of the reaction of azlactone **B1** with cyclic 1,3-enyne **A1** catalyzed by **G-1**, density functional theory (DFT) calculations have been performed at the B3LYP-D3(PCM)/6-311G(d)//B3LYP-D3/6-31G(d) level of theory. Initially, the carbonyl of azlactone (*R*)-**B1** engages in hydrogen bonding with the amide of **G-1**, leading to the formation of **INT1**. Subsequently, a proton from the azlactone is transferred to the basic imine nitrogen of **G-1** via transition state **TS1**, resulting in the hydrogen-bonded enolate intermediate **INT2**. While guanidium is typically considered to possess increased hydrogen-bond donor ability due to its positive charge, our analysis (Figure S6) reveals that in the transition state **TS2-*SS***, where guanidinium prefers bonding with the carbonyl of 1,3-enyne, a lower energy barrier is observed compared to **TS2-*SS′*** (Figure S7). The preferred arrangement in **TS2-*SS*** results in a lower LUMO energy of the 1,3-enyne, facilitating conjugate addition through stronger H-bond activation and avoiding significant steric hindrance between the 2-alkyne substitution of 1,3-enyne and the amide substitution in **G-1** shown in **TS2-*SS′***. Furthermore, the energy of **TS2-*SS*** is lower than that of **TS2-*RR*** by 2.3 kcal/mol. Such a tight activation mechanism leads to high activity and stereoselectivity, yielding **INT4**. Subsequently, prototropy occurs with (*S*)-azlactone to the alkyne group via transition state **TS3**, resulting in allenone intermediate **INT5**. During this step, **TS3-*SSSa*** was found to be unstable by 2.0 kcal/mol compared to the favorable **TS3-*SSRa***, potentially due to electrostatic interactions between the enolate and the guanidinium plane (Figure S11). Next, an inverse-electron- demand cycloaddition between the second enolized azlactone and allenone from **INT5** takes place in a stepwise manner, as shown in **TS4**. The energy of **TS4-*SSR*** was found to be lower by 3.1 kcal/mol compared to **TS4-*SSS***. Eventually, the Michael addition/prototropy/lactonalization pro-product **INT7** is formed with high enantioselectivity and diastereoselectivity.



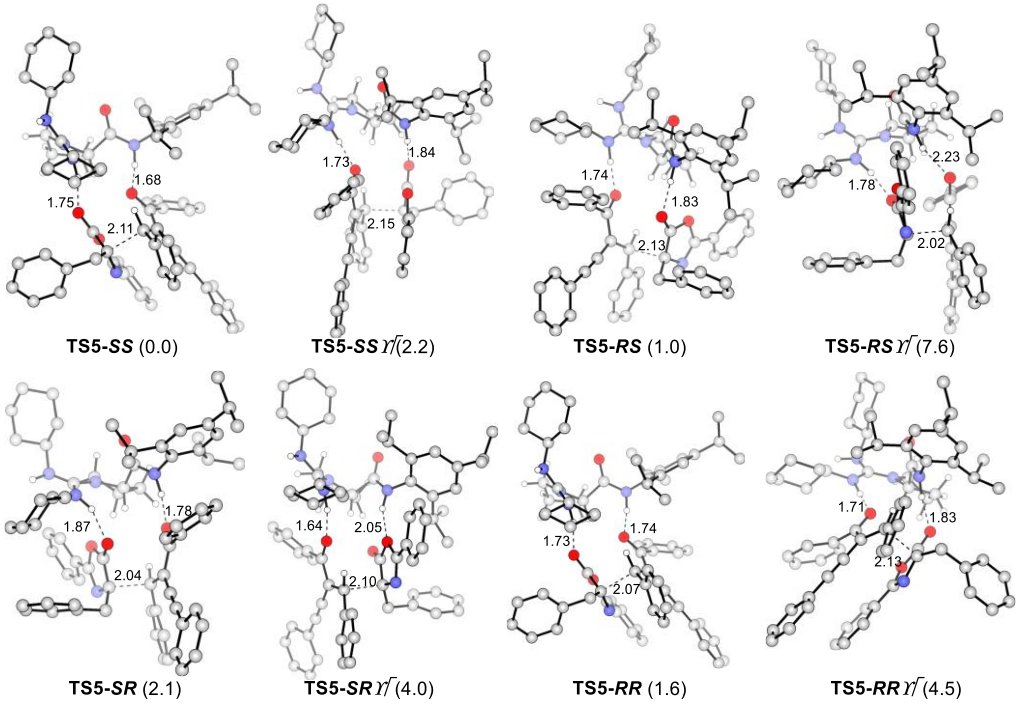


Figure S12. DFT-Calculated relative Gibbs free energies (in kcal/mol), selective bond distances (Å) of the transition states in the reaction of **A1** with **B1** catalyzed by **G-2**.

we have also explored the direct enantioselective inverse-electron-demand hetero-Diels-Alder reaction involving azlactone **B1** and acyclic 1,3-enyne **A1** catalyzed by **G-2**. As shown in above figure, in the favorable transition state leading to the formation of (*S*,*S*)-**D1**, the bifunctional catalytic mode is reversed compared to **TS2** in the cyclic 1,3-enyne case (Figure S8 and S9). Here, guanidinium bonds with the enolized azlactone, while the amide bonds with the 1,3-enyne **A1**. The enol-type activation proceeds through nucleophilic addition to α-alkyne-substituted cyclic enone via *Si*-*Si* facial attacking, with subsequent rapid lactonization instead of prototropy, resulting in the cyclization product **D1**. In this context, the guanidinium-active azlactone facilitates the second cyclization step through a stronger hydrogen bond, while the weaker amide releases the oxygen from the enyne for lactonization.

8.2 Cartesian coordinates

INT0				O	-1.542855000	-2.749890000	-0.079771000
N	2.870756000	0.074190000	-1.025525000	C	-1.222476000	-1.721688000	-0.669644000
N	0.625459000	0.820422000	-1.377380000	N	-1.687573000	-0.478707000	-0.382276000
N	1.137812000	-1.432624000	-1.506660000	C	-2.597142000	-0.171294000	0.677907000
C	1.514428000	-0.119737000	-1.296274000	C	-2.105277000	0.092728000	1.969209000
C	2.054701000	-2.425501000	-2.099690000	C	-3.022864000	0.428315000	2.970726000
H	2.936368000	-1.925201000	-2.506568000	H	-2.667159000	0.627982000	3.977017000
H	2.384498000	-3.142944000	-1.336487000	C	-4.385111000	0.499589000	2.698049000
C	1.208365000	-3.128576000	-3.164819000	C	-4.854620000	0.231254000	1.414887000
C	-0.191555000	-3.103247000	-2.546153000	H	-5.919891000	0.284405000	1.214290000
H	-0.301213000	-3.868664000	-1.772221000	C	-3.973029000	-0.104714000	0.383275000
H	-0.996043000	-3.241204000	-3.273583000	H	-1.142545000	0.272666000	-0.821525000
C	-0.264543000	-1.726189000	-1.883686000	C	-0.629255000	-0.060952000	2.296448000
H	-0.598667000	-0.959460000	-2.593141000	C	-0.395454000	-1.427996000	2.966727000
H	1.568052000	-4.138581000	-3.383028000	H	-0.078600000	-0.054068000	1.351944000

H	-0.950723000	-1.492104000	3.910223000	H	6.016811000	-1.826963000	0.875505000
H	-0.735642000	-2.236562000	2.313546000	H	3.082937000	-1.666790000	3.303761000
H	0.667186000	-1.576887000	3.190772000	H	3.778055000	-2.647907000	2.020494000
C	-4.484205000	-0.448791000	-1.006556000	H	5.598908000	-1.549604000	3.304954000
C	-4.829743000	-1.949008000	-1.080151000	H	4.874008000	0.032277000	3.028520000
H	-3.662034000	-0.266823000	-1.706590000	H	3.078651000	1.060446000	-0.932103000
H	-5.661467000	-2.181755000	-0.403914000	H	-5.084157000	0.761372000	3.487922000
H	-5.132214000	-2.226595000	-2.097468000	**INT1**			
H	-3.974286000	-2.563524000	-0.786439000	N	2.247166000	-2.474266000	1.624564000
H	1.227973000	-2.551172000	-4.096869000	N	0.614805000	-1.173336000	0.446080000
C	-5.673166000	0.413472000	-1.451665000	N	1.773884000	-0.268401000	2.221147000
H	-5.451508000	1.482314000	-1.357988000	C	1.507180000	-1.322925000	1.372530000
H	-5.915242000	0.204438000	-2.499836000	C	2.083393000	-0.406111000	3.647835000
H	-6.574472000	0.202862000	-0.864610000	H	1.740476000	-1.375359000	4.020745000
C	-0.076575000	1.084386000	3.156728000	H	3.165374000	-0.334038000	3.827055000
H	1.005343000	0.966757000	3.287611000	C	1.367179000	0.793653000	4.277600000
H	-0.260095000	2.059959000	2.692998000	C	1.508288000	1.863438000	3.187062000
H	-0.523793000	1.098769000	4.156977000	H	2.525016000	2.268794000	3.178658000
C	0.942546000	2.178882000	-0.972001000	H	0.801465000	2.692088000	3.284526000
C	1.545783000	2.994919000	-2.132131000	C	1.281669000	1.071654000	1.889721000
C	-0.335262000	2.862955000	-0.461164000	H	0.219616000	1.043194000	1.638529000
H	1.668100000	2.189073000	-0.134734000	H	1.804941000	1.091061000	5.235251000
C	1.806037000	4.452924000	-1.731926000	O	3.285381000	1.889369000	0.819572000
H	0.838869000	2.953044000	-2.971673000	C	2.081474000	1.665182000	0.718359000
H	2.470739000	2.521058000	-2.486687000	N	1.341619000	1.927768000	-0.389157000
C	-0.081610000	4.317799000	-0.050777000	C	1.809306000	2.649027000	-1.532649000
H	-1.084867000	2.827279000	-1.264413000	C	2.719480000	2.060883000	-2.426585000
H	-0.746260000	2.293056000	0.379763000	C	3.124701000	2.813129000	-3.536994000
C	0.531377000	5.123933000	-1.203476000	H	3.834480000	2.383227000	-4.237682000
H	2.207572000	5.012301000	-2.585885000	C	2.629993000	4.091850000	-3.760900000
H	2.578592000	4.481758000	-0.948909000	C	1.723752000	4.655740000	-2.864315000
H	-1.016727000	4.781039000	0.286189000	H	1.348276000	5.657242000	-3.045119000
H	0.604034000	4.337289000	0.809437000	C	1.305510000	3.952385000	-1.733208000
H	0.746894000	6.150067000	-0.881001000	H	0.352363000	1.709970000	-0.340252000
H	-0.201132000	5.196645000	-2.020281000	C	3.284664000	0.664840000	-2.221027000
C	3.593229000	-0.710420000	-0.005635000	C	4.775834000	0.741547000	-1.850224000
C	4.962685000	-0.060151000	0.217443000	H	2.751475000	0.204950000	-1.384626000
C	2.824421000	-0.841592000	1.315534000	H	5.351770000	1.219214000	-2.652081000
H	3.766748000	-1.717218000	-0.400449000	H	4.905305000	1.318140000	-0.931892000
C	5.781524000	-0.826052000	1.264623000	H	5.185327000	-0.263566000	-1.697955000
H	4.809535000	0.973802000	0.565217000	C	0.393723000	4.587903000	-0.691686000
H	5.501437000	-0.001620000	-0.735862000	C	1.245522000	5.153521000	0.462510000
C	3.640300000	-1.611511000	2.361271000	H	-0.246570000	3.804911000	-0.276321000
H	2.597314000	0.166991000	1.689761000	H	1.865540000	5.984212000	0.104895000
H	1.867941000	-1.338719000	1.130622000	H	0.604057000	5.529700000	1.268930000
C	5.013004000	-0.964760000	2.585776000	H	1.917439000	4.395991000	0.875936000
H	6.740756000	-0.320986000	1.428658000	H	0.309529000	0.554070000	4.444835000

C	-0.537069000	5.667965000	-1.256162000	C	-2.324787000	-0.271857000	1.450213000
H	-1.114960000	5.293859000	-2.108121000	C	-3.489613000	-1.006868000	-0.261042000
H	-1.242294000	5.991010000	-0.482392000	C	-4.234610000	-1.794724000	-1.238315000
H	0.015081000	6.556953000	-1.582510000	C	-4.428811000	-1.327439000	-2.544901000
C	3.076427000	-0.229151000	-3.455639000	C	-5.089512000	-2.128725000	-3.473786000
H	3.381362000	-1.258283000	-3.230738000	C	-5.556357000	-3.390776000	-3.104551000
H	2.028771000	-0.246433000	-3.771829000	C	-5.365892000	-3.855068000	-1.799229000
H	3.676202000	0.112544000	-4.307059000	C	-4.707246000	-3.062630000	-0.866628000
C	0.492813000	-2.162940000	-0.613352000	C	-2.828363000	0.360476000	2.761574000
C	-0.415837000	-3.347065000	-0.221344000	C	-4.164291000	1.043420000	2.591953000
C	-0.062793000	-1.477494000	-1.869667000	C	-5.352043000	0.302010000	2.623847000
H	1.486089000	-2.574583000	-0.881068000	C	-6.581397000	0.921672000	2.403839000
C	-0.593275000	-4.336887000	-1.381358000	C	-6.639245000	2.292549000	2.146198000
H	-1.390491000	-2.947531000	0.083538000	C	-5.461122000	3.038813000	2.108510000
H	-0.012487000	-3.863413000	0.660263000	C	-4.232050000	2.417015000	2.329287000
C	-0.224004000	-2.456930000	-3.036665000	H	-4.053427000	-0.350080000	-2.825431000
H	-1.037503000	-1.040453000	-1.625196000	H	-5.235307000	-1.768498000	-4.487644000
H	0.590905000	-0.642776000	-2.138503000	H	-6.066231000	-4.014901000	-3.832760000
C	-1.117219000	-3.642225000	-2.645537000	H	-5.727240000	-4.838288000	-1.513047000
H	-1.272578000	-5.145259000	-1.082806000	H	-4.536817000	-3.407690000	0.147350000
H	0.375109000	-4.808813000	-1.606044000	H	-2.070116000	1.076668000	3.096656000
H	-0.641122000	-1.937490000	-3.908464000	H	-2.885864000	-0.437941000	3.508248000
H	0.765736000	-2.829410000	-3.339412000	H	-5.305431000	-0.766720000	2.811936000
H	-1.182789000	-4.361069000	-3.472037000	H	-7.494761000	0.333910000	2.432984000
H	-2.137271000	-3.280358000	-2.461815000	H	-7.597172000	2.775758000	1.975639000
C	3.707076000	-2.433805000	1.832667000	H	-5.497039000	4.105775000	1.907104000
C	4.232660000	-3.873150000	1.815539000	H	-3.314297000	2.997192000	2.286288000
C	4.443335000	-1.565064000	0.802874000	H	2.951423000	4.654604000	-4.633303000
H	3.901849000	-2.023953000	2.830276000	H	-1.312504000	-0.682470000	1.579442000
C	5.750051000	-3.918203000	2.036914000	**TS1**			
H	3.997917000	-4.321553000	0.837050000	N	-2.121754000	-2.272807000	-2.063300000
H	3.708140000	-4.466451000	2.574505000	N	-0.491694000	-1.297843000	-0.643248000
C	5.959685000	-1.606904000	1.028555000	N	-1.496841000	-0.033994000	-2.283619000
H	4.206119000	-1.944623000	-0.202244000	C	-1.350713000	-1.216140000	-1.631822000
H	4.081016000	-0.534528000	0.855550000	C	-1.930902000	0.115877000	-3.674881000
C	6.491610000	-3.045337000	1.015361000	H	-1.685190000	-0.783699000	-4.244861000
H	6.102869000	-4.955365000	1.986830000	H	-3.015088000	0.281733000	-3.730525000
H	5.975811000	-3.558995000	3.051256000	C	-1.179700000	1.372289000	-4.122479000
H	6.464745000	-1.000477000	0.268337000	C	-1.219439000	2.242219000	-2.858454000
H	6.191210000	-1.142829000	1.998371000	H	-2.203282000	2.710905000	-2.758173000
H	7.569467000	-3.059034000	1.218453000	H	-0.455357000	3.022772000	-2.836105000
H	6.354540000	-3.471636000	0.010732000	C	-1.021454000	1.233153000	-1.708469000
H	1.979784000	-3.229206000	1.005712000	H	0.031783000	1.171584000	-1.440907000
O	-1.644654000	1.778433000	0.225139000	H	-1.645024000	1.852525000	-4.987964000
O	-2.987851000	0.218214000	-0.719372000	O	-3.094640000	1.656695000	-0.568016000
N	-3.186626000	-1.329935000	0.935182000	C	-1.868067000	1.620687000	-0.486335000
C	-2.235003000	0.731621000	0.313658000	N	-1.150981000	1.941360000	0.617981000

C	-1.702297000	2.580568000	1.773427000	C	-3.586257000	-2.171610000	-2.238232000
C	-2.597849000	1.898094000	2.613488000	C	-4.135891000	-3.577410000	-2.498401000
C	-3.103126000	2.582833000	3.726413000	C	-4.277350000	-1.515069000	-1.035504000
H	-3.804482000	2.078195000	4.384551000	H	-3.785463000	-1.566060000	-3.128912000
C	-2.714256000	3.885857000	4.009391000	C	-5.658863000	-3.549806000	-2.684441000
C	-1.811198000	4.539337000	3.172610000	H	-3.889405000	-4.217276000	-1.636373000
H	-1.512758000	5.556423000	3.402052000	H	-3.642211000	-4.013595000	-3.375353000
C	-1.297307000	3.907513000	2.038781000	C	-5.798891000	-1.487700000	-1.223015000
H	-0.133334000	1.931488000	0.527539000	H	-4.025605000	-2.093480000	-0.133902000
C	-3.021964000	0.458206000	2.371508000	H	-3.894949000	-0.500501000	-0.891020000
C	-4.517750000	0.374537000	2.024852000	C	-6.359314000	-2.890645000	-1.488353000
H	-2.460193000	0.080080000	1.513822000	H	-6.031445000	-4.569609000	-2.836560000
H	-5.134551000	0.737142000	2.855838000	H	-5.898178000	-2.988999000	-3.599238000
H	-4.731187000	0.976184000	1.139102000	H	-6.269678000	-1.042265000	-0.339646000
H	-4.806565000	-0.664332000	1.824245000	H	-6.044974000	-0.830700000	-2.069780000
C	-0.383729000	4.643300000	1.065550000	H	-7.440956000	-2.845765000	-1.663334000
C	-1.212110000	5.174103000	-0.121475000	H	-6.210023000	-3.514504000	-0.595032000
H	0.345953000	3.930996000	0.670519000	H	-1.845411000	-3.146028000	-1.632230000
H	-1.915545000	5.942979000	0.219400000	O	1.687133000	1.979802000	0.003203000
H	-0.558757000	5.621135000	-0.880505000	O	2.770190000	0.301820000	1.129477000
H	-1.797509000	4.379406000	-0.592812000	N	3.273407000	-1.125305000	-0.541879000
H	-0.146625000	1.116266000	-4.384268000	C	2.261450000	0.895456000	-0.032146000
C	0.421258000	5.779660000	1.708067000	C	2.485799000	-0.076178000	-1.083327000
H	0.978675000	5.429983000	2.583499000	C	3.370665000	-0.879468000	0.720342000
H	1.140847000	6.177457000	0.984281000	C	3.947165000	-1.732740000	1.751055000
H	-0.219245000	6.612637000	2.020727000	C	3.796419000	-1.426943000	3.111309000
C	-2.688957000	-0.433865000	3.580530000	C	4.301601000	-2.293343000	4.078854000
H	-2.900934000	-1.484772000	3.349175000	C	4.962899000	-3.462571000	3.700495000
H	-1.633764000	-0.352617000	3.861304000	C	5.122447000	-3.763925000	2.344151000
H	-3.287927000	-0.161378000	4.456819000	C	4.617644000	-2.907395000	1.372533000
C	-0.416996000	-2.434175000	0.264654000	C	2.642167000	0.310832000	-2.534974000
C	0.522744000	-3.539054000	-0.251772000	C	3.956697000	1.019741000	-2.789608000
C	0.046708000	-1.941521000	1.640900000	C	5.083463000	0.311439000	-3.217775000
H	-1.428850000	-2.856526000	0.388516000	C	6.304654000	0.961171000	-3.399924000
C	0.622170000	-4.697428000	0.750918000	C	6.413104000	2.329947000	-3.151415000
H	1.512838000	-3.095208000	-0.416594000	C	5.294846000	3.043277000	-2.715169000
H	0.180460000	-3.906144000	-1.229697000	C	4.075447000	2.391949000	-2.534922000
C	0.147564000	-3.089630000	2.650500000	H	3.275067000	-0.520455000	3.398154000
H	1.025675000	-1.466177000	1.528467000	H	4.175783000	-2.054958000	5.131081000
H	-0.637090000	-1.164905000	1.990972000	H	5.352989000	-4.136948000	4.457405000
C	1.063804000	-4.207988000	2.136906000	H	5.638696000	-4.671988000	2.045909000
H	1.319677000	-5.455361000	0.374365000	H	4.721236000	-3.130409000	0.316025000
H	-0.359091000	-5.189070000	0.835110000	H	1.810174000	0.964381000	-2.818561000
H	0.518622000	-2.706329000	3.608291000	H	2.571483000	-0.594072000	-3.147346000
H	-0.856969000	-3.495651000	2.842355000	H	5.001802000	-0.757089000	-3.399473000
H	1.075278000	-5.045130000	2.845746000	H	7.171607000	0.397933000	-3.734946000
H	2.091751000	-3.831909000	2.076235000	H	7.363156000	2.837438000	-3.294175000

H	5.372496000	4.108481000	-2.514500000	H	-0.343357000	2.148926000	-6.394567000
H	3.209584000	2.941080000	-2.174475000	C	1.154656000	-3.856012000	-1.914597000
H	-3.111943000	4.395673000	4.882777000	H	1.381316000	-4.341480000	-0.957010000
H	0.909499000	-0.652043000	-0.891922000	H	0.071620000	-3.716046000	-1.979554000
INT2				H	1.446107000	-4.550702000	-2.710054000
N	1.880533000	-0.758480000	2.713544000	C	-0.508919000	-1.756611000	1.413892000
N	0.106715000	-0.433502000	1.235390000	C	-1.404472000	-1.814757000	2.662389000
N	1.883607000	1.054280000	1.239162000	C	-1.304790000	-2.107767000	0.152265000
C	1.289440000	-0.042474000	1.722180000	H	0.314452000	-2.476620000	1.513346000
C	2.882302000	1.856814000	1.962346000	C	-2.056451000	-3.198127000	2.798513000
H	2.676454000	1.824773000	3.035210000	H	-2.172903000	-1.037176000	2.571238000
H	3.889039000	1.461930000	1.778422000	H	-0.823659000	-1.575180000	3.565314000
C	2.718458000	3.239378000	1.328684000	C	-1.961011000	-3.487458000	0.283723000
C	2.430342000	2.904435000	-0.140517000	H	-2.079346000	-1.352468000	-0.002714000
H	3.357476000	2.658922000	-0.666696000	H	-0.643066000	-2.062826000	-0.716349000
H	1.918695000	3.713304000	-0.664614000	C	-2.842610000	-3.575984000	1.536178000
C	1.543904000	1.647383000	-0.078735000	H	-2.714201000	-3.208426000	3.675153000
H	0.490647000	1.925654000	-0.123452000	H	-1.274709000	-3.951266000	2.982409000
H	3.614156000	3.853646000	1.455663000	H	-2.557852000	-3.689455000	-0.612729000
O	3.066532000	0.275234000	-1.331904000	H	-1.179461000	-4.260323000	0.324585000
C	1.902266000	0.651632000	-1.196367000	H	-3.250991000	-4.588497000	1.638340000
N	0.851253000	0.271903000	-1.959558000	H	-3.697071000	-2.899699000	1.425988000
C	0.965376000	-0.428467000	-3.201366000	C	3.307821000	-1.148519000	2.732608000
C	1.478285000	-1.736707000	-3.258404000	C	3.494521000	-2.198166000	3.832800000
C	1.569845000	-2.350665000	-4.514661000	C	3.782064000	-1.677379000	1.372989000
H	1.973442000	-3.356636000	-4.583147000	H	3.905586000	-0.271202000	3.002918000
C	1.141982000	-1.705883000	-5.667219000	C	4.956478000	-2.658458000	3.907887000
C	0.610722000	-0.420043000	-5.585800000	H	2.853024000	-3.063798000	3.606221000
H	0.271939000	0.072827000	-6.490140000	H	3.164780000	-1.791732000	4.797052000
C	0.517854000	0.245164000	-4.362189000	C	5.244245000	-2.132932000	1.448108000
H	-0.042265000	0.751678000	-1.761385000	H	3.143459000	-2.528232000	1.094819000
C	1.913337000	-2.520947000	-2.028773000	H	3.658453000	-0.919284000	0.593619000
C	3.431606000	-2.766227000	-2.036331000	C	5.452045000	-3.177857000	2.551358000
H	1.674731000	-1.925050000	-1.144091000	H	5.059321000	-3.430373000	4.679011000
H	3.725932000	-3.356144000	-2.912275000	H	5.582691000	-1.812678000	4.225146000
H	3.965554000	-1.814898000	-2.054747000	H	5.551567000	-2.529230000	0.474497000
H	3.734819000	-3.326785000	-1.143370000	H	5.884924000	-1.261121000	1.645034000
C	0.003062000	1.678676000	-4.277136000	H	6.509614000	-3.458292000	2.619987000
C	1.186064000	2.659622000	-4.153911000	H	4.899454000	-4.092191000	2.291242000
H	-0.606252000	1.777575000	-3.374084000	H	1.262888000	-1.426009000	3.156202000
H	1.794079000	2.642765000	-5.066332000	O	-1.311022000	1.841039000	-1.183372000
H	0.821134000	3.682485000	-4.003648000	O	-3.184144000	0.619686000	-0.631992000
H	1.840951000	2.404452000	-3.315909000	N	-3.362221000	0.991055000	1.560675000
H	1.870886000	3.763460000	1.776930000	C	-2.129678000	1.490597000	-0.287002000
C	-0.897851000	2.082716000	-5.450833000	C	-2.277885000	1.721754000	1.087193000
H	-1.721812000	1.374124000	-5.587070000	C	-3.862128000	0.364205000	0.532220000
H	-1.330181000	3.070225000	-5.257423000	C	-4.918433000	-0.629343000	0.521175000

C	-5.211899000	-1.365018000	-0.640111000	H	-2.267283000	-5.089894000	-1.746472000
C	-6.177770000	-2.368338000	-0.608772000	C	-3.234147000	-3.562365000	-2.902314000
C	-6.867654000	-2.650701000	0.571725000	C	-3.269697000	-2.206902000	-3.222696000
C	-6.587118000	-1.912737000	1.726582000	H	-4.018343000	-1.842934000	-3.918302000
C	-5.623702000	-0.910893000	1.705962000	C	-2.361174000	-1.308915000	-2.659307000
C	-1.461030000	2.501484000	2.081930000	H	-0.985110000	-0.067041000	-0.639389000
C	-0.932830000	3.886741000	1.746360000	C	-0.368949000	-3.711059000	-0.390229000
C	-0.427067000	4.660165000	2.803684000	C	0.709138000	-4.549145000	-1.098073000
C	0.134295000	5.915384000	2.579954000	H	0.114453000	-2.853908000	0.081612000
C	0.201578000	6.426717000	1.281540000	H	0.256783000	-5.399579000	-1.622662000
C	-0.309257000	5.673449000	0.226012000	H	1.245382000	-3.933149000	-1.823590000
C	-0.876965000	4.415421000	0.452047000	H	1.428297000	-4.950421000	-0.373684000
H	-4.670024000	-1.148154000	-1.554457000	C	-2.369357000	0.158962000	-3.062793000
H	-6.391222000	-2.933911000	-1.511845000	C	-1.485432000	0.358629000	-4.307809000
H	-7.618380000	-3.435477000	0.592808000	H	-1.926028000	0.741147000	-2.254678000
H	-7.122890000	-2.122821000	2.648528000	H	-1.913752000	-0.157471000	-5.175594000
H	-5.390038000	-0.337846000	2.597141000	H	-1.397430000	1.424750000	-4.550099000
H	-0.592850000	1.908601000	2.422689000	H	-0.479825000	-0.044875000	-4.146242000
H	-2.092604000	2.580305000	2.974280000	H	2.063391000	3.367485000	-0.798956000
H	-0.474995000	4.266188000	3.817287000	C	-3.776457000	0.727586000	-3.286246000
H	0.515909000	6.494882000	3.416632000	H	-4.418256000	0.549103000	-2.418195000
H	0.640274000	7.403847000	1.099037000	H	-3.711408000	1.809071000	-3.445227000
H	-0.271006000	6.063508000	-0.787953000	H	-4.264490000	0.295209000	-4.167564000
H	-1.241954000	3.832466000	-0.384583000	C	-1.054180000	-4.521780000	0.721603000
H	1.215503000	-2.203944000	-6.630172000	H	-0.330293000	-4.773592000	1.506697000
H	-0.506082000	0.275377000	0.829797000	H	-1.873324000	-3.958038000	1.178212000
INT3				H	-1.467114000	-5.464002000	0.343215000
N	4.827043000	-0.074946000	-0.014243000	C	3.389352000	-1.761926000	1.929664000
N	2.886554000	-0.590809000	1.195139000	C	3.277050000	-1.521181000	3.440094000
N	2.756243000	0.707199000	-0.724418000	C	2.631216000	-3.022608000	1.497191000
C	3.467321000	-0.011935000	0.140705000	H	4.446910000	-1.899917000	1.677319000
C	3.319235000	1.783480000	-1.558931000	C	3.738864000	-2.755790000	4.226407000
H	4.196499000	2.207272000	-1.067456000	H	2.229807000	-1.296855000	3.673926000
H	3.607636000	1.382847000	-2.538786000	H	3.865168000	-0.637671000	3.718678000
C	2.141084000	2.745934000	-1.694452000	C	3.108046000	-4.248883000	2.282928000
C	0.943287000	1.798003000	-1.798241000	H	1.566557000	-2.852905000	1.683375000
H	0.866928000	1.398317000	-2.815112000	H	2.752255000	-3.162726000	0.418623000
H	-0.005072000	2.258326000	-1.527368000	C	2.978443000	-4.017124000	3.794081000
C	1.285306000	0.657357000	-0.811175000	H	3.610251000	-2.578010000	5.300396000
H	0.836415000	0.887321000	0.156813000	H	4.815884000	-2.910631000	4.062336000
H	2.240934000	3.401780000	-2.563582000	H	2.529428000	-5.128636000	1.977553000
O	1.542646000	-1.490722000	-1.920193000	H	4.158637000	-4.464221000	2.035810000
C	0.792173000	-0.707766000	-1.336494000	H	3.346263000	-4.888581000	4.348747000
N	-0.531444000	-0.861656000	-1.126465000	H	1.915564000	-3.902490000	4.049163000
C	-1.403200000	-1.808253000	-1.748426000	C	5.446553000	-0.539118000	-1.277490000
C	-1.366585000	-3.168062000	-1.396380000	C	6.963455000	-0.587381000	-1.081059000
C	-2.288363000	-4.033842000	-1.999884000	C	4.889878000	-1.895781000	-1.730930000

H	5.231844000	0.203968000	-2.050977000	C	-3.418906000	0.484854000	3.549331000
C	7.664602000	-1.067523000	-2.359605000	C	-2.294892000	1.404318000	3.199536000
H	7.193221000	-1.284609000	-0.259695000	C	-1.052701000	0.984251000	2.809549000
H	7.332351000	0.400302000	-0.779029000	C	-0.810761000	-0.441726000	2.527582000
C	5.590522000	-2.367684000	-3.011297000	C	-1.967721000	-1.396189000	2.710279000
H	5.061904000	-2.628128000	-0.927205000	C	-2.938303000	-0.946864000	3.804932000
H	3.807767000	-1.820210000	-1.881821000	H	-2.462668000	2.471218000	3.313738000
C	7.113302000	-2.420045000	-2.831456000	H	-4.165227000	0.499172000	2.739830000
H	8.745208000	-1.129739000	-2.186650000	H	-3.945588000	0.881191000	4.427359000
H	7.516486000	-0.319065000	-3.150946000	H	-1.555555000	-2.390749000	2.901900000
H	5.201937000	-3.349283000	-3.304330000	H	-2.486535000	-1.437704000	1.742954000
H	5.343229000	-1.678900000	-3.831900000	H	-2.431484000	-0.990911000	4.778174000
H	7.600305000	-2.717659000	-3.767610000	H	-3.791884000	-1.630773000	3.852703000
H	7.363066000	-3.190458000	-2.087510000	O	0.277309000	-0.861363000	2.114059000
H	1.906192000	-0.372833000	1.409923000	C	0.022012000	1.881864000	2.569136000
H	5.294355000	-0.450338000	0.801341000	C	0.988501000	2.589080000	2.357545000
O	-1.496032000	1.403576000	0.037755000	C	2.112307000	3.389475000	2.015091000
O	-3.369643000	0.095354000	0.159314000	C	3.391836000	2.806617000	1.915263000
N	-4.951187000	1.593181000	0.666786000	C	1.972529000	4.760641000	1.721495000
C	-2.728318000	1.347165000	0.245664000	C	4.483215000	3.560246000	1.494629000
C	-3.741097000	2.253000000	0.578744000	H	3.508277000	1.758708000	2.166190000
C	-4.697817000	0.329484000	0.422674000	C	3.070601000	5.508971000	1.306353000
C	-5.592294000	-0.808641000	0.376391000	H	0.996125000	5.223162000	1.812114000
C	-5.117753000	-2.070297000	-0.030598000	C	4.327813000	4.912618000	1.179780000
C	-5.981944000	-3.160513000	-0.073541000	H	5.458334000	3.087899000	1.411240000
C	-7.323499000	-3.015954000	0.285925000	H	2.943230000	6.563130000	1.076682000
C	-7.798839000	-1.762476000	0.687048000	H	5.179694000	5.499186000	0.848597000
C	-6.945522000	-0.666050000	0.733066000	H	-3.949915000	-4.246050000	-3.350618000
C	-3.587535000	3.744039000	0.660724000	**INT3′**			
C	-2.617250000	4.252774000	-0.389073000	N	1.658262000	4.068096000	-0.369692000
C	-2.955474000	4.200539000	-1.746684000	N	1.119924000	1.785031000	-0.469391000
C	-2.045518000	4.596326000	-2.725459000	N	0.333681000	3.091388000	1.279060000
C	-0.778423000	5.058308000	-2.358741000	C	1.025837000	2.962978000	0.138319000
C	-0.432020000	5.115132000	-1.008680000	C	0.514135000	4.187754000	2.239211000
C	-1.345646000	4.708492000	-0.035187000	H	1.533612000	4.574870000	2.176259000
H	-4.082617000	-2.183463000	-0.331131000	H	-0.189886000	5.002207000	2.026145000
H	-5.601115000	-4.124589000	-0.399664000	C	0.165388000	3.519304000	3.570089000
H	-7.995492000	-3.868977000	0.250702000	C	-0.993746000	2.595658000	3.178667000
H	-8.842572000	-1.641636000	0.965248000	H	-1.917661000	3.177841000	3.085821000
H	-7.302630000	0.311247000	1.041562000	H	-1.167382000	1.768369000	3.866383000
H	-3.241795000	4.070628000	1.652580000	C	-0.581160000	2.056049000	1.791028000
H	-4.578147000	4.191126000	0.516565000	H	-0.059578000	1.102765000	1.883143000
H	-3.935713000	3.828008000	-2.032542000	H	-0.104462000	4.246931000	4.340603000
H	-2.325127000	4.547289000	-3.774730000	O	-2.201811000	2.870392000	0.206291000
H	-0.068005000	5.369516000	-3.120127000	C	-1.806388000	1.920065000	0.878733000
H	0.554545000	5.460460000	-0.712529000	N	-2.420043000	0.716481000	0.956430000
H	-1.063610000	4.713034000	1.014032000	C	-3.709030000	0.484548000	0.381000000

C	-3.836091000	0.350015000	-1.012703000	C	1.889008000	6.283105000	-1.366429000
C	-5.120684000	0.184470000	-1.540607000	C	-0.336411000	5.075887000	-1.502624000
H	-5.243888000	0.088224000	-2.615028000	H	0.631754000	5.779548000	0.285426000
C	-6.236115000	0.115548000	-0.712413000	C	1.190856000	7.606974000	-1.706935000
C	-6.083383000	0.206218000	0.668999000	H	2.243248000	5.812084000	-2.296894000
H	-6.955966000	0.134283000	1.311037000	H	2.769824000	6.455133000	-0.736168000
C	-4.822270000	0.405488000	1.240758000	C	-1.032573000	6.401192000	-1.837210000
H	-2.037635000	0.020436000	1.597677000	H	-0.041707000	4.569218000	-2.434012000
C	-2.629035000	0.356885000	-1.935911000	H	-1.014176000	4.405000000	-0.965302000
C	-2.583909000	1.643626000	-2.778110000	C	-0.078573000	7.376781000	-2.538534000
H	-1.735398000	0.325662000	-1.306296000	H	1.887423000	8.265159000	-2.239036000
H	-3.450201000	1.699880000	-3.448801000	H	0.924724000	8.122003000	-0.772832000
H	-2.586079000	2.522442000	-2.129903000	H	-1.913625000	6.207656000	-2.459140000
H	-1.681281000	1.664551000	-3.401913000	H	-1.403336000	6.858320000	-0.908227000
C	-4.664427000	0.489000000	2.751293000	H	-0.580038000	8.332705000	-2.731028000
C	-5.698575000	1.418549000	3.403799000	H	0.202670000	6.965237000	-3.518690000
H	-3.675328000	0.903916000	2.961667000	H	0.867348000	0.913836000	0.051274000
H	-6.717010000	1.022565000	3.319447000	H	2.308505000	3.833754000	-1.108489000
H	-5.480770000	1.530582000	4.472129000	O	0.587258000	-0.611888000	0.710033000
H	-5.684967000	2.412368000	2.943212000	O	2.841754000	-0.770974000	1.172933000
H	1.019692000	2.934367000	3.929896000	N	3.352936000	-2.746246000	0.255025000
C	-4.704702000	-0.918674000	3.373372000	C	1.648657000	-1.284912000	0.609563000
H	-3.910496000	-1.550112000	2.965773000	C	2.003877000	-2.516213000	0.059639000
H	-4.564031000	-0.861999000	4.459064000	C	3.813176000	-1.709950000	0.907832000
H	-5.670281000	-1.401783000	3.178778000	C	5.171835000	-1.440261000	1.332154000
C	-2.599619000	-0.893242000	-2.830564000	C	5.503102000	-0.248607000	2.001121000
H	-1.668150000	-0.925234000	-3.406573000	C	6.816155000	-0.007514000	2.397329000
H	-2.665331000	-1.806318000	-2.233517000	C	7.817601000	-0.944555000	2.136147000
H	-3.431544000	-0.900032000	-3.544235000	C	7.492702000	-2.131623000	1.471071000
C	1.806415000	1.559921000	-1.750153000	C	6.185489000	-2.381013000	1.071107000
C	3.322892000	1.388787000	-1.537950000	C	1.102035000	-3.447311000	-0.688182000
C	1.203186000	0.341111000	-2.457900000	C	1.274716000	-3.451155000	-2.198745000
H	1.621736000	2.436537000	-2.386943000	C	2.539361000	-3.602653000	-2.782791000
C	4.044790000	1.095878000	-2.858368000	C	2.680053000	-3.643069000	-4.169778000
H	3.476444000	0.563637000	-0.834475000	C	1.559515000	-3.531768000	-4.997130000
H	3.746601000	2.280960000	-1.055740000	C	0.296606000	-3.377302000	-4.424056000
C	1.931323000	0.056854000	-3.776329000	C	0.158949000	-3.337279000	-3.035023000
H	1.282044000	-0.534547000	-1.807785000	H	4.723739000	0.478779000	2.202817000
H	0.137637000	0.516458000	-2.629295000	H	7.058934000	0.917777000	2.913428000
C	3.436590000	-0.128131000	-3.551792000	H	8.840822000	-0.753663000	2.446883000
H	5.112877000	0.942532000	-2.664816000	H	8.266058000	-2.866404000	1.263465000
H	3.966410000	1.970846000	-3.521842000	H	5.921391000	-3.297709000	0.554330000
H	1.504405000	-0.838414000	-4.236126000	H	0.069656000	-3.182062000	-0.446685000
H	1.765661000	0.890306000	-4.476358000	H	1.260743000	-4.471948000	-0.320275000
H	3.942690000	-0.319164000	-4.505706000	H	3.409218000	-3.680382000	-2.136969000
H	3.595298000	-1.014819000	-2.926192000	H	3.668242000	-3.760355000	-4.607144000
C	0.925305000	5.322822000	-0.664494000	H	1.671517000	-3.563308000	-6.077585000

H	-0.584010000	-3.284705000	-5.054609000	N	0.393431000	-1.121178000	1.160085000
H	-0.825991000	-3.219354000	-2.594967000	C	0.322251000	-1.241849000	2.583828000
C	1.921133000	-3.150274000	3.553173000	C	1.274983000	-0.597611000	3.392316000
C	0.733820000	-3.394007000	2.677111000	C	1.169098000	-0.745314000	4.779731000
C	-0.363595000	-2.587412000	2.623405000	H	1.899446000	-0.261966000	5.422625000
C	-0.385905000	-1.309083000	3.359377000	C	0.138406000	-1.490537000	5.346518000
C	0.882404000	-0.921183000	4.093663000	C	-0.806013000	-2.102124000	4.527351000
C	1.624368000	-2.135084000	4.661297000	H	-1.615649000	-2.672497000	4.973174000
H	0.742313000	-4.290622000	2.064790000	C	-0.729904000	-1.998264000	3.135324000
H	2.757185000	-2.805334000	2.925464000	H	-0.435724000	-0.780642000	0.669285000
H	2.257434000	-4.103913000	3.980347000	C	2.380213000	0.262401000	2.803246000
H	0.619910000	-0.195408000	4.869768000	C	3.769483000	-0.300763000	3.139464000
H	1.522648000	-0.412638000	3.358851000	H	2.274382000	0.233523000	1.717902000
H	1.002532000	-2.611227000	5.430558000	H	3.965861000	-0.270097000	4.217793000
H	2.553267000	-1.818824000	5.147793000	H	3.843734000	-1.337561000	2.801438000
O	-1.371132000	-0.566769000	3.356222000	H	4.551186000	0.288974000	2.643954000
C	-1.447854000	-2.889819000	1.755157000	C	-1.765747000	-2.695923000	2.264764000
C	-2.313349000	-3.175394000	0.951072000	C	-1.733638000	-4.218296000	2.479281000
C	-3.211402000	-3.553829000	-0.086068000	H	-1.514851000	-2.514034000	1.218422000
C	-4.484571000	-2.971000000	-0.210981000	H	-2.009354000	-4.485988000	3.505857000
C	-2.798454000	-4.508473000	-1.039218000	H	-2.442104000	-4.712553000	1.804204000
C	-5.315065000	-3.327885000	-1.269073000	H	-0.733434000	-4.622353000	2.286338000
H	-4.804654000	-2.226410000	0.507172000	H	0.279204000	-2.976652000	-3.552812000
C	-3.633915000	-4.852687000	-2.096825000	C	-3.174902000	-2.123149000	2.487603000
H	-1.816683000	-4.960418000	-0.942935000	H	-3.194329000	-1.045706000	2.310812000
C	-4.895327000	-4.263384000	-2.216145000	H	-3.887182000	-2.595226000	1.801325000
H	-6.288415000	-2.856074000	-1.358585000	H	-3.521589000	-2.296963000	3.512721000
H	-3.298226000	-5.580149000	-2.830489000	C	2.242430000	1.729743000	3.243441000
H	-5.545278000	-4.531109000	-3.044407000	H	3.015313000	2.348507000	2.773254000
H	-7.225515000	-0.018964000	-1.141913000	H	1.267483000	2.139502000	2.959363000
TS2-*RR*				H	2.345328000	1.832586000	4.329875000
N	4.449648000	-1.564817000	-1.971286000	C	3.819726000	1.202087000	-1.326654000
N	2.881837000	0.172366000	-1.778493000	C	4.546902000	1.883431000	-2.497327000
N	2.174382000	-2.021163000	-1.877809000	C	3.057730000	2.236772000	-0.496329000
C	3.169368000	-1.122112000	-1.874068000	H	4.558267000	0.707329000	-0.682465000
C	2.187574000	-3.299422000	-2.595008000	C	5.493360000	2.980423000	-1.988945000
H	2.720993000	-3.188026000	-3.542110000	H	3.789504000	2.313987000	-3.165466000
H	2.677534000	-4.088256000	-2.008795000	H	5.100284000	1.143845000	-3.093283000
C	0.689435000	-3.582580000	-2.738276000	C	3.998822000	3.324864000	0.027919000
C	0.128835000	-3.104410000	-1.390856000	H	2.284185000	2.681980000	-1.129116000
H	0.306778000	-3.863610000	-0.620266000	H	2.536344000	1.739089000	0.325947000
H	-0.935401000	-2.869045000	-1.407584000	C	4.748812000	4.005654000	-1.123137000
C	0.954895000	-1.833196000	-1.081163000	H	5.980858000	3.473161000	-2.838521000
H	0.414757000	-0.947364000	-1.404889000	H	6.294449000	2.516539000	-1.394018000
H	0.480864000	-4.636769000	-2.941481000	H	3.425832000	4.061218000	0.598184000
O	2.352715000	-2.271511000	0.843891000	H	4.724863000	2.875126000	0.722525000
C	1.322898000	-1.757597000	0.406213000	H	5.450506000	4.753141000	-0.733802000

H	4.023387000	4.547168000	-1.744170000	H	-0.964711000	0.940291000	4.378363000
C	4.958212000	-2.635000000	-1.086196000	H	-0.905526000	1.594575000	1.991112000
C	5.857225000	-3.607033000	-1.851028000	C	-3.637866000	1.018082000	-3.461931000
C	5.679331000	-2.022738000	0.121622000	C	-2.828372000	1.762483000	-2.402248000
H	4.079070000	-3.153898000	-0.701191000	C	-1.388309000	1.697532000	-2.458727000
C	6.384886000	-4.704882000	-0.915858000	C	-0.713940000	0.633922000	-3.123976000
H	6.703948000	-3.051500000	-2.281361000	C	-1.573263000	-0.314009000	-3.950529000
H	5.303443000	-4.040990000	-2.691736000	C	-2.758397000	0.429446000	-4.569687000
C	6.203417000	-3.121565000	1.054255000	H	-3.213561000	2.754198000	-2.176682000
H	6.519282000	-1.403965000	-0.232224000	H	-4.216014000	0.200811000	-3.018507000
H	4.981936000	-1.370543000	0.655633000	H	-4.384616000	1.701031000	-3.882009000
C	7.104884000	-4.109940000	0.302397000	H	-0.925358000	-0.764059000	-4.709942000
H	7.053321000	-5.376135000	-1.467621000	H	-1.937913000	-1.126123000	-3.304963000
H	5.538926000	-5.316676000	-0.571110000	H	-2.377263000	1.233490000	-5.211734000
H	6.742428000	-2.670445000	1.895437000	H	-3.354465000	-0.238298000	-5.203524000
H	5.343979000	-3.655962000	1.481291000	O	0.533096000	0.448880000	-3.118968000
H	7.433790000	-4.911508000	0.974370000	C	-0.625899000	2.694028000	-1.797595000
H	8.012912000	-3.588606000	-0.034342000	C	-0.052224000	3.604637000	-1.222765000
O	-1.800238000	-0.656377000	-0.533393000	C	0.596983000	4.590792000	-0.424756000
O	-4.006399000	-1.088142000	-0.896337000	C	0.457597000	4.575953000	0.978620000
N	-4.910008000	0.967731000	-0.690506000	C	1.408784000	5.583476000	-1.007269000
C	-2.945293000	-0.230227000	-0.608770000	C	1.117597000	5.514505000	1.766715000
C	-3.505508000	1.109556000	-0.598200000	H	-0.172769000	3.821430000	1.438166000
C	-5.140547000	-0.286280000	-0.896027000	C	2.068569000	6.518238000	-0.213197000
C	-6.421906000	-0.942356000	-1.105096000	H	1.513279000	5.604819000	-2.087561000
C	-6.509086000	-2.335113000	-1.252884000	C	1.929229000	6.486980000	1.176167000
C	-7.750031000	-2.938305000	-1.443555000	H	1.001068000	5.484032000	2.846583000
C	-8.909889000	-2.163079000	-1.490614000	H	2.694453000	7.273836000	-0.680230000
C	-8.824863000	-0.774736000	-1.345032000	H	2.446119000	7.215988000	1.793716000
C	-7.590904000	-0.164509000	-1.153594000	H	1.945779000	0.470208000	-2.123545000
C	-2.975400000	2.167953000	0.345216000	H	5.127758000	-0.844471000	-2.189673000
C	-3.040596000	1.765354000	1.801202000	H	0.068012000	-1.588708000	6.426490000
C	-4.265843000	1.623286000	2.466447000	**TS2-*SR***			
C	-4.302234000	1.249568000	3.809216000	N	-0.015492000	-1.251425000	3.273050000
C	-3.115032000	1.012051000	4.506691000	N	0.246374000	-1.638805000	0.974391000
C	-1.891131000	1.143132000	3.852555000	N	0.571073000	0.488074000	1.838404000
C	-1.858978000	1.512895000	2.507621000	C	0.280907000	-0.801940000	2.012572000
H	-5.604152000	-2.931577000	-1.216254000	C	0.299573000	1.546583000	2.823697000
H	-7.811382000	-4.017074000	-1.556151000	H	-0.561436000	1.270766000	3.437009000
H	-9.875956000	-2.636659000	-1.640616000	H	1.172009000	1.680948000	3.475790000
H	-9.725316000	-0.168104000	-1.381907000	C	0.087843000	2.770121000	1.937048000
H	-7.505162000	0.910831000	-1.039385000	C	1.129283000	2.566979000	0.832265000
H	-1.942628000	2.392555000	0.085957000	H	2.117550000	2.882868000	1.182229000
H	-3.559397000	3.079917000	0.174260000	H	0.899049000	3.083081000	-0.099076000
H	-5.187353000	1.799441000	1.918851000	C	1.124655000	1.038681000	0.589257000
H	-5.259553000	1.141230000	4.312443000	H	0.466834000	0.810634000	-0.250844000
H	-3.143869000	0.714931000	5.551351000	H	0.215995000	3.709476000	2.479918000

O	3.218511000	0.024581000	1.259024000	H	1.157694000	-5.652374000	0.979216000
C	2.546035000	0.501202000	0.344541000	H	-0.869997000	-6.806209000	0.117928000
N	2.955870000	0.664056000	-0.932433000	H	-1.196879000	-5.461873000	-0.973467000
C	4.295708000	0.450751000	-1.383232000	C	0.933436000	-1.096919000	4.401571000
C	4.813188000	-0.851056000	-1.482329000	C	0.347468000	-1.810559000	5.621965000
C	6.119872000	-1.007019000	-1.961259000	C	2.333897000	-1.621856000	4.056960000
H	6.541307000	-2.005383000	-2.037674000	H	1.007866000	-0.032138000	4.639864000
C	6.878523000	0.090167000	-2.350088000	C	1.288071000	-1.688014000	6.828897000
C	6.343315000	1.373685000	-2.255584000	H	0.209141000	-2.875804000	5.377901000
H	6.943398000	2.224786000	-2.559376000	H	-0.643181000	-1.401331000	5.853774000
C	5.051903000	1.579774000	-1.766012000	C	3.271059000	-1.490008000	5.264150000
H	2.327745000	1.196684000	-1.561338000	H	2.248065000	-2.682070000	3.773457000
C	4.005736000	-2.076193000	-1.089569000	H	2.729926000	-1.081962000	3.190573000
C	4.613917000	-2.745654000	0.154568000	C	2.698177000	-2.197288000	6.499412000
H	2.998871000	-1.741122000	-0.831414000	H	0.868795000	-2.235747000	7.680779000
H	5.633529000	-3.095570000	-0.045858000	H	1.344784000	-0.632899000	7.132061000
H	4.643174000	-2.033370000	0.982591000	H	4.258071000	-1.893052000	5.011394000
H	4.021397000	-3.617130000	0.460709000	H	3.420060000	-0.424203000	5.489990000
C	4.492968000	2.981896000	-1.564280000	H	3.359105000	-2.057070000	7.362955000
C	4.735015000	3.417829000	-0.105404000	H	2.654806000	-3.279363000	6.308132000
H	3.413876000	2.948389000	-1.734391000	H	0.125747000	-1.260234000	0.026808000
H	5.808387000	3.545489000	0.080556000	H	-0.447007000	-2.166721000	3.266477000
H	4.235836000	4.371728000	0.103713000	O	-0.569007000	-1.161780000	-1.672225000
H	4.367163000	2.668574000	0.602228000	O	-2.030246000	-0.050872000	-0.350183000
H	-0.919066000	2.758363000	1.515252000	N	-3.825988000	0.175242000	-1.686560000
C	5.057075000	4.022398000	-2.539435000	C	-1.688865000	-0.677768000	-1.540917000
H	4.935208000	3.700940000	-3.579309000	C	-2.800954000	-0.451027000	-2.452928000
H	4.526068000	4.972346000	-2.414079000	C	-3.328204000	0.421026000	-0.527402000
H	6.121483000	4.219488000	-2.365075000	C	-3.946261000	1.092739000	0.601734000
C	3.869887000	-3.065301000	-2.258704000	C	-3.268939000	1.218211000	1.823144000
H	3.235563000	-3.912867000	-1.972761000	C	-3.868930000	1.883924000	2.888172000
H	3.418276000	-2.581351000	-3.131478000	C	-5.150758000	2.418229000	2.750160000
H	4.842154000	-3.468742000	-2.563493000	C	-5.835584000	2.280022000	1.538227000
C	0.055935000	-3.090187000	1.061346000	C	-5.238769000	1.625159000	0.466371000
C	-1.430480000	-3.481925000	0.999882000	C	-3.249167000	-1.564798000	-3.378533000
C	0.848797000	-3.778916000	-0.053462000	C	-3.687132000	-2.818986000	-2.641401000
H	0.481703000	-3.420770000	2.017450000	C	-4.699871000	-2.784996000	-1.671210000
C	-1.595101000	-5.004968000	1.090139000	C	-5.085838000	-3.947724000	-1.005697000
H	-1.848609000	-3.120988000	0.052923000	C	-4.479366000	-5.169251000	-1.308032000
H	-1.993346000	-2.980495000	1.798945000	C	-3.477190000	-5.215334000	-2.277179000
C	0.697684000	-5.301628000	0.043375000	C	-3.078714000	-4.046413000	-2.928169000
H	0.479858000	-3.420801000	-1.022292000	H	-2.277697000	0.794338000	1.923390000
H	1.897934000	-3.486865000	0.025381000	H	-3.332849000	1.991471000	3.826869000
C	-0.777251000	-5.718972000	0.005934000	H	-5.615217000	2.940914000	3.581213000
H	-2.655231000	-5.261991000	0.994541000	H	-6.833662000	2.694023000	1.427719000
H	-1.268220000	-5.350477000	2.082736000	H	-5.747636000	1.523205000	-0.486133000
H	1.251963000	-5.778730000	-0.773490000	H	-2.437738000	-1.832883000	-4.057412000

H	-4.074368000	-1.180134000	-3.990192000	H	0.838194000	-0.850286000	1.954929000
H	-5.179719000	-1.839469000	-1.441993000	H	3.811319000	-2.263449000	4.289810000
H	-5.871377000	-3.901715000	-0.256079000	O	3.273113000	-0.363225000	-0.111603000
H	-4.790427000	-6.077216000	-0.798745000	C	2.423424000	0.001147000	0.704625000
H	-3.003648000	-6.160712000	-2.527195000	N	1.921577000	1.251489000	0.815659000
H	-2.289999000	-4.086898000	-3.675536000	C	2.531347000	2.404544000	0.222330000
C	-1.623170000	0.544653000	-4.878540000	C	2.562449000	2.572514000	-1.174648000
C	-2.074330000	1.128614000	-3.555329000	C	3.177752000	3.717880000	-1.690489000
C	-1.085906000	1.868556000	-2.819644000	H	3.213970000	3.857659000	-2.766695000
C	0.310696000	1.651420000	-3.021070000	C	3.711883000	4.691677000	-0.855309000
C	0.784007000	0.767286000	-4.168498000	C	3.643999000	4.524745000	0.524305000
C	-0.274670000	-0.169100000	-4.756430000	H	4.048789000	5.291629000	1.177687000
H	-3.063416000	1.580218000	-3.573531000	C	3.072541000	3.379832000	1.088729000
H	-1.529704000	1.389480000	-5.578546000	H	1.253226000	1.416408000	1.588085000
H	-2.385424000	-0.112904000	-5.304850000	C	1.924456000	1.586632000	-2.136837000
H	1.659367000	0.205840000	-3.822492000	C	2.986865000	0.888899000	-3.002462000
H	1.153624000	1.456117000	-4.943202000	H	1.417776000	0.826182000	-1.541279000
H	-0.379382000	-1.037490000	-4.099435000	H	3.505734000	1.610835000	-3.644459000
H	0.048401000	-0.538861000	-5.737113000	H	3.722564000	0.390884000	-2.367894000
O	1.194509000	2.224157000	-2.327227000	H	2.520433000	0.142578000	-3.658661000
C	-1.467340000	2.810724000	-1.834890000	C	3.018695000	3.244611000	2.603839000
C	-1.744445000	3.660991000	-1.004941000	C	4.391482000	3.475063000	3.255878000
C	-1.985124000	4.653772000	-0.020048000	H	2.712164000	2.228557000	2.852156000
C	-0.972940000	5.579938000	0.315439000	H	4.739558000	4.506723000	3.131042000
C	-3.208354000	4.716781000	0.677771000	H	4.331901000	3.278115000	4.332572000
C	-1.175263000	6.515320000	1.325379000	H	5.151308000	2.812026000	2.826579000
H	-0.032461000	5.544600000	-0.225371000	H	2.078980000	-2.605604000	4.094874000
C	-3.401968000	5.658101000	1.683250000	C	1.950321000	4.183071000	3.191583000
H	-3.990107000	4.008505000	0.432576000	H	0.963903000	3.948678000	2.783021000
C	-2.388600000	6.559652000	2.018038000	H	1.896684000	4.062811000	4.279566000
H	-0.383018000	7.217900000	1.571208000	H	2.185013000	5.232017000	2.972033000
H	-4.349848000	5.679878000	2.214734000	C	0.862806000	2.268208000	-3.015699000
H	-2.542779000	7.291189000	2.806332000	H	0.386781000	1.524094000	-3.666595000
H	7.887809000	-0.051236000	-2.727443000	H	0.092552000	2.752181000	-2.410989000
TS2-*RS*				H	1.304607000	3.033492000	-3.663240000
N	2.602543000	-3.847173000	-0.347082000	C	0.039091000	-2.898067000	-1.519137000
N	0.553790000	-2.712049000	-0.153976000	C	-1.380648000	-3.475960000	-1.460984000
N	2.234138000	-2.360023000	1.396356000	C	0.094715000	-1.564828000	-2.275803000
C	1.789875000	-2.949582000	0.275224000	H	0.682151000	-3.617156000	-2.040146000
C	3.227406000	-2.962886000	2.296530000	C	-1.991376000	-3.583889000	-2.862817000
H	3.066843000	-4.041941000	2.353689000	H	-2.011146000	-2.824324000	-0.848501000
H	4.251017000	-2.781414000	1.945097000	H	-1.364440000	-4.450362000	-0.961110000
C	2.967595000	-2.201449000	3.596767000	C	-0.548854000	-1.669013000	-3.663319000
C	2.707017000	-0.776885000	3.094401000	H	-0.430971000	-0.819405000	-1.672611000
H	3.661462000	-0.286822000	2.869460000	H	1.137028000	-1.240984000	-2.348704000
H	2.147702000	-0.137231000	3.775874000	C	-1.974684000	-2.228690000	-3.580554000
C	1.907430000	-0.973803000	1.779906000	H	-3.014801000	-3.962948000	-2.775278000

H	-1.427231000	-4.318739000	-3.457149000	H	-5.404700000	-1.314690000	2.503587000
H	-0.552041000	-0.681483000	-4.138999000	H	-5.896660000	-1.885066000	-0.042989000
H	0.063122000	-2.322705000	-4.302684000	H	-6.006725000	-3.761852000	-1.660419000
H	-2.401861000	-2.324787000	-4.585864000	H	-4.694471000	-5.836226000	-1.254422000
H	-2.609760000	-1.520120000	-3.033399000	H	-3.277034000	-6.014981000	0.782771000
C	3.968583000	-3.453728000	-0.768740000	H	-3.168292000	-4.128708000	2.386800000
C	4.954339000	-4.605267000	-0.570795000	C	-3.369558000	0.294077000	4.318061000
C	3.956073000	-2.958024000	-2.220351000	C	-3.120779000	0.896330000	2.952090000
H	4.246622000	-2.601971000	-0.146547000	C	-1.806002000	1.424209000	2.703970000
C	6.364369000	-4.193794000	-1.018861000	C	-0.678806000	1.012618000	3.472812000
H	4.618897000	-5.471463000	-1.160813000	C	-0.898296000	0.186301000	4.735189000
H	4.952917000	-4.918516000	0.479729000	C	-2.208518000	-0.600137000	4.757327000
C	5.365505000	-2.546307000	-2.663920000	H	-3.936659000	1.504124000	2.569497000
H	3.580448000	-3.760143000	-2.875546000	H	-3.472372000	1.131218000	5.026355000
H	3.270922000	-2.109222000	-2.300631000	H	-4.322087000	-0.242405000	4.346325000
C	6.370033000	-3.689560000	-2.468634000	H	-0.035195000	-0.477575000	4.858441000
H	7.054159000	-5.037795000	-0.902162000	H	-0.866097000	0.890124000	5.580923000
H	6.729828000	-3.394840000	-0.357974000	H	-2.118912000	-1.447380000	4.069245000
H	5.346143000	-2.223351000	-3.711147000	H	-2.395462000	-1.008295000	5.758199000
H	5.677250000	-1.674969000	-2.072313000	O	0.505802000	1.359157000	3.216888000
H	7.377928000	-3.362164000	-2.749826000	C	-1.594529000	2.337985000	1.641197000
H	6.109626000	-4.520422000	-3.140644000	C	-1.415315000	3.159833000	0.757152000
O	-1.347023000	-1.571516000	1.581945000	C	-1.237998000	4.121239000	-0.274296000
O	-2.148789000	-0.263560000	-0.099999000	C	-0.013025000	4.803466000	-0.428109000
N	-4.261065000	0.120403000	0.582038000	C	-2.285041000	4.410202000	-1.175313000
C	-2.281058000	-0.932420000	1.105254000	C	0.159937000	5.721836000	-1.458678000
C	-3.601716000	-0.603866000	1.614307000	H	0.799796000	4.595991000	0.256377000
C	-3.390572000	0.330234000	-0.339751000	C	-2.100864000	5.329588000	-2.202134000
C	-3.556431000	1.077491000	-1.574658000	H	-3.231073000	3.891404000	-1.069171000
C	-2.484281000	1.291936000	-2.450729000	C	-0.878046000	5.988653000	-2.354040000
C	-2.676665000	2.015968000	-3.624105000	H	1.118371000	6.221540000	-1.563513000
C	-3.933262000	2.537185000	-3.930195000	H	-2.916802000	5.523950000	-2.893068000
C	-5.003833000	2.334763000	-3.052568000	H	-0.736811000	6.702748000	-3.160838000
C	-4.820860000	1.609004000	-1.881533000	H	-0.089324000	-2.230738000	0.494056000
C	-4.418194000	-1.717058000	2.249700000	H	2.127489000	-4.438243000	-1.018966000
C	-4.542082000	-2.887786000	1.292883000	H	4.172734000	5.581205000	-1.276540000
C	-5.334019000	-2.795365000	0.139503000	**TS2-SS**			
C	-5.385923000	-3.848444000	-0.772622000	N	4.753499000	0.911554000	0.044138000
C	-4.648305000	-5.013432000	-0.546245000	N	2.944636000	0.052877000	1.268302000
C	-3.854548000	-5.113093000	0.596869000	N	2.601930000	0.959693000	-0.836877000
C	-3.800235000	-4.055479000	1.505671000	C	3.420275000	0.607385000	0.159104000
H	-1.501100000	0.924187000	-2.191906000	C	2.909082000	2.006841000	-1.823701000
H	-1.835287000	2.196302000	-4.284978000	H	3.586240000	2.740474000	-1.384009000
H	-4.078142000	3.108404000	-4.842664000	H	3.376539000	1.563129000	-2.712067000
H	-5.982226000	2.746465000	-3.283383000	C	1.524313000	2.555170000	-2.164905000
H	-5.637369000	1.445858000	-1.186433000	C	0.648761000	1.297564000	-2.137811000
H	-3.948561000	-2.060571000	3.172968000	H	0.762321000	0.740447000	-3.075072000

H	-0.409822000	1.503525000	-1.982948000	C	3.753528000	-2.639116000	4.514059000
C	1.220612000	0.468642000	-0.963302000	H	3.746312000	-0.827854000	5.720980000
H	0.652897000	0.682358000	-0.056545000	H	5.136236000	-0.983048000	4.652519000
H	1.509953000	3.064327000	-3.132849000	H	3.874385000	-4.143796000	2.946109000
O	2.176861000	-1.627338000	-1.721427000	H	5.215448000	-3.003109000	2.960845000
C	1.189864000	-1.033607000	-1.291521000	H	4.293069000	-3.237049000	5.258500000
N	-0.042900000	-1.566271000	-1.132529000	H	2.681560000	-2.818436000	4.676404000
C	-0.480582000	-2.818333000	-1.663157000	C	5.562232000	0.432376000	-1.099007000
C	-0.012284000	-4.027075000	-1.119304000	C	7.004590000	0.903134000	-0.899437000
C	-0.489381000	-5.222814000	-1.667462000	C	5.480591000	-1.090941000	-1.270784000
H	-0.133365000	-6.167975000	-1.267234000	H	5.176743000	0.906229000	-2.006191000
C	-1.419146000	-5.221586000	-2.702467000	C	7.899604000	0.431157000	-2.053691000
C	-1.888157000	-4.013386000	-3.210690000	H	7.386168000	0.487378000	0.046672000
H	-2.615743000	-4.015479000	-4.017490000	H	7.029119000	1.995357000	-0.804330000
C	-1.428049000	-2.793227000	-2.706961000	C	6.373868000	-1.555850000	-2.427894000
H	-0.768369000	-0.949108000	-0.765703000	H	5.813983000	-1.565626000	-0.335240000
C	0.968078000	-4.060987000	0.040027000	H	4.439462000	-1.384658000	-1.439691000
C	2.315490000	-4.653653000	-0.402374000	C	7.823755000	-1.090567000	-2.240375000
H	1.133076000	-3.032912000	0.363725000	H	8.933624000	0.747032000	-1.872818000
H	2.195290000	-5.682270000	-0.763564000	H	7.578261000	0.926678000	-2.980897000
H	2.744129000	-4.048894000	-1.205424000	H	6.326715000	-2.647052000	-2.516205000
H	3.021348000	-4.678025000	0.436262000	H	5.979805000	-1.151270000	-3.371301000
C	-1.927748000	-1.487518000	-3.310728000	H	8.438286000	-1.395054000	-3.095940000
C	-1.408157000	-1.322238000	-4.749012000	H	8.249931000	-1.583936000	-1.354709000
H	-1.523337000	-0.661110000	-2.724974000	H	1.917561000	-0.019305000	1.420533000
H	-1.793346000	-2.112121000	-5.404572000	H	5.247249000	0.812602000	0.922315000
H	-1.722550000	-0.356569000	-5.162688000	O	-1.888650000	0.380878000	-0.307393000
H	-0.313799000	-1.371305000	-4.777117000	O	-4.021858000	-0.325331000	0.119186000
H	1.214291000	3.265106000	-1.393470000	N	-4.846171000	1.459978000	1.223803000
C	-3.458014000	-1.364502000	-3.243830000	C	-2.980081000	0.602148000	0.188604000
H	-3.807371000	-1.439838000	-2.210233000	C	-3.463523000	1.680205000	1.032514000
H	-3.775872000	-0.391269000	-3.635760000	C	-5.104609000	0.293053000	0.728940000
H	-3.955316000	-2.142353000	-3.835149000	C	-6.370250000	-0.423742000	0.726782000
C	0.390795000	-4.821346000	1.244829000	C	-6.492680000	-1.679029000	0.110940000
H	1.077298000	-4.754201000	2.097699000	C	-7.718054000	-2.341105000	0.121126000
H	-0.572366000	-4.399712000	1.549941000	C	-8.825799000	-1.763114000	0.743402000
H	0.239043000	-5.884346000	1.023108000	C	-8.704899000	-0.513445000	1.359605000
C	3.699483000	-0.741960000	2.245741000	C	-7.486380000	0.154851000	1.354420000
C	3.339778000	-0.284335000	3.665329000	C	-3.008497000	3.105896000	0.785489000
C	3.407507000	-2.234480000	2.043069000	C	-3.094799000	3.481646000	-0.678728000
H	4.772349000	-0.579813000	2.087007000	C	-4.322091000	3.490437000	-1.354665000
C	4.049801000	-1.146805000	4.716998000	C	-4.378179000	3.776624000	-2.717834000
H	2.252897000	-0.366276000	3.779874000	C	-3.207996000	4.059104000	-3.427490000
H	3.595917000	0.775269000	3.788890000	C	-1.982372000	4.055701000	-2.761956000
C	4.126114000	-3.086786000	3.094552000	C	-1.929711000	3.766678000	-1.397516000
H	2.324760000	-2.373403000	2.122268000	H	-5.629217000	-2.125740000	-0.369467000
H	3.698610000	-2.522172000	1.027785000	H	-7.807180000	-3.311988000	-0.357758000

H	-9.779481000	-2.283176000	0.750117000	C	0.420691000	1.105056000	-2.252883000
H	-9.564699000	-0.061494000	1.845997000	H	0.592657000	0.530136000	-3.169767000
H	-7.372759000	1.123926000	1.828535000	H	-0.651635000	1.149060000	-2.068543000
H	-1.979852000	3.231944000	1.126612000	C	1.154716000	0.427187000	-1.071833000
H	-3.645302000	3.756042000	1.396623000	H	0.624920000	0.633581000	-0.140051000
H	-5.230393000	3.256829000	-0.806053000	H	0.953591000	2.944173000	-3.341130000
H	-5.337100000	3.777855000	-3.229280000	O	2.250863000	-1.576847000	-1.882182000
H	-3.253589000	4.279868000	-4.490390000	C	1.279418000	-1.084344000	-1.314084000
H	-1.064917000	4.272887000	-3.303044000	N	0.175423000	-1.760507000	-0.916771000
H	-0.974725000	3.749689000	-0.881479000	C	-0.136424000	-3.121333000	-1.234182000
C	-3.315271000	0.122848000	3.457143000	C	0.569319000	-4.174248000	-0.626847000
C	-2.467346000	1.174541000	2.749787000	C	0.201505000	-5.484869000	-0.956783000
C	-1.090566000	0.862011000	2.448884000	H	0.739524000	-6.313755000	-0.506302000
C	-0.652660000	-0.490443000	2.314049000	C	-0.841800000	-5.742225000	-1.837974000
C	-1.650767000	-1.579134000	2.661179000	C	-1.535506000	-4.684182000	-2.421182000
C	-2.527544000	-1.136290000	3.834365000	H	-2.344717000	-4.892301000	-3.113817000
H	-2.617875000	2.183379000	3.126285000	C	-1.194110000	-3.359783000	-2.137950000
H	-4.165420000	-0.171824000	2.833368000	H	-0.554204000	-1.207319000	-0.478366000
H	-3.765004000	0.576092000	4.348322000	C	1.711481000	-3.933501000	0.344926000
H	-1.086379000	-2.489437000	2.883046000	C	3.050814000	-4.318766000	-0.307182000
H	-2.276052000	-1.790007000	1.781032000	H	1.727809000	-2.868676000	0.582479000
H	-1.883525000	-0.930160000	4.698812000	H	3.058356000	-5.379812000	-0.585687000
H	-3.219604000	-1.933816000	4.129243000	H	3.218737000	-3.719744000	-1.205197000
O	0.508496000	-0.832472000	1.963044000	H	3.880963000	-4.153548000	0.389396000
C	-0.169829000	1.885995000	2.140799000	C	-1.885676000	-2.206106000	-2.850603000
C	0.639448000	2.754750000	1.851499000	C	-1.155427000	-1.912528000	-4.174626000
C	1.526771000	3.762187000	1.393120000	H	-1.801471000	-1.316600000	-2.226194000
C	2.924165000	3.571194000	1.429570000	H	-1.243996000	-2.761718000	-4.862901000
C	1.033670000	4.966555000	0.843337000	H	-1.579761000	-1.028005000	-4.665258000
C	3.787664000	4.523122000	0.897013000	H	-0.088286000	-1.736839000	-4.001771000
H	3.312251000	2.663756000	1.876641000	H	0.719340000	3.160539000	-1.593528000
C	1.905128000	5.916857000	0.319839000	C	-3.386814000	-2.430571000	-3.076665000
H	-0.037987000	5.136381000	0.822343000	H	-3.892588000	-2.668442000	-2.134634000
C	3.285562000	5.698905000	0.332724000	H	-3.839430000	-1.518937000	-3.483030000
H	4.859601000	4.345254000	0.923886000	H	-3.586415000	-3.240819000	-3.787457000
H	1.503364000	6.832182000	-0.106220000	C	1.509208000	-4.684278000	1.670543000
H	3.961397000	6.440745000	-0.082522000	H	2.298088000	-4.408091000	2.380124000
H	-1.781574000	-6.161473000	-3.110441000	H	0.545771000	-4.435255000	2.124360000
INT4				H	1.552071000	-5.771647000	1.536756000
N	4.642617000	1.421741000	-0.332764000	C	4.021148000	-0.165797000	2.055164000
N	3.077856000	0.332365000	1.044280000	C	3.657411000	0.419202000	3.427321000
N	2.467964000	1.089118000	-1.066543000	C	4.006705000	-1.699389000	2.074217000
C	3.384451000	0.914843000	-0.104844000	H	5.035801000	0.157339000	1.793653000
C	2.559020000	2.148646000	-2.086373000	C	4.567309000	-0.144453000	4.526253000
H	3.139249000	2.985716000	-1.696253000	H	2.611377000	0.164517000	3.629549000
H	3.041156000	1.760352000	-2.992474000	H	3.721185000	1.513879000	3.392483000
C	1.092650000	2.477316000	-2.361546000	C	4.922814000	-2.249890000	3.172538000

H	2.974005000	-2.014954000	2.249225000	H	-6.031104000	-1.375561000	-1.436138000
H	4.302877000	-2.070694000	1.087628000	H	-8.346595000	-2.170965000	-1.850777000
C	4.542012000	-1.678677000	4.544516000	H	-10.155078000	-1.622031000	-0.239435000
H	4.260487000	0.256765000	5.499321000	H	-9.646595000	-0.277905000	1.788022000
H	5.600597000	0.196663000	4.359728000	H	-7.317187000	0.515004000	2.196732000
H	4.866734000	-3.345203000	3.182668000	H	-2.113530000	2.841880000	1.421253000
H	5.969812000	-1.992761000	2.949891000	H	-3.749296000	3.073947000	2.048928000
H	5.217775000	-2.060337000	5.319620000	H	-5.687217000	3.203746000	0.359004000
H	3.530298000	-2.018603000	4.805739000	H	-6.359414000	3.900916000	-1.923932000
C	5.436716000	0.972570000	-1.499523000	H	-4.641373000	4.182669000	-3.697682000
C	6.826836000	1.605685000	-1.406624000	H	-2.243605000	3.769492000	-3.168539000
C	5.516438000	-0.557647000	-1.598142000	H	-1.587311000	3.061606000	-0.884588000
H	4.954032000	1.355039000	-2.403851000	C	-3.077024000	-0.863154000	3.056123000
C	7.705220000	1.176972000	-2.589958000	C	-2.492305000	0.503969000	2.643176000
H	7.302700000	1.280727000	-0.467719000	C	-0.996242000	0.433609000	2.351166000
H	6.735134000	2.697489000	-1.360429000	C	-0.250960000	-0.755483000	2.432204000
C	6.392747000	-0.980765000	-2.783920000	C	-0.879381000	-2.005659000	3.025178000
H	5.949349000	-0.945469000	-0.663465000	C	-2.099340000	-1.688548000	3.884194000
H	4.508255000	-0.974598000	-1.693856000	H	-2.679073000	1.218001000	3.458837000
C	7.789761000	-0.351400000	-2.703631000	H	-3.324231000	-1.447617000	2.157353000
H	8.705791000	1.612405000	-2.484858000	H	-4.020746000	-0.699539000	3.583687000
H	7.280867000	1.586842000	-3.517563000	H	-0.093888000	-2.517036000	3.592151000
H	6.462926000	-2.073700000	-2.820354000	H	-1.159200000	-2.686008000	2.206235000
H	5.905956000	-0.669972000	-3.719568000	H	-1.791133000	-1.125758000	4.775483000
H	8.387371000	-0.630755000	-3.579583000	H	-2.581804000	-2.609210000	4.234631000
H	8.315362000	-0.749480000	-1.823439000	O	0.965933000	-0.867456000	2.061799000
H	2.086542000	0.086342000	1.293322000	C	-0.285520000	1.586664000	1.982942000
H	5.202781000	1.450336000	0.509461000	C	0.362095000	2.576102000	1.658277000
O	-2.008453000	0.153139000	-0.443182000	C	1.043865000	3.710126000	1.153780000
O	-4.212142000	-0.278038000	-0.259178000	C	2.455436000	3.771499000	1.144936000
N	-4.784666000	0.823589000	1.641182000	C	0.333782000	4.802791000	0.601934000
C	-3.039516000	0.307560000	0.161400000	C	3.122002000	4.847437000	0.568390000
C	-3.351902000	1.072450000	1.440206000	H	3.011733000	2.957587000	1.593644000
C	-5.186531000	0.099460000	0.672271000	C	1.009652000	5.879007000	0.036060000
C	-6.539089000	-0.383941000	0.408362000	H	-0.751171000	4.786143000	0.609050000
C	-6.824848000	-1.141715000	-0.735611000	C	2.406900000	5.907026000	0.003290000
C	-8.126235000	-1.583988000	-0.964086000	H	4.209069000	4.859097000	0.562788000
C	-9.141848000	-1.274786000	-0.058306000	H	0.439726000	6.701006000	-0.389182000
C	-8.856512000	-0.518420000	1.082753000	H	2.929535000	6.746505000	-0.445735000
C	-7.561101000	-0.072577000	1.318098000	H	-1.115777000	-6.767274000	-2.073349000
C	-3.161494000	2.605047000	1.253685000	**TS3-*SSS*$_a$**			
C	-3.589856000	3.092987000	-0.107361000	N	-3.816353000	1.109156000	-1.524270000
C	-4.935321000	3.331050000	-0.414407000	N	-2.405879000	0.630446000	0.272782000
C	-5.311467000	3.720413000	-1.700331000	N	-1.507058000	1.282201000	-1.774182000
C	-4.346907000	3.878744000	-2.696995000	C	-2.564682000	1.030181000	-0.987180000
C	-3.002689000	3.646798000	-2.400468000	C	-1.548165000	1.241070000	-3.244604000
C	-2.629691000	3.255626000	-1.115738000	H	-2.334708000	0.563732000	-3.573874000

H	-1.738138000	2.246570000	-3.641729000	H	-3.395520000	-1.211562000	1.984306000
C	-0.142127000	0.772621000	-3.609253000	C	-4.147571000	2.521488000	3.105280000
C	0.718898000	1.489893000	-2.566794000	H	-2.122224000	2.270188000	2.378647000
H	0.873118000	2.534465000	-2.860879000	H	-3.190746000	3.030691000	1.208467000
H	1.696975000	1.036536000	-2.406369000	C	-4.092379000	1.418912000	4.171225000
C	-0.133404000	1.435355000	-1.274701000	H	-4.187878000	-0.751519000	4.298358000
H	0.154155000	0.569836000	-0.673152000	H	-5.300103000	-0.041129000	3.133122000
H	0.126365000	1.032922000	-4.637080000	H	-3.953874000	3.503815000	3.553343000
O	-0.771210000	3.645697000	-0.503936000	H	-5.163074000	2.566875000	2.682740000
C	0.050005000	2.735833000	-0.474148000	H	-4.849755000	1.598580000	4.944553000
N	1.247444000	2.775826000	0.164119000	H	-3.113335000	1.452070000	4.671003000
C	1.867705000	3.945242000	0.709810000	C	-4.313019000	2.268689000	-2.292149000
C	1.363454000	4.538801000	1.881249000	C	-5.798563000	2.054574000	-2.589046000
C	2.023912000	5.666336000	2.382613000	C	-4.076532000	3.599514000	-1.564898000
H	1.644183000	6.144905000	3.280530000	H	-3.788011000	2.301604000	-3.251949000
C	3.158368000	6.176390000	1.760715000	C	-6.362467000	3.223511000	-3.407024000
C	3.650395000	5.564935000	0.611498000	H	-6.342911000	1.976600000	-1.637083000
H	4.534445000	5.967125000	0.124936000	H	-5.941319000	1.101540000	-3.110258000
C	3.015832000	4.447093000	0.062238000	C	-4.630794000	4.767979000	-2.389827000
H	1.832857000	1.951586000	0.079450000	H	-4.591162000	3.558332000	-0.594198000
C	0.138133000	4.003967000	2.601656000	H	-3.009282000	3.732799000	-1.358822000
C	-1.032782000	4.992258000	2.467743000	C	-6.118210000	4.569540000	-2.710687000
H	-0.142948000	3.061471000	2.128436000	H	-7.433830000	3.069046000	-3.581176000
H	-0.775152000	5.963675000	2.906806000	H	-5.883278000	3.234538000	-4.396560000
H	-1.283193000	5.138330000	1.414706000	H	-4.474827000	5.709072000	-1.850474000
H	-1.918398000	4.615386000	2.990777000	H	-4.063544000	4.850108000	-3.328654000
C	3.554310000	3.835768000	-1.223857000	H	-6.488873000	5.390645000	-3.335911000
C	3.345604000	4.796740000	-2.406835000	H	-6.694846000	4.600226000	-1.774915000
H	2.985776000	2.931290000	-1.439707000	H	-1.462204000	0.397598000	0.615901000
H	3.906763000	5.727960000	-2.267317000	H	-4.527210000	0.639939000	-0.974166000
H	3.684332000	4.335799000	-3.342523000	O	3.087375000	0.561879000	-0.407956000
H	2.287295000	5.059772000	-2.513310000	O	5.224997000	-0.060284000	-0.046975000
H	-0.076096000	-0.312326000	-3.495951000	N	5.028790000	-2.265891000	0.462843000
C	5.025076000	3.409817000	-1.092994000	C	3.877223000	-0.307180000	-0.134056000
H	5.150987000	2.695482000	-0.274148000	C	3.675299000	-1.787182000	0.175164000
H	5.361752000	2.924954000	-2.016720000	C	5.822455000	-1.281951000	0.300463000
H	5.681220000	4.267765000	-0.906269000	C	7.276682000	-1.267232000	0.419086000
C	0.430199000	3.693913000	4.078922000	C	8.011535000	-0.102308000	0.159465000
H	-0.438094000	3.205083000	4.536918000	C	9.400154000	-0.123435000	0.269901000
H	1.290677000	3.025501000	4.182887000	C	10.056815000	-1.298698000	0.637650000
H	0.639556000	4.603231000	4.654316000	C	9.323328000	-2.460845000	0.896332000
C	-3.372614000	0.870359000	1.361528000	C	7.937711000	-2.449077000	0.787902000
C	-3.258936000	-0.221514000	2.426727000	C	3.133434000	-2.517517000	-1.077162000
C	-3.141435000	2.255119000	1.979329000	C	3.886989000	-2.208382000	-2.347599000
H	-4.382747000	0.832173000	0.940428000	C	5.163233000	-2.731855000	-2.595262000
C	-4.279812000	0.032507000	3.542299000	C	5.856238000	-2.389925000	-3.755909000
H	-2.247221000	-0.197781000	2.845584000	C	5.281672000	-1.525648000	-4.689969000

C	4.004748000	-1.012489000	-4.461200000	C	-4.258381000	-3.387566000	-0.129142000
C	3.314890000	-1.353920000	-3.298505000	C	-5.362979000	-2.556450000	-0.582040000
H	7.494320000	0.805737000	-0.129238000	C	-5.867848000	-2.672535000	-1.887688000
H	9.969517000	0.778802000	0.067871000	C	-6.887662000	-1.826990000	-2.322899000
H	11.139585000	-1.311070000	0.722898000	C	-7.416630000	-0.857557000	-1.468983000
H	9.834586000	-3.375081000	1.182567000	C	-6.917421000	-0.738479000	-0.165777000
H	7.349345000	-3.339043000	0.984065000	C	-5.901892000	-1.579531000	0.277132000
H	2.093693000	-2.219869000	-1.193897000	C	-1.794597000	-4.670305000	2.084968000
H	3.152739000	-3.588220000	-0.846613000	C	-1.898049000	-3.785409000	3.305977000
H	5.612138000	-3.404539000	-1.871558000	C	-0.900358000	-2.856351000	3.615027000
H	6.846024000	-2.801688000	-3.932460000	C	-1.006928000	-2.038705000	4.741131000
H	5.823303000	-1.260929000	-5.593699000	C	-2.112194000	-2.147458000	5.584885000
H	3.543091000	-0.349354000	-5.187683000	C	-3.115356000	-3.071940000	5.285512000
H	2.314618000	-0.968731000	-3.127862000	C	-3.009224000	-3.876874000	4.152428000
C	3.496126000	-1.460183000	2.684728000	H	-5.447616000	-3.422601000	-2.548154000
C	2.745916000	-1.978244000	1.431780000	H	-7.272763000	-1.928253000	-3.333947000
C	1.360846000	-1.356360000	1.245420000	H	-8.212452000	-0.202332000	-1.810944000
C	0.925214000	-0.207146000	2.010441000	H	-7.332991000	0.003723000	0.511201000
C	1.730644000	0.192672000	3.233420000	H	-5.518738000	-1.507794000	1.288125000
C	2.558925000	-0.968221000	3.781666000	H	-0.741602000	-4.871023000	1.850990000
H	2.629671000	-3.065109000	1.521960000	H	-2.249106000	-5.645800000	2.306082000
H	4.144031000	-0.615879000	2.411600000	H	-0.040148000	-2.764873000	2.960198000
H	4.163850000	-2.247215000	3.045140000	H	-0.224080000	-1.319273000	4.963239000
H	1.019595000	0.590732000	3.963441000	H	-2.193428000	-1.516799000	6.466048000
H	2.391545000	1.028115000	2.956204000	H	-3.982032000	-3.164632000	5.934876000
H	1.899416000	-1.778750000	4.115121000	H	-3.796228000	-4.588309000	3.916897000
H	3.138388000	-0.648055000	4.655232000	H	-1.377733000	-3.190752000	0.359481000
O	-0.109627000	0.444303000	1.757701000	**TS3-*SSR*$_a$**			
C	0.462734000	-1.902488000	0.382685000	N	-3.788615000	1.111383000	-1.503646000
C	-0.467532000	-2.453597000	-0.287768000	N	-2.253836000	1.093828000	0.272722000
C	-0.861484000	-2.449259000	-1.704464000	N	-1.517065000	1.128648000	-1.944754000
C	-2.135420000	-1.983697000	-2.062218000	C	-2.497853000	1.113450000	-1.035729000
C	-0.039913000	-2.984345000	-2.710429000	C	-1.693022000	0.690987000	-3.337489000
C	-2.565320000	-2.019015000	-3.385868000	H	-2.498301000	-0.042909000	-3.387942000
H	-2.790861000	-1.608114000	-1.287808000	H	-1.942411000	1.549321000	-3.973878000
C	-0.467820000	-3.010940000	-4.036982000	C	-0.315276000	0.135484000	-3.699111000
H	0.921751000	-3.409434000	-2.450141000	C	0.639170000	1.068050000	-2.941809000
C	-1.729801000	-2.523431000	-4.383906000	H	0.816082000	1.980490000	-3.522099000
H	-3.563907000	-1.663880000	-3.625587000	H	1.605454000	0.616128000	-2.714135000
H	0.185237000	-3.427748000	-4.798561000	C	-0.116678000	1.425323000	-1.636066000
H	-2.065080000	-2.557803000	-5.416510000	H	0.234279000	0.799489000	-0.814842000
H	3.659199000	7.049206000	2.170846000	H	-0.143791000	0.144927000	-4.779500000
O	-2.003198000	-5.808895000	-0.834957000	O	-0.736322000	3.754226000	-1.780364000
O	-3.780718000	-4.348605000	-0.987207000	C	0.050036000	2.921744000	-1.337038000
N	-3.580091000	-3.236039000	0.963193000	N	1.172172000	3.194949000	-0.632783000
C	-2.630102000	-4.898354000	-0.346224000	C	1.661151000	4.491248000	-0.293982000
C	-2.451256000	-4.074078000	0.849192000	C	0.898786000	5.357862000	0.516043000

C	1.439311000	6.614709000	0.810646000	C	-4.139908000	3.585810000	-1.609828000
H	0.863299000	7.307054000	1.417481000	H	-3.668756000	2.274378000	-3.239263000
C	2.702559000	6.987331000	0.362407000	C	-6.286678000	3.103535000	-3.589682000
C	3.454027000	6.100295000	-0.401872000	H	-6.335662000	1.835828000	-1.832968000
H	4.445030000	6.387846000	-0.741508000	H	-5.775238000	1.006151000	-3.285002000
C	2.946264000	4.846162000	-0.752619000	C	-4.695681000	4.725497000	-2.471500000
H	1.724862000	2.394809000	-0.348921000	H	-4.698515000	3.536846000	-0.662941000
C	-0.459925000	4.977874000	1.088349000	H	-3.086832000	3.763104000	-1.372494000
C	-1.584693000	5.798856000	0.434340000	C	-6.150338000	4.457110000	-2.878664000
H	-0.630892000	3.921606000	0.879009000	H	-7.335726000	2.901070000	-3.835764000
H	-1.486976000	6.863877000	0.678935000	H	-5.742712000	3.141226000	-4.544330000
H	-1.557189000	5.682313000	-0.650354000	H	-4.613654000	5.673930000	-1.928477000
H	-2.563314000	5.461503000	0.798816000	H	-4.074738000	4.828689000	-3.372682000
C	3.787750000	3.901356000	-1.599841000	H	-6.522657000	5.260324000	-3.525767000
C	4.177042000	4.538903000	-2.943501000	H	-6.783430000	4.457513000	-1.979368000
H	3.189551000	3.016024000	-1.825779000	H	-1.292510000	0.994462000	0.633474000
H	4.816609000	5.417916000	-2.803975000	H	-4.465277000	0.822899000	-0.808844000
H	4.728864000	3.820192000	-3.560685000	O	2.854868000	0.697685000	-0.414699000
H	3.287681000	4.857167000	-3.497634000	O	4.986749000	-0.018063000	-0.243760000
H	-0.225958000	-0.884940000	-3.324419000	N	4.833901000	-1.726341000	1.246352000
C	5.030176000	3.423173000	-0.829308000	C	3.648510000	-0.075201000	0.064942000
H	4.750347000	2.943526000	0.114057000	C	3.470579000	-1.232993000	1.045074000
H	5.590639000	2.690765000	-1.421027000	C	5.602113000	-1.037067000	0.499915000
H	5.698547000	4.260309000	-0.595832000	C	7.043972000	-1.174980000	0.318187000
C	-0.495180000	5.136419000	2.617629000	C	7.750652000	-0.322529000	-0.540535000
H	-1.466605000	4.810568000	3.007023000	C	9.125768000	-0.483485000	-0.696396000
H	0.278490000	4.531420000	3.099542000	C	9.797318000	-1.489731000	-0.000791000
H	-0.351129000	6.178339000	2.925279000	C	9.091887000	-2.340598000	0.855876000
C	-3.295426000	1.213082000	1.310232000	C	7.719946000	-2.186867000	1.016904000
C	-3.963770000	-0.142787000	1.584721000	C	2.613075000	-2.338154000	0.380029000
C	-2.698746000	1.789970000	2.598220000	C	3.163143000	-2.803865000	-0.947003000
H	-4.047219000	1.923194000	0.940777000	C	4.203952000	-3.739245000	-1.014530000
C	-5.022047000	-0.044102000	2.688808000	C	4.701782000	-4.160704000	-2.246917000
H	-3.183443000	-0.851013000	1.879088000	C	4.166867000	-3.649177000	-3.431124000
H	-4.418284000	-0.543976000	0.674161000	C	3.130971000	-2.715934000	-3.373693000
C	-3.778176000	1.918046000	3.680088000	C	2.633304000	-2.296417000	-2.140447000
H	-1.901630000	1.126110000	2.947299000	H	7.221123000	0.455704000	-1.078337000
H	-2.232732000	2.756135000	2.387200000	H	9.672776000	0.177327000	-1.362201000
C	-4.442627000	0.566167000	3.969634000	H	10.869392000	-1.612698000	-0.125167000
H	-5.427420000	-1.042720000	2.886880000	H	9.614409000	-3.124070000	1.396675000
H	-5.861190000	0.573581000	2.333828000	H	7.152791000	-2.835688000	1.675607000
H	-3.328848000	2.326412000	4.593099000	H	1.603471000	-1.948549000	0.242764000
H	-4.540781000	2.642283000	3.355332000	H	2.569532000	-3.165730000	1.095889000
H	-5.230580000	0.681868000	4.724039000	H	4.620444000	-4.136476000	-0.093809000
H	-3.698315000	-0.119429000	4.389453000	H	5.505033000	-4.891495000	-2.282906000
C	-4.276595000	2.237413000	-2.331290000	H	4.552110000	-3.980780000	-4.391475000
C	-5.723529000	1.955589000	-2.740035000	H	2.698829000	-2.322614000	-4.289901000

H	1.799087000	-1.607994000	-2.090314000	C	0.569227000	-5.251121000	-1.676740000
C	3.818126000	0.258245000	3.105226000	H	-4.659200000	-1.301107000	-2.441784000
C	2.864233000	-0.766788000	2.417666000	H	-7.098367000	-1.069797000	-2.839469000
C	1.436369000	-0.262418000	2.267873000	H	-8.716189000	-2.254300000	-1.371544000
C	1.178020000	1.140741000	2.054844000	H	-7.881775000	-3.689335000	0.480766000
C	2.251334000	2.113808000	2.522679000	H	-5.431954000	-3.921574000	0.864500000
C	3.093117000	1.493436000	3.639048000	H	-0.866691000	-5.022214000	1.307599000
H	2.841504000	-1.683797000	3.014327000	H	0.448510000	-4.050912000	0.654211000
H	4.575594000	0.605660000	2.391819000	H	-2.502736000	-6.086364000	-0.504850000
H	4.374567000	-0.243867000	3.902285000	H	-2.505719000	-7.412074000	-2.600884000
H	1.745945000	3.030811000	2.836581000	H	-0.540885000	-7.340809000	-4.124211000
H	2.897884000	2.393015000	1.679302000	H	1.434932000	-5.941880000	-3.517268000
H	2.439206000	1.220567000	4.476869000	H	1.431620000	-4.645425000	-1.423929000
H	3.822700000	2.216572000	4.021912000	H	-1.163967000	-2.522984000	1.389307000
O	0.110629000	1.594800000	1.595183000	**INT5**			
C	0.367645000	-1.085700000	2.421500000	N	6.027544000	0.547535000	-0.453413000
C	-0.662304000	-1.816310000	2.573452000	N	3.750384000	1.081033000	-0.481753000
C	-1.507595000	-2.079911000	3.741529000	N	4.541597000	-0.655590000	-1.786016000
C	-1.232693000	-1.469912000	4.981140000	C	4.767317000	0.329863000	-0.892317000
C	-2.633136000	-2.916029000	3.644387000	C	5.412098000	-0.933943000	-2.938157000
C	-2.053314000	-1.687510000	6.082931000	H	6.079623000	-0.087041000	-3.113273000
H	-0.366632000	-0.818622000	5.060364000	H	6.011223000	-1.836102000	-2.760083000
C	-3.457108000	-3.127395000	4.750455000	C	4.389039000	-1.163570000	-4.053778000
H	-2.871440000	-3.387917000	2.696502000	C	3.295679000	-1.960662000	-3.332313000
C	-3.173542000	-2.517269000	5.972269000	H	3.607056000	-3.002579000	-3.215940000
H	-1.823962000	-1.205491000	7.029778000	H	2.329084000	-1.930080000	-3.837197000
H	-4.325582000	-3.773726000	4.653881000	C	3.213466000	-1.296925000	-1.939351000
H	-3.818266000	-2.682773000	6.830909000	H	2.433451000	-0.538388000	-1.938443000
H	3.103687000	7.965134000	0.615026000	H	4.814122000	-1.696106000	-4.909482000
O	-0.333834000	-1.649062000	-1.115519000	O	3.841882000	-3.283987000	-0.737741000
O	-2.602462000	-1.929203000	-1.184940000	C	3.033010000	-2.362977000	-0.850189000
N	-2.902998000	-3.555480000	0.348087000	N	1.915864000	-2.243960000	-0.091784000
C	-1.314099000	-2.256748000	-0.725209000	C	1.453043000	-3.257629000	0.812313000
C	-1.509591000	-3.252705000	0.325012000	C	2.074186000	-3.431022000	2.058576000
C	-3.469159000	-2.765860000	-0.495151000	C	1.538849000	-4.383061000	2.936010000
C	-4.894494000	-2.632176000	-0.766446000	H	2.003518000	-4.533426000	3.906137000
C	-5.368190000	-1.826177000	-1.813295000	C	0.416924000	-5.124563000	2.588377000
C	-6.739157000	-1.694646000	-2.026556000	C	-0.176672000	-4.948316000	1.339235000
C	-7.648327000	-2.361666000	-1.204212000	H	-1.045374000	-5.540406000	1.075782000
C	-7.178509000	-3.168918000	-0.163176000	C	0.334129000	-4.027061000	0.420728000
C	-5.812923000	-3.305505000	0.057165000	H	1.384092000	-1.378440000	-0.103544000
C	-0.552520000	-4.432688000	0.438482000	C	3.291717000	-2.628806000	2.481841000
C	-0.531726000	-5.281298000	-0.814512000	C	4.511671000	-3.551959000	2.633240000
C	-1.638339000	-6.068518000	-1.162299000	H	3.513977000	-1.910116000	1.690626000
C	-1.640495000	-6.805633000	-2.345397000	H	4.339813000	-4.313916000	3.402340000
C	-0.536823000	-6.766468000	-3.201524000	H	4.718488000	-4.055541000	1.685130000
C	0.568552000	-5.986521000	-2.862753000	H	5.396684000	-2.976214000	2.927904000

C	-0.260485000	-3.882416000	-0.973835000	H	9.808824000	-2.716732000	1.480452000
C	0.643822000	-4.561594000	-2.022936000	H	8.752488000	-1.647235000	2.399094000
H	-0.300353000	-2.815262000	-1.210764000	H	3.023454000	1.275061000	-1.225805000
H	0.604056000	-5.651496000	-1.906491000	H	6.147515000	1.390661000	0.091096000
H	0.297454000	-4.309314000	-3.031516000	O	-2.378560000	-1.456680000	0.013992000
H	1.690020000	-4.264215000	-1.927931000	O	-4.447837000	-2.216377000	0.521827000
H	3.994901000	-0.198756000	-4.390057000	N	-5.326556000	-0.487154000	1.703967000
C	-1.686522000	-4.429098000	-1.102532000	C	-3.455980000	-1.253487000	0.505248000
H	-2.361938000	-3.977740000	-0.372196000	C	-4.025357000	-0.028492000	1.214706000
H	-2.069174000	-4.199708000	-2.101389000	C	-5.502568000	-1.668969000	1.256046000
H	-1.712229000	-5.519342000	-0.985876000	C	-6.681418000	-2.516360000	1.410847000
C	3.024923000	-1.828640000	3.766471000	C	-6.737451000	-3.787389000	0.823600000
H	3.905274000	-1.233565000	4.035474000	C	-7.880882000	-4.568645000	0.976090000
H	2.181327000	-1.145213000	3.630062000	C	-8.965885000	-4.087866000	1.710422000
H	2.797675000	-2.486374000	4.613056000	C	-8.910045000	-2.819038000	2.295578000
C	3.739978000	1.933644000	0.709561000	C	-7.773375000	-2.032788000	2.147636000
C	2.548225000	2.894404000	0.617765000	C	-4.245633000	1.122768000	0.181663000
C	3.659244000	1.079599000	1.982566000	C	-4.945338000	0.686764000	-1.084687000
H	4.654077000	2.551792000	0.742897000	C	-6.304960000	0.341800000	-1.096383000
C	2.489046000	3.783196000	1.864295000	C	-6.906683000	-0.123999000	-2.264581000
H	1.627571000	2.301916000	0.540681000	C	-6.160578000	-0.244842000	-3.439039000
H	2.620799000	3.494650000	-0.294939000	C	-4.815370000	0.123619000	-3.444003000
C	3.562508000	1.953827000	3.238528000	C	-4.213766000	0.592182000	-2.275528000
H	2.767402000	0.450113000	1.896034000	H	-5.891674000	-4.150047000	0.250677000
H	4.525324000	0.408214000	2.042471000	H	-7.924978000	-5.552703000	0.519183000
C	2.387697000	2.935125000	3.137290000	H	-9.856073000	-4.699459000	1.826378000
H	1.640802000	4.467179000	1.792015000	H	-9.755168000	-2.444624000	2.865548000
H	3.394443000	4.407273000	1.914489000	H	-7.709437000	-1.044729000	2.590739000
H	3.459098000	1.313970000	4.122988000	H	-3.271185000	1.541623000	-0.076105000
H	4.498054000	2.518946000	3.367852000	H	-4.817573000	1.892191000	0.711990000
H	2.344324000	3.579313000	4.023065000	H	-6.889732000	0.436997000	-0.187129000
H	1.447207000	2.368705000	3.109324000	H	-7.959909000	-0.391857000	-2.257234000
C	7.077746000	-0.472288000	-0.285507000	H	-6.629877000	-0.613421000	-4.347231000
C	8.305325000	0.208932000	0.328899000	H	-4.224520000	0.043598000	-4.351467000
C	6.611295000	-1.656253000	0.570790000	H	-3.178124000	0.915270000	-2.291057000
H	7.361622000	-0.845754000	-1.275794000	C	-3.085637000	-0.526106000	3.584021000
C	9.446013000	-0.795442000	0.537735000	C	-3.134074000	0.459928000	2.403553000
H	8.018707000	0.639581000	1.300796000	C	-1.718082000	0.825991000	1.952793000
H	8.631164000	1.038536000	-0.311074000	C	-0.627877000	-0.197222000	1.972947000
C	7.752204000	-2.660716000	0.773569000	C	-0.782190000	-1.367134000	2.930266000
H	6.281433000	-1.266931000	1.544079000	C	-2.215719000	-1.755806000	3.308909000
H	5.752397000	-2.148486000	0.106834000	H	-3.627608000	1.374246000	2.747394000
C	8.991139000	-1.992850000	1.382754000	H	-4.105808000	-0.820680000	3.847497000
H	10.298883000	-0.291697000	1.007068000	H	-2.674895000	0.014069000	4.447561000
H	9.792974000	-1.152621000	-0.442207000	H	-0.248415000	-1.046608000	3.839028000
H	7.404597000	-3.484004000	1.406606000	H	-0.224980000	-2.214273000	2.530583000
H	8.016526000	-3.105765000	-0.196515000	H	-2.189117000	-2.395662000	4.198146000

H	-2.650102000	-2.373194000	2.517190000	H	-1.393127000	3.541114000	0.182383000
O	0.403634000	-0.054312000	1.322673000	**TS4-*SSR***			
C	-1.444842000	2.059087000	1.580187000	N	5.770100000	1.768564000	0.107825000
C	-1.283130000	3.312099000	1.240966000	N	3.512511000	1.396216000	0.594075000
C	-0.962944000	4.429264000	2.141448000	N	4.352801000	0.868830000	-1.498313000
C	-0.794104000	4.246983000	3.523493000	C	4.537180000	1.339426000	-0.251045000
C	-0.816341000	5.715780000	1.600910000	C	4.958967000	1.475326000	-2.694601000
C	-0.464961000	5.322407000	4.341244000	H	5.328672000	2.475130000	-2.456782000
H	-0.911843000	3.252844000	3.946022000	H	5.790666000	0.858057000	-3.057081000
C	-0.488166000	6.791432000	2.424176000	C	3.788733000	1.457853000	-3.681213000
H	-0.949248000	5.867114000	0.536246000	C	3.139005000	0.100066000	-3.389352000
C	-0.306630000	6.599844000	3.794136000	H	3.719342000	-0.703214000	-3.852424000
H	-0.330349000	5.166747000	5.408234000	H	2.104390000	0.033285000	-3.730210000
H	-0.373875000	7.779581000	1.987701000	C	3.233047000	-0.032991000	-1.854674000
H	-0.047150000	7.438170000	4.434513000	H	2.314256000	0.320736000	-1.395031000
H	0.005168000	-5.848554000	3.286535000	H	4.114704000	1.563629000	-4.719852000
O	2.215722000	1.611633000	-2.569916000	O	4.564218000	-2.039872000	-1.914710000
O	0.837163000	3.467146000	-2.397077000	C	3.573253000	-1.474148000	-1.450743000
N	-1.145827000	2.502453000	-2.017769000	N	2.678346000	-2.038938000	-0.609679000
C	1.050421000	2.077213000	-2.388894000	C	2.633404000	-3.438509000	-0.314801000
C	-0.196787000	1.511946000	-2.147127000	C	3.572200000	-4.018085000	0.551463000
C	-0.505922000	3.638467000	-2.169350000	C	3.462410000	-5.387949000	0.821924000
C	-1.030621000	4.978076000	-2.026988000	H	4.183522000	-5.859462000	1.483623000
C	-0.183527000	6.102346000	-2.053944000	C	2.442123000	-6.147957000	0.263854000
C	-0.700084000	7.377966000	-1.840114000	C	1.509782000	-5.551067000	-0.583528000
C	-2.063409000	7.561476000	-1.595558000	H	0.714756000	-6.153590000	-1.008154000
C	-2.912334000	6.449164000	-1.580625000	C	1.588371000	-4.191441000	-0.895198000
C	-2.408461000	5.172257000	-1.797280000	H	1.968455000	-1.440694000	-0.164488000
C	-0.496286000	0.057317000	-2.015070000	C	4.682974000	-3.208602000	1.196758000
C	-0.704286000	-0.701934000	-3.313837000	C	6.058487000	-3.663313000	0.684174000
C	-1.730115000	-1.646215000	-3.426841000	H	4.548036000	-2.165258000	0.902045000
C	-1.895684000	-2.386753000	-4.599901000	H	6.245625000	-4.715231000	0.929768000
C	-1.032347000	-2.192987000	-5.678279000	H	6.108560000	-3.543786000	-0.401212000
C	-0.009773000	-1.245772000	-5.577234000	H	6.856524000	-3.067559000	1.143198000
C	0.150256000	-0.503133000	-4.407278000	C	0.606942000	-3.535338000	-1.859593000
H	0.877021000	5.958044000	-2.229385000	C	1.238725000	-3.391189000	-3.258503000
H	-0.031541000	8.234904000	-1.858865000	H	0.397442000	-2.525637000	-1.489565000
H	-2.461214000	8.557356000	-1.423130000	H	1.378784000	-4.379528000	-3.712624000
H	-3.975478000	6.580349000	-1.397184000	H	0.585374000	-2.800144000	-3.909813000
H	-3.060719000	4.304879000	-1.786684000	H	2.219008000	-2.909485000	-3.216708000
H	-1.359597000	-0.079338000	-1.366678000	H	3.096806000	2.269851000	-3.434963000
H	0.334336000	-0.417430000	-1.479329000	C	-0.737752000	-4.263849000	-1.960048000
H	-2.403094000	-1.798534000	-2.589691000	H	-1.201792000	-4.397885000	-0.977817000
H	-2.704030000	-3.110427000	-4.669840000	H	-1.428418000	-3.679184000	-2.571725000
H	-1.158272000	-2.767594000	-6.592015000	H	-0.628762000	-5.248562000	-2.429732000
H	0.662518000	-1.081174000	-6.415753000	C	4.601808000	-3.269791000	2.730812000
H	0.944143000	0.234017000	-4.329113000	H	5.370259000	-2.631055000	3.182756000

H	3.623253000	-2.929787000	3.087067000	C	-8.943321000	-4.357786000	2.172018000
H	4.758202000	-4.288725000	3.102471000	C	-8.604861000	-3.199880000	2.879258000
C	3.560015000	1.530652000	2.052033000	C	-7.456014000	-2.491059000	2.547583000
C	2.348612000	2.348929000	2.511889000	C	-4.162138000	0.656909000	0.217959000
C	3.598679000	0.148167000	2.718001000	C	-5.157181000	0.482000000	-0.903910000
H	4.464678000	2.084086000	2.342710000	C	-6.524986000	0.298665000	-0.657384000
C	2.333545000	2.475785000	4.038064000	C	-7.411707000	0.076940000	-1.710843000
H	1.439338000	1.843803000	2.168705000	C	-6.944232000	0.040119000	-3.026228000
H	2.362279000	3.332230000	2.028520000	C	-5.587132000	0.239453000	-3.282540000
C	3.542560000	0.262627000	4.246417000	C	-4.701174000	0.462199000	-2.228985000
H	2.742966000	-0.423274000	2.340958000	H	-6.338005000	-4.436590000	-0.017386000
H	4.504336000	-0.381990000	2.400446000	H	-8.391930000	-5.702338000	0.579475000
C	2.334264000	1.092900000	4.701102000	H	-9.842425000	-4.909004000	2.432479000
H	1.459094000	3.051692000	4.351051000	H	-9.239674000	-2.851127000	3.688499000
H	3.220809000	3.036645000	4.370027000	H	-7.175356000	-1.589214000	3.081086000
H	3.514988000	-0.740410000	4.688649000	H	-3.242694000	1.076899000	-0.187089000
H	4.464696000	0.739017000	4.612372000	H	-4.536386000	1.349614000	0.979262000
H	2.329200000	1.192669000	5.793297000	H	-6.891198000	0.326033000	0.364357000
H	1.408547000	0.568656000	4.426705000	H	-8.468992000	-0.066374000	-1.503846000
C	7.043579000	1.169841000	-0.335695000	H	-7.636224000	-0.135176000	-3.845697000
C	8.176914000	1.837786000	0.450344000	H	-5.209652000	0.222839000	-4.301349000
C	7.068866000	-0.354723000	-0.162297000	H	-3.652205000	0.642807000	-2.432398000
H	7.187126000	1.404140000	-1.396733000	C	-2.414863000	-1.683028000	2.891124000
C	9.541753000	1.266794000	0.044331000	C	-2.659523000	-0.456489000	1.991656000
H	8.013379000	1.657469000	1.524094000	C	-1.334881000	0.032897000	1.399544000
H	8.149245000	2.923689000	0.294624000	C	-0.187393000	-0.824561000	1.250340000
C	8.433240000	-0.921253000	-0.575144000	C	-0.212649000	-2.244571000	1.791730000
H	6.872978000	-0.585142000	0.894901000	C	-1.585595000	-2.776301000	2.212743000
H	6.275521000	-0.821929000	-0.751978000	H	-3.048867000	0.341739000	2.633791000
C	9.579114000	-0.259330000	0.199486000	H	-3.376533000	-2.074697000	3.235747000
H	10.330150000	1.737020000	0.643237000	H	-1.877773000	-1.339102000	3.786035000
H	9.743535000	1.531079000	-1.003319000	H	0.463151000	-2.229187000	2.660680000
H	8.437963000	-2.005665000	-0.424273000	H	0.266060000	-2.906575000	1.063346000
H	8.578458000	-0.758027000	-1.652733000	H	-1.456236000	-3.622733000	2.897005000
H	10.546605000	-0.648305000	-0.139245000	H	-2.110364000	-3.173308000	1.339671000
H	9.491301000	-0.516215000	1.265148000	O	0.886487000	-0.393665000	0.764858000
H	2.584025000	1.499738000	0.159687000	C	-1.189103000	1.362705000	1.151355000
H	5.810747000	2.272184000	0.982711000	C	-1.290368000	2.601370000	1.588571000
O	-2.740681000	-1.985947000	-0.843166000	C	-1.213668000	2.991165000	3.006050000
O	-4.657904000	-2.681096000	0.125874000	C	-1.154110000	2.057772000	4.055862000
N	-5.030923000	-1.092652000	1.702227000	C	-1.195324000	4.358760000	3.327131000
C	-3.605939000	-1.794091000	-0.032489000	C	-1.086320000	2.480465000	5.379582000
C	-3.832007000	-0.666130000	0.973029000	H	-1.142376000	0.998604000	3.824346000
C	-5.438463000	-2.174031000	1.162988000	C	-1.119838000	4.780486000	4.652970000
C	-6.635307000	-2.940792000	1.502117000	H	-1.240253000	5.088909000	2.523110000
C	-6.974819000	-4.100270000	0.792842000	C	-1.067120000	3.843655000	5.686808000
C	-8.128527000	-4.804711000	1.130989000	H	-1.040187000	1.742432000	6.175798000

H	-1.104327000	5.843158000	4.879024000	C	-3.396373000	0.163430000	-1.816805000
H	-1.011601000	4.171350000	6.720896000	H	-2.437039000	-0.197353000	-1.452726000
H	2.368041000	-7.208466000	0.489261000	H	-4.645603000	-0.700040000	-4.859037000
O	1.558099000	2.439166000	-0.989841000	O	-4.943126000	1.928981000	-1.293265000
O	-0.205575000	3.889053000	-1.117125000	C	-3.793662000	1.499543000	-1.170717000
N	-1.917063000	2.492811000	-1.518466000	N	-2.777563000	2.137485000	-0.553192000
C	0.336043000	2.595171000	-1.124196000	C	-2.907616000	3.415811000	0.074457000
C	-0.779625000	1.722401000	-1.304202000	C	-2.915056000	3.472867000	1.483355000
C	-1.559870000	3.733193000	-1.362404000	C	-2.995837000	4.727378000	2.093408000
C	-2.407650000	4.909696000	-1.385024000	H	-3.004773000	4.796346000	3.176485000
C	-1.878777000	6.195703000	-1.185947000	C	-3.079569000	5.889863000	1.330632000
C	-2.720217000	7.305798000	-1.196633000	C	-3.069663000	5.811528000	-0.057582000
C	-4.091926000	7.149964000	-1.404020000	H	-3.132145000	6.722732000	-0.644857000
C	-4.620994000	5.870087000	-1.602528000	C	-2.967787000	4.578905000	-0.713038000
C	-3.791067000	4.755725000	-1.592679000	H	-1.933105000	1.586720000	-0.305259000
C	-0.683720000	0.318012000	-1.801573000	C	-2.920637000	2.196417000	2.311672000
C	-0.925999000	0.175000000	-3.294064000	C	-4.376689000	1.765920000	2.569978000
C	-1.729631000	-0.858988000	-3.788976000	H	-2.440484000	1.413051000	1.723160000
C	-1.920184000	-1.020008000	-5.163489000	H	-4.901044000	2.517997000	3.171535000
C	-1.309624000	-0.148038000	-6.064983000	H	-4.919927000	1.654064000	1.627191000
C	-0.513468000	0.892367000	-5.580853000	H	-4.414179000	0.812321000	3.111101000
C	-0.328683000	1.052937000	-4.208397000	C	-2.936112000	4.527185000	-2.232070000
H	-0.812071000	6.310863000	-1.025136000	C	-4.331304000	4.812626000	-2.815346000
H	-2.302460000	8.297108000	-1.042316000	H	-2.655239000	3.510096000	-2.522738000
H	-4.745327000	8.017866000	-1.410568000	H	-4.653870000	5.831488000	-2.568607000
H	-5.687836000	5.741857000	-1.763970000	H	-4.317307000	4.720494000	-3.908429000
H	-4.189604000	3.757424000	-1.742519000	H	-5.062352000	4.108154000	-2.411226000
H	-1.370515000	-0.336307000	-1.260210000	H	-3.575437000	-1.785108000	-3.946130000
H	0.316260000	-0.050119000	-1.561693000	C	-1.880140000	5.477741000	-2.818517000
H	-2.217849000	-1.528649000	-3.089217000	H	-0.883109000	5.259843000	-2.421324000
H	-2.550686000	-1.827390000	-5.527066000	H	-1.843829000	5.376695000	-3.909646000
H	-1.457576000	-0.271905000	-7.134307000	H	-2.109994000	6.525973000	-2.598119000
H	-0.041460000	1.584502000	-6.273489000	C	-2.128338000	2.306768000	3.620985000
H	0.277293000	1.875130000	-3.836229000	H	-2.057625000	1.324668000	4.101041000
H	-1.420416000	3.424163000	0.890800000	H	-1.108757000	2.663529000	3.435537000
TS4-*SSS*				H	-2.600541000	2.988892000	4.337360000
N	-5.823274000	-2.024466000	-0.103876000	C	-3.639783000	-2.195657000	1.758842000
N	-3.574254000	-1.619838000	0.411276000	C	-3.525402000	-3.731156000	1.712795000
N	-4.466060000	-0.825013000	-1.570439000	C	-2.519430000	-1.600714000	2.616742000
C	-4.614449000	-1.485659000	-0.411412000	H	-4.603801000	-1.903652000	2.198543000
C	-5.250372000	-1.074436000	-2.784142000	C	-3.536383000	-4.334323000	3.123542000
H	-5.685001000	-2.075670000	-2.749200000	H	-2.587218000	-3.972591000	1.198532000
H	-6.049920000	-0.329584000	-2.876581000	H	-4.332831000	-4.162877000	1.104403000
C	-4.198604000	-0.887094000	-3.878731000	C	-2.551380000	-2.189398000	4.030976000
C	-3.373187000	0.301870000	-3.362874000	H	-1.560184000	-1.812497000	2.133540000
H	-3.850936000	1.242433000	-3.652516000	H	-2.618510000	-0.513966000	2.643102000
H	-2.349064000	0.301163000	-3.737405000	C	-2.438445000	-3.717397000	3.998695000

H	-3.417712000	-5.422667000	3.061044000	H	9.461321000	2.128119000	4.038161000
H	-4.516657000	-4.152554000	3.589949000	H	7.253334000	1.252848000	3.273012000
H	-1.743270000	-1.759874000	4.627304000	H	3.383558000	-1.309435000	-0.146132000
H	-3.495175000	-1.905734000	4.522355000	H	4.188617000	-1.557319000	1.415939000
H	-2.485629000	-4.126180000	5.015233000	H	6.807104000	-1.510738000	1.389901000
H	-1.455118000	-3.990787000	3.594235000	H	8.799996000	-2.239251000	0.106037000
C	-7.123367000	-1.341051000	-0.274375000	H	8.614615000	-2.684235000	-2.332887000
C	-8.214084000	-2.257208000	0.289376000	H	6.421799000	-2.402136000	-3.474850000
C	-7.145723000	0.039853000	0.393616000	H	4.429870000	-1.666026000	-2.173708000
H	-7.311071000	-1.214955000	-1.345054000	C	2.799345000	2.432353000	1.550182000
C	-9.598516000	-1.608024000	0.159904000	C	2.903682000	0.898746000	1.410077000
H	-8.001878000	-2.445335000	1.353579000	C	1.574764000	0.310154000	0.919038000
H	-8.188162000	-3.227035000	-0.222484000	C	0.473894000	1.137484000	0.483260000
C	-8.531622000	0.684474000	0.263070000	C	0.668133000	2.621184000	0.239618000
H	-6.890156000	-0.083135000	1.456069000	C	2.114178000	3.101976000	0.355021000
H	-6.388242000	0.684931000	-0.060928000	H	3.058917000	0.493509000	2.417686000
C	-9.633405000	-0.224221000	0.822240000	H	3.798405000	2.847436000	1.720236000
H	-10.356507000	-2.266908000	0.598893000	H	2.218898000	2.654165000	2.456506000
H	-9.849137000	-1.507806000	-0.905690000	H	0.025639000	3.142012000	0.963769000
H	-8.533189000	1.654257000	0.772697000	H	0.253437000	2.852018000	-0.749471000
H	-8.732253000	0.892168000	-0.797760000	H	2.133087000	4.191406000	0.474296000
H	-10.618651000	0.235524000	0.680606000	H	2.644276000	2.875750000	-0.572176000
H	-9.492079000	-0.339972000	1.906599000	O	-0.681681000	0.659630000	0.378468000
H	-2.632721000	-1.697700000	-0.021127000	C	1.299214000	-1.000984000	1.159605000
H	-5.798535000	-2.662390000	0.680034000	C	1.121932000	-1.950518000	2.059460000
O	3.951479000	1.249199000	-1.655544000	C	0.928108000	-1.671687000	3.496811000
O	5.776324000	1.800518000	-0.433920000	C	0.647571000	-0.385105000	3.989123000
N	5.352065000	0.821276000	1.567356000	C	1.011778000	-2.731596000	4.413589000
C	4.540247000	1.179251000	-0.616501000	C	0.466348000	-0.169938000	5.351790000
C	4.227750000	0.458374000	0.696015000	H	0.548355000	0.437607000	3.290125000
C	6.160148000	1.520454000	0.869837000	C	0.830057000	-2.515672000	5.778773000
C	7.454686000	2.055038000	1.292182000	H	1.223639000	-3.732788000	4.046440000
C	8.259168000	2.781497000	0.404989000	C	0.557621000	-1.232901000	6.255621000
C	9.492925000	3.269822000	0.830978000	H	0.243064000	0.831582000	5.709432000
C	9.926589000	3.036558000	2.136635000	H	0.899749000	-3.351423000	6.469659000
C	9.123770000	2.310613000	3.022064000	H	0.413219000	-1.062458000	7.318584000
C	7.892149000	1.819680000	2.604187000	H	-3.150195000	6.857338000	1.820321000
C	4.267252000	-1.070872000	0.438780000	O	-1.194003000	-2.538734000	-0.534201000
C	5.489985000	-1.537411000	-0.311417000	O	-0.312623000	-0.853566000	-1.819514000
C	6.726482000	-1.706442000	0.324773000	N	1.861649000	-1.389696000	-1.830583000
C	7.846260000	-2.114007000	-0.399761000	C	-0.189348000	-1.992522000	-1.013801000
C	7.742216000	-2.363928000	-1.769548000	C	1.210741000	-2.269634000	-0.982777000
C	6.512495000	-2.204276000	-2.410043000	C	0.961230000	-0.543700000	-2.245774000
C	5.393153000	-1.790404000	-1.687144000	C	1.100187000	0.596656000	-3.134267000
H	7.914771000	2.953506000	-0.608411000	C	0.089285000	1.570344000	-3.210977000
H	10.116442000	3.831627000	0.141724000	C	0.216967000	2.649656000	-4.082334000
H	10.889138000	3.418186000	2.465416000	C	1.354281000	2.775339000	-4.881306000

C	2.366210000	1.813922000	-4.800438000	C	1.793184000	-3.147173000	-2.929122000
C	2.242851000	0.731268000	-3.938093000	H	2.091086000	-1.218430000	-0.938284000
C	1.795769000	-3.606320000	-0.627522000	C	5.142692000	-3.251345000	-1.002604000
C	1.976749000	-4.478411000	-1.855753000	C	6.457917000	-3.142852000	-1.789466000
C	0.857384000	-5.024631000	-2.496753000	H	4.928285000	-2.264747000	-0.584530000
C	1.005963000	-5.794596000	-3.648444000	H	6.727418000	-4.103468000	-2.244656000
C	2.278138000	-6.026643000	-4.178090000	H	6.358843000	-2.393006000	-2.577008000
C	3.396364000	-5.481974000	-3.547260000	H	7.278740000	-2.849425000	-1.122759000
C	3.245461000	-4.712351000	-2.392121000	C	0.648720000	-2.170053000	-3.182716000
H	-0.780351000	1.487344000	-2.570509000	C	1.005779000	-1.197744000	-4.323304000
H	-0.570978000	3.394090000	-4.132125000	H	0.514194000	-1.567280000	-2.280228000
H	1.454212000	3.618043000	-5.559673000	H	1.086282000	-1.736381000	-5.274939000
H	3.257569000	1.910100000	-5.413835000	H	0.231054000	-0.428840000	-4.425780000
H	3.025176000	-0.014022000	-3.863417000	H	1.963938000	-0.700610000	-4.143867000
H	1.107518000	-4.102249000	0.065477000	H	2.772578000	3.741991000	-1.645870000
H	2.756456000	-3.489493000	-0.115387000	C	-0.695415000	-2.855428000	-3.457430000
H	-0.131791000	-4.830976000	-2.087960000	H	-0.930018000	-3.597020000	-2.685783000
H	0.129429000	-6.215470000	-4.134601000	H	-1.499586000	-2.115643000	-3.457000000
H	2.394624000	-6.626678000	-5.076598000	H	-0.702353000	-3.362893000	-4.429475000
H	4.389883000	-5.653834000	-3.953300000	C	5.274655000	-4.237273000	0.171120000
H	4.117687000	-4.280077000	-1.909612000	H	6.052910000	-3.902321000	0.868205000
H	1.117417000	-2.999821000	1.782868000	H	4.333573000	-4.325394000	0.724406000
INT6				H	5.552051000	-5.239102000	-0.175688000
N	5.385907000	1.699663000	1.316773000	C	3.556896000	-0.261892000	2.504603000
N	3.381793000	0.484492000	1.253462000	C	2.513122000	0.207008000	3.525270000
N	4.149308000	1.599328000	-0.637089000	C	3.454801000	-1.766182000	2.218802000
C	4.284326000	1.246015000	0.647933000	H	4.560642000	-0.061846000	2.897580000
C	4.680331000	2.851802000	-1.197557000	C	2.570581000	-0.627705000	4.808966000
H	4.848256000	3.572551000	-0.394996000	H	1.523306000	0.118919000	3.065328000
H	5.628776000	2.661139000	-1.715389000	H	2.660812000	1.272524000	3.740128000
C	3.589187000	3.257788000	-2.189379000	C	3.494659000	-2.589731000	3.510575000
C	3.141932000	1.906163000	-2.759009000	H	2.520237000	-1.939828000	1.677080000
H	3.860342000	1.553452000	-3.504286000	H	4.268375000	-2.054911000	1.546554000
H	2.147956000	1.930586000	-3.209251000	C	2.422173000	-2.123330000	4.503209000
C	3.185269000	0.952488000	-1.549564000	H	1.784590000	-0.295519000	5.493859000
H	2.213882000	0.900036000	-1.064488000	H	3.532261000	-0.457927000	5.316920000
H	3.960895000	3.942042000	-2.957352000	H	3.366655000	-3.652091000	3.270888000
O	4.713666000	-0.551404000	-2.640625000	H	4.485810000	-2.493522000	3.979067000
C	3.683011000	-0.439976000	-1.974756000	H	2.478422000	-2.708815000	5.428945000
N	2.872513000	-1.448124000	-1.589208000	H	1.427990000	-2.304884000	4.071739000
C	2.905650000	-2.760826000	-2.147360000	C	6.756594000	1.566593000	0.771579000
C	3.981396000	-3.629667000	-1.906739000	C	7.744082000	1.785348000	1.922308000
C	3.948850000	-4.895845000	-2.504773000	C	6.997179000	0.214152000	0.082475000
H	4.776235000	-5.581164000	-2.343079000	H	6.916064000	2.364997000	0.037410000
C	2.871442000	-5.293021000	-3.287584000	C	9.194775000	1.672665000	1.436078000
C	1.796603000	-4.427404000	-3.486765000	H	7.560614000	1.020866000	2.693263000
H	0.954611000	-4.751897000	-4.088531000	H	7.564034000	2.763673000	2.385273000

C	8.447665000	0.107361000	-0.405686000	C	-0.030956000	-2.750328000	0.441714000
H	6.787790000	-0.587918000	0.805781000	C	-1.377839000	-3.435562000	0.659025000
H	6.310279000	0.080382000	-0.758699000	H	-2.680999000	-0.866370000	2.560758000
C	9.446997000	0.330882000	0.735613000	H	-3.021660000	-3.307502000	2.086532000
H	9.878091000	1.801957000	2.283284000	H	-1.448092000	-2.857872000	2.724738000
H	9.403619000	2.493823000	0.735963000	H	0.693744000	-3.122994000	1.182398000
H	8.603935000	-0.870437000	-0.873373000	H	0.393940000	-3.010506000	-0.533377000
H	8.618070000	0.856949000	-1.191824000	H	-1.233167000	-4.507242000	0.842109000
H	10.475471000	0.290601000	0.357901000	H	-1.985699000	-3.361654000	-0.249680000
H	9.347717000	-0.483078000	1.468307000	O	1.059836000	-0.637181000	0.263717000
H	2.446807000	0.337894000	0.834748000	C	-1.034311000	0.899830000	1.264589000
H	5.331727000	1.584830000	2.319420000	C	-1.129525000	1.546954000	2.451282000
O	-2.921521000	-1.146662000	-1.619297000	C	-1.208449000	1.029444000	3.818565000
O	-4.572711000	-2.509749000	-0.908836000	C	-0.890980000	-0.290984000	4.191323000
N	-4.775320000	-1.965721000	1.283113000	C	-1.583164000	1.921078000	4.842867000
C	-3.615573000	-1.524449000	-0.713538000	C	-0.963846000	-0.699803000	5.519921000
C	-3.716448000	-1.101156000	0.750428000	H	-0.562237000	-0.984793000	3.429211000
C	-5.203578000	-2.683073000	0.320295000	C	-1.660493000	1.512185000	6.171002000
C	-6.286452000	-3.664414000	0.357095000	H	-1.820522000	2.949604000	4.581333000
C	-6.670772000	-4.360261000	-0.796453000	C	-1.354138000	0.194916000	6.518584000
C	-7.712537000	-5.283669000	-0.733014000	H	-0.709293000	-1.725152000	5.775402000
C	-8.371772000	-5.515756000	0.474810000	H	-1.959873000	2.222807000	6.936711000
C	-7.988462000	-4.820902000	1.626216000	H	-1.416237000	-0.129009000	7.553619000
C	-6.950511000	-3.897813000	1.570893000	H	2.861868000	-6.281816000	-3.738365000
C	-4.216604000	0.368178000	0.843020000	O	1.410135000	2.751486000	0.340672000
C	-5.369250000	0.689560000	-0.076529000	O	-0.385970000	4.121385000	0.287076000
C	-6.681741000	0.296426000	0.217142000	N	-2.108397000	2.685631000	-0.059502000
C	-7.722128000	0.575839000	-0.669138000	C	0.216457000	2.872741000	0.242657000
C	-7.466707000	1.257675000	-1.860584000	C	-0.902321000	1.849291000	0.022018000
C	-6.164321000	1.661244000	-2.158449000	C	-1.753381000	3.898974000	0.082906000
C	-5.124070000	1.377693000	-1.273566000	C	-2.611470000	5.080050000	0.050008000
H	-6.154484000	-4.170769000	-1.730660000	C	-2.080685000	6.366399000	0.212161000
H	-8.009891000	-5.821627000	-1.628378000	C	-2.925050000	7.474064000	0.168472000
H	-9.183581000	-6.236212000	0.520751000	C	-4.294827000	7.303128000	-0.036575000
H	-8.501253000	-5.000897000	2.566622000	C	-4.823939000	6.018941000	-0.199255000
H	-6.636716000	-3.347062000	2.451220000	C	-3.989626000	4.908120000	-0.157039000
H	-3.392178000	1.038289000	0.618074000	C	-0.707298000	1.127325000	-1.335997000
H	-4.493831000	0.519903000	1.891589000	C	-1.014482000	1.971272000	-2.550562000
H	-6.882505000	-0.234317000	1.142855000	C	-2.065647000	1.597443000	-3.398646000
H	-8.734254000	0.261729000	-0.427982000	C	-2.377530000	2.353045000	-4.529789000
H	-8.278521000	1.474907000	-2.549628000	C	-1.643793000	3.499901000	-4.833958000
H	-5.952591000	2.196525000	-3.080463000	C	-0.589741000	3.879146000	-4.001831000
H	-4.112578000	1.696948000	-1.500393000	C	-0.277102000	3.118556000	-2.875353000
C	-2.094944000	-2.783276000	1.839962000	H	-1.014797000	6.488937000	0.368889000
C	-2.389894000	-1.293155000	1.593636000	H	-2.512691000	8.470982000	0.293993000
C	-1.151981000	-0.563875000	1.080972000	H	-4.950497000	8.168685000	-0.070779000
C	-0.057138000	-1.236287000	0.581597000	H	-5.889298000	5.883806000	-0.360852000

H	-4.385793000	3.906583000	-0.285682000	H	-2.015242000	-2.978677000	3.548817000
H	-1.360082000	0.257489000	-1.326996000	H	-3.478124000	2.322465000	2.724479000
H	0.312934000	0.750551000	-1.359468000	C	1.474237000	-3.157789000	3.612173000
H	-2.639498000	0.707227000	-3.162318000	H	2.276762000	-3.033141000	2.879976000
H	-3.196945000	2.043242000	-5.173111000	H	1.646932000	-2.444992000	4.427142000
H	-1.887528000	4.091150000	-5.712254000	H	1.556228000	-4.162252000	4.043607000
H	-0.006812000	4.767645000	-4.229849000	C	-1.658367000	-3.723040000	-2.924942000
H	0.549271000	3.429158000	-2.243936000	H	-2.285104000	-3.225233000	-3.673117000
H	-1.165221000	2.636108000	2.422363000	H	-0.638601000	-3.337540000	-3.019366000
INT7				H	-1.634307000	-4.789896000	-3.175357000
N	-5.788700000	0.322562000	-0.884358000	C	-3.806931000	0.913128000	-2.664141000
N	-3.540149000	0.746554000	-1.233395000	C	-2.843849000	1.934218000	-3.278026000
N	-4.242363000	0.365770000	0.955144000	C	-3.721619000	-0.439313000	-3.384040000
C	-4.614048000	0.466906000	-0.388386000	H	-4.831622000	1.287256000	-2.780889000
C	-5.021995000	0.966174000	2.036266000	C	-3.087817000	2.081771000	-4.785549000
H	-5.608441000	1.807507000	1.655055000	H	-1.807956000	1.617624000	-3.106986000
H	-5.716516000	0.245090000	2.492444000	H	-2.956248000	2.901960000	-2.772777000
C	-3.942398000	1.381646000	3.039520000	C	-3.963693000	-0.291709000	-4.890052000
C	-2.934354000	0.236126000	2.914715000	H	-2.724737000	-0.865375000	-3.209807000
H	-3.304143000	-0.646768000	3.447252000	H	-4.448855000	-1.121477000	-2.931615000
H	-1.941349000	0.478326000	3.288802000	C	-2.996548000	0.728776000	-5.505387000
C	-2.917967000	-0.054764000	1.398034000	H	-2.370333000	2.793269000	-5.212997000
H	-2.122915000	0.524696000	0.919490000	H	-4.088241000	2.507032000	-4.949202000
H	-4.326862000	1.503916000	4.057047000	H	-3.863060000	-1.264166000	-5.389006000
O	-3.556503000	-2.386552000	1.360767000	H	-4.997211000	0.042193000	-5.060400000
C	-2.684854000	-1.549087000	1.163156000	H	-3.197903000	0.853711000	-6.576928000
N	-1.413621000	-1.875758000	0.777135000	H	-1.967808000	0.345068000	-5.421911000
C	-0.955523000	-3.228626000	0.690262000	C	-6.885638000	-0.279903000	-0.146239000
C	-1.312382000	-4.009309000	-0.424232000	C	-8.178192000	-0.070685000	-0.948505000
C	-0.835071000	-5.324709000	-0.480818000	C	-6.644188000	-1.781813000	0.093820000
H	-1.102719000	-5.951207000	-1.326294000	H	-7.042401000	0.189891000	0.838196000
C	-0.035405000	-5.843421000	0.532055000	C	-9.385775000	-0.729784000	-0.271456000
C	0.297442000	-5.055509000	1.633252000	H	-8.027915000	-0.498494000	-1.949561000
H	0.908207000	-5.474709000	2.426553000	H	-8.345896000	1.004266000	-1.090382000
C	-0.162173000	-3.740277000	1.736552000	C	-7.848497000	-2.447826000	0.771022000
H	-0.703745000	-1.153508000	0.785599000	H	-6.461921000	-2.253049000	-0.883072000
C	-2.228625000	-3.483768000	-1.518435000	H	-5.737081000	-1.922679000	0.687856000
C	-3.634524000	-4.098337000	-1.390280000	C	-9.140503000	-2.224964000	-0.025967000
H	-2.334802000	-2.404627000	-1.378827000	H	-10.288728000	-0.584624000	-0.878652000
H	-3.601855000	-5.182057000	-1.559217000	H	-9.576721000	-0.235550000	0.693303000
H	-4.043271000	-3.906983000	-0.396633000	H	-7.659251000	-3.520920000	0.902374000
H	-4.307699000	-3.657786000	-2.135074000	H	-7.973345000	-2.029367000	1.781385000
C	0.097256000	-2.911232000	2.985082000	H	-9.997262000	-2.673344000	0.494230000
C	-1.034596000	-3.146342000	4.003733000	H	-9.056181000	-2.737725000	-0.995593000
H	0.062459000	-1.858236000	2.700469000	H	-2.881593000	1.415294000	-0.848602000
H	-1.010850000	-4.178030000	4.374700000	O	1.499635000	-1.010949000	0.820644000
H	-0.927443000	-2.471259000	4.861930000	O	2.649206000	-2.786838000	0.054030000

N	4.287567000	-1.839009000	-1.199566000	C	5.590165000	3.304554000	-1.467535000
C	2.418696000	-1.441753000	0.168488000	C	4.854234000	2.922300000	-4.129494000
C	3.522266000	-0.732428000	-0.622664000	H	2.823270000	2.928306000	-3.398951000
C	3.767634000	-2.925030000	-0.777675000	C	6.569305000	3.224150000	-2.456363000
C	4.180605000	-4.296230000	-1.049464000	H	5.875893000	3.456170000	-0.429681000
C	3.427443000	-5.375319000	-0.566358000	C	6.204833000	3.027988000	-3.789817000
C	3.837915000	-6.676916000	-0.844665000	H	4.562348000	2.788480000	-5.167328000
C	4.991855000	-6.904844000	-1.595856000	H	7.617581000	3.316112000	-2.186326000
C	5.741609000	-5.826401000	-2.077009000	H	6.967822000	2.968198000	-4.560481000
C	5.339226000	-4.523491000	-1.807964000	H	0.319547000	-6.869498000	0.471720000
C	4.443899000	0.054222000	0.359668000	O	-1.349090000	2.909557000	0.454758000
C	4.854614000	-0.738002000	1.576967000	O	0.322062000	4.783636000	-1.254295000
C	5.805007000	-1.765196000	1.491685000	N	1.078265000	4.216257000	0.799082000
C	6.123907000	-2.532050000	2.611641000	C	-0.335820000	2.428182000	0.014530000
C	5.507024000	-2.277554000	3.837936000	C	1.084449000	2.802465000	0.489174000
C	4.576223000	-1.243803000	3.939403000	C	0.645335000	5.133629000	-0.123155000
C	4.253958000	-0.483586000	2.815836000	C	0.615524000	6.559603000	0.322605000
H	2.527993000	-5.191622000	0.009820000	C	0.641333000	7.544188000	-0.672283000
H	3.252494000	-7.513572000	-0.475084000	C	0.619575000	8.892014000	-0.325893000
H	5.308475000	-7.921793000	-1.809316000	C	0.557183000	9.267969000	1.017962000
H	6.638495000	-6.005011000	-2.662601000	C	0.510702000	8.291277000	2.013901000
H	5.903252000	-3.672339000	-2.174700000	C	0.540917000	6.941199000	1.668938000
H	3.921787000	0.963167000	0.660109000	C	1.446074000	1.999859000	1.768562000
H	5.313710000	0.358253000	-0.231375000	C	0.543498000	1.969679000	2.988255000
H	6.288269000	-1.965317000	0.540922000	C	0.708625000	0.876896000	3.855284000
H	6.857463000	-3.328801000	2.526382000	C	0.021935000	0.806103000	5.065700000
H	5.754975000	-2.877085000	4.709025000	C	-0.861256000	1.825051000	5.426815000
H	4.096317000	-1.030366000	4.890235000	C	-1.056974000	2.899191000	4.559727000
H	3.529156000	0.319290000	2.901392000	C	-0.361573000	2.974943000	3.350706000
C	2.536751000	-0.533719000	-3.009682000	H	0.675879000	7.226754000	-1.708786000
C	2.999903000	0.228489000	-1.758838000	H	0.647275000	9.650623000	-1.102575000
C	1.896690000	1.160965000	-1.270675000	H	0.535678000	10.319764000	1.288415000
C	0.627129000	0.740507000	-1.421854000	H	0.441640000	8.579869000	3.058592000
C	0.132465000	-0.431839000	-2.208967000	H	0.465861000	6.194495000	2.455100000
C	1.251467000	-1.324438000	-2.761784000	H	2.430637000	2.390768000	2.066796000
H	3.879678000	0.804990000	-2.037401000	H	1.617738000	0.971331000	1.454050000
H	3.335494000	-1.197293000	-3.349314000	H	1.379176000	0.070640000	3.571969000
H	2.368423000	0.208926000	-3.799578000	H	0.165559000	-0.052060000	5.716209000
H	-0.466666000	-0.021300000	-3.032271000	H	-1.406356000	1.771526000	6.364555000
H	-0.575055000	-1.002012000	-1.598644000	H	-1.763578000	3.683216000	4.816515000
H	0.915204000	-1.794077000	-3.691219000	H	-0.563193000	3.795090000	2.673251000
H	1.441268000	-2.149606000	-2.068585000	H	3.273662000	4.110813000	-0.087045000
O	-0.455696000	1.427570000	-0.896967000	H	1.388871000	4.511913000	1.710622000
C	2.138052000	2.436913000	-0.577306000	**TS1′**			
C	3.197628000	3.251981000	-0.749981000	N	-2.142360000	-2.607162000	-1.135449000
C	4.231777000	3.168703000	-1.792653000	N	-0.615183000	-1.539956000	0.315699000
C	3.875737000	2.996564000	-3.141141000	N	-0.829163000	-0.835649000	-1.877669000

C	-1.187312000	-1.664282000	-0.867583000	H	-2.363342000	-2.009947000	1.351923000
C	-0.814112000	-1.194655000	-3.301197000	C	-1.561268000	-3.933780000	3.192866000
H	-0.656193000	-2.270451000	-3.411894000	H	0.198223000	-3.538442000	1.999496000
H	-1.764890000	-0.927108000	-3.781393000	H	-1.146607000	-4.165020000	1.070630000
C	0.324146000	-0.331608000	-3.849156000	C	-1.649901000	-1.539827000	3.988998000
C	0.170606000	0.962769000	-3.040916000	H	0.093384000	-0.972281000	2.830775000
H	-0.659699000	1.560655000	-3.428183000	H	-1.340393000	-0.071373000	2.411697000
H	1.075131000	1.573499000	-3.028522000	C	-1.238766000	-2.973673000	4.344543000
C	-0.196143000	0.473121000	-1.628913000	H	-1.243910000	-4.954166000	3.439056000
H	0.698971000	0.347102000	-1.034934000	H	-2.651459000	-3.969841000	3.048503000
H	0.245073000	-0.172087000	-4.928191000	H	-1.392447000	-0.852206000	4.803155000
O	-2.169090000	1.846971000	-1.528896000	H	-2.743071000	-1.497887000	3.878614000
C	-1.172307000	1.437959000	-0.937173000	H	-1.741913000	-3.300127000	5.262707000
N	-0.828790000	1.797954000	0.326256000	H	-0.158662000	-3.003264000	4.547678000
C	-1.425788000	2.885777000	1.040472000	C	-3.370724000	-2.377668000	-1.919005000
C	-2.754423000	2.809728000	1.487074000	C	-4.298488000	-3.579302000	-1.707033000
C	-3.278085000	3.915063000	2.170376000	C	-4.076538000	-1.066355000	-1.548368000
H	-4.306845000	3.885114000	2.517508000	H	-3.107789000	-2.345930000	-2.982941000
C	-2.501963000	5.039180000	2.421838000	C	-5.602664000	-3.418932000	-2.498740000
C	-1.177074000	5.083378000	1.989913000	H	-4.532547000	-3.656750000	-0.633922000
H	-0.578425000	5.963039000	2.198952000	H	-3.781278000	-4.503562000	-1.993942000
C	-0.615274000	4.016060000	1.287211000	C	-5.375966000	-0.903208000	-2.346185000
H	0.017689000	1.410077000	0.734975000	H	-4.301860000	-1.090481000	-0.472412000
C	-3.626324000	1.582524000	1.273820000	H	-3.418477000	-0.209717000	-1.717923000
C	-4.797477000	1.895389000	0.328350000	C	-6.311300000	-2.102787000	-2.151152000
H	-3.012437000	0.810613000	0.802702000	H	-6.259655000	-4.274872000	-2.305290000
H	-5.440535000	2.678337000	0.747405000	H	-5.373956000	-3.435714000	-3.573808000
H	-4.418982000	2.230522000	-0.639345000	H	-5.871973000	0.027587000	-2.050910000
H	-5.417198000	1.003470000	0.176960000	H	-5.133192000	-0.800196000	-3.413884000
C	0.812066000	4.071650000	0.753813000	H	-7.215118000	-1.988853000	-2.761443000
C	0.807689000	4.418027000	-0.748080000	H	-6.640789000	-2.136529000	-1.102515000
H	1.257693000	3.079581000	0.869451000	H	-2.242745000	-3.297586000	-0.404333000
H	0.439530000	5.439040000	-0.903886000	O	1.699224000	0.828050000	1.878835000
H	1.822591000	4.354787000	-1.159297000	O	2.728463000	0.880261000	-0.158113000
H	0.163448000	3.745619000	-1.321233000	N	2.756437000	-1.301818000	-0.728260000
H	1.288633000	-0.802196000	-3.637115000	C	2.161504000	0.199420000	0.936950000
C	1.721723000	5.038618000	1.520879000	C	2.107380000	-1.202919000	0.543948000
H	1.710268000	4.829526000	2.595616000	C	3.064321000	-0.103264000	-1.079504000
H	2.752639000	4.931540000	1.166709000	C	3.668809000	0.342462000	-2.329342000
H	1.431957000	6.085443000	1.370699000	C	3.869420000	1.706497000	-2.590071000
C	-4.136794000	1.017942000	2.610835000	C	4.419853000	2.110299000	-3.805111000
H	-4.668756000	0.072683000	2.445836000	C	4.775037000	1.163125000	-4.766643000
H	-3.314393000	0.831279000	3.307825000	C	4.582420000	-0.197260000	-4.506095000
H	-4.835660000	1.707602000	3.097513000	C	4.034143000	-0.608408000	-3.296283000
C	-1.276086000	-2.032863000	1.528052000	C	2.495159000	-2.268073000	1.564018000
C	-0.889250000	-3.479317000	1.890518000	C	3.949350000	-2.159618000	1.967053000
C	-0.987957000	-1.068903000	2.689000000	C	4.319646000	-1.382369000	3.071096000

C	5.662846000	-1.226548000	3.413147000	H	1.685542000	0.608557000	1.417465000
C	6.655490000	-1.846532000	2.652768000	H	3.332811000	2.113657000	3.525033000
C	6.295734000	-2.617420000	1.545905000	H	2.411553000	2.854788000	2.195502000
C	4.952062000	-2.770466000	1.205587000	H	1.570344000	1.983762000	3.501468000
H	3.589217000	2.437572000	-1.839465000	C	4.709703000	0.649053000	-2.605641000
H	4.569789000	3.168147000	-4.001163000	C	5.660953000	1.641758000	-3.291714000
H	5.201803000	1.481318000	-5.713484000	H	3.691824000	0.933102000	-2.880102000
H	4.862621000	-0.938124000	-5.249665000	H	6.712960000	1.372794000	-3.142867000
H	3.878642000	-1.659324000	-3.075511000	H	5.477014000	1.650756000	-4.372287000
H	2.292097000	-3.252790000	1.128508000	H	5.517763000	2.658665000	-2.909452000
H	1.862627000	-2.161082000	2.449971000	H	-1.076674000	2.333045000	-4.140698000
H	3.547748000	-0.884634000	3.652602000	C	4.926692000	-0.785182000	-3.120443000
H	5.933790000	-0.620624000	4.273645000	H	4.185825000	-1.466632000	-2.694324000
H	7.702218000	-1.727603000	2.918964000	H	4.821734000	-0.818549000	-4.210993000
H	7.063129000	-3.099044000	0.945525000	H	5.930239000	-1.144617000	-2.860577000
H	4.672054000	-3.355605000	0.334021000	C	2.589026000	-0.539908000	2.970696000
H	-2.925177000	5.883240000	2.959721000	H	1.658166000	-0.591029000	3.547707000
H	0.669509000	-1.341519000	0.373745000	H	2.690726000	-1.461485000	2.392419000
TS2-*SS′*				H	3.420795000	-0.501979000	3.683190000
N	-2.041336000	3.936187000	-0.019989000	C	-1.970360000	1.654417000	1.717789000
N	-1.343173000	1.737953000	0.392064000	C	-3.460562000	1.283305000	1.614084000
N	-0.583161000	2.866084000	-1.489175000	C	-1.216486000	0.655127000	2.601334000
C	-1.303237000	2.833642000	-0.362693000	H	-1.873172000	2.642194000	2.187292000
C	-0.816918000	3.819065000	-2.585519000	C	-4.105464000	1.195084000	3.003189000
H	-1.872518000	4.098859000	-2.615973000	H	-3.536462000	0.318389000	1.100183000
H	-0.214572000	4.724153000	-2.438083000	H	-3.994997000	2.009405000	0.984902000
C	-0.315601000	3.047846000	-3.806519000	C	-1.855978000	0.590962000	3.993218000
C	0.904607000	2.312821000	-3.244898000	H	-1.235946000	-0.338319000	2.141036000
H	1.747059000	3.008184000	-3.150603000	H	-0.167818000	0.954320000	2.665910000
H	1.226417000	1.443696000	-3.817864000	C	-3.341077000	0.219365000	3.906843000
C	0.447731000	1.869780000	-1.837441000	H	-5.153725000	0.890057000	2.903613000
H	0.014386000	0.868532000	-1.877490000	H	-4.111139000	2.193704000	3.465787000
H	-0.074207000	3.710669000	-4.642098000	H	-1.318142000	-0.140627000	4.602725000
O	1.823575000	2.908745000	-0.151728000	H	-1.748179000	1.566295000	4.491346000
C	1.620665000	1.912059000	-0.844419000	H	-3.788743000	0.202001000	4.907940000
N	2.396437000	0.807172000	-0.885050000	H	-3.428091000	-0.797114000	3.502989000
C	3.681332000	0.743935000	-0.260767000	C	-1.422145000	5.273192000	0.149120000
C	3.787886000	0.720788000	1.141515000	C	-2.501207000	6.241715000	0.639407000
C	5.067791000	0.691970000	1.704510000	C	-0.218733000	5.238154000	1.100843000
H	5.169874000	0.679706000	2.785520000	H	-1.083757000	5.618402000	-0.832002000
C	6.206241000	0.649430000	0.907424000	C	-1.921227000	7.649063000	0.838818000
C	6.078998000	0.631197000	-0.478755000	H	-2.897363000	5.874806000	1.599514000
H	6.969076000	0.578566000	-1.098337000	H	-3.337815000	6.259433000	-0.069414000
C	4.821634000	0.690200000	-1.088777000	C	0.360607000	6.645691000	1.290866000
H	2.161205000	0.083025000	-1.582633000	H	-0.555565000	4.846364000	2.072801000
C	2.571390000	0.693146000	2.051540000	H	0.539410000	4.549181000	0.714983000
C	2.464810000	1.993984000	2.865461000	C	-0.708420000	7.631816000	1.779525000

H	-2.699742000	8.317563000	1.224194000	H	-2.064462000	-4.210368000	-3.597967000
H	-1.617618000	8.052171000	-0.137827000	H	0.145348000	-0.809373000	-5.129263000
H	1.200547000	6.606903000	1.993259000	H	-1.098345000	-0.596155000	-3.894353000
H	0.772655000	6.998350000	0.334244000	H	-0.235013000	-3.295104000	-5.067894000
H	-0.288310000	8.640638000	1.868568000	H	-1.764389000	-2.476060000	-5.409049000
H	-1.037771000	7.337555000	2.786583000	O	1.687174000	-0.653039000	-3.168646000
H	-1.004623000	0.842405000	0.007490000	C	1.669160000	-2.835885000	-1.411458000
H	-2.712359000	3.740146000	0.711704000	C	2.550128000	-3.056635000	-0.596470000
O	-0.549219000	-0.831701000	-0.322379000	C	3.465217000	-3.320769000	0.456416000
O	-2.746693000	-1.109781000	-0.860115000	C	4.678243000	-2.613448000	0.574094000
N	-2.955304000	-3.351985000	-0.754522000	C	3.148375000	-4.281559000	1.442807000
C	-1.488154000	-1.596790000	-0.501265000	C	5.529026000	-2.847777000	1.649118000
C	-1.583197000	-3.046278000	-0.563263000	H	4.931858000	-1.867455000	-0.168586000
C	-3.564509000	-2.232934000	-0.953761000	C	4.004654000	-4.504258000	2.516417000
C	-4.974585000	-2.002934000	-1.222101000	H	2.222106000	-4.840996000	1.356954000
C	-5.486403000	-0.702043000	-1.352246000	C	5.199019000	-3.787858000	2.627816000
C	-6.844575000	-0.508864000	-1.592825000	H	6.450117000	-2.277836000	1.725551000
C	-7.701673000	-1.604461000	-1.709396000	H	3.737696000	-5.240735000	3.269819000
C	-7.193143000	-2.901368000	-1.584355000	H	5.865050000	-3.961708000	3.468344000
C	-5.839591000	-3.103749000	-1.342604000	H	7.191761000	0.618960000	1.364775000
C	-0.834501000	-3.907726000	0.436238000	**TS2-*RR′***			
C	-1.159283000	-3.580494000	1.877442000	N	1.634049000	0.239901000	3.481665000
C	-2.442403000	-3.792773000	2.401034000	N	0.210785000	-0.533522000	1.783092000
C	-2.718456000	-3.508865000	3.738033000	N	2.073864000	0.721993000	1.241049000
C	-1.715300000	-3.007939000	4.572530000	C	1.304849000	0.130531000	2.157630000
C	-0.439415000	-2.781480000	4.055784000	C	3.071664000	1.761838000	1.523839000
C	-0.166290000	-3.060476000	2.715402000	H	2.786116000	2.319554000	2.418352000
H	-4.815305000	0.145422000	-1.265365000	H	4.054774000	1.302296000	1.688642000
H	-7.234883000	0.500191000	-1.691707000	C	3.063733000	2.576703000	0.231349000
H	-8.760141000	-1.450538000	-1.898487000	C	2.916367000	1.494156000	-0.846129000
H	-7.856735000	-3.756404000	-1.676528000	H	3.890029000	1.040002000	-1.056540000
H	-5.427901000	-4.102382000	-1.242708000	H	2.485204000	1.851055000	-1.781684000
H	0.236352000	-3.794058000	0.271882000	C	1.971435000	0.449691000	-0.205550000
H	-1.096625000	-4.949595000	0.215923000	H	0.955994000	0.627330000	-0.559298000
H	-3.219681000	-4.184871000	1.751481000	H	3.966914000	3.179573000	0.110419000
H	-3.715336000	-3.686636000	4.133182000	O	3.137709000	-1.612906000	0.287400000
H	-1.929445000	-2.795241000	5.616447000	C	2.422207000	-0.992501000	-0.500736000
H	0.349482000	-2.392348000	4.693766000	N	1.994352000	-1.446990000	-1.696584000
H	0.826967000	-2.882362000	2.316726000	C	2.427137000	-2.673225000	-2.289174000
C	-1.606721000	-3.238529000	-3.387451000	C	1.966920000	-3.901400000	-1.788221000
C	-0.587057000	-3.389976000	-2.263312000	C	2.398771000	-5.074696000	-2.418672000
C	0.614493000	-2.590661000	-2.320081000	H	2.062118000	-6.036092000	-2.040911000
C	0.734340000	-1.475689000	-3.199134000	C	3.239424000	-5.027234000	-3.524405000
C	-0.332452000	-1.294513000	-4.271582000	C	3.672078000	-3.797339000	-4.017690000
C	-0.990854000	-2.621850000	-4.644941000	H	4.327108000	-3.770479000	-4.882081000
H	-0.417164000	-4.421569000	-1.960885000	C	3.281922000	-2.602342000	-3.409356000
H	-2.433334000	-2.588272000	-3.077043000	H	1.487319000	-0.783103000	-2.311322000

C	1.024400000	-3.983251000	-0.600052000	H	3.227285000	-1.795153000	2.549003000
C	1.733606000	-4.611361000	0.611408000	C	4.618881000	-1.905947000	5.748235000
H	0.744380000	-2.962386000	-0.330315000	H	4.304208000	-0.305027000	7.191101000
H	2.037062000	-5.643468000	0.399056000	H	5.120185000	0.197803000	5.715278000
H	2.623340000	-4.028995000	0.863200000	H	4.744893000	-3.185480000	3.991072000
H	1.070097000	-4.635589000	1.485372000	H	5.385838000	-1.566544000	3.753052000
C	3.817415000	-1.256037000	-3.877029000	H	5.597791000	-2.194822000	6.148885000
C	5.046793000	-0.875411000	-3.028159000	H	3.875745000	-2.555775000	6.232937000
H	3.040945000	-0.505532000	-3.706832000	O	-1.183353000	0.225435000	-0.473065000
H	5.878033000	-1.560945000	-3.233385000	O	-3.310540000	-0.580500000	-0.401392000
H	5.379678000	0.143558000	-3.260514000	N	-4.510166000	1.275494000	-0.845355000
H	4.828661000	-0.937244000	-1.957642000	C	-2.382513000	0.447314000	-0.554092000
H	2.206598000	3.254943000	0.218722000	C	-3.136781000	1.623838000	-0.960192000
C	4.155908000	-1.207885000	-5.371833000	C	-4.555627000	0.017331000	-0.565508000
H	3.302932000	-1.520818000	-5.983358000	C	-5.722580000	-0.829116000	-0.370964000
H	4.421056000	-0.184357000	-5.658659000	C	-5.586624000	-2.193133000	-0.067011000
H	5.010116000	-1.847564000	-5.623547000	C	-6.719985000	-2.978259000	0.131263000
C	-0.270040000	-4.732131000	-0.957096000	C	-7.992862000	-2.415880000	0.023285000
H	-0.961352000	-4.735498000	-0.105933000	C	-8.130410000	-1.058967000	-0.286661000
H	-0.775576000	-4.256864000	-1.804863000	C	-7.005208000	-0.267124000	-0.483363000
H	-0.073168000	-5.776166000	-1.225600000	C	-2.771542000	3.012540000	-0.442700000
C	-0.699916000	-1.282208000	2.657682000	C	-2.283719000	3.023395000	0.988211000
C	-1.779525000	-0.354601000	3.237636000	C	-3.178564000	3.028809000	2.065392000
C	-1.316118000	-2.433876000	1.852938000	C	-2.711463000	3.079961000	3.379388000
H	-0.105058000	-1.718043000	3.471075000	C	-1.338686000	3.119422000	3.633532000
C	-2.828971000	-1.127834000	4.042669000	C	-0.438492000	3.087749000	2.566969000
H	-2.263523000	0.170674000	2.406198000	C	-0.907382000	3.035075000	1.254344000
H	-1.319170000	0.428091000	3.849810000	H	-4.596057000	-2.628452000	0.004766000
C	-2.373502000	-3.190933000	2.665799000	H	-6.608151000	-4.032764000	0.366584000
H	-1.775896000	-2.024814000	0.946909000	H	-8.874781000	-3.031129000	0.176602000
H	-0.517319000	-3.106790000	1.533966000	H	-9.119776000	-0.619208000	-0.374393000
C	-3.456314000	-2.246817000	3.203059000	H	-7.092532000	0.787175000	-0.723301000
H	-3.597721000	-0.432173000	4.398670000	H	-2.005654000	3.460978000	-1.073361000
H	-2.360367000	-1.564397000	4.937727000	H	-3.678841000	3.617397000	-0.539360000
H	-2.819653000	-3.972717000	2.039189000	H	-4.246999000	3.007383000	1.865675000
H	-1.890128000	-3.706256000	3.509028000	H	-3.418910000	3.099597000	4.204214000
H	-4.188216000	-2.806228000	3.797819000	H	-0.973592000	3.175098000	4.655805000
H	-4.003802000	-1.803871000	2.360762000	H	0.630075000	3.117621000	2.758535000
C	2.947590000	-0.212628000	3.996158000	H	-0.213112000	3.015707000	0.420012000
C	2.978440000	0.017086000	5.508619000	C	-3.375569000	0.597079000	-3.582985000
C	3.232180000	-1.677576000	3.637392000	C	-2.609580000	1.701908000	-2.850974000
H	3.721235000	0.413799000	3.543499000	C	-1.166787000	1.709566000	-2.960714000
C	4.316411000	-0.443638000	6.103799000	C	-0.431752000	0.523557000	-3.269911000
H	2.160089000	-0.556988000	5.971443000	C	-1.227630000	-0.698951000	-3.698668000
H	2.794062000	1.075339000	5.728927000	C	-2.478702000	-0.272992000	-4.470419000
C	4.572026000	-2.130440000	4.231176000	H	-3.063447000	2.684837000	-2.964540000
H	2.420622000	-2.300031000	4.044802000	H	-3.888517000	-0.058689000	-2.871369000

H	-4.175844000	1.053930000	-4.175763000	C	-4.370841000	-2.545814000	-0.839305000
H	-0.567186000	-1.333983000	-4.298038000	H	-1.753112000	-1.456776000	0.497377000
H	-1.509968000	-1.276010000	-2.805763000	C	-1.156004000	-1.111747000	-2.408235000
H	-2.171284000	0.292583000	-5.358756000	C	-1.483902000	0.163518000	-3.208435000
H	-3.040841000	-1.147003000	-4.820918000	H	-0.798300000	-0.802232000	-1.423574000
O	0.825263000	0.466770000	-3.236001000	H	-1.856793000	-0.089148000	-4.208218000
C	-0.396473000	2.835082000	-2.597314000	H	-2.259026000	0.745174000	-2.697812000
C	0.336159000	3.754188000	-2.265146000	H	-0.593033000	0.791026000	-3.329658000
C	1.209204000	4.767916000	-1.794018000	C	-5.143655000	-2.460635000	0.466646000
C	2.526828000	4.866101000	-2.291469000	C	-6.281993000	-1.430040000	0.348775000
C	0.808038000	5.661962000	-0.777596000	H	-4.447309000	-2.098605000	1.229712000
C	3.410852000	5.808141000	-1.775201000	H	-7.017717000	-1.752951000	-0.397883000
H	2.838817000	4.187158000	-3.078681000	H	-6.802845000	-1.317269000	1.307868000
C	1.699197000	6.603014000	-0.270501000	H	-5.889538000	-0.456268000	0.042581000
H	-0.200642000	5.593245000	-0.382688000	H	-2.296516000	1.758489000	4.279727000
C	3.005240000	6.679966000	-0.760913000	C	-5.669551000	-3.824098000	0.938578000
H	4.422317000	5.865793000	-2.168968000	H	-4.862373000	-4.562338000	1.001997000
H	1.373225000	7.278436000	0.516137000	H	-6.124917000	-3.729108000	1.930988000
H	3.697956000	7.414874000	-0.360905000	H	-6.437456000	-4.222256000	0.265853000
H	-0.194107000	-0.307986000	0.868900000	C	-0.025820000	-1.921076000	-3.058249000
H	0.873038000	-0.030185000	4.092340000	H	0.886779000	-1.317746000	-3.103136000
H	3.558361000	-5.947841000	-4.005899000	H	0.192933000	-2.825262000	-2.482730000
TS2-*SR′*				H	-0.271943000	-2.220751000	-4.083602000
N	-1.920884000	4.031213000	0.338147000	C	0.612298000	2.932744000	-0.506288000
N	-0.212119000	2.438146000	0.599769000	C	1.591280000	4.021962000	-0.045361000
N	-2.263872000	2.153443000	1.641407000	C	1.363215000	1.786854000	-1.189573000
C	-1.445028000	2.868787000	0.850731000	H	-0.079452000	3.357036000	-1.245616000
C	-3.211163000	2.735318000	2.595857000	C	2.409191000	4.562066000	-1.227601000
H	-2.854597000	3.715029000	2.920451000	H	2.253655000	3.582486000	0.707974000
H	-4.209495000	2.849947000	2.153039000	H	1.047592000	4.838706000	0.450557000
C	-3.215735000	1.667972000	3.692675000	C	2.106719000	2.340069000	-2.413812000
C	-3.198732000	0.364800000	2.879781000	H	2.068493000	1.337887000	-0.481892000
H	-4.211429000	0.125205000	2.537737000	H	0.655386000	1.003901000	-1.473469000
H	-2.818678000	-0.493219000	3.437462000	C	3.098972000	3.438242000	-2.012601000
C	-2.293334000	0.688279000	1.660136000	H	3.155288000	5.276585000	-0.862227000
H	-1.294022000	0.280187000	1.789967000	H	1.738735000	5.118237000	-1.900758000
H	-4.080406000	1.747019000	4.357738000	H	2.633737000	1.534132000	-2.933363000
O	-3.768192000	0.847455000	-0.254474000	H	1.372913000	2.742711000	-3.129176000
C	-2.952901000	0.168777000	0.372279000	H	3.587589000	3.853469000	-2.902567000
N	-2.620040000	-1.111065000	0.084477000	H	3.887306000	2.996522000	-1.396452000
C	-3.159624000	-1.852602000	-1.015019000	C	-3.247109000	4.103247000	-0.309564000
C	-2.431866000	-1.916090000	-2.215610000	C	-3.976396000	5.394867000	0.061990000
C	-2.948852000	-2.693386000	-3.256663000	C	-3.106534000	3.948762000	-1.829837000
H	-2.404974000	-2.759554000	-4.193722000	H	-3.807272000	3.237532000	0.048064000
C	-4.150588000	-3.379697000	-3.109329000	C	-5.352313000	5.451214000	-0.617804000
C	-4.857156000	-3.301158000	-1.911630000	H	-3.371559000	6.256725000	-0.258095000
H	-5.793862000	-3.839728000	-1.806260000	H	-4.075348000	5.464087000	1.151592000

C	-4.483235000	3.998510000	-2.504389000	C	0.151011000	-0.468598000	4.471938000
H	-2.469404000	4.757495000	-2.221231000	C	0.245818000	-1.990558000	4.373707000
H	-2.607319000	2.998665000	-2.048381000	H	3.443661000	-2.023766000	2.960009000
C	-5.236913000	5.284479000	-2.139406000	H	2.244581000	-2.123835000	5.173478000
H	-5.852276000	6.395211000	-0.371266000	H	1.805881000	-3.507358000	4.190659000
H	-5.982131000	4.645889000	-0.213775000	H	-0.887399000	-0.127334000	4.446534000
H	-4.369237000	3.914909000	-3.591416000	H	0.564220000	-0.133223000	5.435716000
H	-5.061370000	3.123398000	-2.178737000	H	-0.305410000	-2.316262000	3.484709000
H	-6.234389000	5.282289000	-2.594686000	H	-0.224174000	-2.464408000	5.244278000
H	-4.701695000	6.149626000	-2.557524000	O	0.503642000	1.397520000	3.028518000
H	0.241821000	1.892368000	1.363545000	C	3.023984000	0.448501000	2.141758000
H	-1.219662000	4.650028000	-0.050712000	C	3.857446000	1.130370000	1.566385000
O	-0.006591000	-1.379276000	0.953377000	C	4.824783000	1.938443000	0.913837000
O	1.908695000	-1.369981000	-0.268645000	C	4.918339000	3.319325000	1.193383000
N	3.088638000	-3.018108000	0.720773000	C	5.704179000	1.388649000	-0.042784000
C	1.087569000	-1.874811000	0.725210000	C	5.831050000	4.121105000	0.514173000
C	1.862476000	-2.882608000	1.428923000	H	4.266116000	3.745981000	1.948837000
C	3.082673000	-2.113878000	-0.195930000	C	6.616823000	2.197329000	-0.711965000
C	4.141325000	-1.766751000	-1.128685000	H	5.651122000	0.329340000	-0.258942000
C	3.904807000	-0.873816000	-2.182978000	C	6.681593000	3.567841000	-0.446627000
C	4.938458000	-0.518870000	-3.044639000	H	5.882978000	5.183141000	0.739767000
C	6.215893000	-1.052438000	-2.864736000	H	7.273681000	1.751157000	-1.453722000
C	6.453131000	-1.952198000	-1.819939000	H	7.390347000	4.196909000	-0.977624000
C	5.424473000	-2.310731000	-0.954954000	H	-4.538766000	-3.977549000	-3.929602000
C	1.161624000	-4.184994000	1.789686000	**TS2-*RS′***			
C	0.450008000	-4.733087000	0.566462000	N	-4.159658000	-2.599358000	-0.394014000
C	1.172067000	-5.316369000	-0.483149000	N	-2.874914000	-1.753071000	1.394062000
C	0.525028000	-5.717722000	-1.651910000	N	-1.874523000	-2.292733000	-0.618344000
C	-0.853080000	-5.537980000	-1.790977000	C	-2.972939000	-2.193796000	0.144388000
C	-1.582301000	-4.960190000	-0.751702000	C	-1.655318000	-3.308325000	-1.655615000
C	-0.932514000	-4.562552000	0.416980000	H	-2.240959000	-4.201408000	-1.427871000
H	2.913380000	-0.459134000	-2.307324000	H	-1.945736000	-2.922790000	-2.638844000
H	4.748699000	0.182324000	-3.852229000	C	-0.138978000	-3.495056000	-1.567160000
H	7.023958000	-0.769896000	-3.533470000	C	0.391087000	-2.070176000	-1.318149000
H	7.446449000	-2.367417000	-1.675734000	H	0.627259000	-1.580924000	-2.267262000
H	5.593527000	-2.994970000	-0.130473000	H	1.280663000	-2.066899000	-0.689512000
H	0.430960000	-4.030902000	2.585211000	C	-0.772050000	-1.316549000	-0.612154000
H	1.916270000	-4.887772000	2.157733000	H	-0.496905000	-1.043386000	0.405877000
H	2.247418000	-5.433051000	-0.384875000	H	0.280223000	-3.949294000	-2.468937000
H	1.099765000	-6.165707000	-2.458314000	O	-1.917109000	-0.260432000	-2.462552000
H	-1.356516000	-5.835182000	-2.706357000	C	-1.211914000	-0.106535000	-1.460684000
H	-2.650710000	-4.803987000	-0.859034000	N	-0.716386000	1.070724000	-1.035239000
H	-1.501229000	-4.099403000	1.219931000	C	-0.806977000	2.306298000	-1.754122000
C	1.710350000	-2.419901000	4.256581000	C	-1.852206000	3.195486000	-1.450746000
C	2.404128000	-1.739009000	3.097136000	C	-1.891524000	4.423545000	-2.118003000
C	2.123965000	-0.343076000	2.893364000	H	-2.687374000	5.129156000	-1.900394000
C	0.923452000	0.263184000	3.379768000	C	-0.919523000	4.752047000	-3.060379000

C	0.113401000	3.861557000	-3.338837000	H	-6.516013000	-3.009330000	-1.688467000
H	0.872972000	4.132507000	-4.065050000	H	-5.223472000	-3.892587000	-2.505769000
C	0.196234000	2.627506000	-2.685815000	C	-5.581317000	0.043752000	-2.787517000
H	-0.234830000	1.090867000	-0.127565000	H	-5.993455000	-0.606863000	-0.754810000
C	-2.862136000	2.847698000	-0.371781000	H	-4.359499000	0.037730000	-0.998256000
C	-4.287596000	3.316439000	-0.688375000	C	-6.614638000	-0.841352000	-3.497317000
H	-2.885417000	1.756560000	-0.299438000	H	-6.861081000	-2.904280000	-4.146784000
H	-4.375346000	4.408652000	-0.669388000	H	-5.238296000	-2.258938000	-4.373747000
H	-4.608639000	2.967276000	-1.675532000	H	-5.988143000	1.047243000	-2.616434000
H	-4.986677000	2.923387000	0.059574000	H	-4.690578000	0.165919000	-3.417322000
C	1.323070000	1.652338000	-2.983547000	H	-6.880989000	-0.409785000	-4.469380000
C	0.980153000	0.796642000	-4.217102000	H	-7.538786000	-0.868772000	-2.901263000
H	1.396290000	0.981866000	-2.124731000	O	0.542644000	1.280691000	1.399564000
H	0.919201000	1.421951000	-5.116264000	O	2.256291000	0.424796000	0.172669000
H	1.757225000	0.040411000	-4.386494000	N	4.046187000	1.043546000	1.394130000
H	0.017061000	0.292596000	-4.090650000	C	1.752921000	1.142936000	1.245399000
H	0.107341000	-4.136859000	-0.718249000	C	2.882884000	1.472020000	2.088531000
C	2.689357000	2.333871000	-3.135295000	C	3.641434000	0.423622000	0.341273000
H	2.920630000	2.952532000	-2.263103000	C	4.438012000	-0.260472000	-0.663213000
H	3.472482000	1.574867000	-3.234510000	C	3.847243000	-0.842476000	-1.794003000
H	2.733930000	2.970126000	-4.027253000	C	4.635584000	-1.500241000	-2.734294000
C	-2.381542000	3.388209000	0.988251000	C	6.016705000	-1.586671000	-2.556784000
H	-3.100624000	3.149904000	1.780778000	C	6.610056000	-1.007132000	-1.430135000
H	-1.413930000	2.956620000	1.260943000	C	5.829334000	-0.347081000	-0.487649000
H	-2.272274000	4.478680000	0.949431000	C	2.941631000	2.874577000	2.676860000
C	-3.941527000	-1.185644000	2.222277000	C	2.772815000	3.869022000	1.541241000
C	-3.889179000	-1.829008000	3.615781000	C	3.849684000	4.203160000	0.711348000
C	-3.793513000	0.342436000	2.279765000	C	3.651632000	4.985269000	-0.427341000
H	-4.911489000	-1.412477000	1.764013000	C	2.370491000	5.428531000	-0.762703000
C	-4.888672000	-1.174867000	4.577269000	C	1.291140000	5.104686000	0.060304000
H	-2.867705000	-1.727837000	4.000906000	C	1.495671000	4.341696000	1.208820000
H	-4.080637000	-2.904836000	3.523498000	H	2.775580000	-0.785592000	-1.924217000
C	-4.793230000	0.974548000	3.254745000	H	4.166936000	-1.957137000	-3.600840000
H	-2.767067000	0.584340000	2.581046000	H	6.629167000	-2.105143000	-3.288888000
H	-3.925681000	0.747935000	1.271977000	H	7.684692000	-1.074289000	-1.286383000
C	-4.688046000	0.344306000	4.648809000	H	6.271222000	0.103010000	0.394731000
H	-4.788468000	-1.623928000	5.572100000	H	2.149024000	3.022983000	3.412928000
H	-5.914556000	-1.386615000	4.240653000	H	3.904179000	3.001032000	3.182399000
H	-4.624340000	2.056541000	3.305150000	H	4.839487000	3.822642000	0.947017000
H	-5.814699000	0.835530000	2.870593000	H	4.497239000	5.234124000	-1.063199000
H	-5.424427000	0.793297000	5.325750000	H	2.210412000	6.011155000	-1.665156000
H	-3.696139000	0.559983000	5.070262000	H	0.288685000	5.426717000	-0.205299000
C	-4.609623000	-1.997394000	-1.672229000	H	0.651279000	4.077011000	1.837859000
C	-5.644330000	-2.892266000	-2.351148000	C	2.097745000	0.666949000	4.742001000
C	-5.143703000	-0.574869000	-1.454825000	C	2.582176000	-0.065559000	3.511575000
H	-3.726925000	-1.912238000	-2.307019000	C	1.732099000	-1.091172000	2.978949000
C	-6.093387000	-2.273445000	-3.683679000	C	0.324248000	-1.092700000	3.214760000

C	-0.234620000	-0.190199000	4.309176000	H	-1.804573000	7.370233000	1.343989000
C	0.616497000	1.038271000	4.636409000	C	-0.093194000	7.521317000	0.058430000
H	3.645254000	-0.288756000	3.494114000	C	0.805756000	6.830849000	-0.748499000
H	2.245741000	-0.008675000	5.599619000	H	1.600796000	7.372375000	-1.253358000
H	2.713109000	1.549211000	4.942029000	C	0.692903000	5.449941000	-0.935262000
H	-1.248407000	0.107897000	4.023645000	H	0.385134000	2.802659000	-0.238422000
H	-0.341785000	-0.824781000	5.203062000	C	-2.344681000	4.719885000	1.337879000
H	0.480733000	1.772065000	3.837289000	C	-3.733120000	5.059959000	0.770045000
H	0.273245000	1.501184000	5.569738000	H	-2.172340000	3.649873000	1.218095000
O	-0.465804000	-1.883767000	2.627976000	H	-3.944733000	6.131251000	0.875891000
C	2.260095000	-2.070270000	2.102149000	H	-3.785835000	4.791360000	-0.286291000
C	2.710405000	-2.940848000	1.376365000	H	-4.512638000	4.511534000	1.312298000
C	3.189913000	-3.974909000	0.529595000	C	1.669168000	4.737360000	-1.861528000
C	2.429226000	-5.148836000	0.338282000	C	1.483596000	5.204393000	-3.315139000
C	4.419230000	-3.855647000	-0.150311000	H	1.454476000	3.668610000	-1.837966000
C	2.872754000	-6.150415000	-0.519871000	H	1.706123000	6.272203000	-3.423666000
H	1.494999000	-5.257728000	0.880635000	H	2.152346000	4.650893000	-3.985068000
C	4.856132000	-4.864262000	-1.002549000	H	0.452078000	5.044138000	-3.647442000
H	5.013959000	-2.960750000	-0.011645000	H	-0.142678000	-0.815437000	-3.228146000
C	4.086763000	-6.013945000	-1.198171000	C	3.124878000	4.905120000	-1.397184000
H	2.271171000	-7.045601000	-0.655777000	H	3.254814000	4.537882000	-0.374629000
H	5.801682000	-4.744067000	-1.524376000	H	3.797452000	4.332212000	-2.045960000
H	4.430845000	-6.797101000	-1.867962000	H	3.439645000	5.954726000	-1.424956000
H	-1.932093000	-1.751467000	1.846101000	C	-2.291883000	5.025276000	2.844339000
H	-4.904774000	-2.718646000	0.282710000	H	-2.998298000	4.381523000	3.381853000
H	-0.964832000	5.708403000	-3.574743000	H	-1.292736000	4.853004000	3.256312000
TS3-*SSR*$_a$′				H	-2.565315000	6.065077000	3.058482000
N	-4.237665000	-0.579130000	-1.403309000	C	-3.853359000	0.069043000	1.414598000
N	-2.819350000	-0.060426000	0.368308000	C	-3.430105000	-0.698546000	2.671858000
N	-2.203813000	0.446183000	-1.833260000	C	-4.091428000	1.553169000	1.728022000
C	-3.074758000	-0.045228000	-0.943715000	H	-4.781943000	-0.365982000	1.030364000
C	-2.149351000	-0.032418000	-3.224869000	C	-4.438377000	-0.503888000	3.810787000
H	-2.543486000	-1.049540000	-3.271899000	H	-2.442027000	-0.337402000	2.975456000
H	-2.756018000	0.618086000	-3.867757000	H	-3.322456000	-1.763666000	2.449261000
C	-0.666496000	0.073431000	-3.581762000	C	-5.116542000	1.732162000	2.852622000
C	-0.207447000	1.305721000	-2.794408000	H	-3.131151000	1.979566000	2.032254000
H	-0.441657000	2.220505000	-3.350759000	H	-4.402328000	2.074668000	0.816083000
H	0.860227000	1.306016000	-2.570696000	C	-4.675590000	0.980529000	4.115236000
C	-1.038070000	1.268680000	-1.484844000	H	-4.079092000	-1.033104000	4.701055000
H	-0.459383000	0.790390000	-0.695518000	H	-5.395923000	-0.971153000	3.534920000
H	-0.513583000	0.181969000	-4.659582000	H	-5.248174000	2.800089000	3.065679000
O	-2.491185000	3.205627000	-1.472160000	H	-6.097740000	1.354416000	2.527195000
C	-1.433084000	2.701030000	-1.110479000	H	-5.423196000	1.091868000	4.910188000
N	-0.439859000	3.352085000	-0.451612000	H	-3.742765000	1.426257000	4.488848000
C	-0.347391000	4.767687000	-0.270558000	C	-5.127894000	0.035772000	-2.403217000
C	-1.249951000	5.443673000	0.573331000	C	-6.488037000	-0.666496000	-2.340493000
C	-1.110041000	6.829288000	0.707964000	C	-5.289203000	1.546728000	-2.186266000

H	-4.716567000	-0.134249000	-3.406681000	C	3.129397000	1.659841000	3.146336000
C	-7.455758000	-0.075102000	-3.373838000	C	2.685854000	0.316295000	2.493865000
H	-6.904267000	-0.537650000	-1.329971000	C	1.175035000	0.156272000	2.390908000
H	-6.357467000	-1.740657000	-2.504260000	C	0.313537000	1.300989000	2.253880000
C	-6.243440000	2.141493000	-3.228883000	C	0.865558000	2.634814000	2.736628000
H	-5.701732000	1.702997000	-1.178921000	C	1.968632000	2.428696000	3.776593000
H	-4.320440000	2.053317000	-2.209377000	H	3.074701000	-0.511854000	3.094409000
C	-7.608575000	1.442288000	-3.203700000	H	3.586105000	2.316376000	2.394570000
H	-8.429618000	-0.572379000	-3.293498000	H	3.915536000	1.462462000	3.881248000
H	-7.076624000	-0.290997000	-4.383051000	H	0.019731000	3.202559000	3.133078000
H	-6.357189000	3.216850000	-3.051601000	H	1.254410000	3.211811000	1.886269000
H	-5.798991000	2.036817000	-4.229687000	H	1.563390000	1.871536000	4.630592000
H	-8.263210000	1.846082000	-3.985504000	H	2.324333000	3.392501000	4.159592000
H	-8.100276000	1.648829000	-2.242113000	O	-0.868785000	1.249859000	1.847503000
H	-1.881805000	0.193919000	0.704377000	C	0.607220000	-1.073493000	2.509475000
H	-4.646181000	-1.294414000	-0.816087000	C	0.107289000	-2.233704000	2.603428000
O	2.031481000	1.680430000	-0.292037000	C	-0.499756000	-3.026511000	3.666782000
O	4.276002000	1.871758000	-0.172274000	C	-1.123688000	-2.408321000	4.767467000
N	4.848343000	0.215475000	1.275493000	C	-0.515471000	-4.430331000	3.587602000
C	3.080293000	1.279839000	0.152490000	C	-1.748565000	-3.169137000	5.751186000
C	3.397055000	0.131005000	1.104825000	H	-1.112507000	-1.324539000	4.832891000
C	5.262813000	1.167833000	0.538561000	C	-1.135847000	-5.188552000	4.580003000
C	6.635147000	1.621116000	0.333938000	H	-0.043237000	-4.919604000	2.740508000
C	6.921045000	2.710483000	-0.499917000	C	-1.758402000	-4.564134000	5.661886000
C	8.242137000	3.115496000	-0.678611000	H	-2.225958000	-2.673596000	6.592855000
C	9.276819000	2.439293000	-0.030847000	H	-1.135976000	-6.272687000	4.504065000
C	8.991136000	1.351936000	0.800741000	H	-2.247143000	-5.157580000	6.429612000
C	7.676066000	0.941301000	0.984506000	H	0.001363000	8.596556000	0.184022000
C	3.019566000	-1.208324000	0.422521000	O	-0.240350000	-1.490341000	-0.983387000
C	3.712629000	-1.412389000	-0.902539000	O	1.109467000	-3.304151000	-1.273731000
C	5.012587000	-1.926770000	-0.968967000	N	0.167267000	-4.817797000	0.108773000
C	5.649142000	-2.096356000	-2.198383000	C	0.011468000	-2.654789000	-0.717661000
C	4.992415000	-1.750046000	-3.380701000	C	-0.538270000	-3.584644000	0.259346000
C	3.695867000	-1.234190000	-3.324310000	C	1.123078000	-4.580290000	-0.721630000
C	3.062106000	-1.066497000	-2.093775000	C	2.222536000	-5.444183000	-1.130020000
H	6.111511000	3.230127000	-1.000011000	C	3.231137000	-4.963593000	-1.980078000
H	8.463215000	3.959789000	-1.324779000	C	4.289814000	-5.794761000	-2.337949000
H	10.305648000	2.757526000	-0.173043000	C	4.351036000	-7.104559000	-1.859864000
H	9.796425000	0.825206000	1.304150000	C	3.345537000	-7.584362000	-1.013854000
H	7.431357000	0.099874000	1.623755000	C	2.287388000	-6.760987000	-0.646323000
H	1.939890000	-1.197824000	0.280924000	C	-2.013354000	-3.585003000	0.576996000
H	3.263806000	-2.011675000	1.124229000	C	-2.997302000	-3.788529000	-0.557435000
H	5.523640000	-2.195267000	-0.049414000	C	-4.365641000	-3.833978000	-0.244394000
H	6.656554000	-2.502016000	-2.232807000	C	-5.329412000	-3.987541000	-1.239677000
H	5.485958000	-1.884747000	-4.339328000	C	-4.941288000	-4.087393000	-2.578799000
H	3.172681000	-0.971925000	-4.240058000	C	-3.586014000	-4.042721000	-2.901829000
H	2.040572000	-0.705094000	-2.046394000	C	-2.623482000	-3.900711000	-1.899115000

H	3.188215000	-3.944460000	-2.344583000	C	4.238608000	5.095531000	-0.250882000
H	5.070958000	-5.409672000	-2.987096000	H	3.399640000	3.136717000	-0.162386000
H	5.178946000	-7.749848000	-2.140465000	H	4.856924000	5.779878000	0.341444000
H	3.391026000	-8.602812000	-0.638209000	H	4.753175000	4.915266000	-1.202327000
H	1.503216000	-7.113609000	0.015510000	H	3.289961000	5.601649000	-0.460971000
H	-2.235499000	-2.616879000	1.035853000	H	0.232265000	1.174977000	-3.697722000
H	-2.191781000	-4.335470000	1.354305000	C	5.316675000	3.021092000	0.748584000
H	-4.670628000	-3.765318000	0.798218000	H	5.132278000	2.065688000	1.248203000
H	-6.381851000	-4.034031000	-0.971925000	H	5.823608000	2.810354000	-0.200200000
H	-5.688079000	-4.210532000	-3.358179000	H	5.999777000	3.608546000	1.373071000
H	-3.270629000	-4.132555000	-3.937936000	C	-0.363647000	2.491697000	4.671240000
H	-1.573233000	-3.890493000	-2.169143000	H	-1.361390000	2.041215000	4.735708000
H	-0.073049000	-2.967122000	1.338410000	H	0.376185000	1.687437000	4.720245000
TS3-*SSS*$_a$′				H	-0.230209000	3.126802000	5.554734000
N	-3.533164000	2.566825000	-1.766333000	C	-3.683315000	1.272979000	0.802901000
N	-2.475550000	1.406010000	-0.031334000	C	-4.425099000	-0.034701000	0.492274000
N	-1.212336000	2.399752000	-1.713753000	C	-3.297832000	1.377372000	2.283420000
C	-2.392871000	2.126087000	-1.143464000	H	-4.334424000	2.127311000	0.578261000
C	-1.051935000	2.806106000	-3.118566000	C	-5.640316000	-0.224287000	1.409560000
H	-1.866237000	2.399419000	-3.717199000	H	-3.738651000	-0.880350000	0.619602000
H	-1.051104000	3.901094000	-3.194249000	H	-4.739539000	-0.041496000	-0.562441000
C	0.321400000	2.241413000	-3.473117000	C	-4.519609000	1.179789000	3.188263000
C	1.109353000	2.469884000	-2.179650000	H	-2.530326000	0.630941000	2.504740000
H	1.425170000	3.517456000	-2.112068000	H	-2.837638000	2.353991000	2.456162000
H	1.993346000	1.842067000	-2.074760000	C	-5.238353000	-0.141467000	2.887001000
C	0.083137000	2.166911000	-1.061380000	H	-6.103514000	-1.192631000	1.196297000
H	0.166975000	1.124947000	-0.742588000	H	-6.394691000	0.548931000	1.195088000
H	0.763980000	2.744099000	-4.337753000	H	-4.203805000	1.217803000	4.238061000
O	-0.373892000	4.141233000	0.263076000	H	-5.221437000	2.015134000	3.044202000
C	0.292733000	3.120758000	0.125902000	H	-6.123588000	-0.245750000	3.525829000
N	1.326269000	2.745412000	0.917100000	H	-4.575971000	-0.983672000	3.124118000
C	1.905135000	3.536287000	1.959936000	C	-3.756462000	4.000099000	-2.066273000
C	1.183669000	3.792453000	3.141861000	C	-5.174875000	4.158523000	-2.618936000
C	1.809240000	4.550853000	4.137865000	C	-3.524238000	4.896073000	-0.841591000
H	1.267678000	4.768516000	5.053634000	H	-3.056791000	4.296432000	-2.853373000
C	3.109456000	5.019900000	3.983013000	C	-5.469770000	5.627254000	-2.953412000
C	3.808610000	4.744462000	2.812129000	H	-5.892580000	3.808817000	-1.860284000
H	4.822240000	5.115762000	2.690803000	H	-5.303561000	3.521792000	-3.502544000
C	3.221196000	4.008359000	1.778962000	C	-3.812105000	6.363380000	-1.184269000
H	1.820033000	1.900247000	0.649444000	H	-4.199539000	4.568327000	-0.036908000
C	-0.234164000	3.290671000	3.363866000	H	-2.498989000	4.771174000	-0.477801000
C	-1.223515000	4.469517000	3.342369000	C	-5.230094000	6.540536000	-1.743202000
H	-0.482965000	2.606619000	2.550848000	H	-6.500988000	5.724280000	-3.311932000
H	-0.994118000	5.185154000	4.141182000	H	-4.819211000	5.943193000	-3.781355000
H	-1.173716000	4.986920000	2.382105000	H	-3.667209000	6.986271000	-0.294541000
H	-2.250141000	4.118053000	3.501135000	H	-3.080668000	6.710332000	-1.928630000
C	3.999166000	3.770078000	0.492278000	H	-5.404692000	7.586551000	-2.021676000

H	-5.960394000	6.297253000	-0.957971000	O	-0.497679000	0.273827000	1.457733000
H	-1.652346000	0.882123000	0.317807000	C	0.024972000	-1.577598000	-0.529373000
H	-4.365346000	2.122186000	-1.399547000	C	-0.834914000	-1.813164000	-1.436323000
O	3.014808000	0.630135000	-0.285835000	C	-1.101136000	-1.302299000	-2.784806000
O	5.004472000	-0.404601000	-0.046947000	C	-2.269031000	-0.558662000	-3.026064000
N	4.461146000	-2.600100000	-0.268461000	C	-0.255928000	-1.585296000	-3.871404000
C	3.651153000	-0.395362000	-0.274841000	C	-2.565144000	-0.084334000	-4.301517000
C	3.221887000	-1.846116000	-0.468240000	H	-2.941185000	-0.360339000	-2.199268000
C	5.392288000	-1.754225000	-0.067105000	C	-0.552437000	-1.105200000	-5.146912000
C	6.814403000	-2.009117000	0.137139000	H	0.625598000	-2.197035000	-3.719538000
C	7.719254000	-0.954370000	0.318835000	C	-1.703820000	-0.347277000	-5.369625000
C	9.072634000	-1.229894000	0.501662000	H	-3.473866000	0.490981000	-4.458503000
C	9.525635000	-2.549924000	0.504237000	H	0.119656000	-1.331396000	-5.970096000
C	8.622400000	-3.602013000	0.323210000	H	-1.935286000	0.019398000	-6.365429000
C	7.270504000	-3.336333000	0.139666000	H	3.577314000	5.600016000	4.773817000
C	2.726526000	-2.060654000	-1.919242000	O	-1.833126000	-5.712721000	-1.299223000
C	3.678560000	-1.561107000	-2.978435000	O	-1.475855000	-4.821807000	0.793548000
C	4.859081000	-2.248072000	-3.292965000	N	-2.834752000	-3.023053000	0.737522000
C	5.741458000	-1.741841000	-4.246309000	C	-2.059618000	-4.825340000	-0.505359000
C	5.454735000	-0.544830000	-4.905722000	C	-2.801960000	-3.573200000	-0.564904000
C	4.274835000	0.138799000	-4.612114000	C	-2.013465000	-3.732301000	1.440550000
C	3.395283000	-0.368791000	-3.656227000	C	-1.598962000	-3.489986000	2.813634000
H	7.359304000	0.068323000	0.313856000	C	-0.932978000	-4.475544000	3.559633000
H	9.773781000	-0.412701000	0.642012000	C	-0.556267000	-4.217373000	4.876163000
H	10.581550000	-2.760747000	0.647294000	C	-0.830430000	-2.978074000	5.459758000
H	8.975018000	-4.629065000	0.325972000	C	-1.487016000	-1.992306000	4.716546000
H	6.552467000	-4.137106000	-0.001353000	C	-1.864093000	-2.243255000	3.402291000
H	1.777574000	-1.537525000	-2.013963000	C	-3.970827000	-3.410601000	-1.508403000
H	2.529784000	-3.132702000	-2.027565000	C	-5.264378000	-3.999577000	-0.981753000
H	5.084624000	-3.178159000	-2.781468000	C	-5.359534000	-5.366454000	-0.686764000
H	6.653901000	-2.284783000	-4.476655000	C	-6.540808000	-5.901045000	-0.176472000
H	6.143587000	-0.152406000	-5.648483000	C	-7.649290000	-5.080105000	0.047333000
H	4.036322000	1.065025000	-5.127837000	C	-7.567726000	-3.720743000	-0.251205000
H	2.469737000	0.154961000	-3.438544000	C	-6.382337000	-3.189512000	-0.764140000
C	2.828505000	-2.220932000	2.006990000	H	-0.720866000	-5.434307000	3.099144000
C	2.153360000	-2.256928000	0.611139000	H	-0.043253000	-4.985440000	5.448216000
C	0.869500000	-1.429139000	0.525763000	H	-0.529546000	-2.779326000	6.484465000
C	0.465098000	-0.520702000	1.569946000	H	-1.691933000	-1.020552000	5.158021000
C	1.219307000	-0.546102000	2.883592000	H	-2.344640000	-1.481920000	2.802744000
C	1.858544000	-1.908512000	3.139820000	H	-3.691236000	-3.896985000	-2.451009000
H	1.903826000	-3.297343000	0.372502000	H	-4.125438000	-2.350593000	-1.732559000
H	3.608674000	-1.447207000	2.025771000	H	-4.500542000	-6.008092000	-0.862012000
H	3.344345000	-3.171320000	2.169310000	H	-6.597794000	-6.963207000	0.046785000
H	0.510332000	-0.269301000	3.666099000	H	-8.568394000	-5.498779000	0.448224000
H	1.990897000	0.239715000	2.858481000	H	-8.424547000	-3.072281000	-0.086170000
H	1.079447000	-2.672964000	3.204535000	H	-6.322829000	-2.130056000	-1.001646000
H	2.390524000	-1.908780000	4.098077000	H	-1.743480000	-2.709439000	-1.086921000

TS5-*SS*

N	-4.793716000	-2.482168000	-0.890315000
N	-2.548145000	-2.252445000	-0.233842000
N	-3.323806000	-1.166774000	-2.117611000
C	-3.548559000	-1.968671000	-1.063673000
C	-4.090668000	-1.183128000	-3.366868000
H	-4.411776000	-2.202271000	-3.592860000
H	-4.975538000	-0.538564000	-3.299987000
C	-3.073927000	-0.601754000	-4.352028000
C	-2.393274000	0.503062000	-3.526446000
H	-2.982274000	1.424420000	-3.572988000
H	-1.382189000	0.732844000	-3.868597000
C	-2.383554000	-0.038796000	-2.071113000
H	-1.383993000	-0.363963000	-1.776950000
H	-3.547198000	-0.221652000	-5.261553000
O	-4.150259000	1.150138000	-0.922740000
C	-2.935005000	1.030279000	-1.106095000
N	-1.963961000	1.812275000	-0.605929000
C	-2.175488000	2.908974000	0.286521000
C	-2.151540000	2.676734000	1.672079000
C	-2.307679000	3.769507000	2.526792000
H	-2.298022000	3.601817000	3.600136000
C	-2.477383000	5.067707000	2.039248000
C	-2.482989000	5.261515000	0.656763000
H	-2.603176000	6.270573000	0.273180000
C	-2.323743000	4.202230000	-0.240750000
H	-1.020888000	1.377816000	-0.592545000
C	-2.019464000	1.269104000	2.232479000
C	-3.392328000	0.787317000	2.735318000
H	-1.713756000	0.612703000	1.414833000
H	-3.746816000	1.407165000	3.567393000
H	-4.130202000	0.850768000	1.928722000
H	-3.342723000	-0.250668000	3.088656000
C	-2.335908000	4.425305000	-1.744395000
C	-3.774995000	4.330273000	-2.287024000
H	-1.755011000	3.610624000	-2.189142000
H	-4.387401000	5.148704000	-1.888810000
H	-3.781781000	4.407488000	-3.381855000
H	-4.246679000	3.387542000	-1.994950000
H	-2.349977000	-1.373616000	-4.633424000
C	-1.672374000	5.741487000	-2.168659000
H	-0.665099000	5.827608000	-1.750504000
H	-2.254912000	6.614833000	-1.853009000
C	-0.933985000	1.158986000	3.312905000
H	-0.854320000	0.124967000	3.669154000
H	0.043212000	1.450780000	2.915033000
H	-1.152195000	1.787288000	4.183755000
C	-2.639402000	6.244150000	2.986580000
C	-1.382724000	6.447120000	3.849622000
C	-3.894239000	6.097384000	3.863134000
H	-2.768318000	7.143495000	2.369525000
H	-0.493600000	6.578170000	3.224014000
H	-1.488550000	7.330888000	4.489850000
H	-1.207993000	5.581616000	4.499228000
H	-3.817685000	5.220829000	4.516986000
H	-4.028099000	6.978975000	4.501046000
H	-4.792096000	5.976944000	3.247704000
C	-2.667524000	-3.011271000	1.015009000
C	-2.561347000	-4.524160000	0.752447000
C	-1.572658000	-2.561595000	1.988017000
H	-3.644685000	-2.773431000	1.456208000
C	-2.624477000	-5.323156000	2.061399000
H	-1.609861000	-4.703251000	0.237004000
H	-3.353566000	-4.853164000	0.065644000
C	-1.660697000	-3.339882000	3.305168000
H	-0.604198000	-2.739704000	1.509933000
H	-1.653472000	-1.485602000	2.157110000
C	-1.563241000	-4.851256000	3.064274000
H	-2.503193000	-6.391578000	1.847920000
H	-3.621820000	-5.205051000	2.510703000
H	-0.863056000	-3.012974000	3.980992000
H	-2.611848000	-3.106926000	3.806332000
H	-1.668539000	-5.397033000	4.009197000
H	-0.563146000	-5.086340000	2.675352000
C	-5.978604000	-1.590685000	-0.856543000
C	-7.156634000	-2.204726000	-1.612820000
C	-6.347190000	-1.262736000	0.596094000
H	-5.670946000	-0.653713000	-1.323961000
C	-8.375120000	-1.271301000	-1.561337000
H	-7.412930000	-3.172353000	-1.156044000
H	-6.866285000	-2.411216000	-2.649419000
C	-7.560733000	-0.325425000	0.644290000
H	-6.577801000	-2.197004000	1.132556000
H	-5.486047000	-0.800127000	1.089610000
C	-8.754096000	-0.918779000	-0.116315000
H	-9.222627000	-1.735354000	-2.079035000
H	-8.139428000	-0.347122000	-2.107946000
H	-7.831512000	-0.120596000	1.686458000
H	-7.275988000	0.636235000	0.196808000
H	-9.596041000	-0.216627000	-0.108272000
H	-9.097034000	-1.827932000	0.398951000
H	-1.584252000	-2.162657000	-0.587097000
H	-1.592590000	5.783550000	-3.261211000
H	-4.842640000	-3.253898000	-0.236256000

O	0.059430000	-2.663614000	-0.936530000	H	9.528010000	3.567616000	0.154917000
O	1.746540000	-1.450886000	-1.889251000	C	1.565368000	2.150887000	-0.774476000
N	3.498794000	-2.074733000	-0.605245000	C	1.072793000	2.269946000	-2.081829000
C	1.222996000	-2.276782000	-0.912206000	C	2.197650000	3.253120000	-0.185106000
C	2.328161000	-2.542095000	0.008999000	C	1.232790000	3.452474000	-2.798570000
C	3.111442000	-1.353757000	-1.609738000	H	0.583994000	1.412030000	-2.530305000
C	3.906503000	-0.462207000	-2.432399000	C	2.342647000	4.443643000	-0.895801000
C	3.348660000	0.217767000	-3.525616000	H	2.568331000	3.178415000	0.830040000
C	4.115932000	1.130487000	-4.243268000	C	1.870046000	4.544397000	-2.206202000
C	5.443560000	1.370277000	-3.882369000	H	0.862151000	3.524135000	-3.817589000
C	6.006216000	0.686173000	-2.801361000	H	2.825586000	5.294893000	-0.424212000
C	5.244685000	-0.223203000	-2.076703000	H	1.993781000	5.470236000	-2.761120000
C	2.348298000	-3.829935000	0.795322000	H	0.924136000	-1.110357000	1.473175000
C	2.271796000	-5.051208000	-0.099569000	C	2.742893000	-1.475222000	2.574004000
C	1.202659000	-5.946496000	-0.002357000	C	2.019644000	-1.832845000	3.722532000
C	1.121156000	-7.061435000	-0.838015000	C	4.141131000	-1.623003000	2.591500000
C	2.113564000	-7.293543000	-1.789624000	C	2.665625000	-2.304379000	4.864148000
C	3.185951000	-6.404374000	-1.896155000	H	0.939582000	-1.714653000	3.720488000
C	3.264288000	-5.292924000	-1.059106000	C	4.784744000	-2.102662000	3.729355000
H	2.314535000	0.035119000	-3.793605000	H	4.704211000	-1.393653000	1.696304000
H	3.673487000	1.663969000	-5.079874000	C	4.053782000	-2.441090000	4.871367000
H	6.036632000	2.091838000	-4.437449000	H	2.085154000	-2.565462000	5.745126000
H	7.031500000	0.883041000	-2.504844000	H	5.865278000	-2.219635000	3.723418000
H	5.657045000	-0.739723000	-1.218961000	H	4.562590000	-2.812944000	5.756433000
H	3.266508000	-3.847628000	1.389352000	**TS5-*RR***			
H	1.515143000	-3.841925000	1.505842000	N	4.982953000	-2.478288000	0.333848000
H	0.428330000	-5.769394000	0.739185000	N	2.742836000	-2.138991000	-0.327316000
H	0.281795000	-7.746112000	-0.745880000	N	3.419966000	-1.578844000	1.798590000
H	2.053757000	-8.159445000	-2.443347000	C	3.709362000	-2.062203000	0.582287000
H	3.964132000	-6.577713000	-2.634811000	C	4.153887000	-1.890510000	3.028362000
H	4.090218000	-4.593371000	-1.150180000	H	4.536818000	-2.912535000	2.984656000
C	1.999348000	-0.981318000	1.396123000	H	4.998265000	-1.204091000	3.171836000
C	2.348425000	0.250398000	0.742417000	C	3.078409000	-1.651546000	4.091811000
C	1.334799000	0.859317000	-0.057996000	C	2.353953000	-0.402916000	3.563473000
O	0.209926000	0.298312000	-0.222025000	H	2.905845000	0.496723000	3.851758000
C	3.647004000	0.795266000	0.772888000	H	1.327256000	-0.302481000	3.919688000
C	4.760510000	1.289135000	0.736785000	C	2.373516000	-0.570271000	2.023629000
C	6.030979000	1.901537000	0.606982000	H	1.401252000	-0.921360000	1.679495000
C	7.138830000	1.462264000	1.359305000	H	3.504304000	-1.508078000	5.088829000
C	6.210340000	2.958865000	-0.311103000	O	3.970895000	0.991489000	1.097746000
C	8.385146000	2.058715000	1.192583000	C	2.784826000	0.737810000	1.325277000
H	7.003502000	0.651594000	2.068884000	N	1.735526000	1.539031000	1.062256000
C	7.459303000	3.550931000	-0.465230000	C	1.824415000	2.900060000	0.638098000
H	5.360805000	3.287892000	-0.900618000	C	2.245465000	3.223033000	-0.661422000
C	8.553490000	3.104543000	0.281550000	C	2.244756000	4.568591000	-1.040102000
H	9.230727000	1.706566000	1.777596000	H	2.569904000	4.828234000	-2.043723000
H	7.582735000	4.362868000	-1.177351000	C	1.812529000	5.579146000	-0.180707000

C	1.388606000	5.220440000	1.100360000	H	1.202369000	-1.495918000	-4.603932000
H	1.038678000	6.000056000	1.769644000	H	2.908024000	-1.923682000	-4.498290000
C	1.387983000	3.895012000	1.533779000	H	1.586787000	-3.902294000	-5.228621000
H	0.800345000	1.179362000	1.330404000	H	0.554554000	-3.769172000	-3.804426000
C	2.662691000	2.160251000	-1.663491000	C	6.103268000	-1.520805000	0.511651000
C	4.173079000	2.227025000	-1.940857000	C	7.364428000	-2.234276000	0.995464000
H	2.447621000	1.185268000	-1.217642000	C	6.348346000	-0.744949000	-0.788222000
H	4.444812000	3.183723000	-2.402972000	H	5.771590000	-0.795117000	1.256151000
H	4.728633000	2.119459000	-1.006412000	C	8.517309000	-1.233502000	1.165538000
H	4.476410000	1.426966000	-2.628642000	H	7.648642000	-3.002343000	0.260423000
C	0.970506000	3.521150000	2.948271000	H	7.156976000	-2.757114000	1.936455000
C	2.224350000	3.417446000	3.838475000	C	7.495670000	0.257067000	-0.612039000
H	0.501832000	2.533010000	2.909497000	H	6.596815000	-1.455544000	-1.592723000
H	2.684769000	4.404993000	3.962458000	H	5.427842000	-0.225372000	-1.070431000
H	1.967084000	3.034150000	4.833394000	C	8.772649000	-0.440063000	-0.123819000
H	2.977087000	2.759112000	3.393322000	H	9.425777000	-1.761097000	1.478579000
H	2.396157000	-2.507704000	4.124317000	H	8.265059000	-0.533741000	1.974997000
C	-0.059800000	4.474642000	3.564226000	H	7.679047000	0.783444000	-1.555799000
H	-0.929725000	4.588742000	2.911242000	H	7.186230000	1.017691000	0.117381000
H	0.363436000	5.467523000	3.757168000	H	9.569108000	0.295628000	0.038875000
C	1.851675000	2.263862000	-2.966023000	H	9.132294000	-1.126215000	-0.904561000
H	2.092951000	1.431953000	-3.639018000	H	1.773671000	-2.169568000	0.037320000
H	0.776658000	2.240193000	-2.764385000	O	0.248679000	-2.595542000	0.724634000
H	2.070433000	3.192956000	-3.504074000	O	-0.857628000	-1.215464000	-0.726957000
C	1.749808000	7.026465000	-0.636303000	N	-2.932824000	-2.111154000	-0.664006000
C	0.641537000	7.216659000	-1.686766000	C	-0.805171000	-2.232085000	0.205163000
C	3.102399000	7.534716000	-1.158872000	C	-2.173841000	-2.700541000	0.363704000
H	1.482770000	7.631835000	0.240189000	C	-2.183713000	-1.198597000	-1.187116000
H	-0.325252000	6.883420000	-1.295200000	C	-2.521781000	-0.201515000	-2.185692000
H	0.553285000	8.269686000	-1.979475000	C	-1.524770000	0.490912000	-2.890626000
H	0.856141000	6.632292000	-2.589430000	C	-1.877416000	1.472229000	-3.811705000
H	3.412067000	6.989111000	-2.057742000	C	-3.223078000	1.777741000	-4.030500000
H	3.041385000	8.597383000	-1.421160000	C	-4.217913000	1.083576000	-3.337459000
H	3.887635000	7.409938000	-0.405788000	C	-3.873656000	0.092329000	-2.423927000
C	2.879019000	-2.528096000	-1.733452000	C	-2.380670000	-4.163731000	0.683235000
C	2.570447000	-4.026546000	-1.891755000	C	-1.686833000	-5.032065000	-0.349342000
C	1.932874000	-1.666545000	-2.580374000	C	-0.563274000	-5.793052000	-0.010151000
H	3.909393000	-2.319883000	-2.048352000	C	0.104955000	-6.552496000	-0.973032000
C	2.549719000	-4.457022000	-3.362574000	C	-0.337704000	-6.552016000	-2.296057000
H	1.592301000	-4.224358000	-1.437533000	C	-1.452395000	-5.785657000	-2.648080000
H	3.300689000	-4.617757000	-1.321835000	C	-2.120912000	-5.033817000	-1.682971000
C	1.921484000	-2.108773000	-4.047899000	H	-0.481469000	0.261863000	-2.704658000
H	0.921860000	-1.750257000	-2.168592000	H	-1.100933000	2.004890000	-4.353505000
H	2.226421000	-0.616226000	-2.487387000	H	-3.495125000	2.555959000	-4.738131000
C	1.574201000	-3.597424000	-4.175394000	H	-5.264371000	1.327624000	-3.490406000
H	2.270584000	-5.514406000	-3.424709000	H	-4.631605000	-0.440707000	-1.865217000
H	3.559617000	-4.367139000	-3.790279000	H	-3.455299000	-4.363491000	0.706832000

H	-1.987661000	-4.382739000	1.680559000
H	-0.206146000	-5.781250000	1.015986000
H	0.973171000	-7.141661000	-0.688951000
H	0.177053000	-7.145684000	-3.046650000
H	-1.804961000	-5.779073000	-3.676093000
H	-2.978062000	-4.426463000	-1.958193000
C	-2.701626000	-1.554116000	2.003147000
C	-2.904603000	-0.204962000	1.544753000
C	-1.774967000	0.670826000	1.489227000
O	-0.615159000	0.310159000	1.841697000
C	-4.135483000	0.254259000	1.032601000
C	-5.154504000	0.713373000	0.545855000
C	-6.269526000	1.302799000	-0.099340000
C	-7.529935000	0.672028000	-0.118238000
C	-6.119918000	2.539000000	-0.766142000
C	-8.601691000	1.256636000	-0.786679000
H	-7.650489000	-0.276539000	0.396270000
C	-7.199476000	3.115101000	-1.427292000
H	-5.147967000	3.021466000	-0.759793000
C	-8.444449000	2.478941000	-1.444472000
H	-9.566310000	0.755860000	-0.794121000
H	-7.068827000	4.066600000	-1.936548000
H	-9.283722000	2.932065000	-1.964549000
C	-1.958897000	2.055462000	0.938243000
C	-1.201150000	2.444853000	-0.170573000
C	-2.866213000	2.964406000	1.496852000
C	-1.355177000	3.712125000	-0.728233000
H	-0.507554000	1.737189000	-0.607557000
C	-3.007524000	4.240307000	0.953191000
H	-3.465431000	2.664992000	2.350130000
C	-2.255855000	4.614548000	-0.164815000
H	-0.758709000	3.997436000	-1.588571000
H	-3.710326000	4.940029000	1.397274000
H	-2.374526000	5.606140000	-0.593422000
H	-0.403302000	4.076747000	4.525749000
H	5.072114000	-3.045687000	-0.501445000
H	-1.766286000	-1.665470000	2.547959000
C	-3.808861000	-2.364489000	2.562011000
C	-3.609309000	-3.028263000	3.782248000
C	-5.042617000	-2.526164000	1.907119000
C	-4.616431000	-3.806105000	4.352064000
H	-2.654918000	-2.919650000	4.291782000
C	-6.044934000	-3.309197000	2.473598000
H	-5.191670000	-2.058878000	0.942618000
C	-5.841075000	-3.947427000	3.699761000
H	-4.442384000	-4.303156000	5.302654000
H	-6.990465000	-3.428006000	1.950967000
H	-6.627653000	-4.555701000	4.137777000

TS5-*SR*

N	-3.146419000	-3.388200000	0.748175000
N	-1.680067000	-1.603134000	1.180344000
N	-2.423326000	-2.003351000	-0.977757000
C	-2.410508000	-2.314970000	0.318591000
C	-2.868991000	-2.891653000	-2.060106000
H	-2.759514000	-3.934783000	-1.761950000
H	-3.920944000	-2.688927000	-2.297550000
C	-1.959442000	-2.474940000	-3.215783000
C	-1.866214000	-0.954090000	-3.036714000
H	-2.749895000	-0.469671000	-3.464558000
H	-0.974519000	-0.506316000	-3.476796000
C	-1.847193000	-0.758600000	-1.503452000
H	-0.815385000	-0.639820000	-1.177301000
H	-2.366942000	-2.769157000	-4.186924000
O	-3.901903000	0.331499000	-0.847698000
C	-2.697973000	0.448172000	-1.082389000
N	-1.987478000	1.591580000	-1.073225000
C	-2.536314000	2.901186000	-0.907045000
C	-2.871070000	3.375309000	0.371762000
C	-3.307768000	4.697340000	0.487197000
H	-3.560803000	5.079170000	1.471497000
C	-3.406182000	5.545155000	-0.616795000
C	-3.084438000	5.034371000	-1.875804000
H	-3.166675000	5.687434000	-2.739485000
C	-2.649571000	3.719165000	-2.046296000
H	-1.008146000	1.513944000	-1.398754000
C	-2.794160000	2.482977000	1.598896000
C	-4.194689000	1.948247000	1.953899000
H	-2.161240000	1.629964000	1.335968000
H	-4.856592000	2.773983000	2.242770000
H	-4.632935000	1.428730000	1.099238000
H	-4.141378000	1.252259000	2.801575000
C	-2.347702000	3.149903000	-3.424994000
C	-3.587815000	2.403299000	-3.955943000
H	-1.540385000	2.418612000	-3.314227000
H	-4.404409000	3.110999000	-4.142951000
H	-3.359659000	1.890789000	-4.898651000
H	-3.951388000	1.667026000	-3.232996000
H	-0.978309000	-2.943890000	-3.093442000
C	-1.871110000	4.195520000	-4.440292000
H	-1.019976000	4.769606000	-4.057956000
H	-1.558110000	3.700816000	-5.366248000
H	-2.665402000	4.903812000	-4.702510000
C	-2.152854000	3.179803000	2.807414000
H	-2.023405000	2.466858000	3.630235000

H	-1.173891000	3.590203000	2.549593000	O	0.920508000	-0.566241000	0.719454000
H	-2.779353000	3.995774000	3.185686000	O	0.658577000	-2.512725000	-0.442279000
C	-3.815324000	6.998531000	-0.453214000	N	2.791373000	-3.046360000	-0.925588000
C	-2.740339000	7.784319000	0.318284000	C	1.446471000	-1.486153000	0.103926000
C	-5.191836000	7.142838000	0.214961000	C	2.809256000	-1.770351000	-0.311415000
H	-3.886750000	7.433014000	-1.459442000	C	1.556447000	-3.404384000	-1.012334000
H	-1.767763000	7.710752000	-0.180392000	C	1.011786000	-4.617765000	-1.598844000
H	-3.008919000	8.844558000	0.395929000	C	-0.268605000	-5.079196000	-1.252276000
H	-2.623521000	7.389903000	1.334404000	C	-0.764816000	-6.250561000	-1.818630000
H	-5.179180000	6.749298000	1.237872000	C	0.006835000	-6.972353000	-2.731791000
H	-5.488613000	8.196888000	0.267995000	C	1.286673000	-6.521021000	-3.069272000
H	-5.959103000	6.596007000	-0.343186000	C	1.791247000	-5.352920000	-2.507761000
C	-1.613521000	-1.829670000	2.629378000	C	3.954493000	-1.468607000	0.630317000
C	-0.558131000	-2.890392000	2.989974000	C	3.721190000	-2.060810000	2.005406000
C	-1.317679000	-0.501287000	3.332801000	C	3.557463000	-3.442432000	2.181978000
H	-2.605513000	-2.165324000	2.959784000	C	3.312020000	-3.973319000	3.447957000
C	-0.475782000	-3.089228000	4.508803000	C	3.234048000	-3.131963000	4.560660000
H	0.413402000	-2.554417000	2.610512000	C	3.395784000	-1.755752000	4.394374000
H	-0.779727000	-3.840154000	2.484014000	C	3.628383000	-1.225600000	3.124149000
C	-1.241178000	-0.697508000	4.851729000	H	-0.858001000	-4.528382000	-0.528303000
H	-0.365977000	-0.108424000	2.954166000	H	-1.753485000	-6.605247000	-1.539477000
H	-2.095981000	0.220134000	3.073289000	H	-0.383538000	-7.883920000	-3.174874000
C	-0.203005000	-1.761642000	5.227251000	H	1.890938000	-7.081939000	-3.776433000
H	0.314683000	-3.812191000	4.736302000	H	2.781232000	-4.986319000	-2.759007000
H	-1.420317000	-3.518767000	4.876122000	H	4.083079000	-0.388947000	0.720542000
H	-1.001959000	0.258569000	5.331829000	H	4.865480000	-1.873419000	0.178134000
H	-2.230222000	-0.997648000	5.228985000	H	3.622021000	-4.096546000	1.317316000
H	-0.190600000	-1.915485000	6.313174000	H	3.191312000	-5.046863000	3.568293000
H	0.795142000	-1.408593000	4.942375000	H	3.052675000	-3.545765000	5.548911000
C	-4.605892000	-3.474180000	0.493920000	H	3.341794000	-1.093094000	5.254116000
C	-5.148132000	-4.702275000	1.228373000	H	3.745928000	-0.152857000	2.994524000
C	-5.340448000	-2.192577000	0.910598000	C	2.978474000	-0.410445000	-1.825818000
H	-4.755152000	-3.631123000	-0.578295000	C	2.788558000	0.901956000	-1.269601000
C	-6.660901000	-4.844494000	1.010174000	C	1.481359000	1.480642000	-1.375859000
H	-4.947518000	-4.589012000	2.305460000	O	0.553177000	0.977479000	-2.074959000
H	-4.617058000	-5.601785000	0.894066000	C	3.785598000	1.621859000	-0.578697000
C	-6.850957000	-2.339107000	0.686992000	C	4.589539000	2.289436000	0.052289000
H	-5.142316000	-2.008758000	1.977535000	C	5.450050000	3.093036000	0.840073000
H	-4.945960000	-1.337722000	0.351061000	C	6.748225000	2.662671000	1.184774000
C	-7.410939000	-3.567972000	1.415184000	C	5.006130000	4.348289000	1.310945000
H	-7.035044000	-5.707662000	1.572607000	C	7.571243000	3.462180000	1.971562000
H	-6.850844000	-5.056060000	-0.051712000	H	7.095314000	1.696926000	0.829616000
H	-7.362026000	-1.427884000	1.016753000	C	5.837449000	5.137388000	2.098620000
H	-7.047925000	-2.432163000	-0.390796000	H	4.006226000	4.681051000	1.050893000
H	-8.481912000	-3.680768000	1.209347000	C	7.122857000	4.702252000	2.433069000
H	-7.312342000	-3.421099000	2.500508000	H	8.569036000	3.115448000	2.227409000
H	-0.875623000	-1.072888000	0.823093000	H	5.481058000	6.100940000	2.453679000

H	7.768773000	5.323436000	3.047063000	C	2.750296000	-2.046809000	4.783220000
C	1.189784000	2.771663000	-0.669604000	C	1.933791000	-2.869071000	4.007764000
C	1.394367000	2.914153000	0.709039000	H	1.573104000	-3.801986000	4.434014000
C	0.640761000	3.835852000	-1.392906000	C	1.569458000	-2.537402000	2.699402000
C	1.072918000	4.112946000	1.342869000	H	0.633486000	-0.868139000	0.670145000
H	1.795558000	2.079638000	1.272463000	C	3.290431000	0.894988000	2.403332000
C	0.323323000	5.036240000	-0.759620000	C	4.815805000	0.944650000	2.223849000
H	0.471366000	3.714841000	-2.457956000	H	2.832855000	1.027241000	1.421097000
C	0.537914000	5.177446000	0.610514000	H	5.330636000	0.842808000	3.186708000
H	1.236272000	4.216436000	2.412305000	H	5.141078000	0.135852000	1.565503000
H	-0.111130000	5.850053000	-1.331571000	H	5.122345000	1.903049000	1.784594000
H	0.278887000	6.107388000	1.108879000	C	0.680560000	-3.481475000	1.903339000
H	-2.912306000	-3.665029000	1.693042000	C	1.311952000	-4.877120000	1.768631000
H	2.088709000	-0.724136000	-2.367658000	H	0.577642000	-3.078319000	0.894725000
C	4.217968000	-0.895576000	-2.479272000	H	1.427044000	-5.365185000	2.743031000
C	5.506413000	-0.432820000	-2.167644000	H	0.676578000	-5.523354000	1.150927000
C	4.091381000	-1.888765000	-3.466820000	H	2.303052000	-4.819862000	1.304450000
C	6.623706000	-0.949380000	-2.822373000	H	0.922817000	-1.988852000	-4.068276000
H	5.629056000	0.341303000	-1.421860000	C	-0.731585000	-3.559251000	2.507539000
C	5.205963000	-2.402909000	-4.121150000	H	-1.184901000	-2.567979000	2.583065000
H	3.100393000	-2.256136000	-3.717301000	H	-1.385053000	-4.181289000	1.885756000
C	6.481835000	-1.936101000	-3.798205000	H	-0.710631000	-3.995715000	3.512879000
H	7.611291000	-0.573508000	-2.568661000	C	2.792294000	2.040260000	3.299733000
H	5.080097000	-3.165422000	-4.885291000	H	3.040992000	3.012742000	2.858701000
H	7.355828000	-2.334630000	-4.306096000	H	1.706332000	1.992247000	3.425495000
TS5-*RS*				H	3.248624000	1.999313000	4.295294000
N	4.260019000	1.107865000	-3.197148000	C	3.136422000	-2.444187000	6.197370000
N	2.386307000	1.838139000	-1.949894000	C	2.588820000	-1.446873000	7.232070000
N	2.591494000	-0.376356000	-2.620926000	C	4.658296000	-2.610399000	6.341581000
C	3.064899000	0.875899000	-2.567864000	H	2.674250000	-3.419865000	6.398852000
C	2.949139000	-1.329767000	-3.684022000	H	1.501530000	-1.348980000	7.146162000
H	3.005216000	-0.809871000	-4.642648000	H	2.827002000	-1.773306000	8.251279000
H	3.920855000	-1.799643000	-3.487729000	H	3.025818000	-0.451755000	7.088673000
C	1.827194000	-2.360703000	-3.574350000	H	5.176450000	-1.660833000	6.163754000
C	1.611428000	-2.447634000	-2.060373000	H	4.918595000	-2.949536000	7.351192000
H	2.397277000	-3.061735000	-1.605915000	H	5.044083000	-3.340208000	5.621974000
H	0.644222000	-2.853762000	-1.783532000	C	2.925818000	3.172941000	-1.659418000
C	1.751717000	-0.985827000	-1.575880000	C	2.332122000	4.223723000	-2.607627000
H	0.779535000	-0.490639000	-1.529775000	C	2.707672000	3.551374000	-0.192834000
H	2.096657000	-3.320392000	-4.023543000	H	4.008344000	3.129865000	-1.817595000
O	3.709163000	-0.998239000	-0.168576000	C	2.927719000	5.608533000	-2.318733000
C	2.479331000	-0.954567000	-0.224547000	H	1.244562000	4.242275000	-2.466818000
N	1.641901000	-0.966973000	0.837064000	H	2.514064000	3.930054000	-3.649878000
C	2.035212000	-1.319889000	2.168498000	C	3.292881000	4.939106000	0.100475000
C	2.837063000	-0.453573000	2.932402000	H	1.639336000	3.540313000	0.032410000
C	3.191990000	-0.845148000	4.224484000	H	3.179636000	2.797270000	0.441350000
H	3.819779000	-0.183452000	4.815152000	C	2.735518000	6.006907000	-0.849428000

H	2.472412000	6.354162000	-2.980985000	H	-4.168073000	0.259779000	0.681217000
H	4.002438000	5.595022000	-2.555713000	H	-5.271067000	-0.913451000	-0.046653000
H	3.078331000	5.208105000	1.141079000	H	-5.092014000	-3.382006000	0.898099000
H	4.388385000	4.899857000	0.003910000	H	-4.921675000	-4.704197000	2.992101000
H	3.215313000	6.973924000	-0.655632000	H	-3.988243000	-3.663032000	5.049052000
H	1.665537000	6.133388000	-0.649476000	H	-3.242870000	-1.290528000	4.998100000
C	5.461547000	0.392508000	-2.692560000	H	-3.420522000	0.020557000	2.898500000
C	6.486810000	0.205171000	-3.809099000	C	-2.988983000	0.222519000	-1.928262000
C	6.060893000	1.119155000	-1.481562000	C	-2.635580000	1.425170000	-1.235747000
H	5.113946000	-0.579145000	-2.336987000	C	-1.257134000	1.791457000	-1.147347000
C	7.727197000	-0.534356000	-3.285075000	O	-0.320528000	1.240063000	-1.794752000
H	6.783523000	1.192352000	-4.194918000	C	-3.551730000	2.244841000	-0.535524000
H	6.029349000	-0.337616000	-4.644484000	C	-4.254985000	3.004213000	0.109799000
C	7.293178000	0.371454000	-0.958210000	C	-5.018755000	3.899114000	0.900081000
H	6.346074000	2.141548000	-1.776330000	C	-6.420797000	3.784083000	0.993654000
H	5.301493000	1.192591000	-0.697420000	C	-4.373785000	4.927882000	1.620389000
C	8.335895000	0.173619000	-2.066453000	C	-7.150419000	4.670246000	1.779937000
H	8.470039000	-0.629342000	-4.085634000	H	-6.922941000	2.992127000	0.446277000
H	7.438657000	-1.556364000	-3.000826000	C	-5.114082000	5.807586000	2.402863000
H	7.726896000	0.915399000	-0.111239000	H	-3.294170000	5.015804000	1.554915000
H	6.971035000	-0.605117000	-0.572315000	C	-6.503771000	5.686242000	2.487714000
H	9.190794000	-0.398711000	-1.687347000	H	-8.230480000	4.566882000	1.842245000
H	8.725909000	1.154216000	-2.376384000	H	-4.603354000	6.593845000	2.952910000
O	-1.173306000	-0.573693000	0.688166000	H	-7.077119000	6.375589000	3.101026000
O	-1.271077000	-2.438191000	-0.637628000	H	1.365727000	1.682094000	-1.779487000
N	-3.457721000	-2.485842000	-1.169197000	C	-0.927025000	2.941763000	-0.233068000
C	-1.847307000	-1.318874000	-0.010850000	C	-0.587134000	2.687387000	1.101128000
C	-3.225930000	-1.294356000	-0.453768000	C	-0.991058000	4.261516000	-0.690734000
C	-2.319650000	-3.083958000	-1.278707000	C	-0.305070000	3.748014000	1.962810000
C	-2.031443000	-4.326760000	-1.975918000	H	-0.572564000	1.661227000	1.453206000
C	-0.871105000	-5.070019000	-1.705269000	C	-0.714271000	5.320463000	0.174652000
C	-0.631067000	-6.261397000	-2.385763000	H	-1.292760000	4.456953000	-1.715961000
C	-1.542686000	-6.724632000	-3.336234000	C	-0.364938000	5.065665000	1.502997000
C	-2.704652000	-5.992131000	-3.599701000	H	-0.047936000	3.546966000	2.998455000
C	-2.952024000	-4.801130000	-2.926425000	H	-0.785236000	6.343988000	-0.183375000
C	-4.313108000	-0.800532000	0.470257000	H	-0.152158000	5.889761000	2.178255000
C	-4.287065000	-1.586832000	1.765622000	H	4.440799000	2.086892000	-3.385384000
C	-4.702219000	-2.924356000	1.803041000	H	-2.121264000	-0.225503000	-2.407996000
C	-4.596139000	-3.667231000	2.977982000	C	-4.234193000	-0.012669000	-2.685503000
C	-4.072241000	-3.083292000	4.133821000	C	-5.449515000	0.641084000	-2.422208000
C	-3.655828000	-1.752150000	4.105067000	C	-4.203089000	-0.961726000	-3.723882000
C	-3.760934000	-1.010938000	2.927244000	C	-6.587772000	0.351077000	-3.172406000
H	-0.175852000	-4.722649000	-0.949681000	H	-5.496060000	1.381395000	-1.634329000
H	0.266302000	-6.833047000	-2.166242000	C	-5.338948000	-1.249452000	-4.472849000
H	-1.352353000	-7.653341000	-3.866516000	H	-3.271252000	-1.478088000	-3.935868000
H	-3.417546000	-6.351191000	-4.336615000	C	-6.541142000	-0.594097000	-4.197753000
H	-3.846023000	-4.217115000	-3.119321000	H	-7.517205000	0.869989000	-2.953583000

H	-5.286930000	-1.983567000	-5.272561000	H	1.764811000	-0.203578000	-3.599657000
H	-7.431664000	-0.816275000	-4.779292000	H	3.295607000	-0.208965000	-4.484833000
TS5-*SS′*				C	4.426265000	4.457581000	-4.294702000
N	3.873882000	-3.034084000	2.578271000	C	3.795989000	4.121422000	-5.656713000
N	2.002502000	-2.618545000	1.190848000	C	5.957629000	4.329059000	-4.348253000
N	2.732862000	-1.032282000	2.722006000	H	4.187536000	5.505219000	-4.067466000
C	2.856894000	-2.227506000	2.131257000	H	2.707654000	4.238720000	-5.625538000
C	3.256783000	-0.721220000	4.060180000	H	4.191859000	4.776687000	-6.441622000
H	3.185785000	-1.602661000	4.700432000	H	4.012001000	3.085991000	-5.945074000
H	4.308252000	-0.411260000	4.010652000	H	6.257851000	3.301516000	-4.584620000
C	2.375957000	0.456568000	4.477385000	H	6.376831000	4.986010000	-5.119534000
C	2.227359000	1.240195000	3.167040000	H	6.408265000	4.594620000	-3.386142000
H	3.125796000	1.842616000	2.990546000	C	2.147441000	-3.785998000	0.309647000
H	1.356320000	1.893231000	3.132769000	C	0.896103000	-4.669059000	0.409705000
C	2.113160000	0.139629000	2.083573000	C	2.417848000	-3.343845000	-1.132328000
H	1.067393000	-0.052135000	1.844374000	H	3.010872000	-4.370886000	0.643924000
H	2.825945000	1.045460000	5.281557000	C	0.999318000	-5.874891000	-0.532740000
O	4.092557000	0.205165000	0.703217000	H	0.021234000	-4.068282000	0.138203000
C	2.911234000	0.528119000	0.827296000	H	0.757273000	-4.991416000	1.448920000
N	2.191511000	1.275181000	-0.045301000	C	2.505444000	-4.549879000	-2.075256000
C	2.747989000	2.047115000	-1.113080000	H	1.605277000	-2.684922000	-1.451449000
C	3.424215000	1.419458000	-2.176110000	H	3.342060000	-2.759935000	-1.160938000
C	3.970803000	2.220768000	-3.180800000	C	1.254731000	-5.432444000	-1.978991000
H	4.502375000	1.739041000	-3.997036000	H	0.078691000	-6.466353000	-0.470859000
C	3.834071000	3.609619000	-3.182608000	H	1.817753000	-6.530965000	-0.199552000
C	3.117655000	4.195100000	-2.139681000	H	2.646868000	-4.197561000	-3.103890000
H	2.980946000	5.273150000	-2.140986000	H	3.395806000	-5.145817000	-1.823541000
C	2.572411000	3.446571000	-1.092782000	H	1.360666000	-6.309805000	-2.628610000
H	1.242241000	1.506908000	0.266770000	H	0.387029000	-4.868862000	-2.340982000
C	3.519459000	-0.091397000	-2.307314000	C	5.270496000	-2.562982000	2.383408000
C	4.977867000	-0.573442000	-2.278441000	C	6.202647000	-3.261721000	3.371644000
H	3.005035000	-0.535618000	-1.455379000	C	5.724342000	-2.757131000	0.930815000
H	5.545340000	-0.173936000	-3.127170000	H	5.267943000	-1.488823000	2.576398000
H	5.458827000	-0.250889000	-1.352414000	C	7.651409000	-2.789714000	3.179104000
H	5.025622000	-1.668331000	-2.338197000	H	6.147605000	-4.349150000	3.209460000
C	1.752595000	4.147898000	-0.018495000	H	5.861230000	-3.075887000	4.396653000
C	2.451951000	5.385989000	0.562702000	C	7.169728000	-2.279874000	0.744801000
H	1.596788000	3.456547000	0.811261000	H	5.648746000	-3.823853000	0.667240000
H	2.576854000	6.177633000	-0.184710000	H	5.055007000	-2.196188000	0.273193000
H	1.847747000	5.798564000	1.378438000	C	8.119152000	-2.975807000	1.728838000
H	3.443585000	5.135953000	0.956313000	H	8.312319000	-3.327193000	3.869018000
H	1.400986000	0.091524000	4.819746000	H	7.717937000	-1.725185000	3.445460000
C	0.361571000	4.511393000	-0.571273000	H	7.488071000	-2.453618000	-0.289482000
H	-0.143136000	3.630986000	-0.979094000	H	7.202851000	-1.193360000	0.903547000
H	0.448957000	5.251132000	-1.376699000	H	9.139360000	-2.592027000	1.610534000
C	2.796749000	-0.569710000	-3.578257000	H	8.157935000	-4.050283000	1.497118000
H	2.774676000	-1.665092000	-3.621248000	H	1.136887000	-2.065294000	1.025794000

O	-0.170938000	1.906116000	1.368694000	H	-9.394457000	-3.026072000	-2.903876000
O	-1.477379000	1.413544000	-0.436657000	C	-1.475246000	-2.161081000	-1.051154000
N	-3.540837000	1.677382000	0.446620000	C	-0.595345000	-1.656690000	-2.020102000
C	-1.287808000	1.715452000	0.899080000	C	-2.297727000	-3.247167000	-1.380535000
C	-2.612207000	1.725102000	1.493771000	C	-0.569899000	-2.195575000	-3.304732000
C	-2.864894000	1.390233000	-0.621226000	H	0.045472000	-0.822609000	-1.752320000
C	-3.360624000	1.055937000	-1.940708000	C	-2.256242000	-3.799412000	-2.660514000
C	-2.488028000	0.870694000	-3.023828000	H	-2.970613000	-3.656617000	-0.637340000
C	-2.989810000	0.480261000	-4.261712000	C	-1.404396000	-3.265916000	-3.630487000
C	-4.360748000	0.277404000	-4.432758000	H	0.098888000	-1.779174000	-4.051576000
C	-5.234039000	0.473979000	-3.359132000	H	-2.895375000	-4.644576000	-2.900791000
C	-4.740393000	0.858197000	-2.118113000	H	-1.386548000	-3.686779000	-4.631997000
C	-2.866086000	2.566086000	2.718718000	H	-0.268945000	4.931749000	0.217176000
C	-2.462436000	4.008875000	2.484115000	H	3.762578000	-4.005538000	2.312692000
C	-1.336661000	4.548662000	3.113879000	H	-1.622000000	-0.327198000	2.545409000
C	-0.942372000	5.865242000	2.869545000	C	-3.699791000	-0.273224000	3.121893000
C	-1.668495000	6.658560000	1.980760000	C	-3.359387000	-0.424438000	4.476100000
C	-2.787712000	6.124387000	1.337215000	C	-5.048464000	-0.040798000	2.795609000
C	-3.179755000	4.810043000	1.585966000	C	-4.331355000	-0.378932000	5.474213000
H	-1.424364000	1.021619000	-2.883513000	H	-2.318041000	-0.591024000	4.741926000
H	-2.307258000	0.325721000	-5.092490000	C	-6.016780000	0.012303000	3.794331000
H	-4.748193000	-0.035928000	-5.398345000	H	-5.316746000	0.135954000	1.763010000
H	-6.298419000	0.301268000	-3.482536000	C	-5.667107000	-0.163409000	5.135881000
H	-5.400149000	0.989353000	-1.269403000	H	-4.044241000	-0.507186000	6.514457000
H	-3.927140000	2.491370000	2.972496000	H	-7.052426000	0.202079000	3.524598000
H	-2.303496000	2.160458000	3.565801000	H	-6.428200000	-0.121929000	5.910155000
H	-0.763490000	3.928246000	3.797831000	**TS5-*RR′***			
H	-0.066924000	6.269419000	3.371276000	N	4.619093000	-3.007501000	1.155670000
H	-1.362035000	7.682461000	1.785557000	N	2.588015000	-2.314818000	0.211321000
H	-3.354818000	6.733015000	0.638017000	N	3.480625000	-1.184203000	2.042910000
H	-4.039137000	4.387349000	1.072727000	C	3.547288000	-2.151623000	1.119214000
C	-2.620450000	-0.328958000	2.115463000	C	4.220121000	-1.209722000	3.313549000
C	-2.702326000	-1.118038000	0.919473000	H	4.420953000	-2.242384000	3.606688000
C	-1.471106000	-1.494069000	0.289701000	H	5.174362000	-0.678106000	3.208167000
O	-0.344680000	-1.210727000	0.793273000	C	3.287408000	-0.444594000	4.252453000
C	-3.935248000	-1.452822000	0.321658000	C	2.738435000	0.659359000	3.341496000
C	-4.983619000	-1.749526000	-0.223944000	H	3.474872000	1.464721000	3.246626000
C	-6.163803000	-2.100780000	-0.924834000	H	1.792939000	1.085981000	3.675357000
C	-7.433905000	-1.973937000	-0.327039000	C	2.548505000	-0.045404000	1.978911000
C	-6.083191000	-2.571035000	-2.253204000	H	1.519308000	-0.392714000	1.880279000
C	-8.583844000	-2.303130000	-1.038424000	H	3.811520000	-0.057044000	5.130539000
H	-7.499190000	-1.616288000	0.696135000	O	4.031433000	0.919250000	0.322747000
C	-7.238883000	-2.902924000	-2.952239000	C	2.903573000	0.893421000	0.813692000
H	-5.107512000	-2.649705000	-2.721192000	N	1.875010000	1.695904000	0.469419000
C	-8.494382000	-2.769602000	-2.352341000	C	1.929229000	2.753694000	-0.487581000
H	-9.556219000	-2.196705000	-0.564773000	C	2.087158000	2.475437000	-1.856834000
H	-7.161303000	-3.261364000	-3.975536000	C	2.131615000	3.555581000	-2.744937000

H	2.267297000	3.351314000	-3.802873000	H	1.916651000	-6.553608000	-1.566904000
C	1.998136000	4.877004000	-2.317174000	H	3.360080000	-5.701347000	-2.109796000
C	1.802151000	5.112555000	-0.954201000	H	1.442195000	-3.140944000	-4.178060000
H	1.686876000	6.137314000	-0.615218000	H	3.068677000	-3.611530000	-3.696429000
C	1.772791000	4.074749000	-0.021591000	H	1.637822000	-5.635465000	-3.894573000
H	1.016854000	1.584738000	1.014956000	H	0.466804000	-4.944167000	-2.769588000
C	2.219199000	1.057715000	-2.390755000	C	6.015303000	-2.513617000	1.081974000
C	3.656432000	0.807981000	-2.882057000	C	6.948430000	-3.724741000	1.008434000
H	2.012639000	0.374146000	-1.563997000	C	6.233650000	-1.560313000	-0.101019000
H	3.897068000	1.461352000	-3.729426000	H	6.236826000	-1.976729000	2.009079000
H	4.368550000	0.999006000	-2.076368000	C	8.415522000	-3.279763000	0.928783000
H	3.778077000	-0.228831000	-3.220585000	H	6.698894000	-4.310358000	0.109500000
C	1.665200000	4.351565000	1.471955000	H	6.783461000	-4.376905000	1.874539000
C	3.076669000	4.364430000	2.091700000	C	7.699154000	-1.113012000	-0.170931000
H	1.111555000	3.525271000	1.928400000	H	5.967764000	-2.089827000	-1.028636000
H	3.650213000	5.218539000	1.712402000	H	5.565926000	-0.697602000	-0.010873000
H	3.020520000	4.448849000	3.183732000	C	8.650277000	-2.314709000	-0.241660000
H	3.632282000	3.456311000	1.838856000	H	9.063533000	-4.159374000	0.840159000
H	2.478845000	-1.100602000	4.593878000	H	8.689694000	-2.782318000	1.869989000
C	0.911671000	5.642893000	1.812784000	H	7.843138000	-0.454785000	-1.034932000
H	-0.079710000	5.666761000	1.348884000	H	7.935257000	-0.512061000	0.719204000
H	1.462453000	6.534241000	1.491278000	H	9.693971000	-1.978763000	-0.247421000
C	1.192251000	0.754861000	-3.495437000	H	8.486214000	-2.849778000	-1.188265000
H	1.314877000	-0.273496000	-3.853887000	H	1.674066000	-1.816488000	0.309215000
H	0.166614000	0.863358000	-3.133171000	O	-0.205100000	1.347411000	2.361445000
H	1.316684000	1.417227000	-4.359372000	O	-1.875974000	-0.206540000	2.383894000
C	2.052830000	6.036078000	-3.298379000	N	-3.504715000	0.888178000	1.259263000
C	0.791590000	6.083406000	-4.176990000	C	-1.324660000	0.997041000	1.994122000
C	3.325329000	6.003465000	-4.159810000	C	-2.320098000	1.627255000	1.134064000
H	2.077501000	6.960415000	-2.705875000	C	-3.183544000	-0.199824000	1.880223000
H	-0.107006000	6.188644000	-3.560437000	C	-3.991488000	-1.385659000	2.089019000
H	0.830547000	6.929109000	-4.873737000	C	-3.512648000	-2.479764000	2.824483000
H	0.690596000	5.164080000	-4.765841000	C	-4.282079000	-3.634462000	2.935140000
H	3.342773000	5.122632000	-4.811711000	C	-5.535235000	-3.705716000	2.323433000
H	3.379123000	6.890862000	-4.801011000	C	-6.021430000	-2.611912000	1.601696000
H	4.223904000	5.974168000	-3.534660000	C	-5.255376000	-1.459057000	1.479635000
C	2.699826000	-3.218512000	-0.944799000	C	-2.363673000	3.131201000	1.028914000
C	2.215351000	-4.639035000	-0.607004000	C	-2.829280000	3.764120000	2.324385000
C	1.927510000	-2.640717000	-2.133866000	C	-1.930829000	4.025984000	3.366360000
H	3.759223000	-3.254604000	-1.232074000	C	-2.376326000	4.577976000	4.567114000
C	2.305044000	-5.562551000	-1.828583000	C	-3.729158000	4.871106000	4.746029000
H	1.179539000	-4.576890000	-0.262296000	C	-4.633452000	4.602704000	3.717178000
H	2.792857000	-5.054185000	0.231200000	C	-4.184914000	4.051995000	2.517034000
C	2.024616000	-3.565980000	-3.352418000	H	-2.536308000	-2.421816000	3.290070000
H	0.878415000	-2.512212000	-1.854846000	H	-3.898135000	-4.483765000	3.493242000
H	2.322677000	-1.650577000	-2.364660000	H	-6.129831000	-4.611601000	2.403617000
C	1.534772000	-4.981139000	-3.020716000	H	-6.986739000	-2.669500000	1.108921000

H	-5.604722000	-0.612766000	0.900985000	H	-1.589908000	4.535859000	-3.595414000
H	-3.038048000	3.409388000	0.216581000	H	-5.401166000	2.679011000	-2.877186000
H	-1.364778000	3.492993000	0.760584000	H	-4.041401000	4.421606000	-4.020099000
H	-0.882541000	3.779051000	3.236829000	**TS5-*SR′***			
H	-1.665351000	4.778979000	5.364503000	N	-2.727558000	-4.128124000	0.810409000
H	-4.076570000	5.303194000	5.680620000	N	-1.481612000	-2.175113000	1.115910000
H	-5.689686000	4.822264000	3.849107000	N	-1.527412000	-3.166400000	-0.958946000
H	-4.889499000	3.832552000	1.719360000	C	-1.916830000	-3.152233000	0.325090000
C	-1.636710000	0.895398000	-0.744087000	C	-1.466816000	-4.351410000	-1.821856000
C	-1.882531000	-0.525872000	-0.745746000	H	-1.218766000	-5.231910000	-1.224114000
C	-0.873922000	-1.369457000	-0.192112000	H	-2.430936000	-4.509070000	-2.321438000
O	0.233508000	-0.907964000	0.224200000	C	-0.382517000	-3.973619000	-2.831763000
C	-3.098577000	-1.093327000	-1.180083000	C	-0.588705000	-2.465480000	-3.027893000
C	-4.131866000	-1.634894000	-1.532487000	H	-1.386740000	-2.281072000	-3.752183000
C	-5.316475000	-2.323910000	-1.891200000	H	0.315887000	-1.948089000	-3.353948000
C	-6.343057000	-1.687073000	-2.617232000	C	-1.035851000	-1.947704000	-1.646168000
C	-5.495093000	-3.668872000	-1.502016000	H	-0.191376000	-1.511983000	-1.111518000
C	-7.510281000	-2.373860000	-2.937577000	H	-0.478885000	-4.538069000	-3.763716000
H	-6.208127000	-0.653421000	-2.921152000	O	-3.231635000	-1.293729000	-2.384011000
C	-6.662830000	-4.347416000	-1.833993000	C	-2.205461000	-0.958083000	-1.794155000
H	-4.715332000	-4.153294000	-0.923801000	N	-1.993986000	0.252842000	-1.232828000
C	-7.677376000	-3.705858000	-2.550077000	C	-2.832867000	1.405040000	-1.372183000
H	-8.294394000	-1.867728000	-3.494518000	C	-4.107126000	1.453762000	-0.773110000
H	-6.787296000	-5.382021000	-1.524513000	C	-4.825869000	2.649589000	-0.852953000
H	-8.589881000	-4.238363000	-2.802867000	H	-5.808887000	2.696142000	-0.393579000
C	-1.101063000	-2.838654000	-0.006474000	C	-4.317621000	3.785178000	-1.485324000
C	-0.718483000	-3.393943000	1.223325000	C	-3.060423000	3.695239000	-2.080020000
C	-1.626313000	-3.682080000	-0.994938000	H	-2.656325000	4.568929000	-2.582474000
C	-0.888280000	-4.753440000	1.475626000	C	-2.301257000	2.523103000	-2.045147000
H	-0.307591000	-2.735790000	1.981425000	H	-1.085148000	0.420021000	-0.813050000
C	-1.772623000	-5.047945000	-0.751314000	C	-4.737163000	0.271488000	-0.053295000
H	-1.916336000	-3.269975000	-1.953525000	C	-5.897234000	-0.297730000	-0.888839000
C	-1.414591000	-5.586610000	0.486736000	H	-3.978908000	-0.509088000	0.048292000
H	-0.608976000	-5.163433000	2.442548000	H	-6.664714000	0.467634000	-1.053028000
H	-2.173349000	-5.690839000	-1.530194000	H	-5.528804000	-0.641308000	-1.857370000
H	-1.544097000	-6.648244000	0.677811000	H	-6.371969000	-1.139220000	-0.370804000
H	0.773228000	5.719523000	2.896297000	C	-0.956030000	2.477347000	-2.753678000
H	4.480089000	-3.827623000	0.579792000	C	-1.162951000	2.251770000	-4.262642000
H	-0.586211000	1.130979000	-0.605493000	H	-0.391496000	1.619676000	-2.386836000
C	-2.334321000	1.836669000	-1.643671000	H	-1.725953000	3.079949000	-4.709433000
C	-1.586692000	2.855497000	-2.259541000	H	-0.193416000	2.184032000	-4.769599000
C	-3.722559000	1.796751000	-1.871990000	H	-1.720115000	1.326968000	-4.450081000
C	-2.193147000	3.771215000	-3.117098000	H	0.600278000	-4.173977000	-2.404155000
H	-0.521906000	2.928414000	-2.065205000	C	-0.102384000	3.726091000	-2.494147000
C	-4.326610000	2.721747000	-2.718899000	H	-0.014142000	3.936582000	-1.424406000
H	-4.321992000	1.062976000	-1.352339000	H	0.901111000	3.580906000	-2.896880000
C	-3.565623000	3.705501000	-3.355479000	H	-0.523495000	4.615694000	-2.976825000

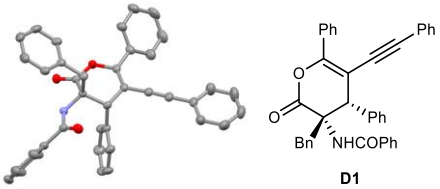
C	-5.220055000	0.643136000	1.359790000	H	-7.221641000	-4.533164000	0.709590000
H	-5.532617000	-0.257839000	1.902037000	H	-0.509578000	-1.809892000	0.974493000
H	-4.436353000	1.136494000	1.941518000	O	1.380803000	0.224142000	-1.215307000
H	-6.083735000	1.316459000	1.325864000	O	0.236055000	1.624209000	0.194455000
C	-5.096144000	5.088619000	-1.506114000	N	1.896925000	2.962223000	0.916000000
C	-5.253322000	5.660856000	-0.086660000	C	1.417468000	1.139836000	-0.410665000
C	-6.460958000	4.930679000	-2.195439000	C	2.488883000	1.913609000	0.187745000
H	-4.508016000	5.808265000	-2.090712000	C	0.626083000	2.723512000	0.945878000
H	-4.279379000	5.784997000	0.397510000	C	-0.399724000	3.448184000	1.679616000
H	-5.756279000	6.634656000	-0.113160000	C	-1.764762000	3.191981000	1.479597000
H	-5.854989000	4.991041000	0.539774000	C	-2.722555000	3.901059000	2.200292000
H	-7.104148000	4.234391000	-1.644688000	C	-2.331631000	4.871166000	3.125304000
H	-6.981872000	5.893753000	-2.248641000	C	-0.971436000	5.132257000	3.323986000
H	-6.345843000	4.544128000	-3.213542000	C	-0.008947000	4.428639000	2.608791000
C	-2.046765000	-1.769752000	2.405458000	C	3.780289000	2.137695000	-0.557371000
C	-1.352153000	-2.484988000	3.577319000	C	3.581092000	2.903543000	-1.847996000
C	-1.887618000	-0.246545000	2.530186000	C	3.557525000	4.302948000	-1.853756000
H	-3.117928000	-2.016027000	2.398062000	C	3.364083000	5.006729000	-3.042344000
C	-1.860569000	-1.970076000	4.930306000	C	3.186396000	4.318377000	-4.244140000
H	-0.275757000	-2.296996000	3.481707000	C	3.193223000	2.922227000	-4.246018000
H	-1.491932000	-3.573519000	3.502700000	C	3.387274000	2.220966000	-3.055222000
C	-2.397204000	0.266022000	3.880127000	H	-2.074602000	2.454892000	0.752931000
H	-0.825675000	-0.005362000	2.414584000	H	-3.774337000	3.696818000	2.025735000
H	-2.410396000	0.235191000	1.700945000	H	-3.080145000	5.422862000	3.687036000
C	-1.696973000	-0.448284000	5.042685000	H	-0.662411000	5.886685000	4.042062000
H	-1.327106000	-2.476866000	5.743042000	H	1.050170000	4.616107000	2.751751000
H	-2.924239000	-2.228821000	5.043395000	H	4.228683000	1.162883000	-0.772325000
H	-2.242061000	1.349078000	3.937474000	H	4.463583000	2.677378000	0.103914000
H	-3.481873000	0.099006000	3.953430000	H	3.686526000	4.837076000	-0.916178000
H	-2.092304000	-0.095961000	6.002926000	H	3.351884000	6.093369000	-3.030699000
H	-0.626878000	-0.199161000	5.027706000	H	3.037412000	4.865738000	-5.170846000
C	-3.902451000	-4.695160000	0.119377000	H	3.049614000	2.377933000	-5.175851000
C	-4.644731000	-5.599324000	1.108711000	H	3.378724000	1.134894000	-3.051631000
C	-4.825068000	-3.605233000	-0.437967000	C	3.010360000	0.537728000	1.693028000
H	-3.551706000	-5.322541000	-0.706847000	C	3.245021000	-0.731049000	1.060726000
C	-5.889930000	-6.217041000	0.458585000	C	2.091771000	-1.559734000	0.895139000
H	-4.951105000	-4.995286000	1.976905000	O	0.968459000	-1.232501000	1.392021000
H	-3.970166000	-6.381515000	1.478501000	C	4.501814000	-1.151952000	0.578215000
C	-6.067445000	-4.222562000	-1.090552000	C	5.567155000	-1.554305000	0.140289000
H	-5.127992000	-2.957448000	0.396906000	C	6.762891000	-2.074779000	-0.414801000
H	-4.289272000	-2.974835000	-1.153998000	C	7.920635000	-1.279668000	-0.541790000
C	-6.818194000	-5.138000000	-0.115389000	C	6.808999000	-3.412091000	-0.864783000
H	-6.420985000	-6.833594000	1.192802000	C	9.081377000	-1.807013000	-1.098439000
H	-5.574502000	-6.892808000	-0.348913000	H	7.892117000	-0.248437000	-0.203045000
H	-6.722440000	-3.424360000	-1.456109000	C	7.973781000	-3.927310000	-1.423787000
H	-5.761598000	-4.801932000	-1.973752000	H	5.920763000	-4.028291000	-0.765811000
H	-7.676683000	-5.605805000	-0.611467000	C	9.115841000	-3.131022000	-1.543124000

H	9.964747000	-1.180447000	-1.188442000	C	-5.089694000	2.229657000	-1.013509000
H	7.993001000	-4.958858000	-1.765875000	H	-6.017656000	2.232958000	-0.448865000
H	10.024100000	-3.538280000	-1.978030000	C	-4.861062000	3.241860000	-1.945883000
C	2.184076000	-2.883590000	0.202349000	C	-3.653829000	3.222177000	-2.641526000
C	2.897810000	-3.070147000	-0.990483000	H	-3.452182000	4.011974000	-3.359273000
C	1.519452000	-3.980404000	0.770305000	C	-2.702561000	2.216691000	-2.458599000
C	2.994499000	-4.337734000	-1.563525000	H	-0.996591000	0.502409000	-1.335377000
H	3.370202000	-2.219314000	-1.463897000	C	-4.494995000	0.204816000	0.335055000
C	1.614196000	-5.247800000	0.197142000	C	-5.717056000	-0.643940000	-0.055819000
H	0.952886000	-3.831117000	1.683780000	H	-3.645056000	-0.469920000	0.450684000
C	2.366584000	-5.433946000	-0.964643000	H	-6.602176000	-0.013344000	-0.198826000
H	3.556743000	-4.468188000	-2.484160000	H	-5.516969000	-1.187563000	-0.980323000
H	1.115930000	-6.092587000	0.665834000	H	-5.953191000	-1.365650000	0.735370000
H	2.452274000	-6.422015000	-1.408561000	C	-1.392723000	2.273621000	-3.233017000
H	-2.797060000	-4.128168000	1.819566000	C	-1.588395000	2.604989000	-4.720245000
H	2.021102000	0.569763000	2.139184000	H	-0.909455000	1.295815000	-3.193185000
C	3.989971000	1.332421000	2.460415000	H	-1.957298000	3.625473000	-4.873075000
C	5.379717000	1.308490000	2.251911000	H	-0.630005000	2.522984000	-5.244693000
C	3.486438000	2.188665000	3.458498000	H	-2.297682000	1.915607000	-5.191178000
C	6.227674000	2.106363000	3.018385000	H	0.901105000	-3.832142000	-2.758189000
H	5.794030000	0.657351000	1.494839000	C	-0.434290000	3.277671000	-2.566322000
C	4.333082000	2.983838000	4.222893000	H	-0.285748000	3.034897000	-1.511130000
H	2.414167000	2.226075000	3.624186000	H	0.543539000	3.258242000	-3.057774000
C	5.712099000	2.947112000	4.004925000	H	-0.839041000	4.295589000	-2.619994000
H	7.299350000	2.067944000	2.842077000	C	-4.737634000	0.890173000	1.692674000
H	3.917922000	3.632673000	4.989446000	H	-4.917005000	0.134510000	2.466790000
H	6.377582000	3.566843000	4.599721000	H	-3.885222000	1.498609000	2.006750000
TS5-*RS'*				H	-5.617199000	1.542683000	1.662470000
N	-2.075636000	-4.334153000	0.845401000	C	-5.880307000	4.341678000	-2.189963000
N	-0.973459000	-2.293642000	1.211498000	C	-6.018196000	5.265696000	-0.967926000
N	-1.037212000	-3.222731000	-0.909175000	C	-7.245478000	3.772394000	-2.608552000
C	-1.357711000	-3.269579000	0.389800000	H	-5.504495000	4.950708000	-3.022806000
C	-0.957054000	-4.390388000	-1.801325000	H	-5.053069000	5.707697000	-0.700171000
H	-0.472712000	-5.219981000	-1.280061000	H	-6.725557000	6.078061000	-1.171942000
H	-1.954917000	-4.712938000	-2.120177000	H	-6.388820000	4.711271000	-0.097088000
C	-0.165582000	-3.834360000	-2.986065000	H	-7.688822000	3.173754000	-1.804345000
C	-0.690166000	-2.397893000	-3.100509000	H	-7.946160000	4.581404000	-2.845630000
H	-1.663477000	-2.391271000	-3.602070000	H	-7.150176000	3.129000000	-3.489461000
H	-0.011504000	-1.722399000	-3.618377000	C	-1.516821000	-2.067346000	2.557590000
C	-0.870883000	-1.949711000	-1.635019000	C	-0.716136000	-2.808322000	3.639999000
H	0.006665000	-1.403852000	-1.291735000	C	-1.549427000	-0.566761000	2.863926000
H	-0.325711000	-4.419623000	-3.895742000	H	-2.550588000	-2.435899000	2.552751000
O	-3.251890000	-1.695511000	-1.585763000	C	-1.325357000	-2.561593000	5.028183000
C	-2.160347000	-1.134306000	-1.499832000	H	0.318083000	-2.443794000	3.611118000
N	-1.968408000	0.197145000	-1.325743000	H	-0.676064000	-3.885965000	3.426047000
C	-2.969324000	1.203698000	-1.512303000	C	-2.200829000	-0.318255000	4.228221000
C	-4.162890000	1.213097000	-0.759696000	H	-0.522325000	-0.187909000	2.881763000

H	-2.073433000	-0.036244000	2.065807000	H	-1.096067000	6.985509000	2.105792000
C	-1.447606000	-1.062855000	5.337697000	H	0.660694000	5.221157000	1.979378000
H	-0.714550000	-3.058702000	5.790853000	H	3.978623000	0.420775000	1.369669000
H	-2.322013000	-3.026269000	5.072094000	H	4.051213000	1.988839000	2.178427000
H	-2.219099000	0.758005000	4.433388000	H	2.378043000	2.268466000	4.235213000
H	-3.249028000	-0.649924000	4.199747000	H	1.712501000	1.164459000	6.357576000
H	-1.949015000	-0.919910000	6.302603000	H	1.962535000	-1.297556000	6.612342000
H	-0.442280000	-0.635762000	5.431099000	H	2.873775000	-2.642888000	4.727612000
C	-3.377855000	-4.678485000	0.225530000	H	3.534855000	-1.524992000	2.612200000
C	-3.523969000	-6.191174000	0.054095000	C	2.821246000	1.968112000	-0.659512000
C	-4.528934000	-4.090977000	1.052898000	C	3.234972000	0.728247000	-1.255379000
H	-3.397261000	-4.181704000	-0.747033000	C	2.231034000	-0.017113000	-1.959677000
C	-4.881955000	-6.540334000	-0.571235000	O	1.062977000	0.400028000	-2.182887000
H	-3.437783000	-6.670591000	1.040469000	C	4.525385000	0.175949000	-1.125503000
H	-2.699989000	-6.576142000	-0.556999000	C	5.614342000	-0.370213000	-1.042295000
C	-5.885410000	-4.440940000	0.427726000	C	6.840839000	-1.074376000	-0.968233000
H	-4.479143000	-4.491941000	2.077548000	C	7.912957000	-0.607443000	-0.179143000
H	-4.406535000	-3.004668000	1.115389000	C	7.007347000	-2.279076000	-1.686939000
C	-6.042861000	-5.956062000	0.245027000	C	9.105803000	-1.320422000	-0.113820000
H	-4.983093000	-7.628167000	-0.659778000	H	7.793396000	0.316434000	0.378889000
H	-4.919816000	-6.136543000	-1.593121000	C	8.203693000	-2.984188000	-1.611558000
H	-6.694973000	-4.040460000	1.048835000	H	6.185749000	-2.642330000	-2.295962000
H	-5.962678000	-3.941132000	-0.547042000	C	9.259656000	-2.511769000	-0.827196000
H	-6.998710000	-6.181421000	-0.242200000	H	9.921314000	-0.944710000	0.498702000
H	-6.070080000	-6.440204000	1.232093000	H	8.315320000	-3.909399000	-2.171353000
O	1.159973000	-0.558737000	0.705749000	H	10.192714000	-3.065489000	-0.773177000
O	-0.027101000	1.403910000	0.842767000	H	-0.216320000	-1.657805000	0.914138000
N	1.573052000	2.799131000	1.608180000	C	2.634350000	-1.371838000	-2.482418000
C	1.144110000	0.651156000	0.914662000	C	3.020278000	-2.389265000	-1.599991000
C	2.200829000	1.593060000	1.226200000	C	2.647468000	-1.619787000	-3.858345000
C	0.325694000	2.673908000	1.305638000	C	3.440992000	-3.625263000	-2.090091000
C	-0.714259000	3.684499000	1.371146000	H	3.000346000	-2.191489000	-0.533630000
C	-2.043277000	3.376769000	1.052433000	C	3.076629000	-2.853001000	-4.351115000
C	-3.025740000	4.359966000	1.122803000	H	2.341337000	-0.830476000	-4.539291000
C	-2.690009000	5.659590000	1.504243000	C	3.482161000	-3.856421000	-3.468338000
C	-1.361674000	5.973064000	1.814707000	H	3.748515000	-4.404535000	-1.397725000
C	-0.375381000	4.995693000	1.749654000	H	3.102689000	-3.028236000	-5.423251000
C	3.413325000	1.119910000	1.991181000	H	3.822017000	-4.814894000	-3.851328000
C	3.021259000	0.447960000	3.290022000	H	-2.063822000	-4.441399000	1.852510000
C	2.491991000	1.194334000	4.351753000	H	1.840255000	2.254393000	-1.028909000
C	2.111879000	0.570512000	5.539628000	C	3.690337000	3.151102000	-0.450614000
C	2.250030000	-0.812866000	5.683173000	C	5.065259000	3.083536000	-0.174181000
C	2.760870000	-1.566512000	4.625360000	C	3.087887000	4.420195000	-0.517229000
C	3.139066000	-0.938818000	3.436922000	C	5.807333000	4.247114000	0.023681000
H	-2.297136000	2.376553000	0.732661000	H	5.553153000	2.119204000	-0.128197000
H	-4.047658000	4.104511000	0.867978000	C	3.829381000	5.581011000	-0.322075000
H	-3.457177000	6.427283000	1.556023000	H	2.023922000	4.487454000	-0.723183000

C	5.196046000	5.499153000	-0.047732000	H	3.340972000	6.549819000	-0.384537000
H	6.871373000	4.172367000	0.231961000	H	5.779145000	6.403150000	0.106020000

9. Determination of absolute configurations of the compounds D1, E1 and G1



D1

The colourless crystal in block-shape, with approximate dimensions of 0.096 × 0.138 × 0.470 mm^3, was selected and mounted for the single-crystal X-ray diffraction. The data set was collected by Bruker D8 Venture Photon II diffractometer at 173(2)K equipped with micro-focus Cu radiation source (K_α = 1.54178Å). Applied with face-indexed numerical absorption correction, the structure solution was solved and refinement was processed by SHELXTL (version 6.14) and OLEX 2.3 program package[13-16]. The structure was analyzed by ADDSYM routine implemented in PLATON suite and no higher symmetry was suggested[17]. The crystal data and further details are listed in Table S12. The crystal of product **D1** was obtained in the solvents of dichloromethane and isopropanol. CCDC: 2290734.

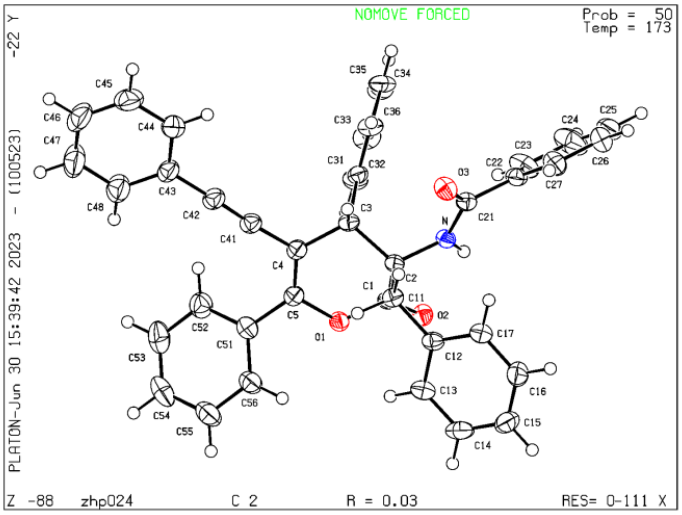


Figure S13. The thermal ellipsoid figure of **D1** with 50% probabilities

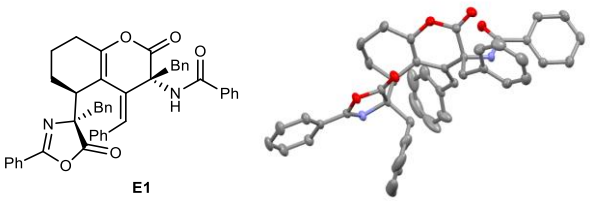
Table S12 Crystallographic Data for $C_{39}H_{29}NO_3$.

Formula	$C_{39}H_{29}NO_3$
Formula mass (amu)	559.67
Space group	C 2
a (Å)	21.1267 (9)
b (Å)	6.7221 (3)
c (Å)	22.0658 (10)
α (deg)	90
β (deg)	100.794 (2)
γ (deg)	90
V (Å^3)	3078.2 (2)
Z	4
λ (Å)	1.54178
T (K)	173
ρ_{calcd} (g cm^{-3})	1.208
μ (mm^{-1})	0.599
Transmission factors	0.715-1.000
θ_{max} (deg)	68.237
No. of unique data, including $F_o^2 < 0$	5595
No. of unique data, with $F_o^2 > 2\sigma(F_o^2)$	5352
No. of variables	393
$R(F)$ for $F_o^2 > 2\sigma(F_o^2)$ [a]	0.0310

$R_w(F_o^2)$ [b]	0.0752
Goodness of fit	1.054

[a] $R(F) = \sum||F_o| - |F_c|| / \sum|F_o|$.

[b] $R_w(F_o^2) = [\sum[w(F_o^2 - F_c^2)^2] / \sum wF_o^4]^{1/2}$; $w^{-1} = [\sigma^2(F_o^2) + (Ap)^2 + Bp]$, where $p = [\max(F_o^2,0) + 2F_c^2] / 3$.



The colourless crystal in block-shape, with approximate dimensions of 0.157 × 0.169 × 0.265 mm^3, was selected and mounted for the single-crystal X-ray diffraction. The data set was collected by Bruker D8 Venture Photon II diffractometer at 173(2)K equipped with micro-focus Cu radiation source (K_α = 1.54178Å). Applied with face-indexed numerical absorption correction, the structure solution was solved and refinement was processed by SHELXTL (version 6.14) and OLEX 2.3 program package[13], [14], [15], [16]. The structure was analyzed by ADDSYM routine implemented in PLATON suite and no higher symmetry was suggested[17]. The crystal data and further details are listed in Table S13. The crystal of product **E1** was obtained in the solvents of dichloromethane and isopropanol. CCDC: 2290736.

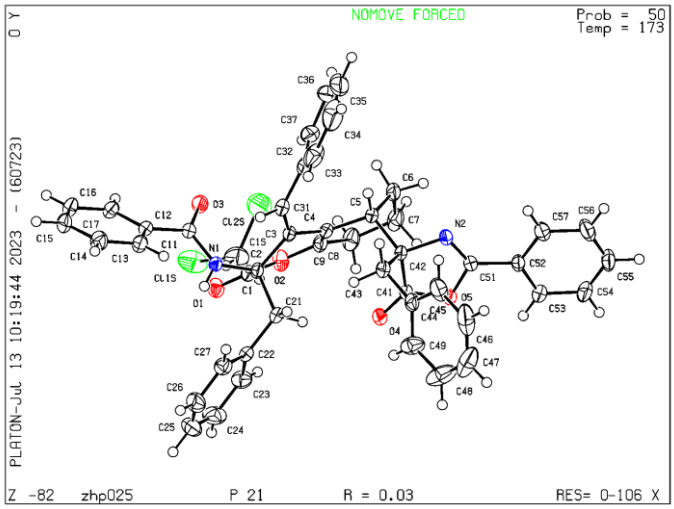


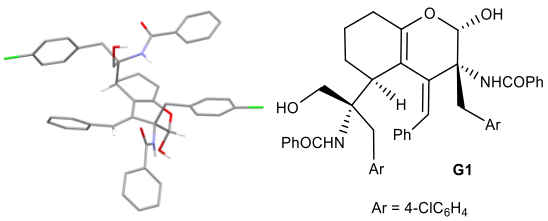
Figure S14. The thermal ellipsoid figure of **E1** with 50% probabilities

Table S13 Crystallographic Data for $C_{46}H_{38}N_2O_5$.

Formula	$C_{46}H_{38}N_2O_5$
Formula mass (amu)	698.82
Space group	P 21
a (Å)	13.1610 (3)
b (Å)	11.3464 (2)
c (Å)	13.7532 (3)
α (deg)	90
β (deg)	105.382 (1)
γ (deg)	90
V (Å^3)	1980.20 (7)
Z	2
λ (Å)	1.54178
T (K)	173
ρ_{calcd} (g cm^{-3})	1.314
μ (mm^{-1})	1.878
Transmission factors	0.840-0.965
θ_{max} (deg)	68.261
No. of unique data, including $F_o^2 < 0$	7234
No. of unique data, with $F_o^2 > 2\sigma(F_o^2)$	7036
No. of variables	510
$R(F)$ for $F_o^2 > 2\sigma(F_o^2)$ [a]	0.0275
$R_w(F_o^2)$ [b]	0.0655
Goodness of fit	1.030

[a] $R(F) = \sum||F_o| - |F_c|| / \sum|F_o|$.

[b] $R_w(F_o^2) = [\sum[w(F_o^2 - F_c^2)^2] / \sum wF_o^4]^{1/2}$; $w^{-1} = [\sigma^2(F_o^2) + (Ap)^2 + Bp]$, where $p = [\max(F_o^2,0) + 2F_c^2] / 3$.



The colourless crystal in block-shape, with approximate dimensions of 0.174 × 0.220 × 0.332 mm^3, was selected and mounted for the single-crystal X-ray diffraction. The data set was collected by Bruker D8 Venture Photon II diffractometer at 173(2)K equipped with micro-focus Cu radiation source ($K\alpha$ = 1.54178Å). Applied with face-indexed numerical absorption correction, the structure solution was solved and refinement was processed by SHELXTL (version 6.14) and OLEX 2.3 program package[13], [14], [15], [16]. The structure was analyzed by ADDSYM routine implemented in PLATON suite and no higher symmetry was suggested[17]. The crystal data and further details are listed in Table S14. The crystal of product **G1** was obtained in the solvents of tetrahydrofuran and petroleum ether. CCDC: 2310080.

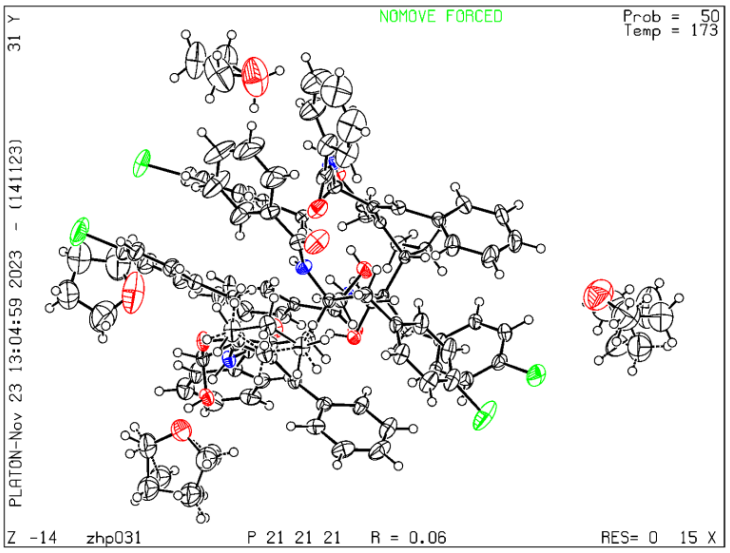


Figure S15. The thermal ellipsoid figure of **G1** with 50% probabilities

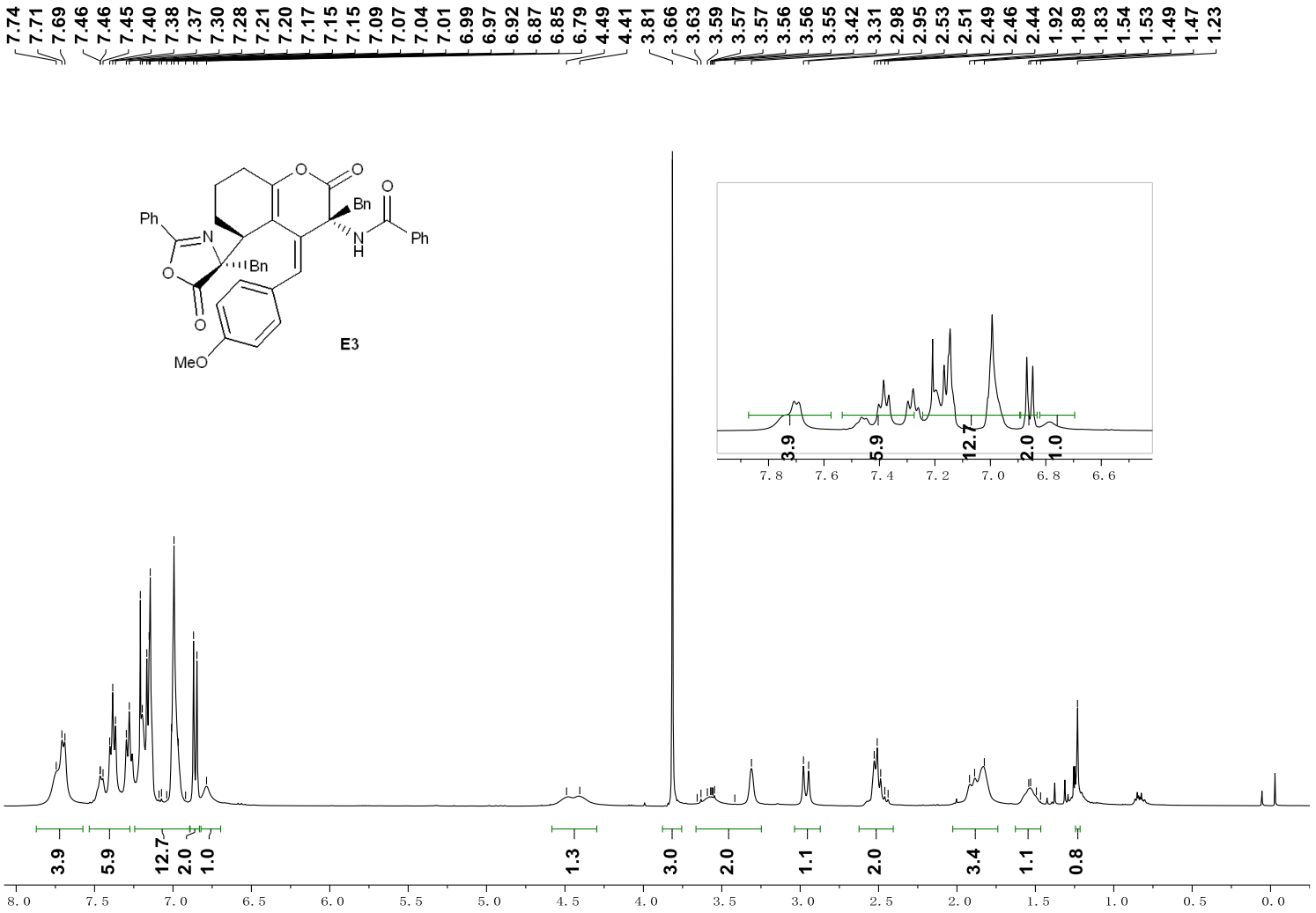
Table S14 Crystallographic Data for $C_{46}H_{42}Cl_2N_2O_5$.

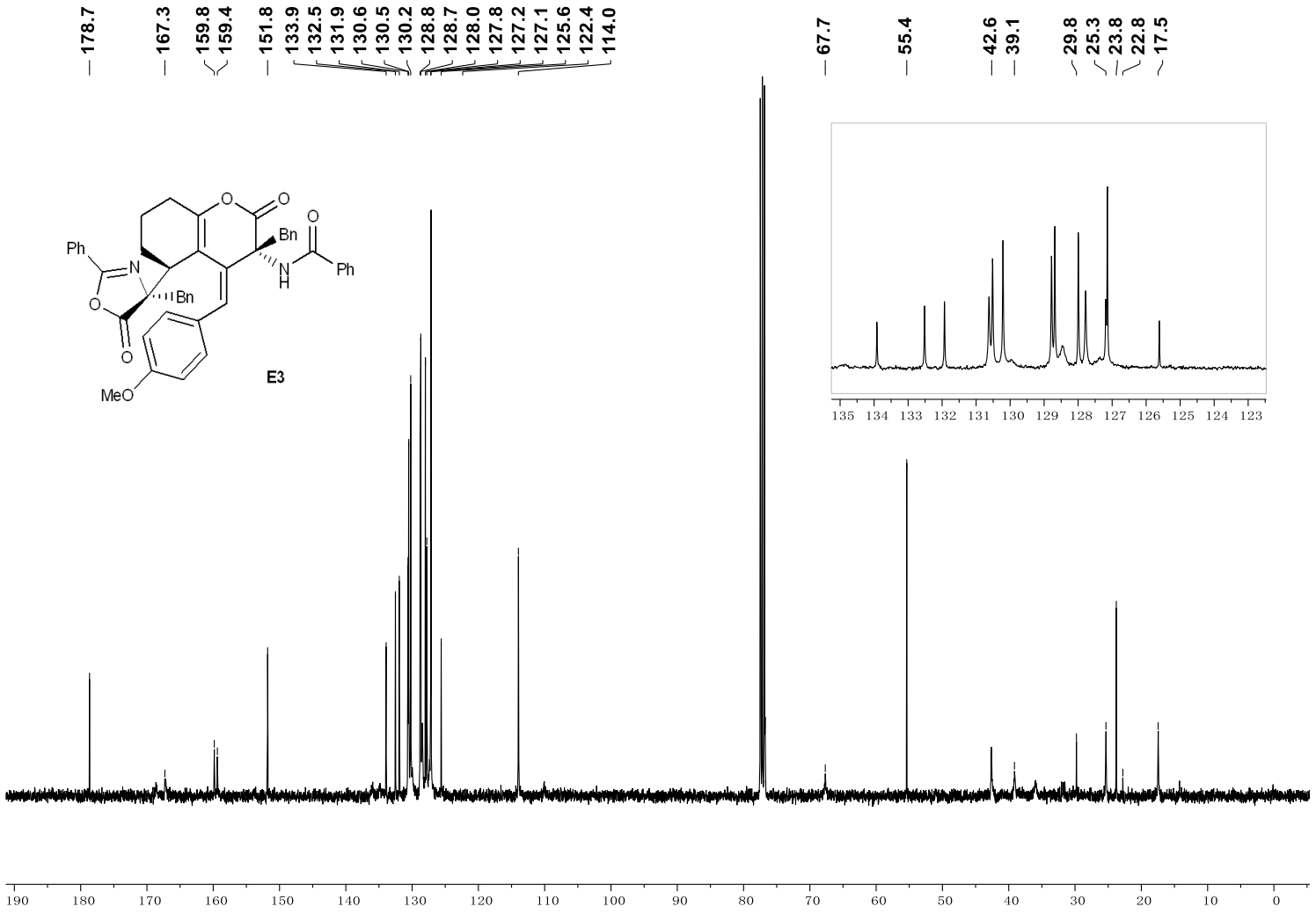
Formula	$C_{46}H_{42}Cl_2N_2O_5$
Formula mass (amu)	773.75
Space group	P 21 21 21
a (Å)	15.6884 (5)
b (Å)	16.7218 (6)
c (Å)	36.4564 (12)
α (deg)	90
β (deg)	90
γ (deg)	90
V (Å^3)	9563.9 (6)
Z	4
λ (Å)	1.54178
T (K)	173
ρ_{calcd} (g cm^{-3})	1.275
μ (mm^{-1})	1.660
Transmission factors	0.655-0.869
θ_{max} (deg)	68.326
No. of unique data, including $F_o^2 < 0$	17245
No. of unique data, with $F_o^2 > 2\sigma(F_o^2)$	15873
No. of variables	1225
$R(F)$ for $F_o^2 > 2\sigma(F_o^2)$ [a]	0.0565
$R_w(F_o^2)$ [b]	0.1399
Goodness of fit	1.041

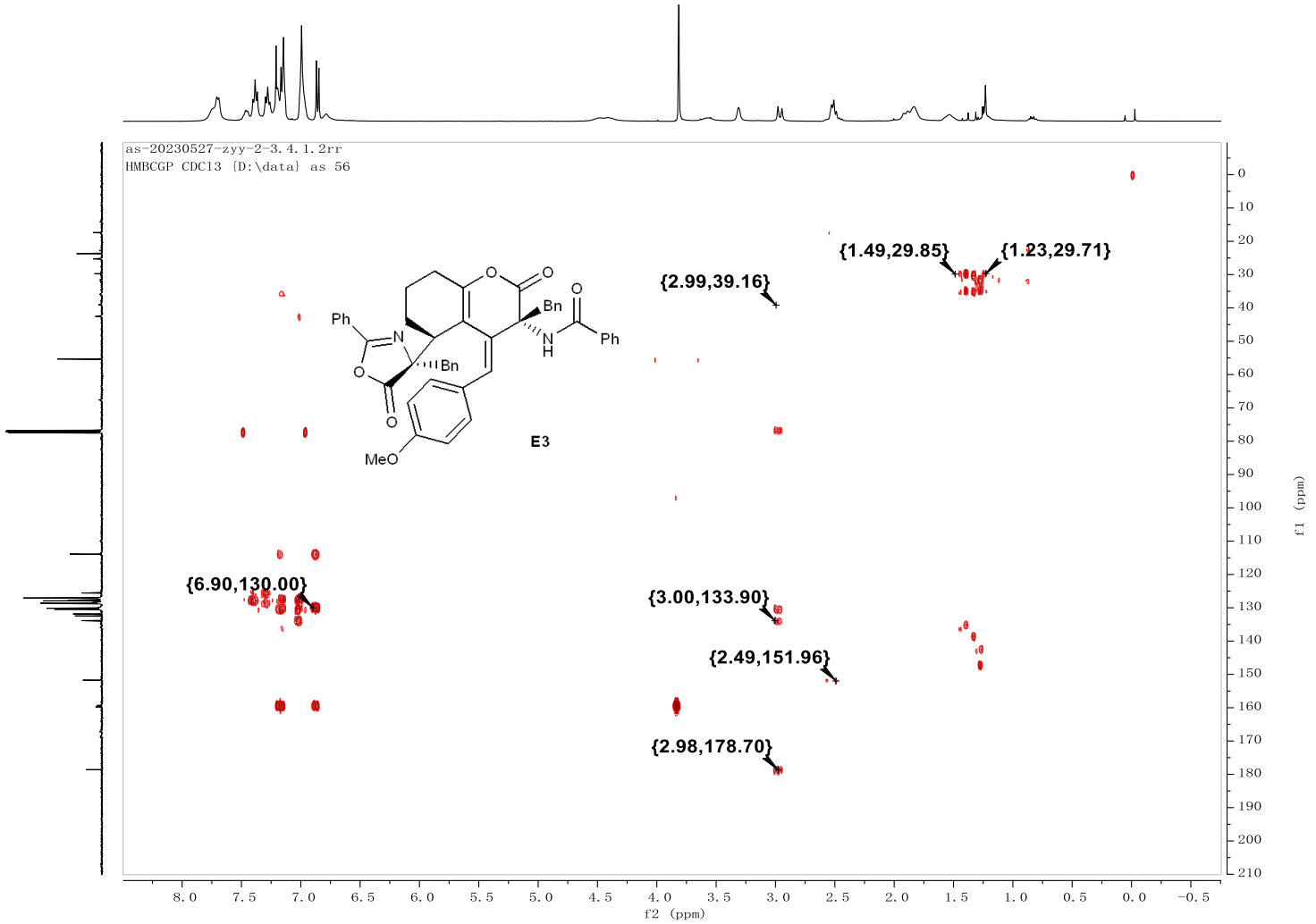
[a] $R(F) = \sum||F_o| - |F_c|| / \sum|F_o|$.

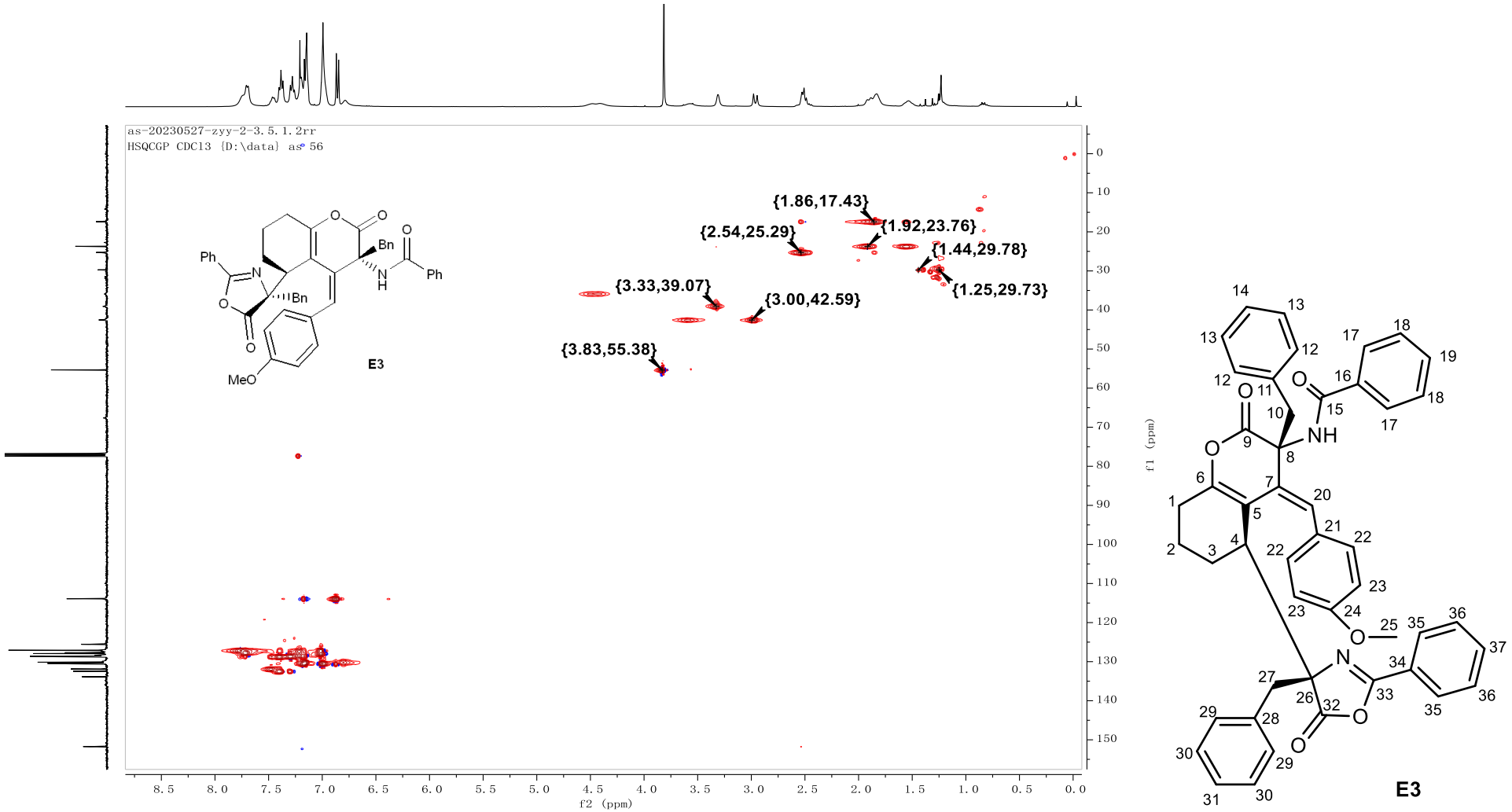
[b] $R_w(F_o^2) = [\sum[w(F_o^2 - F_c^2)^2] / \sum wF_o^4]^{1/2}$; $w^{-1} = [\sigma^2(F_o^2) + (Ap)^2 + Bp]$, where $p = [\max(F_o^2,0) + 2F_c^2] / 3$.

10. Analysis result of 2D NMR spectra of the product E3




178.7
167.3
159.8
159.4
151.8
133.9
132.5
131.9
130.6
130.5
130.2
128.8
128.7
128.0
127.8
127.2
127.1
125.6
122.4
114.0
67.7
55.4
42.6
39.1
29.8
25.3
23.8
22.8
17.5
Ph
N
O
Bn
Bn
O
O
O
O
N
H
Ph
MeO
E3
135 134 133 132 131 130 129 128 127 126 125 124 123
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


as-20230527-zyy-2-3.4.1.2rr
HMBCGP CDCl3 (D:\data) as 56
{1.49,29.85}
{1.23,29.71}
{2.99,39.16}
{6.90,130.00}
{3.00,133.90}
{2.49,151.96}
{2.98,178.70}
Ph
N
O
Bn
O
O
O
N
H
Ph
Bn
O
MeO
E3
f2 (ppm)
f1 (ppm)



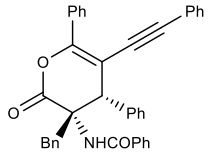
HSQC-Correlation Peak: (1.25, 29.7); (1.44, 29.8); (1.86, 17.4); (1.92, 23.8); (2.54, 25.3); (3.00, 42.6); (3.33, 39.1); (3.83, 55.4).
HMBC-Correlation Peak: (1.23, 29.7); (1.49, 29.9); (2.99, 39.2); (3.00, 133.9); (2.49, 152.0); (2.98, 178.7); (6.90, 130.0).

Number of Atom	H (ppm)	C (ppm)
1	1.21-1.62	29.8
2	1.75-2.05	17.5
3	3.24-3.68	39.1
4	2.90-3.03	42.6
5	-	114.0-132.5
6	-	133.9

7	-	114.0-132.5
8	-	67.7
9	-	167.3
10	1.75-2.05, 4.38-4.52	23.8
11	-	114.0-132.5
12	6.82-7.81	114.0-132.5
13	6.82-7.81	114.0-132.5
14	6.82-7.81	114.0-132.5
15	-	159.8
16	-	114.0-132.5
17	6.82-7.81	114.0-132.5
18	6.82-7.81	114.0-132.5
19	6.82-7.81	114.0-132.5
20	6.82-7.81	114.0-132.5
21	-	114.0-132.5
22	6.82-7.81	114.0-132.5
23	6.82-7.81	114.0-132.5
24	-	159.4
25	3.81(s)	55.4
26	-	22.8
27	2.41-2.57	25.3
28	-	114.0-132.5
29	6.82-7.81	114.0-132.5
30	6.82-7.81	114.0-132.5
31	6.82-7.81	114.0-132.5
32	-	178.7
33	-	151.8
34	-	114.0-132.5
35	6.82-7.81	114.0-132.5
36	6.82-7.81	114.0-132.5
37	6.82-7.81	114.0-132.5

11. Characterization of the products

***N*-((3*S*,4*S*)-3-benzyl-2-oxo-4,6-diphenyl-5-(phenylethynyl)-3,4-dihydro-2H-pyran-3-yl)benzamide (D1)**



D1

49.8 mg, 89% yield; white solid, melting point: 186.3 – 189.2 °C, $[\alpha]^{22}_D$ = 40.2 (*c* = 0.87, CH_2Cl_2).

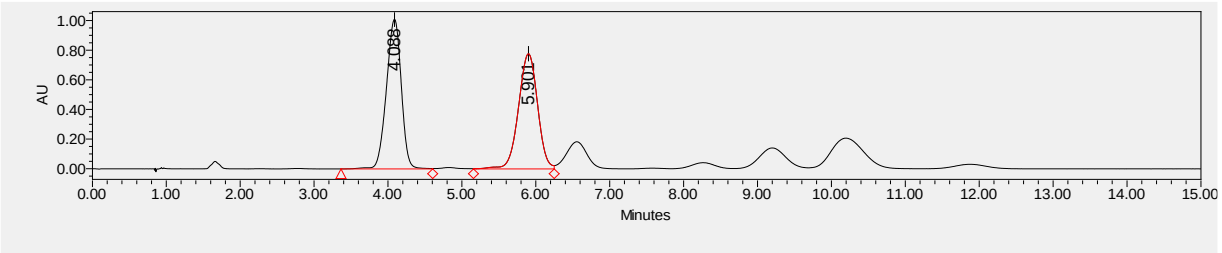
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IC-3, CO_2/IPROH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 3.94 min, t_{minor} = 5.68 min. er = 95:5. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 – 8.22 (m, 2H), 7.58 – 7.43 (m, 3H), 7.44 – 7.08 (m, 20H), 6.65 (s, 1H), 5.18 (s, 1H), 4.37 (d, *J* = 12.0 Hz, 1H), 3.60 (d, *J* = 16.0 Hz, 1H).

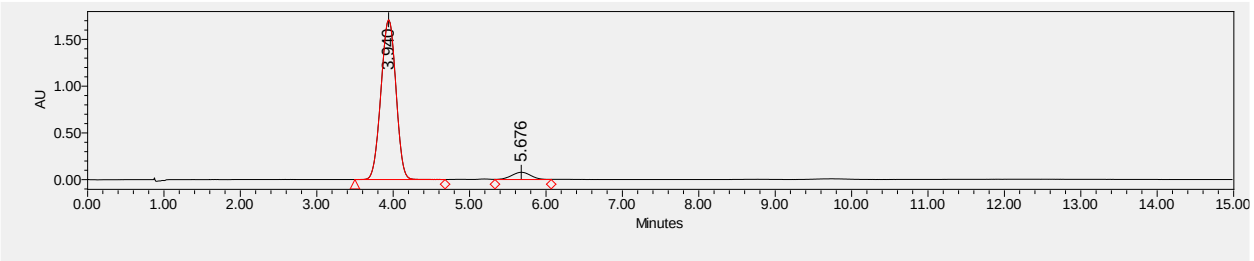
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.0, 168.0, 151.9, 136.3, 135.1, 134.8, 131.7, 131.5, 131.4, 130.4, 130.1, 128.9, 128.7, 128.6, 128.5, 128.5, 128.2, 127.7, 127.6, 126.7, 122.9, 102.7, 96.6, 86.3, 64.7, 52.6, 38.5.

IR (neat): ν (cm^{-1}): 3416, 2923, 1768, 1665, 1485, 1165, 692, 528.

HRMS (ESI-TOF) calcd for $C_{39}H_{29}NO_3^+$ ([M]+H^+) = 560.2220, found 560.2224.

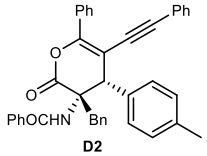


	Retention Time	Area	% Area
1	4.088	14105758	50.37
2	5.901	13898569	49.63



	Retention Time	Area	% Area
1	3.940	23205226	94.50
2	5.676	1351045	5.50

***N*-((3*S*,4*S*)-3-benzyl-2-oxo-6-phenyl-5-(phenylethynyl)-4-(p-tolyl)-3,4-dihydro-2H-pyran-3-yl)benzamide (D2)**



D2

49.3 mg, 86% yield; white solid, melting point: 91.2 – 94.7 °C, $[\alpha]^{19}_{D}$ = 33.0 (*c* = 0.71, CH_2Cl_2).

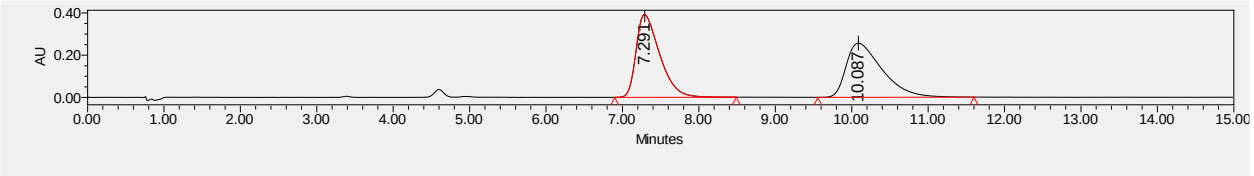
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 9.99 min, t_{minor} = 7.41 min. er = 89:11. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 – 8.22 (m, 2H), 7.59 – 7.45 (m, 3H), 7.48 – 7.18 (m, 15H), 7.14 – 7.01 (m, 4H), 6.64 (s, 1H), 5.14 (s, 1H), 4.34 (d, *J* = 12.0 Hz, 1H), 3.58 (d, *J* = 12.0 Hz, 1H), 2.23 (s, 3H).

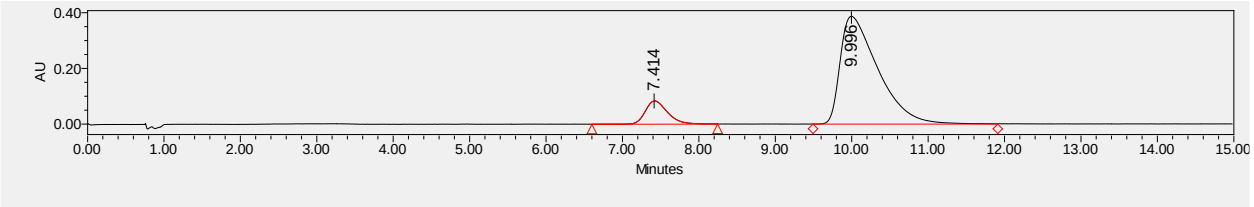
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.1, 168.0, 151.8, 137.9, 135.2, 134.9, 133.1, 131.7, 131.5, 130.4, 130.1, 129.6, 128.7, 128.6, 128.5, 128.1, 127.7, 127.6, 126.8, 123.0, 103.0, 96.6, 86.4, 64.9, 52.2, 38.5, 21.2.

IR (neat): ν (cm^{-1}): 3419, 3029, 1768, 1666, 1512, 1166, 753, 528.

HRMS (ESI-TOF) calcd for $C_{40}H_{31}NO_3^+$ ([M]+H^+) = 574.2377, found 574.2379.

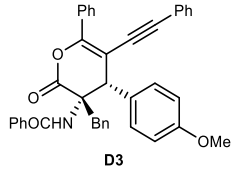


	Retention Time	Area	% Area
1	7.291	8417752	50.12
2	10.087	8376888	49.88



	Retention Time	Area	% Area
1	7.414	1696537	11.30
2	9.996	13318101	88.70

***N*-((3*S*,4*S*)-3-benzyl-4-(4-methoxyphenyl)-2-oxo-6-phenyl-5-(phenylethynyl)-3,4-dihydro-2H-pyran-3-yl)benzamide (D3)**



D3

24.1 mg, 41% yield; pale yellow solid, melting point: 93.2 – 97.5 °C, $[\alpha]^{20}_{D}$ = 30.8 (*c* = 0.40, CH_2Cl_2).

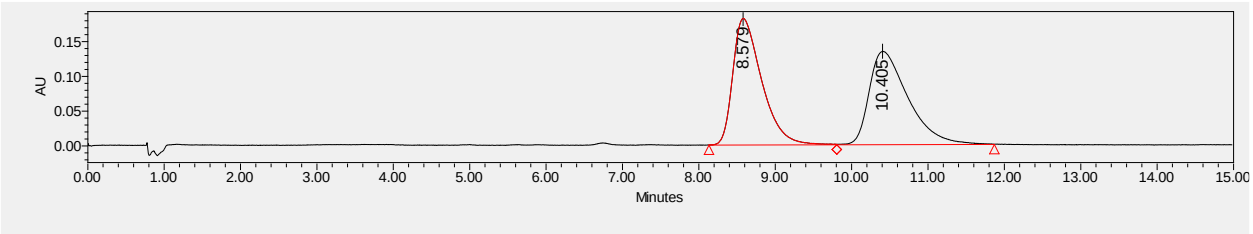
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 10.48 min, t_{minor} = 8.73 min. er = 93:7. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.28 – 8.23 (m, 2H), 7.59 – 7.46 (m, 3H), 7.47 – 7.41 (m, 3H), 7.42 – 7.26 (m, 7H), 7.29 – 7.18 (m, 5H), 7.15 – 7.07 (m, 2H), 6.79 – 6.74 (m, 2H), 6.65 (s, 1H), 5.12 (s, 1H), 4.33 (d, *J* = 12.0 Hz, 1H), 3.70 (s, 3H), 3.57 (d, *J* = 12.0 Hz, 1H).

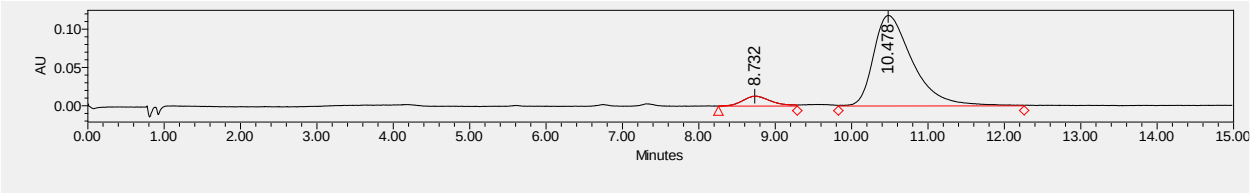
^{13}C NMR (101 MHz, $CDCl_3$) *δ* 168.1, 168.0, 159.4, 151.7, 135.2, 135.0, 131.7, 131.5, 131.5, 130.4, 130.1, 129.4, 128.7, 128.6, 128.5, 128.5, 128.1, 127.7, 127.6, 126.8, 123.0, 114.3, 103.1, 96.6, 86.4, 65.0, 55.3, 51.8, 38.5.

IR (neat): ν (cm^{-1}): 3418, 2928, 1768, 1666, 1512, 1261, 755, 528.

HRMS (ESI-TOF) calcd for $C_{40}H_{31}NO_4^+$ ([M]+H^+) = 590.2326, found 590.2328.

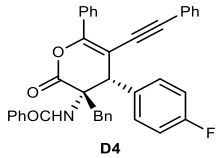


	Retention Time	Area	% Area
1	8.579	4786115	50.24
2	10.405	4740546	49.76



	Retention Time	Area	% Area
1	8.732	332242	7.31
2	10.478	4214833	92.69

_N_-((3_S_,4_S_)-3-benzyl-4-(4-fluorophenyl)-2-oxo-6-phenyl-5-(phenylethynyl)-3,4-dihydro-2H-pyran-3-yl)benzamide (D4)



D4

49.6 mg, 86% yield; white solid, melting point: 98.6 – 101.4 °C, $[\alpha]^{20}_D$ = 49.0 (*c* = 0.87, CH_2Cl_2).

Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 6.64 min, t_{minor} = 4.79 min. er = 92:8. dr >19:1.

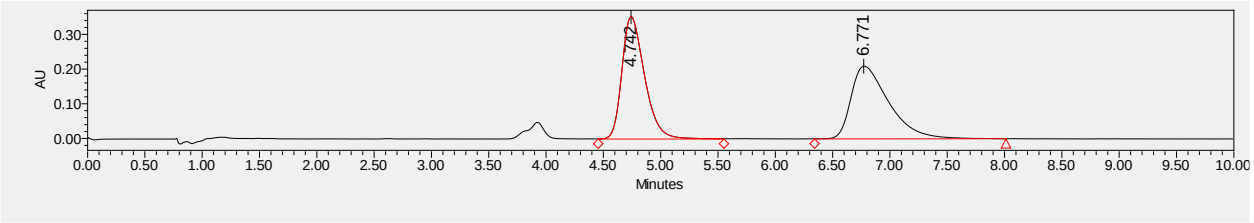
^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.29 – 8.22 (m, 2H), 7.59 – 7.27 (m, 15H), 7.25 – 7.20 (m, 3H), 7.13 – 7.09 (m, 2H), 6.96 – 6.90 (m, 2H), 6.67 (s, 1H), 5.18 (s, 1H), 4.32 (d, *J* = 12.0 Hz, 1H), 3.58 (d, *J* = 12.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) *δ* 168.0, 167.9, 162.6 (d, *J* = 240.0 Hz), 151.9, 134.9, 134.7, 132.2 (d, *J* = 10.0 Hz), 131.9, 131.5, 131.3, 130.5, 130.1, 130.0, 129.9, 128.8, 128.8, 128.6, 128.5, 127.7, 127.7, 126.7, 122.8, 115.9 (d, *J* = 20.0 Hz), 102.6, 96.8, 86.1, 64.7, 51.9, 38.6.

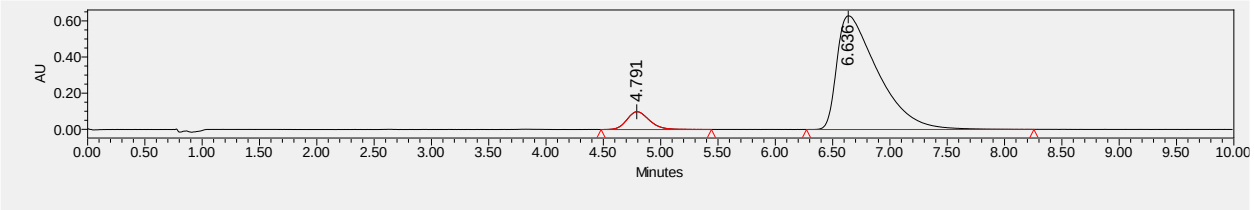
^{19}F NMR (376 MHz, $CDCl_3$) δ -113.74.

IR (neat): ν (cm^{-1}): 3415, 3061, 1766, 1663, 1509, 1161, 690, 528.

HRMS (ESI-TOF) calcd for $C_{39}H_{28}FNO_3^+$ ([M]+H^+) = 578.2126, found 578.2129.

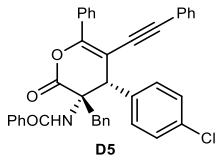


	Retention Time	Area	% Area
1	4.742	4850723	50.22
2	6.771	4809094	49.78



	Retention Time	Area	% Area
1	4.791	1347749	7.93
2	6.636	15642650	92.07

***N*-((3*S*,4*S*)-3-benzyl-4-(4-chlorophenyl)-2-oxo-6-phenyl-5-(phenylethynyl)-3,4-dihydro-2H-pyran-3-yl)benzamide (D5)**



D5

53.5 mg, 90% yield; white solid, melting point: 100.2 – 104.7 °C, $[\alpha]^{19}_D$ = 25.9 (*c* = 0.90, CH_2Cl_2).

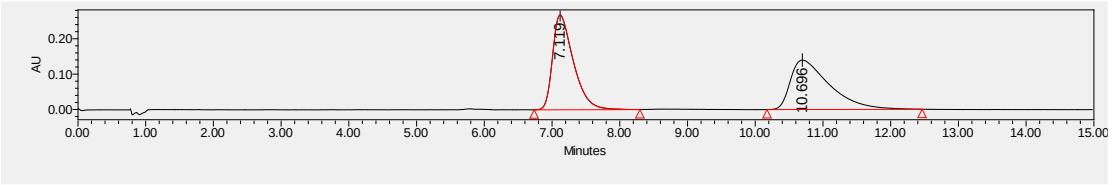
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 10.50 min, t_{minor} = 7.26 min. er = 91:9. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 – 8.22 (m, 2H), 7.59 – 7.40 (m, 6H), 7.42 – 7.17 (m, 14H), 7.15 – 7.06 (m, 2H), 6.68 (s, 1H), 5.18 (s, 1H), 4.32 (d, J = 12.0 Hz, 1H), 3.58 (d, J = 12.0 Hz, 1H).

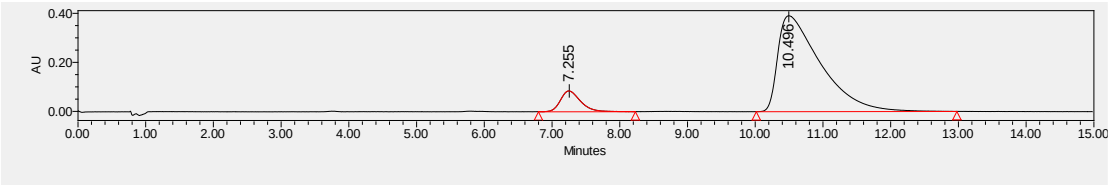
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.0, 167.8, 152.0, 134.9, 134.8, 134.6, 134.1, 131.9, 131.5, 131.2, 130.6, 130.1, 129.7, 129.1, 128.9, 128.8, 128.6, 128.5, 127.7, 126.8, 122.7, 102.4, 96.9, 86.0, 64.6, 52.0, 38.6.

IR (neat): ν (cm^{-1}): 3416, 3030, 1769, 1666, 1488, 1166, 753, 529.

HRMS (ESI-TOF) calcd for $C_{39}H_{28}ClNO_3^+$ ([M]+H^+) = 594.1830, 595.1864, found 594.1837, 595.1865.

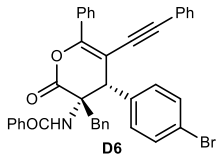


	Retention Time	Area	% Area
1	7.119	5722630	50.55
2	10.696	5597601	49.45



	Retention Time	Area	% Area
1	7.255	1755465	9.27
2	10.496	17177644	90.73

***N*-((3*S*,4*S*)-3-benzyl-4-(4-bromophenyl)-2-oxo-6-phenyl-5-(phenylethynyl)-3,4-dihydro-2H-pyran-3-yl)benzamide (D6)**



D6

47.9 mg, 75% yield; pale yellow solid, melting point: 97.3 – 99.8 °C, $[\alpha]^{19}_D$ = 16.0 (c = 0.60, CH_2Cl_2).

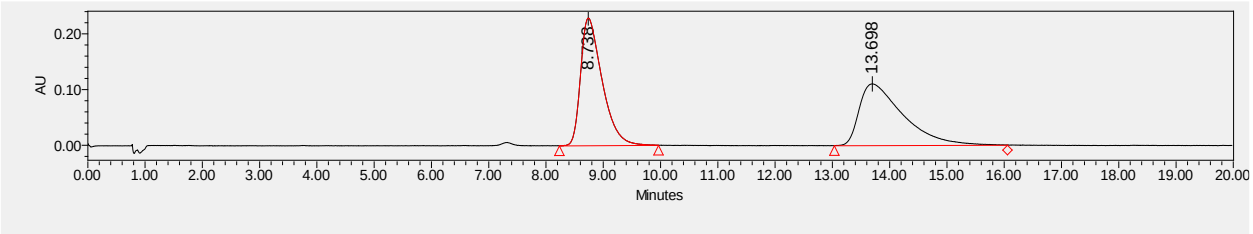
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 13.46 min, t_{minor} = 8.87 min. er = 92:8. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 – 8.20 (m, 2H), 7.59 – 7.27 (m, 15H), 7.27 – 7.17 (m, 5H), 7.14 – 7.06 (m, 2H), 6.68 (s, 1H), 5.16 (s, 1H), 4.31 (d, *J* = 16.0 Hz, 1H), 3.57 (d, *J* = 16.0 Hz, 1H).

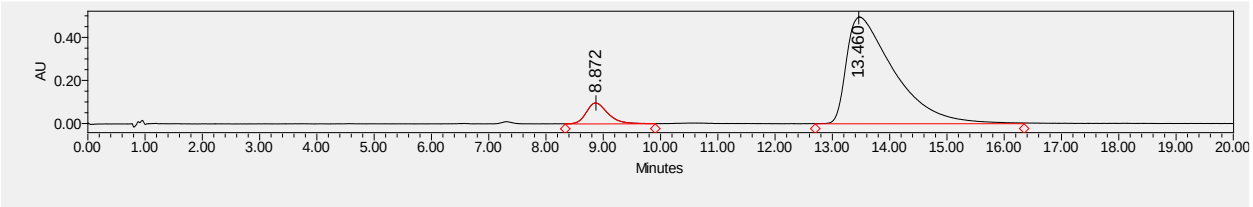
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.0, 167.8, 152.0, 135.5, 134.8, 134.6, 132.1, 131.9, 131.5, 131.2, 130.6, 130.1, 130.0, 128.9, 128.8, 128.6, 128.6, 127.7, 126.8, 122.7, 122.4, 102.3, 96.9, 86.0, 64.5, 52.1, 38.6.

IR (neat): ν (cm^{-1}): 3415, 3030, 1769, 1666, 1486, 1166, 754, 528.

HRMS (ESI-TOF) calcd for $C_{39}H_{28}BrNO_3^+$ ([M]+H^+) = 638.1325, 640.1305, found 638.1329, 640.1302.

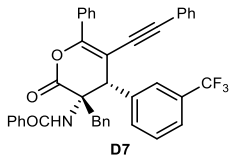


	Retention Time	Area	% Area
1	8.738	5989133	50.25
2	13.698	5928445	49.75



	Retention Time	Area	% Area
1	8.872	2561746	8.18
2	13.460	28764468	91.82

***N*-((3*S*,4*S*)-3-benzyl-2-oxo-6-phenyl-5-(phenylethynyl)-4-(3-(trifluoromethyl)phenyl)-3,4-dihydro-2H-pyran-3-yl)benzamide (D7)**



D7

52.7 mg, 84% yield; pale yellow solid, melting point: 88.5 – 90.4 °C, $[\alpha]^{19}_D$ = 51.1 (*c* = 0.90, CH_2Cl_2).

Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 9.87 min, t_{minor} = 8.02 min. er = 86:14. dr >19:1.

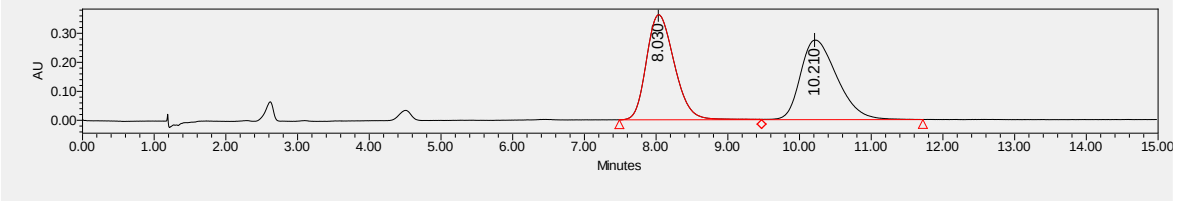
^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.28 – 8.25 (m, 2H), 7.72 – 7.67 (m, 1H), 7.61 – 7.20 (m, 19H), 7.15 – 7.08 (m, 2H), 6.65 (s, 1H), 5.29 (s, 1H), 4.34 (d, *J* = 16.0 Hz, 1H), 3.60 (d, *J* = 12.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) *δ* 168.2, 167.6, 152.4, 137.4, 134.7, 134.5, 131.9, 131.5, 131.3, 131.2, 131.0, 130.8, 130.7, 130.1, 129.6, 129.1, 128.9, 128.7, 128.7, 128.6, 127.8, 126.8, 126.0 (q, *J* = 3.3 Hz), 125.2 (q, *J* = 3.3 Hz), 122.6, 122.6, 101.9, 97.0, 85.9, 64.6, 52.3, 38.6.

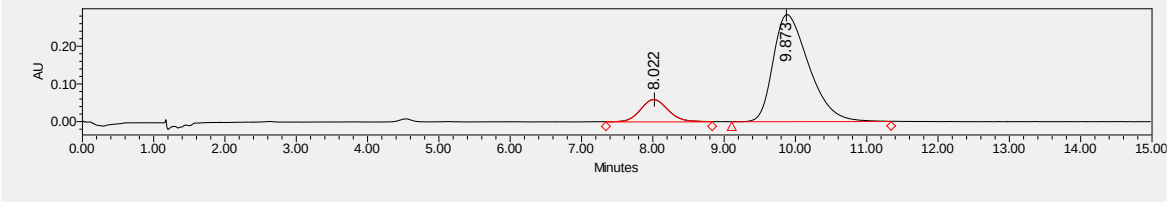
^{19}F NMR (377 MHz, $CDCl_3$) δ -62.56.

IR (neat): *ν* (cm^{-1}): 3416, 3031, 1769, 1665, 1327, 1165, 755, 529.

HRMS (ESI-TOF) calcd for $C_{40}H_{28}F_3NO_3^+$ ([M]+H^+) = 628.2094, found 628.2095.

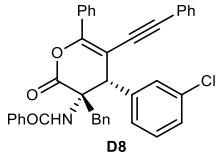


	Retention Time	Area	% Area
1	8.030	9787718	50.15
2	10.210	9727338	49.85



	Retention Time	Area	% Area
1	8.022	1605504	13.93
2	9.873	9916634	86.07

***N*-((3*S*,4*S*)-3-benzyl-4-(3-chlorophenyl)-2-oxo-6-phenyl-5-(phenylethynyl)-3,4-dihydro-2H-pyran-3-yl)benzamide (D8)**



D8

37.4 mg, 63% yield; white solid, melting point: 91.0 – 92.7 °C, $[\alpha]^{19}_{D}$ = 46.4 (*c* = 0.60, CH_2Cl_2).

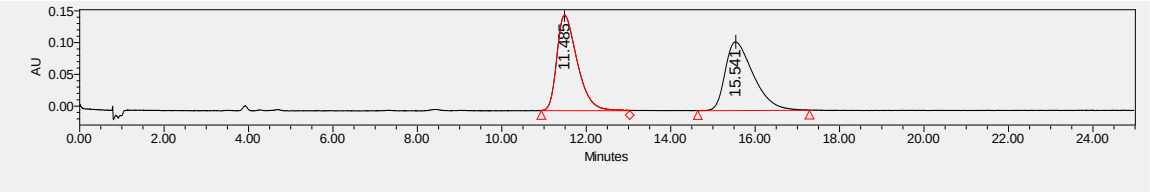
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 15.15 min, t_{minor} = 11.56 min. er = 88:12. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 – 8.24 (m, 2H), 7.60 – 7.47 (m, 3H), 7.50 – 7.28 (m, 11H), 7.27 – 7.06 (m, 8H), 6.65 (s, 1H), 5.17 (s, 1H), 4.33 (d, *J* = 16.0 Hz, 1H), 3.57 (d, *J* = 16.0 Hz, 1H).

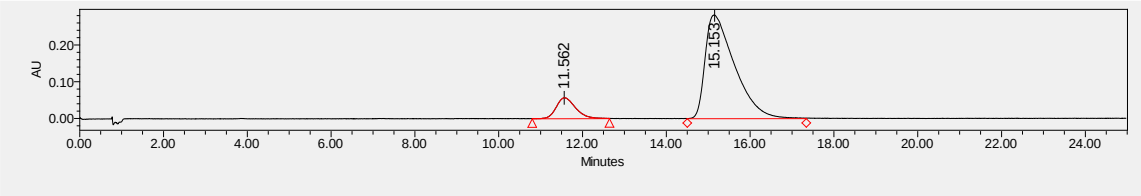
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.3, 167.6, 152.2, 138.3, 135.0, 134.7, 134.6, 131.8, 131.5, 131.2, 130.6, 130.2, 130.1, 128.9, 128.8, 128.7, 128.6, 128.6, 127.8, 127.7, 126.8, 126.2, 122.7, 102.0, 96.9, 86.0, 64.6, 52.2, 38.6.

IR (neat): ν (cm^{-1}): 3415, 3029, 1770, 1666, 1485, 1166, 752, 532.

HRMS (ESI-TOF) calcd for $C_{39}H_{28}ClNO_3^+$ ([M]+H^+) = 594.1830, 595.1864, found 594.1833, 595.1865.

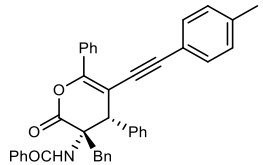


	Retention Time	Area	% Area
1	11.485	5035647	50.08
2	15.541	5020458	49.92



	Retention Time	Area	% Area
1	11.562	1842215	11.76
2	15.153	13819510	88.24

***N*-((3*S*,4*S*)-3-benzyl-2-oxo-4,6-diphenyl-5-(p-tolylethynyl)-3,4-dihydro-2H-pyran-3-yl)benzamide (D9)**



D9

48.1 mg, 84% yield; pale yellow solid, melting point: 157.2 – 160.4 °C, $[\alpha]^{19}_{D}$ = 34.8 (*c* = 0.72, CH_2Cl_2).

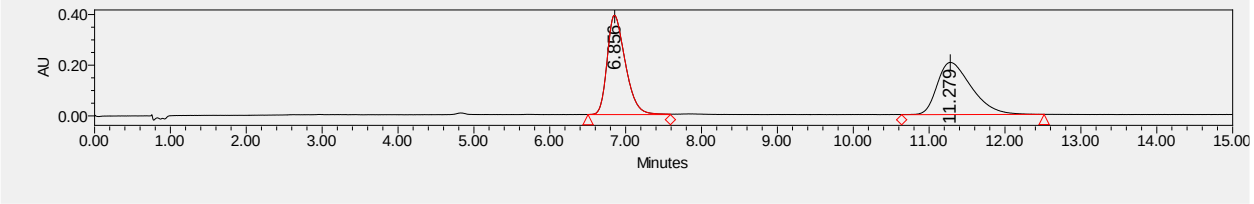
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 11.29 min, t_{minor} = 6.95 min. er = 90:10. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.29 – 8.22 (m, 2H), 7.58 – 7.44 (m, 3H), 7.47 – 7.34 (m, 3H), 7.36 – 7.15 (m, 12H), 7.16 – 7.07 (m, 4H), 6.63 (s, 1H), 5.16 (s, 1H), 4.36 (d, *J* = 12.0 Hz, 1H), 3.59 (d, *J* = 16.0 Hz, 1H), 2.33 (s, 3H).

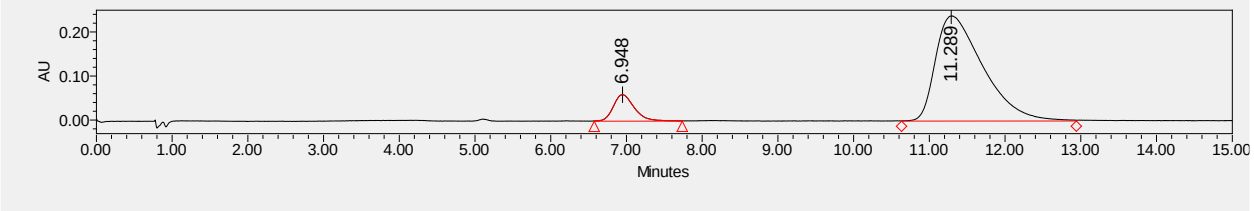
^{13}C NMR (101 MHz, $CDCl_3$) *δ* 168.1, 151.5, 139.0, 136.4, 135.2, 134.9, 131.7, 131.5, 131.4, 130.3, 130.1, 129.3, 128.9, 128.7, 128.6, 128.5, 128.3, 128.2, 127.7, 127.6, 126.8, 119.9, 103.0, 97.0, 85.7, 64.8, 52.7, 38.6, 21.7.

IR (neat): *ν* (cm^{-1}): 3418, 3030, 1770, 1666, 1511, 1167, 753, 528.

HRMS (ESI-TOF) calcd for $C_{40}H_{31}NO_3^+$ ([M]+H^+) = 574.2377, found 574.2379.

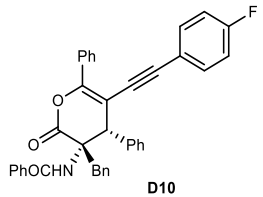


	Retention Time	Area	% Area
1	6.856	6518930	50.22
2	11.279	6460883	49.78



	Retention Time	Area	% Area
1	6.948	1165666	10.08
2	11.289	10401995	89.92

_N_-((3_S_,4_S_)-3-benzyl-5-((4-fluorophenyl)ethynyl)-2-oxo-4,6-diphenyl-3,4-dihydro-2H-pyran-3-yl)benzamide (D10)



D10

45.0 mg, 78% yield; white solid, melting point: 92.7 – 95.3 °C, $[\alpha]^{19}_D$ = 47.9 (*c* = 0.72, CH_2Cl_2).

Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 7.11 min, t_{minor} = 5.72 min. er = 91:9. dr >19:1.

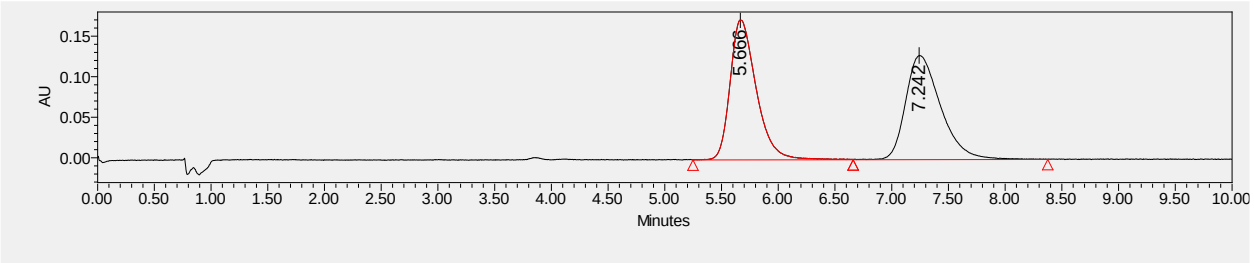
^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.25 – 8.21 (m, 2H), 7.59 – 7.45 (m, 3H), 7.47 – 7.27 (m, 9H), 7.29 – 7.16 (m, 6H), 7.13 – 7.10 (m, 2H), 7.05 – 6.94 (m, 2H), 6.63 (s, 1H), 5.15 (s, 1H), 4.36 (d, *J* = 12.0 Hz, 1H), 3.58 (d, *J* = 16.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) *δ* 168.1, 168.0, 162.8 (d, *J* = 250.6 Hz), 152.0, 136.3, 135.1, 134.8, 133.4 (d, *J* = 8.3 Hz), 131.7, 131.4, 130.5, 130.1, 129.0, 128.7, 128.6, 128.5, 128.3, 128.3, 127.7, 127.6, 126.8, 119.04 (d, *J* = 3.5 Hz), 115.87 (d, *J* = 22.1 Hz), 102.6, 95.4, 86.0, 64.8, 52.6, 38.6.

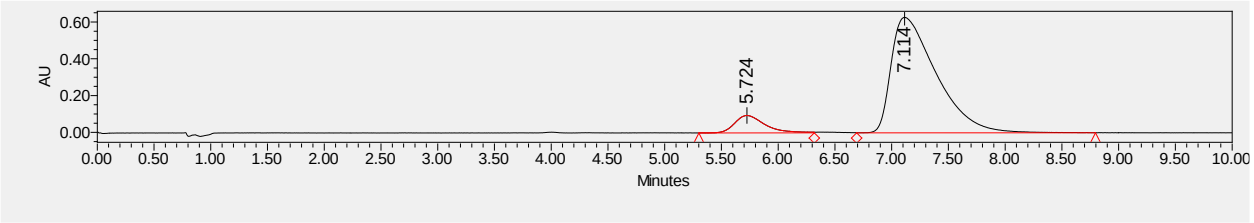
^{19}F NMR (376 MHz, $CDCl_3$) *δ* -109.96.

IR (neat): *ν* (cm^{-1}): 3417, 3031, 1768, 1665, 1452, 1156, 696, 529.

HRMS (ESI-TOF) calcd for $C_{39}H_{28}FNO_3^+$ ([M]+H^+) = 578.2126, found 578.2128.

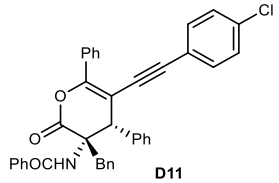


	Retention Time	Area	% Area
1	5.666	2771112	50.10
2	7.242	2760374	49.90



	Retention Time	Area	% Area
1	5.724	1763982	9.22
2	7.114	17366612	90.78

***N*-((3*S*,4*S*)-3-benzyl-5-((4-chlorophenyl)ethynyl)-2-oxo-4,6-diphenyl-3,4-dihydro-2H-pyran-3-yl)benzamide (D11)**



D11

48.1 mg, 81% yield; white solid, melting point: 93.5 – 96.7 °C, $[\alpha]^{19}_{D}$ = 36.9 (*c* = 0.80, CH_2Cl_2).

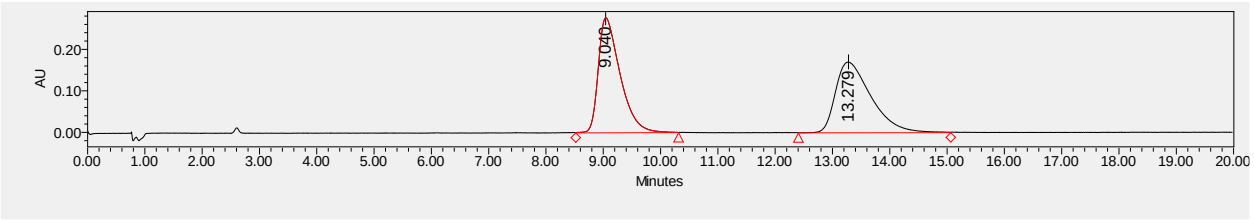
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 13.98 min, t_{minor} = 9.65 min. er = 93:7. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.24 – 8.20 (m, 2H), 7.59 – 7.46 (m, 3H), 7.48 – 7.17 (m, 17H), 7.14 – 7.09 (m, 2H), 6.63 (s, 1H), 5.16 (s, 1H), 4.36 (d, *J* = 12.0 Hz, 1H), 3.58 (d, *J* = 12.0 Hz, 1H).

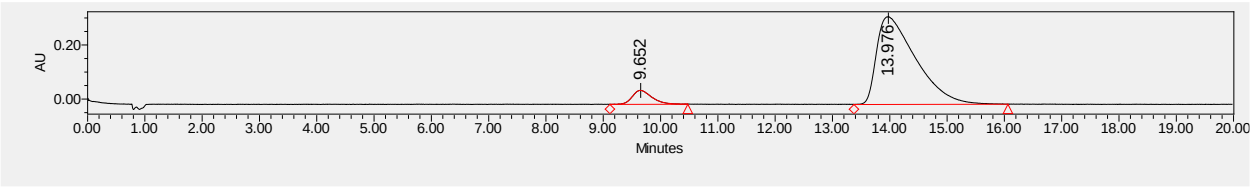
^{13}C NMR (101 MHz, $CDCl_3$) *δ* 168.1, 167.9, 152.3, 136.2, 135.1, 134.8, 134.8, 132.7, 131.7, 131.4, 130.6, 130.1, 129.0, 128.9, 128.7, 128.6, 128.5, 128.3, 128.2, 127.7, 127.6, 126.8, 121.4, 102.5, 95.3, 87.3, 64.7, 52.5, 38.6.

IR (neat): *ν* (cm^{-1}): 3417, 3030, 1770, 1667, 1486, 1083, 749, 525.

HRMS (ESI-TOF) calcd for $C_{39}H_{28}ClNO_3^+$ ([M]+Na^+) = 616.1650, 617.1683, found 616.1653, 617.1682.

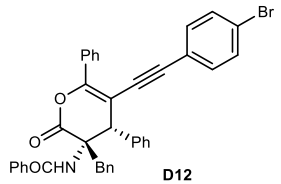


	Retention Time	Area	% Area
1	9.040	7325228	49.91
2	13.279	7351792	50.09



	Retention Time	Area	% Area
1	9.652	1236713	7.43
2	13.976	15407674	92.57

***N*-((3*S*,4*S*)-3-benzyl-5-((4-bromophenyl)ethynyl)-2-oxo-4,6-diphenyl-3,4-dihydro-2H-pyran-3-yl)benzamide (D12)**



D12

53.0 mg, 83% yield; white solid, melting point: 184.3 – 187.9 °C, $[\alpha]^{19}_{D}$ = 24.3 (*c* = 0.92, CH_2Cl_2).

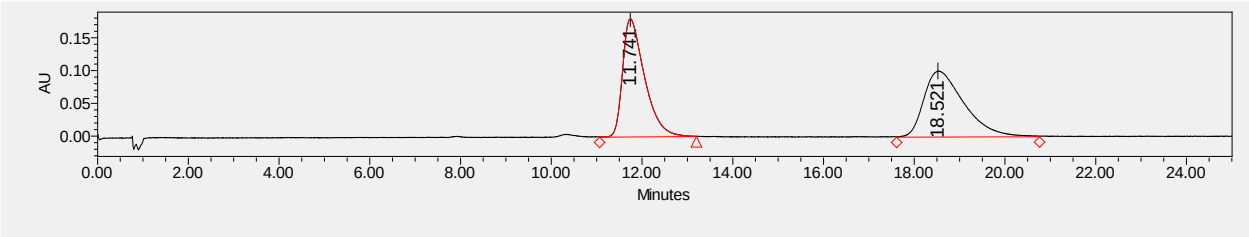
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 18.33 min, t_{minor} = 11.99 min. er = 91:9. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.23 – 8.20 (m, 2H), 7.59 – 7.46 (m, 3H), 7.47 – 7.34 (m, 5H), 7.36 – 7.27 (m, 4H), 7.28 – 7.17 (m, 8H), 7.13 – 7.09 (m, 2H), 6.63 (s, 1H), 5.15 (s, 1H), 4.36 (d, *J* = 12.0 Hz, 1H), 3.57 (d, *J* = 12.0 Hz, 1H).

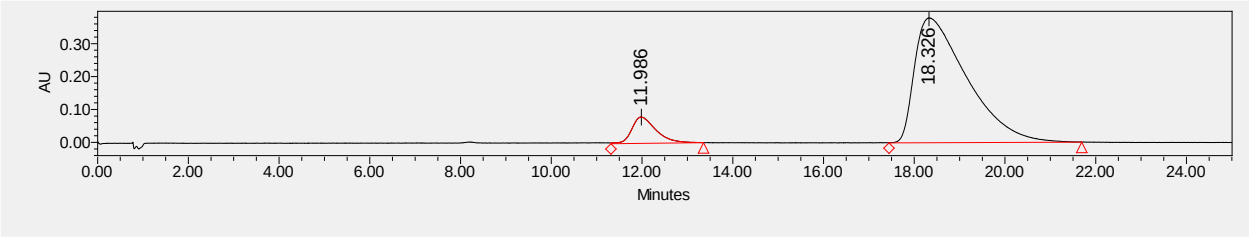
^{13}C NMR (101 MHz, $CDCl_3$) *δ* 168.1, 167.9, 152.3, 136.2, 135.1, 134.8, 132.9, 131.8, 131.7, 131.4, 130.6, 130.1, 129.0, 128.7, 128.6, 128.5, 128.3, 128.2, 127.7, 127.6, 126.8, 123.1, 121.8, 102.5, 95.4, 87.5, 64.7, 52.5, 38.6.

IR (neat): ν (cm^{-1}): 3416, 3030, 1768, 1664, 1483, 1163, 695, 523.

HRMS (ESI-TOF) calcd for $C_{39}H_{28}BrNO_3^+$ ([M]+H^+) = 638.1325, 640.1305, found 638.1323, 640.1305.

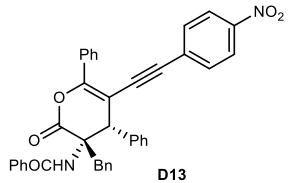


	Retention Time	Area	% Area
1	11.741	6057230	49.41
2	18.521	6201365	50.59



	Retention Time	Area	% Area
1	11.986	2973587	8.90
2	18.326	30455381	91.10

***N*-((3*S*,4*S*)-3-benzyl-5-((4-nitrophenyl)ethynyl)-2-oxo-4,6-diphenyl-3,4-dihydro-2H-pyran-3-yl)benzamide (D13)**



D13

30.8 mg, 51% yield; yellow solid, melting point: 102.9 – 106.3 °C, $[\alpha]^{19}_D$ = 11.1 (*c* = 0.41, CH_2Cl_2).

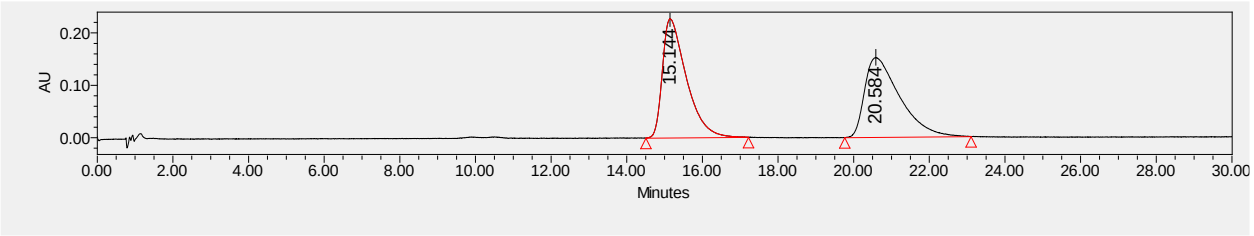
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 20.47 min, t_{minor} = 15.42 min. er = 82:18. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 – 8.13 (m, 4H), 7.61 – 7.53 (m, 3H), 7.51 – 7.18 (m, 15H), 7.15 – 7.08 (m, 2H), 6.62 (s, 1H), 5.19 (s, 1H), 4.37 (d, *J* = 16.0 Hz, 1H), 3.57 (d, *J* = 12.0 Hz, 1H).

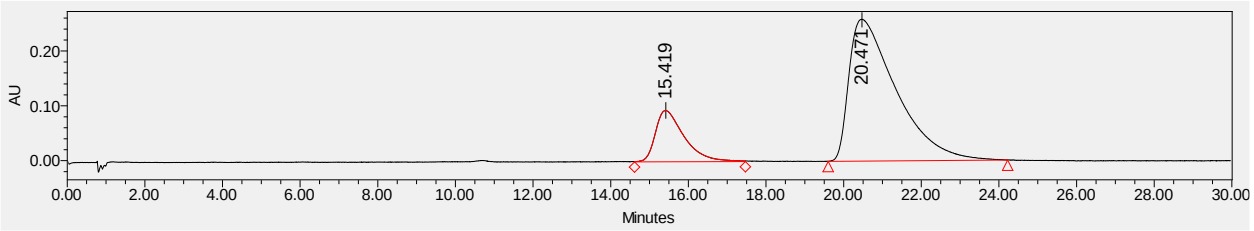
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.2, 167.7, 153.8, 147.2, 136.0, 135.0, 134.6, 132.1, 131.8, 131.2, 131.0, 130.1, 129.7, 129.1, 128.7, 128.6, 128.6, 128.5, 128.2, 127.9, 127.7, 126.8, 123.8, 101.9, 94.1, 91.7, 64.8, 52.3, 38.7.

IR (neat): ν (cm^{-1}): 3417, 2925, 1771, 1665, 1515, 1261, 696, 571.

HRMS (ESI-TOF) calcd for $C_{39}H_{28}N_2O_5^+$ ([M]+H^+) = 605.2071, found 605.2069.

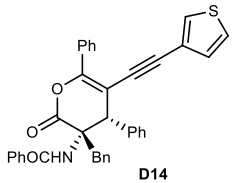


	Retention Time	Area	% Area
1	15.144	10026844	50.43
2	20.584	9857065	49.57



	Retention Time	Area	% Area
1	15.419	4815553	18.11
2	20.471	21772688	81.89

***N*-((3*S*,4*S*)-3-benzyl-2-oxo-4,6-diphenyl-5-(thiophen-3-ylethynyl)-3,4-dihydro-2H-pyran-3-yl)benzamide (D14)**



D14

45.2 mg, 80% yield; pale yellow solid, melting point: 155.9 – 159.1 °C, $[\alpha]^{18}_{D}$ = 52.7 (*c* = 0.66, CH_2Cl_2).

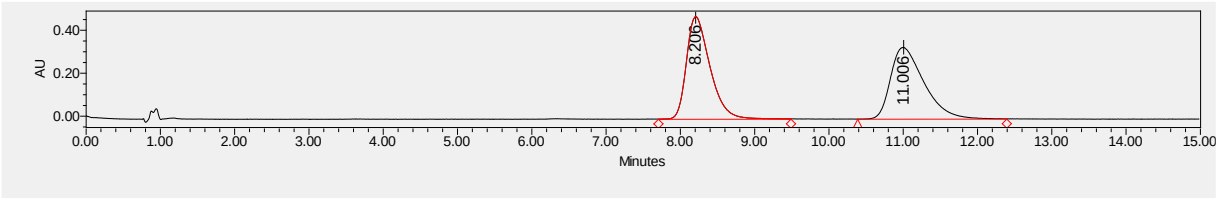
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 10.73 min, t_{minor} = 8.23 min. er = 92:8. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 – 8.21 (m, 2H), 7.58 – 7.44 (m, 3H), 7.47 – 7.27 (m, 8H), 7.28 – 7.17 (m, 7H), 7.15 – 7.02 (m, 3H), 6.62 (s, 1H), 5.15 (s, 1H), 4.35 (d, *J* = 12.0 Hz, 1H), 3.58 (d, *J* = 16.0 Hz, 1H).

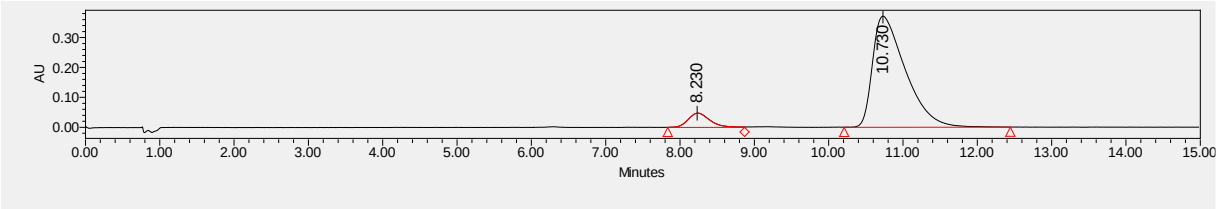
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.1, 168.0, 151.8, 136.3, 135.2, 134.9, 131.7, 131.4, 130.4, 130.1, 129.6, 129.2, 128.9, 128.7, 128.6, 128.5, 128.3, 127.6, 127.6, 126.8, 125.7, 122.0, 102.7, 91.9, 85.8, 64.8, 52.5, 38.5.

IR (neat): ν (cm^{-1}): 3416, 3030, 1771, 1665, 1512, 1166, 696, 552.

HRMS (ESI-TOF) calcd for $C_{37}H_{27}NO_3S^+$ ([M]+H^+) = 566.1784, found 566.1784.

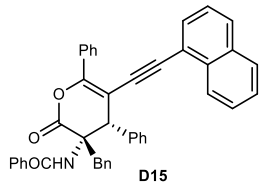


	Retention Time	Area	% Area
1	8.206	10579726	50.23
2	11.006	10481918	49.77



	Retention Time	Area	% Area
1	8.230	970843	7.83
2	10.730	11431362	92.17

***N*-((3*S*,4*S*)-3-benzyl-5-(naphthalen-1-ylethynyl)-2-oxo-4,6-diphenyl-3,4-dihydro-2H-pyran-3-yl)benzamide (D15)**



D15

51.8 mg, 85% yield; pale yellow solid, melting point: 88.5 – 91.4 °C, $[\alpha]^{19}_{D}$ = 7.7 (*c* = 0.88, CH_2Cl_2).

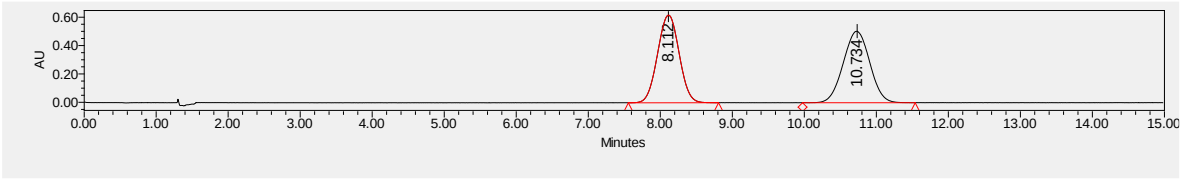
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IC-3, CO_2/IPROH = 80/20, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 10.70 min, t_{minor} = 8.13 min. er = 83:17. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 – 8.30 (m, 2H), 8.04 – 7.97 (m, 1H), 7.82 – 7.77 (m, 2H), 7.62 – 7.49 (m, 4H), 7.52 – 7.34 (m, 8H), 7.36 – 7.11 (m, 10H), 6.69 (s, 1H), 5.29 (s, 1H), 4.42 (d, *J* = 16.0 Hz, 1H), 3.66 (d, *J* = 16.0 Hz, 1H).

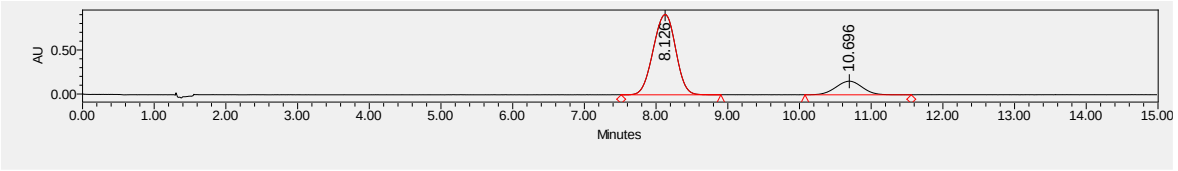
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.1, 168.0, 151.9, 136.6, 135.1, 134.8, 133.2, 133.0, 131.7, 131.6, 130.5, 130.1, 129.2, 129.0, 128.7, 128.6, 128.3, 127.9, 127.6, 126.9, 126.8, 126.6, 126.2, 125.3, 120.5, 103.1, 95.0, 91.0, 64.8, 53.1, 38.8.

IR (neat): ν (cm^{-1}): 3417, 3060, 1769, 1666, 1511, 1167, 752, 550.

HRMS (ESI-TOF) calcd for $C_{43}H_{31}NO_3^+$ ([M]+Na^+) = 632.2196, found 632.2197.

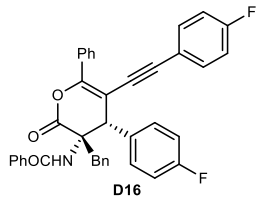


	Retention Time	Area	% Area
1	8.112	12834441	49.89
2	10.734	12890277	50.11



	Retention Time	Area	% Area
1	8.126	19770001	83.36
2	10.696	3945164	16.64

***N*-((3*S*,4*S*)-3-benzyl-4-(4-fluorophenyl)-5-((4-fluorophenyl)ethynyl)-2-oxo-6-phenyl-3,4-dihydro-2H-pyran-3-yl)benzamide (D16)**



D16

58.3 mg, 98% yield; white solid, melting point: 92.4 – 96.8 °C, $[\alpha]^{20}_{D}$ = 47.3 (*c* = 0.90, CH_2Cl_2).

Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 5.22 min, t_{minor} = 4.19 min. er = 90:10. dr >19:1.

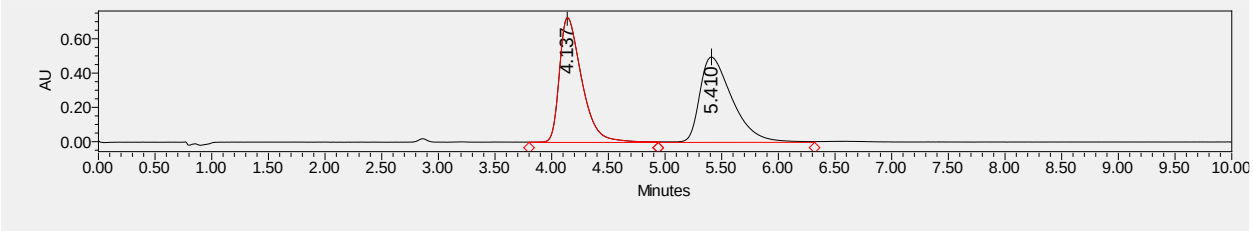
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 – 8.19 (m, 2H), 7.59 – 7.38 (m, 6H), 7.39 – 7.26 (m, 6H), 7.25 – 7.20 (m, 3H), 7.13 – 7.09 (m, 2H), 7.05 – 6.88 (m, 4H), 6.67 (s, 1H), 5.16 (s, 1H), 4.32 (d, *J* = 16.0 Hz, 1H), 3.57 (d, *J* = 12.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.0, 167.8, 164.0 (d, *J* = 250.0 Hz), 161.5 (d, *J* = 240.0 Hz), 152.0, 134.9, 134.7, 133.5, 133.4, 132.1 (d, *J* = 3.3 Hz), 131.9, 131.3, 130.6, 130.1, 130.0, 129.9, 128.8, 128.6, 128.5, 127.7, 126.7, 118.9 (d, *J* = 3.6 Hz), 115.9 (d, *J* = 22.1 Hz), 102.5, 95.6, 85.8, 64.8, 51.8, 38.6.

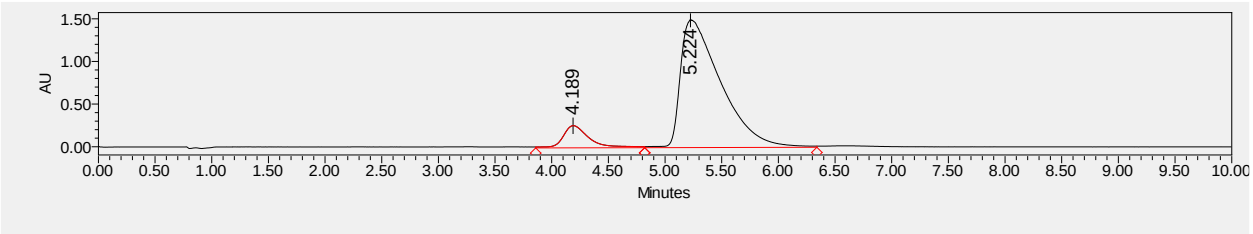
^{19}F NMR (376 MHz, $CDCl_3$) δ -109.76, -113.64.

IR (neat): ν (cm^{-1}): 3415, 2925, 1768, 1664, 1511, 1157, 694, 528.

HRMS (ESI-TOF) calcd for $C_{39}H_{27}F_2NO_3^+$ ([M]+H^+) = 596.2032, found 596.2032.

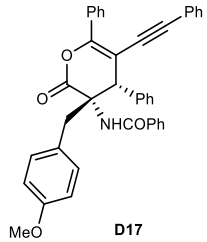


	Retention Time	Area	% Area
1	4.137	9988864	50.09
2	5.410	9952668	49.91



	Retention Time	Area	% Area
1	4.189	4154213	10.08
2	5.224	37072869	89.92

_N_-((3_S_,4_S_)-3-(4-methoxybenzyl)-2-oxo-4,6-diphenyl-5-(phenylethynyl)-3,4-dihydro-2H-pyran-3-yl)benzamide (D17)



D17

40.0 mg, 68% yield; white solid, melting point: 88.4 – 92.3 °C, $[\alpha]^{21}_D$ = 61.2 (*c* = 0.64, CH_2Cl_2).

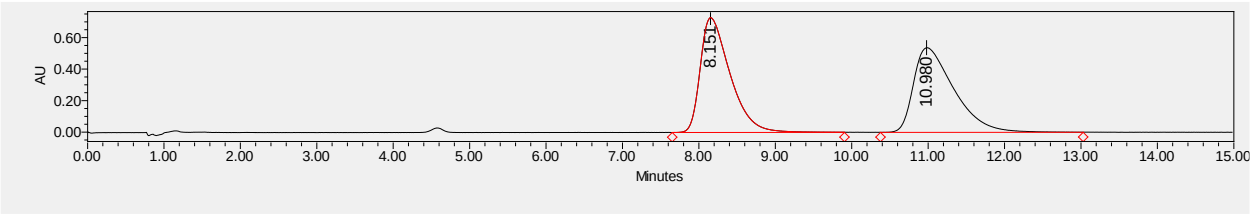
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 11.02 min, t_{minor} = 8.41 min. er = 94:6. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 – 8.22 (m, 2H), 7.59 – 7.45 (m, 3H), 7.48 – 7.26 (m, 12H), 7.28 – 7.16 (m, 3H), 7.06 – 7.01 (m, 2H), 6.79 – 6.73 (m, 2H), 6.64 (s, 1H), 5.13 (s, 1H), 4.29 (d, *J* = 12.0 Hz, 1H), 3.73 (s, 3H), 3.54 (d, *J* = 12.0 Hz, 1H).

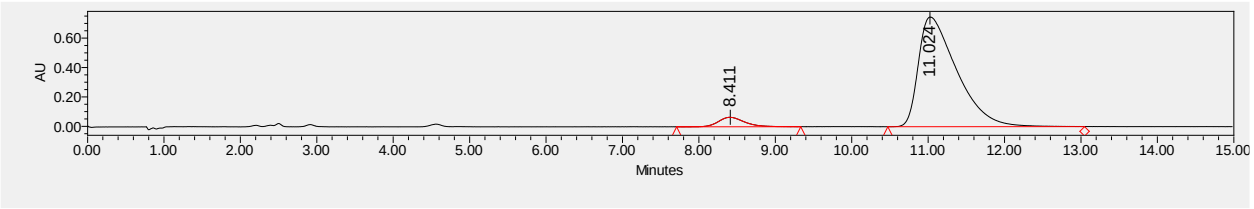
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.1, 168.0, 159.0, 151.9, 136.5, 135.2, 131.7, 131.5, 131.2, 130.4, 129.0, 128.9, 128.7, 128.7, 128.5, 128.5, 128.3, 128.2, 127.7, 126.9, 126.8, 123.0, 114.0, 102.8, 96.6, 86.4, 64.9, 55.3, 52.6, 37.8.

IR (neat): ν (cm^{-1}): 3418, 2930, 1768, 1666, 1512, 1252, 753, 527.

HRMS (ESI-TOF) calcd for $C_{40}H_{31}NO_4^+$ ([M]+H^+) = 590.2326, found 590.2328.

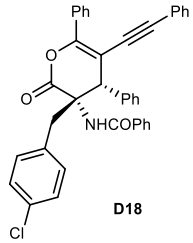


	Retention Time	Area	% Area
1	8.151	19768584	50.00
2	10.980	19768479	50.00



	Retention Time	Area	% Area
1	8.411	1547903	5.61
2	11.024	26034472	94.39

***N*-((3*S*,4*S*)-3-(4-chlorobenzyl)-2-oxo-4,6-diphenyl-5-(phenylethynyl)-3,4-dihydro-2H-pyran-3-yl)benzamide (D18)**



D18

50.5 mg, 85% yield; white solid, melting point: 99.2 – 102.9 °C, $[\alpha]^{20}_{D}$ = 63.2 (*c* = 0.88, CH_2Cl_2).

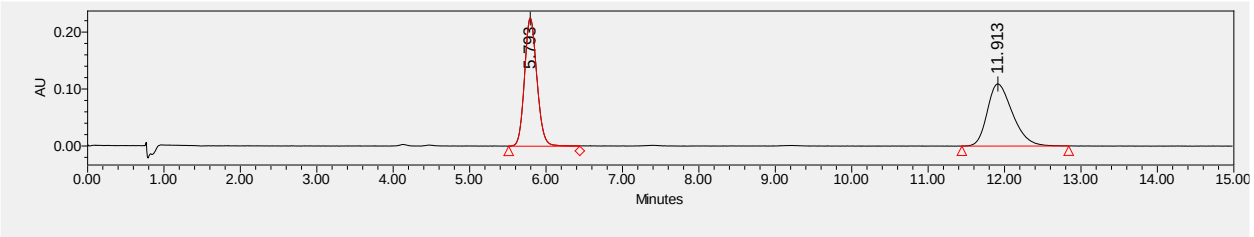
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/IPROH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 12.27 min, t_{minor} = 5.97 min. er = 91:9. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 – 8.22 (m, 2H), 7.59 – 7.46 (m, 3H), 7.49 – 7.15 (m, 17H), 7.07 – 7.02 (m, 2H), 6.62 (s, 1H), 5.14 (s, 1H), 4.35 (d, *J* = 16.0 Hz, 1H), 3.56 (d, *J* = 16.0 Hz, 1H).

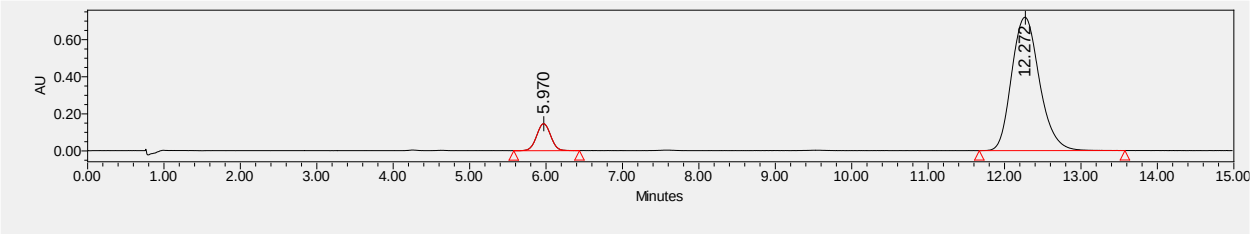
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.1, 167.9, 151.8, 136.2, 134.9, 133.6, 133.3, 131.9, 131.5, 131.4, 131.3, 130.5, 129.0, 128.8, 128.8, 128.5, 128.4, 128.2, 127.7, 126.7, 122.8, 102.7, 96.8, 86.2, 64.6, 52.6, 38.0.

IR (neat): ν (cm^{-1}): 3415, 3061, 1767, 1665, 1486, 1162, 691, 528.

HRMS (ESI-TOF) calcd for $C_{39}H_{28}ClNO_3^+$ ([M]+Na^+) = 616.1650, 617.1683, found 616.1658, 617.1694.

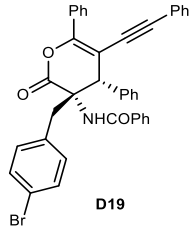


	Retention Time	Area	% Area
1	5.793	2530728	50.28
2	11.913	2502913	49.72



	Retention Time	Area	% Area
1	5.970	1856190	9.27
2	12.272	18169076	90.73

***N*-((3*S*,4*S*)-3-(4-bromobenzyl)-2-oxo-4,6-diphenyl-5-(phenylethynyl)-3,4-dihydro-2H-pyran-3-yl)benzamide (D19)**



D19

58.7 mg, 92% yield; pale yellow solid, melting point: 102.3 – 105.7 °C, $[\alpha]^{20}_D$ = 61.1 (*c* = 0.93, CH_2Cl_2).

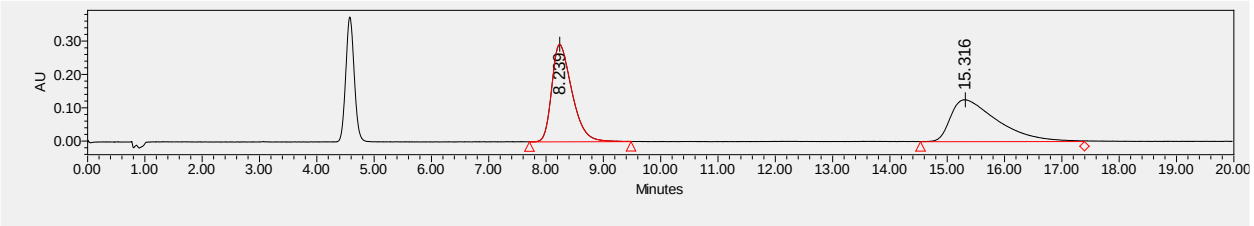
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 14.72 min, t_{minor} = 8.37 min. er = 89:11. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 – 8.20 (m, 2H), 7.59 – 7.45 (m, 3H), 7.49 – 7.25 (m, 14H), 7.26 – 7.16 (m, 3H), 7.01 – 6.96 (m, 2H), 6.62 (s, 1H), 5.14 (s, 1H), 4.34 (d, *J* = 12.0 Hz, 1H), 3.54 (d, *J* = 12.0 Hz, 1H).

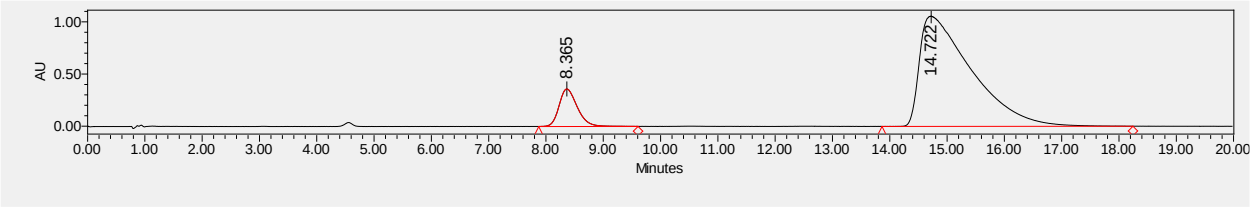
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.1, 167.8, 151.8, 136.1, 134.9, 133.9, 131.9, 131.8, 131.7, 131.5, 131.3, 130.5, 129.0, 128.8, 128.8, 128.5, 128.4, 128.2, 127.7, 126.7, 122.8, 121.8, 102.7, 96.8, 86.2, 64.5, 52.6, 38.1.

IR (neat): ν (cm^{-1}): 3416, 3061, 1767, 1665, 1486, 1163, 692, 527.

HRMS (ESI-TOF) calcd for $C_{39}H_{28}BrNO_3^+$ ([M]+H^+) = 638.1325, 640.1305, found 638.1321, 640.1307.

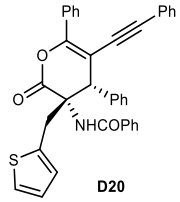


	Retention Time	Area	% Area
1	8.239	7154132	49.98
2	15.316	7158787	50.02



	Retention Time	Area	% Area
1	8.365	7946904	10.66
2	14.722	66621256	89.34

***N*-((3*S*,4*S*)-2-oxo-4,6-diphenyl-5-(phenylethynyl)-3-(thiophen-2-ylmethyl)-3,4-dihydro-2H-pyran-3-yl)benzamide (D20)**



D20

45.2 mg, 80% yield; pale yellow solid, melting point: 97.4 – 100.5 °C, $[\alpha]^{20}_{D}$ = 71.4 (*c* = 0.75, CH_2Cl_2).

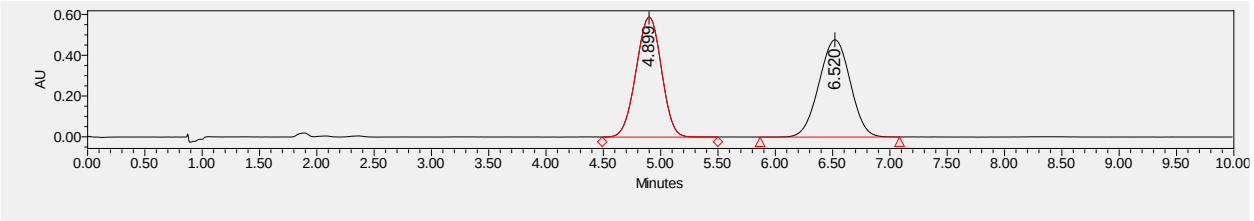
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IC-3, CO_2/IPROH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 4.93 min, t_{minor} = 6.57 min. er = 89:11. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 – 8.20 (m, 2H), 7.58 – 7.40 (m, 6H), 7.40 – 7.17 (m, 12H), 7.17 – 7.11 (m, 1H), 6.91 – 6.88 (m, 1H), 6.83 – 6.80 (m, 2H), 5.12 (s, 1H), 4.63 (d, *J* = 16.0 Hz, 1H), 3.85 (d, *J* = 12.0 Hz, 1H).

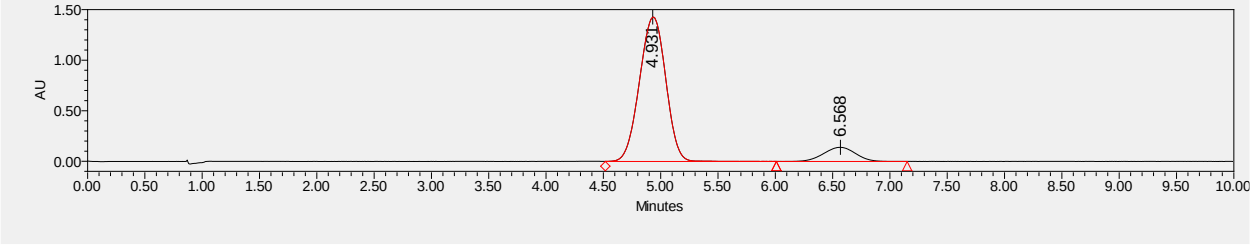
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.0, 167.6, 152.1, 136.1, 135.0, 131.8, 131.5, 131.4, 130.4, 129.0, 128.8, 128.7, 128.5, 128.5, 128.3, 128.3, 127.7, 127.0, 126.9, 125.6, 122.9, 102.4, 96.6, 86.2, 64.8, 52.2, 32.8.

IR (neat): ν (cm^{-1}): 3417, 3062, 1767, 1666, 1485, 1145, 692, 527.

HRMS (ESI-TOF) calcd for $C_{37}H_{27}SNO_3^+$ ([M]+H^+) = 566.1784, found 566.1788.

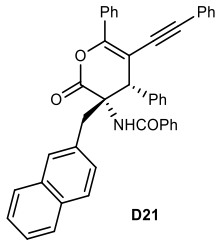


	Retention Time	Area	% Area
1	4.899	9038233	49.99
2	6.520	9040820	50.01



	Retention Time	Area	% Area
1	4.931	22713108	89.37
2	6.568	2700279	10.63

***N*-((3*S*,4*S*)-3-(naphthalen-2-ylmethyl)-2-oxo-4,6-diphenyl-5-(phenylethynyl)-3,4-dihydro-2H-pyran-3-yl)benzamide (D21)**



D21

43.3 mg, 71% yield; pale yellow solid, melting point: 95.1 – 97.2 °C, $[\alpha]^{20}_{D}$ = 64.7 (*c* = 0.78, CH_2Cl_2).

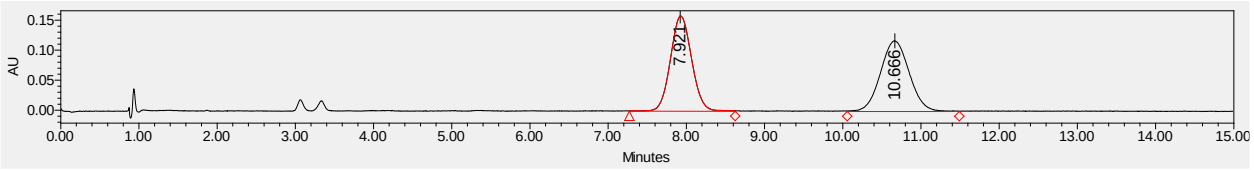
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IC-3, CO_2/IPROH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 8.03 min, t_{minor} = 10.81 min. er = 79:21. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.32 – 8.26 (m, 2H), 7.80 – 7.62 (m, 3H), 7.61 – 7.48 (m, 4H), 7.46 – 7.26 (m, 14H), 7.28 – 7.17 (m, 4H), 6.64 (s, 1H), 5.22 (s, 1H), 4.52 (d, *J* = 12.0 Hz, 1H), 3.76 (d, *J* = 16.0 Hz, 1H).

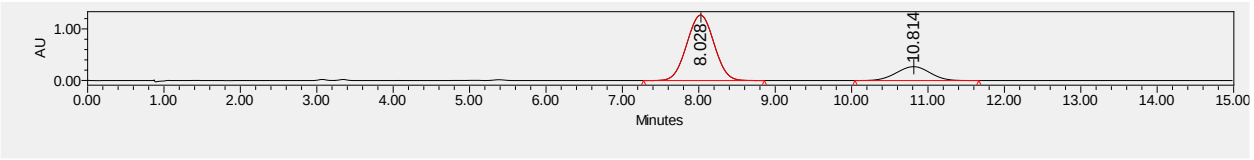
^{13}C NMR (101 MHz, $CDCl_3$) *δ* 168.3, 168.0, 151.9, 136.4, 135.2, 133.4, 132.8, 132.4, 131.7, 131.5, 131.5, 130.5, 129.3, 129.0, 128.8, 128.7, 128.5, 128.3, 128.2, 128.0, 127.9, 127.8, 127.8, 126.8, 126.2, 126.0, 123.0, 102.8, 96.7, 86.4, 64.8, 52.7, 38.8.

IR (neat): *ν* (cm^{-1}): 3415, 3058, 1767, 1665, 1511, 1167, 692, 531.

HRMS (ESI-TOF) calcd for $C_{43}H_{31}NO_3^+$ ([M]+H^+) = 610.2377, found 610.2375.

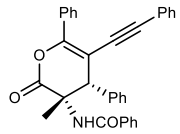


	Retention Time	Area	% Area
1	7.921	2998018	49.89
2	10.666	3011120	50.11



	Retention Time	Area	% Area
1	8.028	31468123	79.19
2	10.814	8271116	20.81

***N*-((3*S*,4*S*)-3-methyl-2-oxo-4,6-diphenyl-5-(phenylethynyl)-3,4-dihydro-2H-pyran-3-yl)benzamide (D22)**



D22

33.3 mg, 69% yield; white solid, melting point: 72.9 – 75.3 °C, $[\alpha]^{19}_{D}$ = -67.0 (*c* = 0.61, CH_2Cl_2).

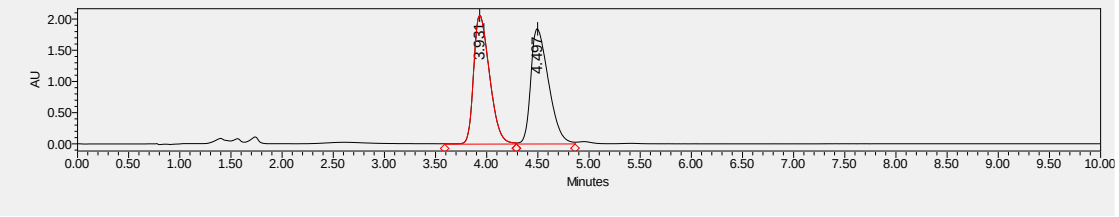
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 4.03 min, t_{minor} = 4.62 min. er = 70:30. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 – 8.14 (m, 2H), 7.54 – 7.41 (m, 6H), 7.40 – 7.29 (m, 4H), 7.33 – 7.16 (m, 8H), 6.99 (s, 1H), 4.99 (s, 1H), 2.15 (s, 3H).

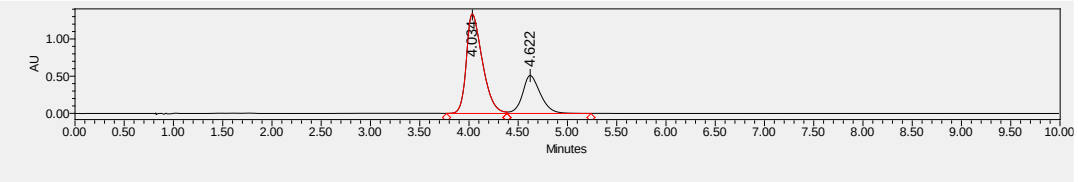
^{13}C NMR (101 MHz, $CDCl_3$) δ 170.2, 167.4, 152.0, 136.5, 134.9, 131.7, 131.5, 131.4, 130.3, 129.0, 128.7, 128.7, 128.5, 128.4, 128.2, 128.0, 127.7, 126.9, 122.9, 102.8, 96.5, 86.3, 59.4, 52.3, 22.1.

IR (neat): ν (cm^{-1}): 3419, 3061, 1767, 1666, 1513, 1093, 692, 529.

HRMS (ESI-TOF) calcd for $C_{33}H_{25}NO_3^+$ ([M]+H^+) = 484.1907, found 484.1911.

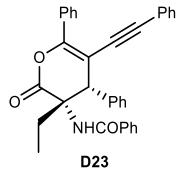


	Retention Time	Area	% Area
1	3.931	22301486	49.93
2	4.497	22364139	50.07



	Retention Time	Area	% Area
1	4.034	15136522	70.06
2	4.622	6468650	29.94

_N_-((3_S_,4_S_)-3-ethyl-2-oxo-4,6-diphenyl-5-(phenylethynyl)-3,4-dihydro-2H-pyran-3-yl)benzamide (D23)



D23

31.8 mg, 64% yield; pale yellow solid, melting point: 67.9 – 70.3 °C, $[\alpha]^{21}_D$ = 54.7 (*c* = 0.51, CH_2Cl_2).

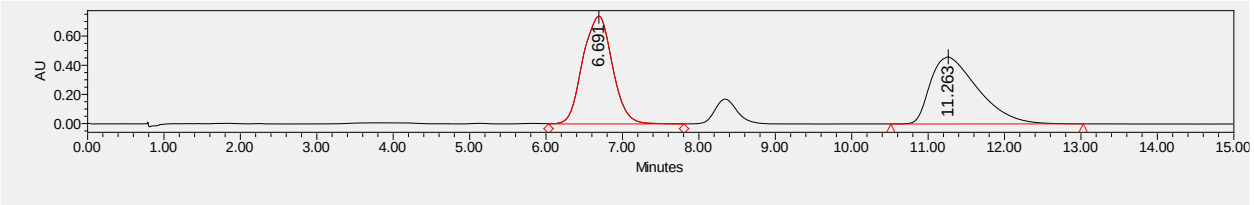
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/IPROH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 11.95 min, t_{minor} = 7.11 min. er = 69:31. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 – 8.13 (m, 2H), 7.54 – 7.41 (m, 6H), 7.40 – 7.16 (m, 12H), 6.85 (s, 1H), 4.97 (s, 1H), 3.15 – 3.02 (m, 1H), 2.41 – 2.27 (m, 1H), 0.97 (t, *J* = 4.0 Hz, 3H).

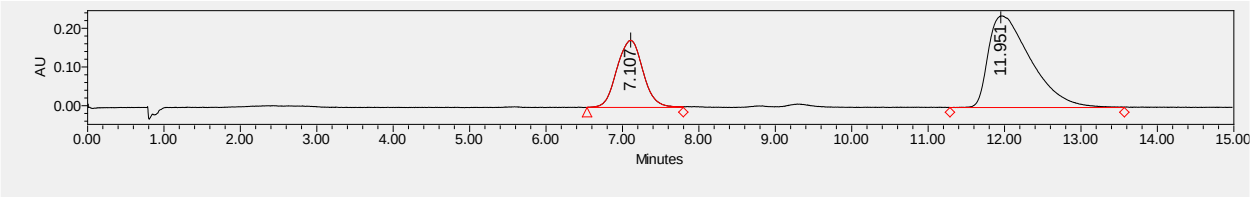
^{13}C NMR (101 MHz, $CDCl_3$) δ 169.0, 167.4, 151.9, 136.8, 134.9, 131.7, 131.5, 130.3, 128.9, 128.7, 128.7, 128.5, 128.4, 128.2, 127.7, 126.8, 123.0, 102.7, 96.3, 86.4, 64.0, 52.6, 26.3, 8.9.

IR (neat): ν (cm^{-1}): 3420, 2932, 1762, 1666, 1485, 1095, 692, 528.

HRMS (ESI-TOF) calcd for $C_{34}H_{27}NO_3^+$ ([M]+H^+) = 498.2064, found 498.2064.

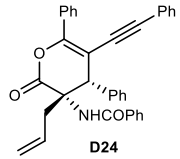


	Retention Time	Area	% Area
1	6.691	19955672	50.17
2	11.263	19820169	49.83



	Retention Time	Area	% Area
1	7.107	4112459	30.99
2	11.951	9156188	69.01

***N*-((3*S*,4*S*)-3-allyl-2-oxo-4,6-diphenyl-5-(phenylethynyl)-3,4-dihydro-2H-pyran-3-yl)benzamide (D24)**



D24

29.0 mg, 57% yield; pale yellow solid, melting point: 134.2 – 138.5 °C, $[\alpha]^{21}_{D}$ = 76.5 (*c* = 0.51, CH_2Cl_2).

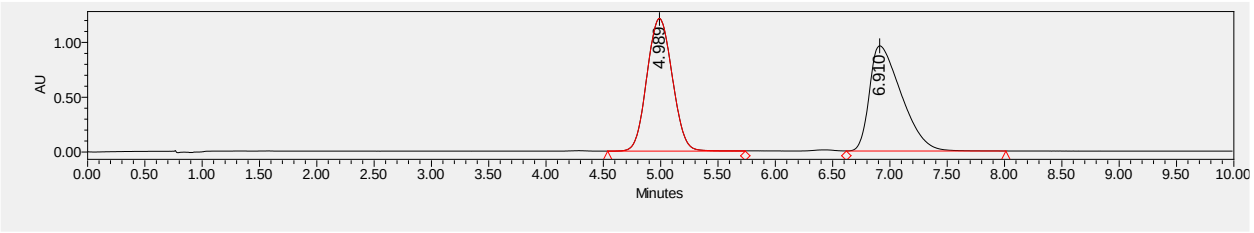
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 7.05 min, t_{minor} = 4.98 min. er = 79:21. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 – 8.14 (m, 2H), 7.55 – 7.40 (m, 6H), 7.40 – 7.16 (m, 12H), 6.86 (s, 1H), 5.82 – 5.67 (m, 1H), 5.23 – 5.12 (m, 2H), 5.01 (s, 1H), 3.91 – 3.82 (m, 1H), 3.04 – 2.94 (m, 1H).

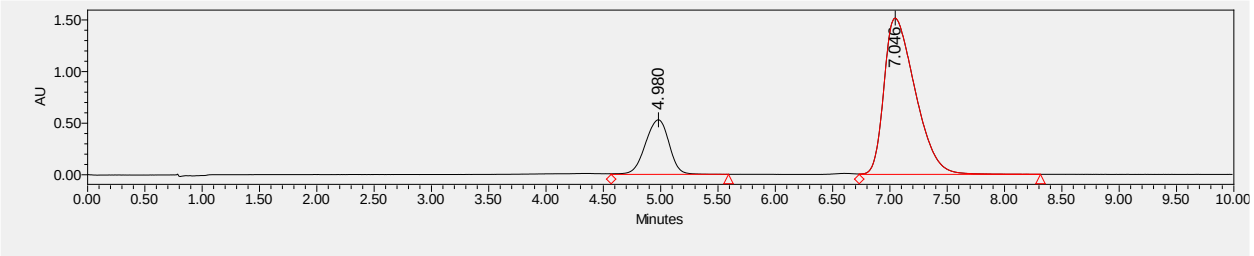
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.4, 167.5, 152.0, 136.3, 134.9, 131.7, 131.5, 131.4, 131.1, 130.3, 129.0, 128.7, 128.5, 128.4, 128.3, 128.2, 127.7, 126.8, 122.9, 120.6, 102.6, 96.5, 86.3, 63.5, 52.3, 37.3.

IR (neat): ν (cm^{-1}): 3418, 3062, 1762, 1666, 1485, 1145, 692, 530.

HRMS (ESI-TOF) calcd for $C_{35}H_{27}NO_3^+$ ([M]+H^+) = 510.2064, found 510.2067.

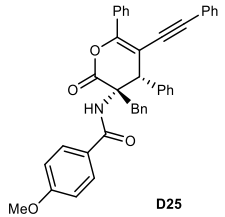


	Retention Time	Area	% Area
1	4.989	18616533	50.06
2	6.910	18569888	49.94



	Retention Time	Area	% Area
1	4.980	7617998	21.05
2	7.046	28567167	78.95

***N*-((3*S*,4*S*)-3-benzyl-2-oxo-4,6-diphenyl-5-(phenylethynyl)-3,4-dihydro-2H-pyran-3-yl)-4-methoxybenzamide (D25)**



D25

53.0 mg, 90% yield; white solid, melting point: 88.4 – 90.2 °C, $[\alpha]^{20}_{D}$ = 42.8 (*c* = 0.86, CH_2Cl_2).

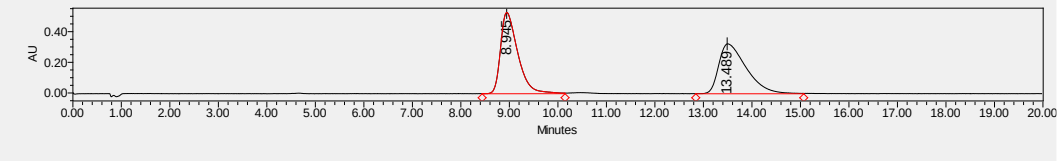
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 13.26 min, t_{minor} = 9.10 min. er = 94:6. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.28 – 8.23 (m, 2H), 7.59 – 7.45 (m, 3H), 7.43 – 7.25 (m, 9H), 7.27 – 7.16 (m, 6H), 7.13 – 7.09 (m, 2H), 6.84 – 6.78 (m, 2H), 6.57 (s, 1H), 5.16 (s, 1H), 4.36 (d, *J* = 12.0 Hz, 1H), 3.79 (s, 3H), 3.57 (d, *J* = 12.0 Hz, 1H).

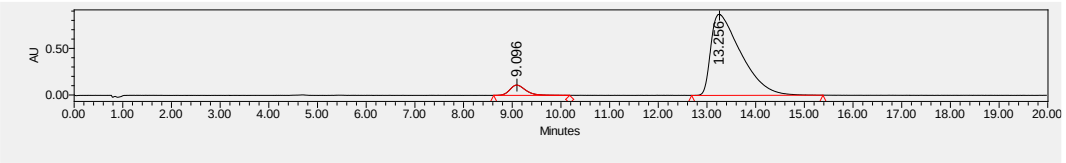
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.1, 167.4, 162.4, 151.9, 136.4, 135.0, 131.5, 130.4, 130.1, 128.9, 128.7, 128.6, 128.5, 128.5, 128.5, 128.3, 128.2, 127.7, 127.5, 127.4, 122.9, 113.9, 102.8, 96.6, 86.4, 64.7, 55.5, 52.6, 38.6.

IR (neat): ν (cm^{-1}): 3422, 3031, 1767, 1660, 1485, 1254, 763, 527.

HRMS (ESI-TOF) calcd for $C_{40}H_{31}NO_4^+$ ([M]+H^+) = 590.2326, found 590.2328.

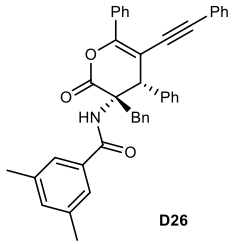


	Retention Time	Area	% Area
1	8.945	13103249	50.52
2	13.489	12831757	49.48



	Retention Time	Area	% Area
1	9.096	2559778	6.41
2	13.256	37400261	93.59

***N*-((3*S*,4*S*)-3-benzyl-2-oxo-4,6-diphenyl-5-(phenylethynyl)-3,4-dihydro-2H-pyran-3-yl)-3,5-dimethylbenzamide (D26)**



D26

35.2 mg, 60% yield; white solid, melting point: 162.4 – 166.5 °C, $[\alpha]^{20}_D$ = 45.4 (*c* = 0.54, CH_2Cl_2).

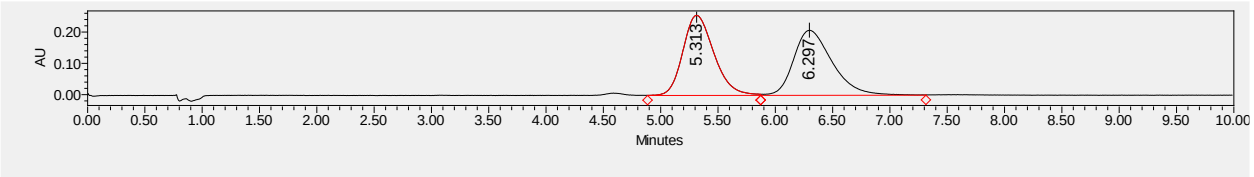
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 6.23 min, t_{minor} = 5.37 min. er = 88:12. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 – 8.23 (m, 2H), 7.59 – 7.45 (m, 3H), 7.40 – 7.16 (m, 13H), 7.14 – 7.11 (m, 2H), 7.06 – 7.04 (m, 1H), 6.98 – 6.93 (m, 2H), 6.60 (s, 1H), 5.15 (s, 1H), 4.36 (d, *J* = 16.0 Hz, 1H), 3.57 (d, *J* = 12.0 Hz, 1H), 2.26 (s, 6H).

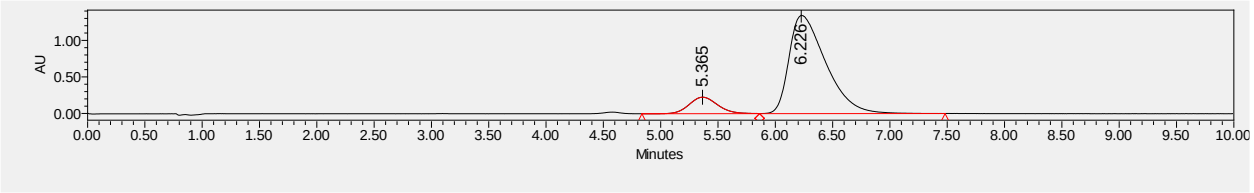
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.4, 168.1, 151.9, 138.4, 136.4, 135.2, 134.9, 133.3, 131.5, 130.4, 130.2, 129.0, 128.7, 128.6, 128.5, 128.5, 128.3, 128.2, 127.7, 127.6, 124.5, 123.0, 102.9, 96.6, 86.4, 64.7, 52.7, 38.6, 21.3.

IR (neat): ν (cm^{-1}): 3421, 2923, 1769, 1664, 1496, 1166, 763, 553.

HRMS (ESI-TOF) calcd for $C_{41}H_{33}NO_3^+$ ([M]+H^+) = 588.2533, found 588.2535.

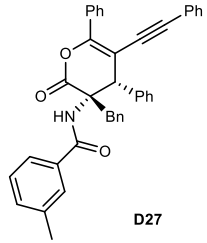


	Retention Time	Area	% Area
1	5.313	4809008	49.74
2	6.297	4860157	50.26



	Retention Time	Area	% Area
1	5.365	3921881	11.60
2	6.226	29882859	88.40

***N*-((3*S*,4*S*)-3-benzyl-2-oxo-4,6-diphenyl-5-(phenylethynyl)-3,4-dihydro-2H-pyran-3-yl)-3-methylbenzamide (D27)**



D27

35.0 mg, 61% yield; pale pink solid, melting point: 131.8 – 134.9 °C, $[\alpha]^{19}_{D}$ = 47.9 (*c* = 0.56, CH_2Cl_2).

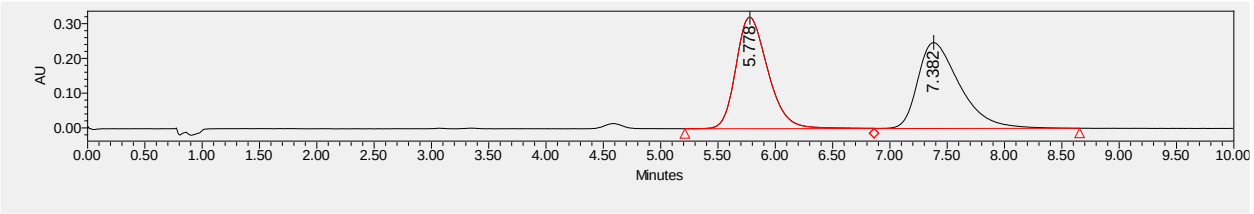
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 7.34 min, t_{minor} = 5.89 min. er = 92:8. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 – 8.24 (m, 2H), 7.59 – 7.45 (m, 3H), 7.41 – 7.15 (m, 16H), 7.15 – 7.10 (m, 3H), 6.62 (s, 1H), 5.16 (s, 1H), 4.36 (d, *J* = 16.0 Hz, 1H), 3.58 (d, *J* = 12.0 Hz, 1H), 2.32 (s, 3H).

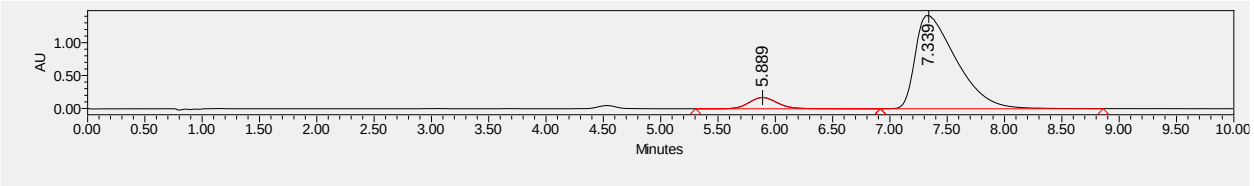
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.3, 168.0, 151.9, 138.6, 136.4, 135.1, 134.9, 132.5, 131.5, 131.5, 130.4, 130.1, 129.0, 128.7, 128.6, 128.5, 128.5, 128.3, 128.2, 127.7, 127.6, 127.4, 123.8, 122.9, 102.8, 96.6, 86.3, 64.7, 52.6, 38.6, 21.4.

IR (neat): ν (cm^{-1}): 3419, 3031, 1768, 1665, 1506, 1165, 751, 526.

HRMS (ESI-TOF) calcd for $C_{40}H_{31}NO_3^+$ ([M]+H^+) = 574.2377, found 574.2376.

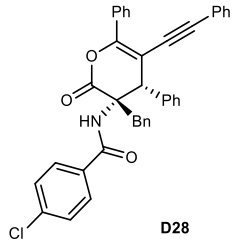


	Retention Time	Area	% Area
1	5.778	6227542	49.75
2	7.382	6289379	50.25



	Retention Time	Area	% Area
1	5.889	3001894	7.81
2	7.339	35410614	92.19

***N*-((3*S*,4*S*)-3-benzyl-2-oxo-4,6-diphenyl-5-(phenylethynyl)-3,4-dihydro-2H-pyran-3-yl)-4-chlorobenzamide (D28)**



D28

51.1 mg, 86% yield; pale yellow solid, melting point: 100.3 – 102.9 °C, $[\alpha]^{19}_{D}$ = 33.8 (*c* = 0.79, CH_2Cl_2).

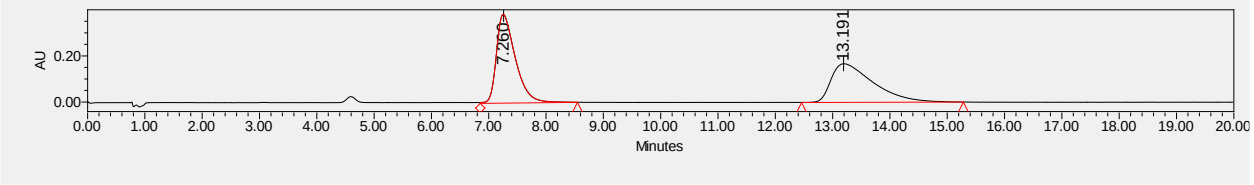
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 12.70 min, t_{minor} = 7.39 min. er = 91:9. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 – 8.23 (m, 2H), 7.59 – 7.45 (m, 3H), 7.40 – 7.18 (m, 17H), 7.11 – 7.08 (m, 2H), 6.59 (s, 1H), 5.13 (s, 1H), 4.32 (d, *J* = 16.0 Hz, 1H), 3.59 (d, *J* = 16.0 Hz, 1H).

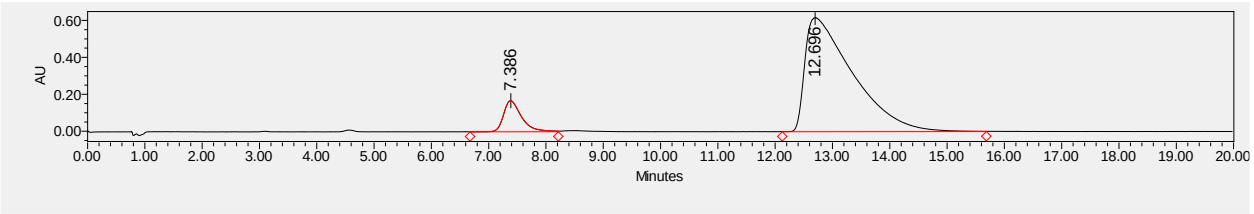
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.0, 166.9, 151.9, 138.0, 136.3, 134.7, 133.4, 131.5, 131.4, 130.5, 130.1, 129.0, 128.8, 128.6, 128.5, 128.3, 128.2, 127.7, 127.7, 122.9, 102.7, 96.7, 86.2, 64.8, 52.7, 38.6.

IR (neat): ν (cm^{-1}): 3412, 3030, 1768, 1667, 1481, 1167, 751, 529.

HRMS (ESI-TOF) calcd for $C_{39}H_{28}ClNO_3^+$ ([M]+H^+) = 594.1830, 595.1864, found 594.1835, 595.1866.

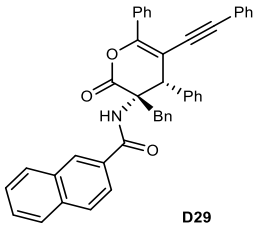


	Retention Time	Area	% Area
1	7.260	8823029	50.65
2	13.191	8597080	49.35



	Retention Time	Area	% Area
1	7.386	3697892	9.36
2	12.696	35808717	90.64

_N_-((3_S_,4_S_)-3-benzyl-2-oxo-4,6-diphenyl-5-(phenylethynyl)-3,4-dihydro-2H-pyran-3-yl)-2-naphthamide (D29)



D29

28.0 mg, 46% yield; white solid, melting point: 231.2 – 235.6 °C, $[\alpha]^{19}_{D}$ = 30.4 (*c* = 0.90, CH_2Cl_2).

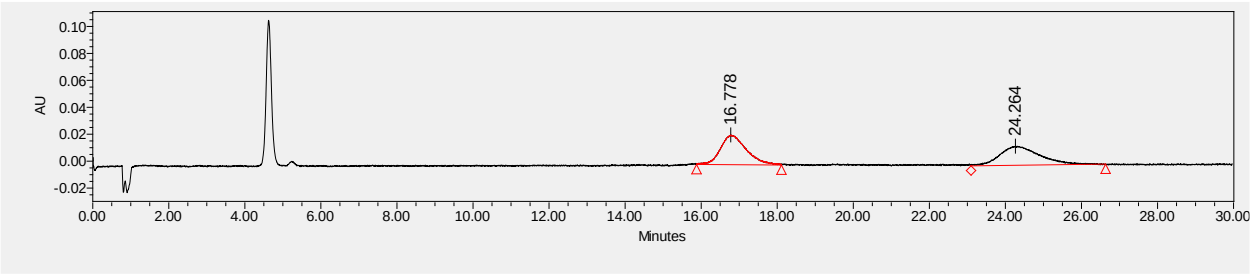
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 23.11 min, t_{minor} = 16.84 min. er = 96:4. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 – 8.25 (m, 2H), 7.87 – 7.76 (m, 4H), 7.60 – 7.45 (m, 6H), 7.42 – 7.11 (m, 15H), 6.80 (s, 1H), 5.21 (s, 1H), 4.42 (d, *J* = 12.0 Hz, 1H), 3.62 (d, *J* = 12.0 Hz, 1H).

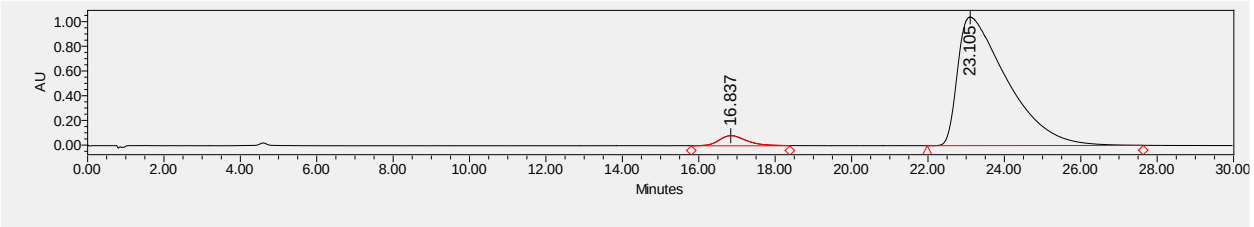
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.1, 168.0, 151.9, 136.4, 134.9, 132.6, 132.2, 131.5, 131.5, 130.4, 130.2, 129.0, 129.0, 128.8, 128.7, 128.6, 128.5, 128.3, 128.3, 127.8, 127.8, 127.6, 127.3, 126.9, 123.4, 122.9, 102.8, 96.7, 86.4, 64.9, 52.7, 38.7.

IR (neat): ν (cm^{-1}): 3416, 3060, 1768, 1664, 1496, 1166, 759, 529.

HRMS (ESI-TOF) calcd for $C_{43}H_{31}NO_3^+$ ([M]+H^+) = 610.2377, found 610.2379.

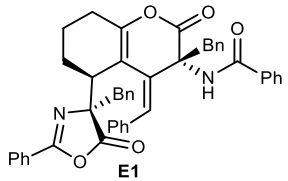


	Retention Time	Area	% Area
1	16.778	1039152	50.11
2	24.264	1034592	49.89



	Retention Time	Area	% Area
1	16.837	4148403	4.25
2	23.105	93520130	95.75

***N*-((3*R*,5*S*)-3-benzyl-5-((*S*)-4-benzyl-5-oxo-2-phenyl-4,5-dihydrooxazol-4-yl)-4-((*E*)-benzylidene)-2-oxo-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)benzamide (E1)**



E1

69.2 mg, 99% yield; pale yellow solid, melting point: 131.6 – 133.9 °C, $[\alpha]^{23}_{D}$ = -232.2 (*c* = 1.09, CH_2Cl_2).

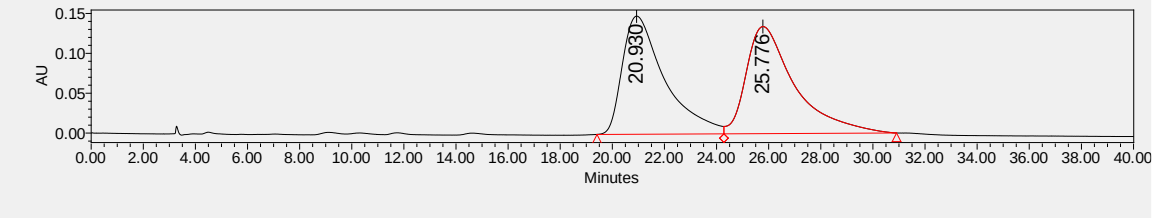
Dissolved in *i*PrOH for HPLC; HPLC (Chiralcel IC, hexane/*i*PrOH = 95/5, flow rate 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 26.04 min, t_{minor} = 21.17 min. er >99:1. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.08 – 7.57 (m, 4H), 7.52 – 7.11 (m, 17H), 7.05 – 6.57 (m, 6H), 4.71 – 4.36 (m, 1H), 3.75 – 3.46 (m, 1H), 3.29 – 3.19 (m, 1H), 3.07 – 2.92 (m, 1H), 2.71 – 2.40 (m, 2H), 2.07 – 1.79 (m, 3H), 1.66 – 1.47 (m, 1H), 1.32 – 1.20 (m, 1H).

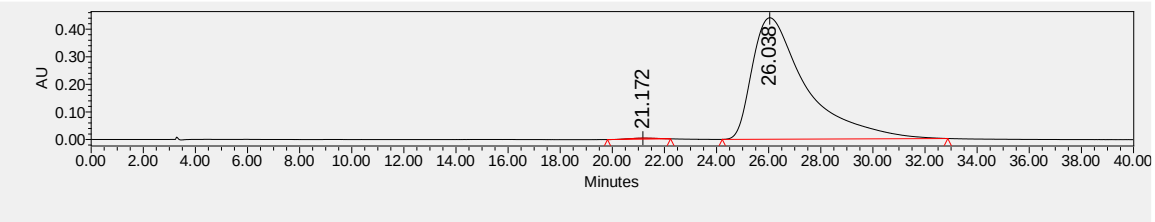
13C NMR (101 MHz, $CDCl_3$) *δ* 178.6, 167.2, 159.7, 152.0, 137.4, 135.8, 133.8, 132.5, 131.9, 130.4, 130.1, 129.1, 128.7, 128.6, 128.4, 127.9, 127.7, 127.1, 127.0, 125.5, 67.7, 42.4, 39.2, 36.0, 29.7, 25.3, 23.5, 17.3.

IR (neat): ν (cm^{-1}): 3409, 2925, 1761, 1655, 1481, 1137, 968, 779.

HRMS (ESI-TOF) calcd for $C_{46}H_{38}N_2O_5^+$ ([M]+H^+) = 699.2853, found 699.2853.

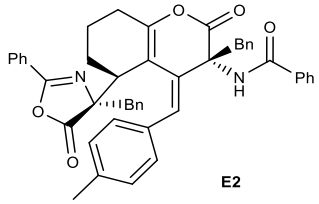


	Retention Time	Area	% Area
1	20.930	16721621	49.01
2	25.776	17399757	50.99



	Retention Time	Area	% Area
1	21.172	277579	0.44
2	26.038	63041412	99.56

***N*-((3*R*,5*S*)-3-benzyl-5-((*S*)-4-benzyl-5-oxo-2-phenyl-4,5-dihydrooxazol-4-yl)-4-((*E*)-4-methylbenzylidene)-2-oxo-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)benzamide (E2)**



E2

70.5 mg, 99% yield; pale yellow solid, melting point: 137.2 – 139.4 °C, $[\alpha]^{22}_D$ = -263.4 (*c* = 1.10, CH_2Cl_2).

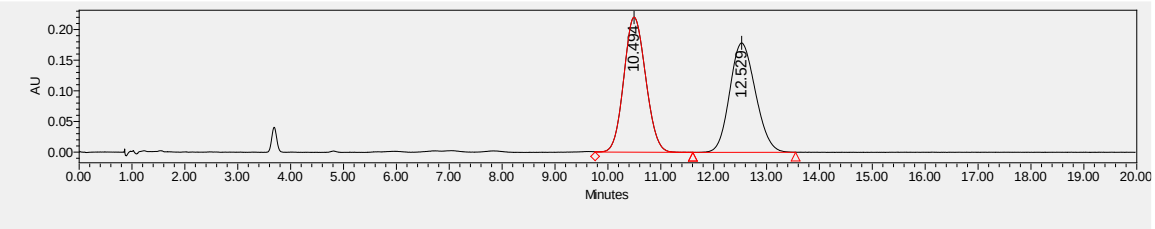
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IC-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 10.23 min, t_{minor} = 12.57 min. er = 99:1. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 – 7.61 (m, 4H), 7.56 – 7.39 (m, 4H), 7.36 – 7.10 (m, 12H), 7.06 – 6.96 (m, 5H), 6.90 – 6.73 (s, 1H), 4.63 – 4.39 (m, 1H), 3.76 – 3.50 (m, 1H), 3.38 – 3.25 (m, 1H), 3.06 – 2.91 (m, 1H), 2.66 – 2.47 (m, 2H), 2.38 (s, 3H), 2.11 – 1.81 (m, 3H), 1.64 – 1.49 (m, 1H), 1.29 – 1.24 (m, 1H).

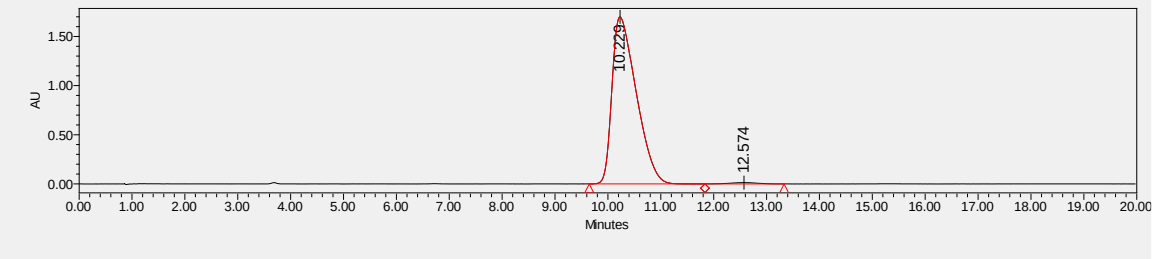
^{13}C NMR (101 MHz, $CDCl_3$) δ 178.7, 167.2, 159.8, 151.9, 137.9, 133.9, 132.5, 131.9, 130.5, 130.2, 129.3, 129.2, 128.8, 128.7, 128.5, 128.0, 127.8, 127.2, 127.2, 125.6, 67.8, 42.6, 39.2, 35.9, 29.8, 25.3, 23.7, 21.5, 17.5.

IR (neat): ν (cm^{-1}): 3410, 2924, 1761, 1657, 1481, 1137, 970, 749.

HRMS (ESI-TOF) calcd for $C_{47}H_{40}N_2O_5^+$ ([M]+H^+) = 713.3010, found 713.3010.

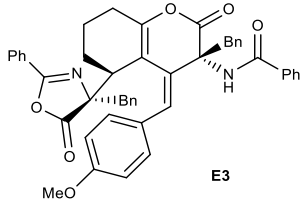


	Retention Time	Area	% Area
1	10.494	6319737	51.14
2	12.529	6037940	48.86



	Retention Time	Area	% Area
1	10.229	54076108	99.12
2	12.574	482206	0.88

***N*-((3*R*,5*S*)-3-benzyl-5-((*S*)-4-benzyl-5-oxo-2-phenyl-4,5-dihydrooxazol-4-yl)-4-((*E*)-4-methoxybenzylidene)-2-oxo-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)benzamide (E3)**



E3

72.1 mg, 99% yield; pale yellow solid, melting point: 139.8 – 142.1 °C, $[\alpha]^{22}_D$ = -300.8 (*c* = 1.14, CH_2Cl_2).

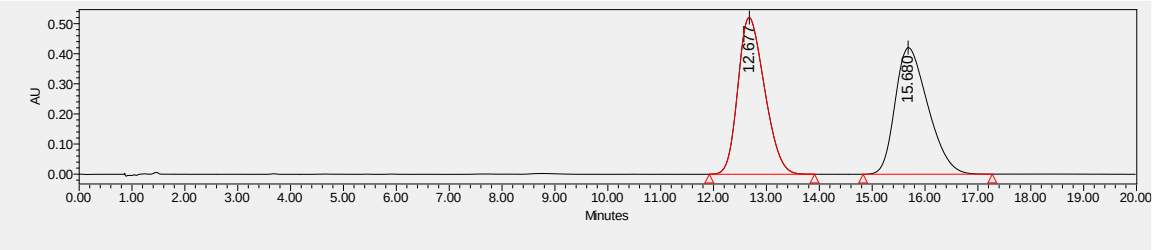
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IC-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 12.55 min, t_{minor} = 15.91 min. er = 99:1. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.81 – 7.65 (m, 4H), 7.51 – 7.25 (m, 6H), 7.24 – 6.89 (m, 13H), 6.89 – 6.82 (m, 2H), 6.79 (s, 1H), 4.52 – 4.38 (m, 1H), 3.81 (s, 3H), 3.68 – 3.24 (m, 2H), 3.03 – 2.90 (m, 1H), 2.57 – 2.41 (m, 2H), 2.05 – 1.75 (m, 3H), 1.62 – 1.46 (m, 1H), 1.24 – 1.21 (m, 1H).

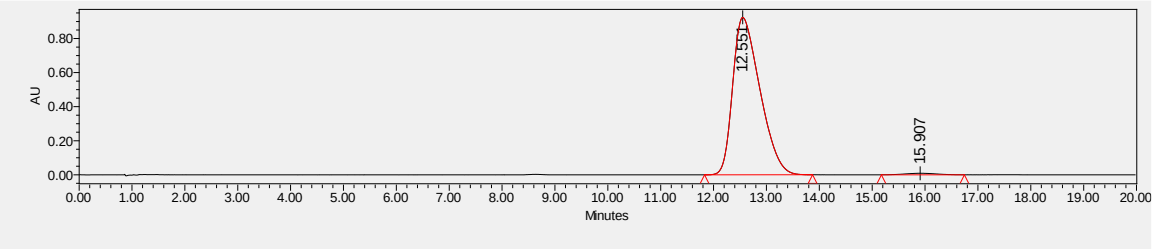
^{13}C NMR (101 MHz, $CDCl_3$) *δ* 178.7, 167.3, 159.8, 159.4, 151.8, 133.9, 132.5, 131.9, 130.6, 130.5, 130.2, 128.8, 128.7, 128.0, 127.8, 127.2, 127.1, 125.6, 122.4, 114.0, 67.7, 55.4, 42.6, 39.1, 29.8, 25.3, 23.8, 22.8, 17.5.

IR (neat): *ν* (cm^{-1}): 3409, 2927, 1759, 1657, 1508, 1252, 970, 697.

HRMS (ESI-TOF) calcd for $C_{47}H_{40}N_2O_6^+$ ([M]+H^+) = 729.2959, found 729.2959.

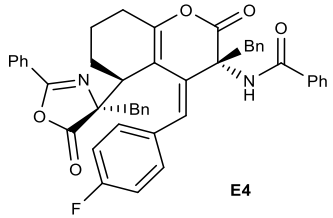


	Retention Time	Area	% Area
1	12.677	18179735	50.08
2	15.680	18119339	49.92



	Retention Time	Area	% Area
1	12.551	32976873	98.87
2	15.907	377754	1.13

***N*-((3*R*,5*S*)-3-benzyl-5-((*S*)-4-benzyl-5-oxo-2-phenyl-4,5-dihydrooxazol-4-yl)-4-((*E*)-4-fluorobenzylidene)-2-oxo-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)benzamide (E4)**



E4

61.7 mg, 86% yield; pale yellow solid, melting point: 134.3 – 137.2 °C, $[\alpha]^{22}_{D}$ = -220.1 (*c* = 0.94, CH_2Cl_2).

Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IC-3, CO_2/MeOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 23.43 min, t_{minor} = 26.78 min. er = 99:1. dr >19:1.

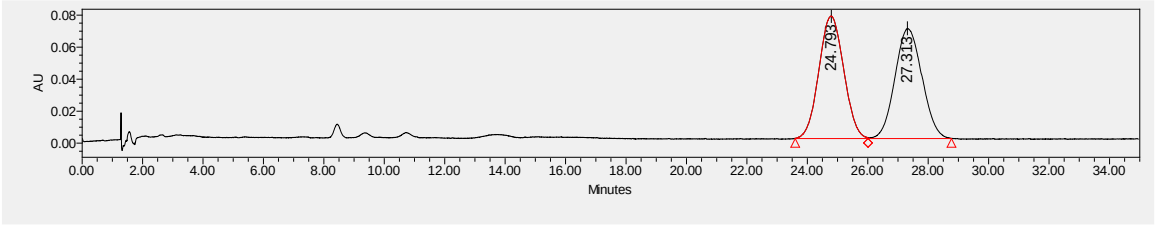
^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.80 – 7.66 (m, 4H), 7.53 – 7.38 (m, 4H), 7.37 – 7.27 (m, 4H), 7.25 – 7.14 (m, 5H), 7.07 – 6.93 (m, 8H), 6.82 (s, 1H), 4.62 – 4.36 (m, 1H), 3.68 – 3.44 (m, 1H), 3.20 – 3.16 (m, 1H), 3.05 – 2.95 (m, 1H), 2.66 – 2.45 (m, 2H), 2.04 – 1.84 (m, 3H), 1.61 – 1.50 (m, 1H), 1.32 – 1.24 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) *δ* 178.6, 164.1, 161.5, 152.6, 133.7, 132.6, 132.1, 130.5, 130.2, 130.0, 128.8, 128.7, 128.6, 128.1, 127.8, 127.3, 127.2, 125.3 (d, *J* = 50.0 Hz), 116.0 (d, *J* = 20.0 Hz), 67.9, 42.6, 39.6, 36.2, 29.8, 25.4, 23.6, 17.5.

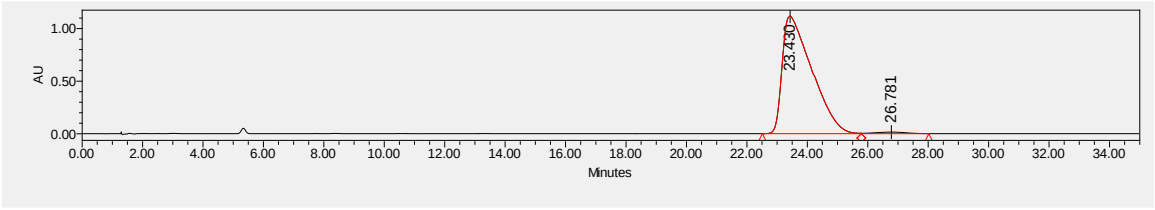
^{19}F NMR (376 MHz, $CDCl_3$) *δ* -112.61.

IR (neat): *ν* (cm^{-1}): 3410, 2926, 1763, 1657, 1505, 1227, 971, 698.

HRMS (ESI-TOF) calcd for $C_{46}H_{37}FN_2O_5^+$ ([M]+H^+) = 717.2759, found 717.2759.

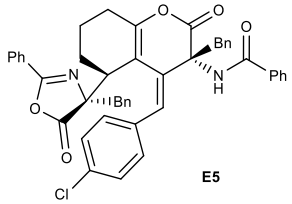


	Retention Time	Area	% Area
1	24.793	4366910	50.56
2	27.313	4270151	49.44



	Retention Time	Area	% Area
1	23.430	76002427	98.59
2	26.781	1083171	1.41

***N*-((3*R*,5*S*)-3-benzyl-5-((*S*)-4-benzyl-5-oxo-2-phenyl-4,5-dihydrooxazol-4-yl)-4-((*E*)-4-chlorobenzylidene)-2-oxo-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)benzamide (E5)**



E5

63.8 mg, 87% yield; pale yellow solid, melting point: 142.3 – 144.6 °C, $[\alpha]^{21}_{D}$ = -220.7 (*c* = 0.99, CH_2Cl_2).

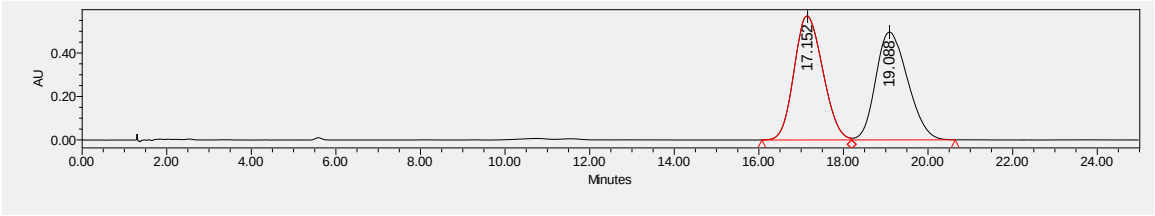
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IC-3, CO_2/MeOH = 85/15, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 16.97 min, t_{minor} = 19.34 min. er = 98:2. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.92 – 7.62 (m, 4H), 7.56 – 7.08 (m, 16H), 7.07 – 6.91 (m, 5H), 6.80 (s, 1H), 4.62 – 4.23 (m, 1H), 3.74 – 3.37 (m, 1H), 3.23 – 3.13 (m, 1H), 3.03 – 2.93 (m, 1H), 2.68 – 2.45 (m, 2H), 2.28 – 1.81 (m, 3H), 1.64 – 1.43 (m, 1H), 1.29 – 1.23 (m, 1H).

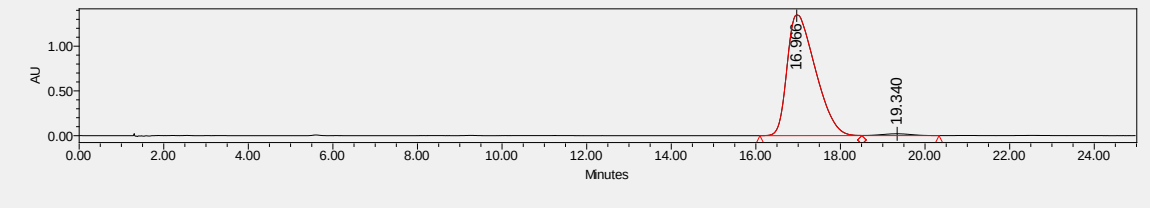
^{13}C NMR (101 MHz, $CDCl_3$) *δ* 178.6, 167.2, 159.9, 152.5, 135.8, 133.7, 132.6, 132.0, 130.6, 130.5, 130.2, 128.8, 128.7, 128.6, 128.1, 127.8, 127.3, 127.1, 125.5, 124.9, 67.7, 42.7, 39.1, 36.2, 29.8, 25.4, 23.7, 17.3.

IR (neat): *ν* (cm^{-1}): 3410, 2925, 1763, 1656, 1483, 1138, 970, 697.

HRMS (ESI-TOF) calcd for $C_{46}H_{37}ClN_2O_5^+$ ([M]+K^+) = 771.2023, 772.2056, found 771.2025, 772.2059.

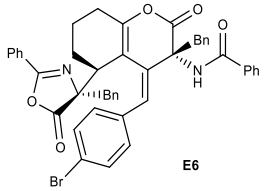


	Retention Time	Area	% Area
1	17.152	26885041	50.84
2	19.088	25996435	49.16



	Retention Time	Area	% Area
1	16.966	62616730	98.40
2	19.340	1016100	1.60

_N_-((3_R_,5_S_)-3-benzyl-5-((_S_)-4-benzyl-5-oxo-2-phenyl-4,5-dihydrooxazol-4-yl)-4-((_E_)-4-bromobenzylidene)-2-oxo-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)benzamide (E6)



E6

74.7 mg, 96% yield; pale yellow solid, melting point: 148.2 – 151.3 °C, $[\alpha]^{21}_D$ = -225.0 (*c* = 1.21, CH_2Cl_2).

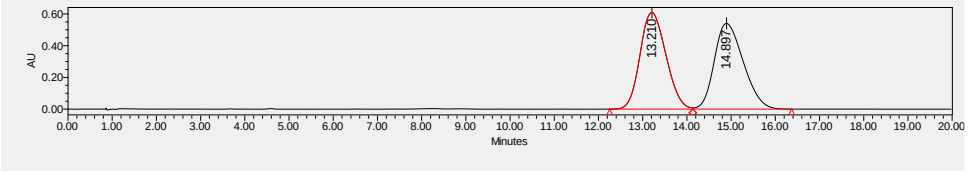
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IC-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 13.16 min, t_{minor} = 15.18 min. er = 98:2. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.84 – 7.67 (m, 4H), 7.53 – 7.28 (m, 9H), 7.26 – 7.10 (m, 7H), 7.07 – 6.90 (m, 5H), 6.76 (s, 1H), 4.61 – 4.22 (m, 1H), 3.68 – 3.41 (m, 1H), 3.23 – 3.15 (m, 1H), 3.04 – 2.93 (m, 1H), 2.66 – 2.44 (m, 2H), 2.11 – 1.84 (m, 3H), 1.61 – 1.46 (m, 1H), 1.33 – 1.19 (m, 1H).

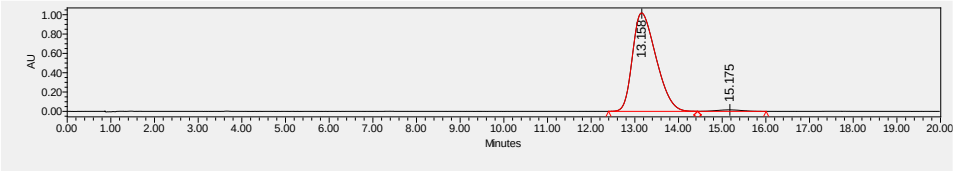
^{13}C NMR (101 MHz, $CDCl_3$) *δ* 178.6, 167.2, 160.0, 152.5, 133.7, 132.6, 132.0, 131.7, 130.9, 130.5, 130.2, 128.8, 128.7, 128.5, 128.1, 127.8, 127.3, 127.1, 125.5, 122.0, 67.7, 42.6, 39.3, 36.1, 29.8, 25.4, 23.7, 17.3.

IR (neat): *ν* (cm^{-1}): 3410, 2926, 1764, 1656, 1482, 1138, 969, 697.

HRMS (ESI-TOF) calcd for $C_{46}H_{37}BrN_2O_5^+$ ([M]+Na^+) = 799.1778, 801.1758, found 799.1779, 801.1768.

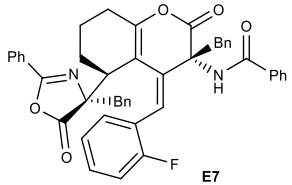


	Retention Time	Area	% Area
1	13.210	24804168	50.17
2	14.897	24638847	49.83



	Retention Time	Area	% Area
1	13.158	38159677	98.34
2	15.175	644292	1.66

***N*-((3*R*,5*S*)-3-benzyl-5-((*S*)-4-benzyl-5-oxo-2-phenyl-4,5-dihydrooxazol-4-yl)-4-((*E*)-2-fluorobenzylidene)-2-oxo-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)benzamide (E7)**



E7

68.8 mg, 96% yield; pale yellow solid, melting point: 138.1 – 141.6 °C, $[\alpha]^{22}_{D}$ = -210.3 (*c* = 0.99, CH_2Cl_2).

Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IC-3, CO_2/MeOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 23.25 min, t_{minor} = 26.46 min. er = 98:2. dr >19:1.

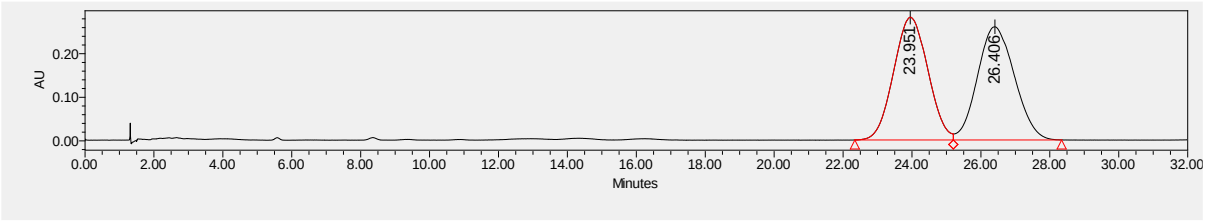
^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.84 – 7.65 (m, 4H), 7.52 – 6.95 (m, 21H), 6.86 – 6.78 (s, 1H), 4.55 – 4.34 (m, 1H), 3.61 – 3.47 (m, 1H), 3.21 – 3.15 (m, 1H), 3.03 – 2.94 (m, 1H), 2.58 – 2.44 (m, 2H), 2.08 – 1.82 (m, 3H), 1.62 – 1.48 (m, 1H), 1.31 – 1.23 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) *δ* 178.6, 167.3, 162.40 (d, *J* = 240.0 Hz), 159.9, 152.3, 133.7, 132.6, 132.0, 131.0, 130.9, 130.5, 130.2, 128.8, 128.7, 128.5, 128.0, 127.8, 127.3, 127.1, 125.5, 115.59 (d, *J* = 20.0 Hz), 67.8, 42.6, 38.3, 31.4, 29.8, 25.4, 23.7, 17.4.

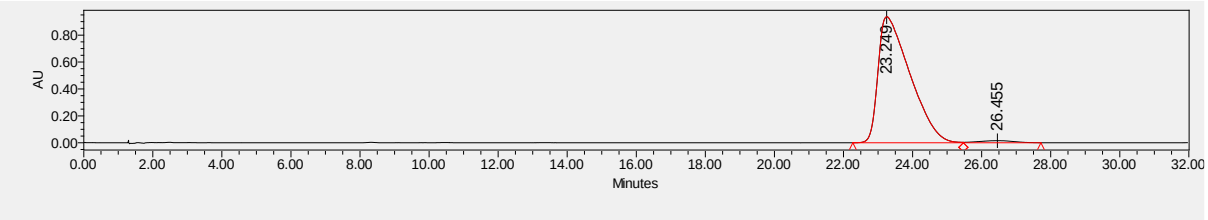
^{19}F NMR (376 MHz, $CDCl_3$) *δ* -112.78.

IR (neat): *ν* (cm^{-1}): 3410, 2926, 1765, 1657, 1505, 1228, 971, 750.

HRMS (ESI-TOF) calcd for $C_{46}H_{37}FN_2O_5^+$ ([M]+Na^+) = 739.2579, found 739.2579.

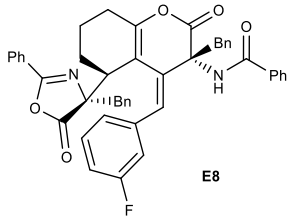


	Retention Time	Area	% Area
1	23.951	19436202	50.04
2	26.406	19406716	49.96



	Retention Time	Area	% Area
1	23.249	60049288	98.22
2	26.455	1090584	1.78

***N*-((3*R*,5*S*)-3-benzyl-5-((*S*)-4-benzyl-5-oxo-2-phenyl-4,5-dihydrooxazol-4-yl)-4-((*E*)-3-fluorobenzylidene)-2-oxo-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)benzamide (E8)**



E8

69.5 mg, 97% yield; pale yellow solid, melting point: 134.1 – 136.8 °C, $[\alpha]^{22}_{D}$ = -212.2 (*c* = 1.06, CH_2Cl_2).

Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IC-3, CO_2/MeOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 21.43 min, t_{minor} = 24.48 min. er = 98:2. dr >19:1.

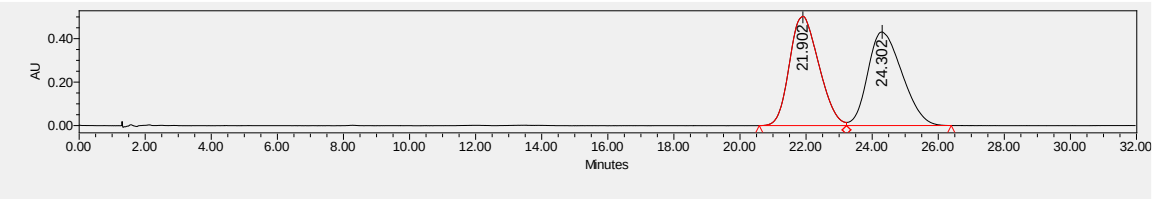
^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.77 – 7.69 (m, 4H), 7.53 – 7.27 (m, 8H), 7.27 – 7.11 (m, 5H), 7.08 – 6.93 (m, 8H), 6.82 (s, 1H), 4.59 – 4.34 (m, 1H), 3.61 – 3.47 (m, 1H), 3.23 – 3.14 (m, 1H), 3.06 – 2.96 (m, 1H), 2.60 – 2.47 (m, 2H), 1.99 – 1.84 (m, 3H), 1.61 – 1.50 (m, 1H), 1.34 – 1.23 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) *δ* 178.6, 167.2, 162.8 (d, *J* = 250.0 Hz), 159.9, 152.6, 133.7, 132.6, 132.1, 130.5, 130.2, 130.0, 130.0, 128.8, 128.7, 128.6, 128.1, 127.8, 127.3, 127.2, 125.3 (d, *J* = 50.0 Hz), 116.0 (d, *J* = 20.0 Hz), 67.7, 42.7, 39.6, 36.0, 29.8, 25.4, 23.6, 17.4.

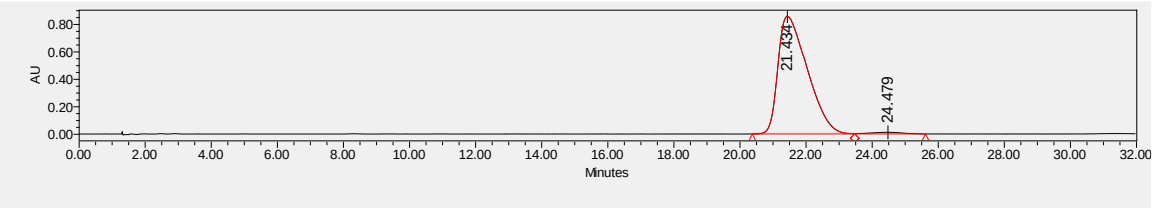
^{19}F NMR (376 MHz, $CDCl_3$) *δ* -112.61.

IR (neat): *ν* (cm^{-1}): 3410, 2926, 1765, 1656, 1481, 1139, 972, 696.

HRMS (ESI-TOF) calcd for $C_{46}H_{37}FN_2O_5^+$ ([M]+K^+) = 755.2318, found 755.2318.

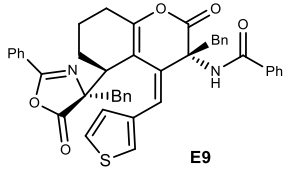


	Retention Time	Area	% Area
1	21.902	31084315	50.07
2	24.302	31001150	49.93



	Retention Time	Area	% Area
1	21.434	52744755	98.44
2	24.479	835102	1.56

_N_-((3_R_,5_S_,_E_)-3-benzyl-5-((_S_)-4-benzyl-5-oxo-2-phenyl-4,5-dihydrooxazol-4-yl)-2-oxo-4-(thiophen-3-ylmethylene)-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)benzamide (E9)



E9

60.6 mg, 86% yield; pale yellow solid, melting point: 137.5 – 140.2 °C, $[\alpha]^{22}_{D}$ = -249.4 (*c* = 0.89, CH_2Cl_2).

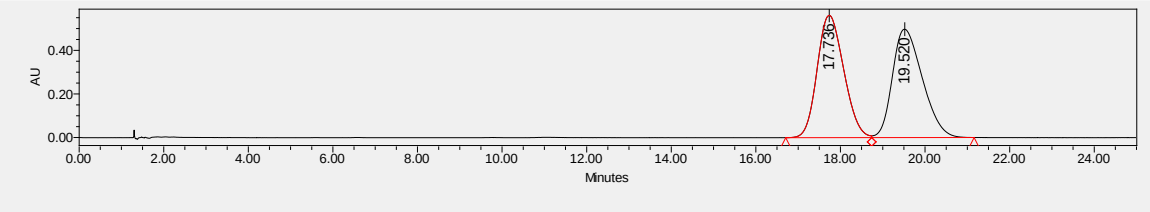
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IC-3, CO_2/MeOH = 85/15, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 17.59 min, t_{minor} = 19.78 min. er = 98:2. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.04 – 7.66 (m, 4H), 7.55 – 6.95 (m, 20H), 6.76 (s, 1H), 4.66 – 4.29 (m, 1H), 3.76 – 3.51 (m, 1H), 3.44 – 3.31 (m, 1H), 3.11 – 2.98 (m, 1H), 2.68 – 2.43 (m, 2H), 2.20 – 1.80 (m, 3H), 1.62 – 1.50 (m, 1H), 1.33 – 1.24 (m, 1H).

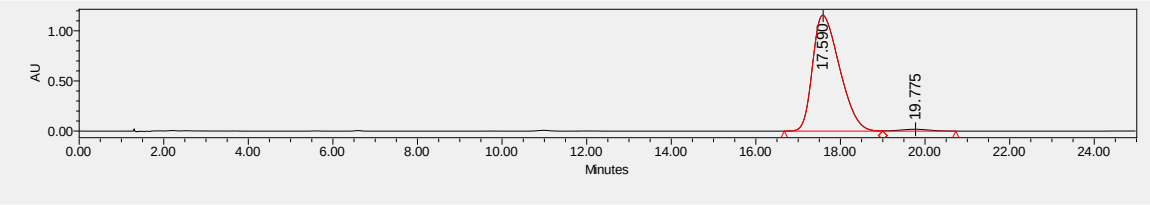
^{13}C NMR (101 MHz, $CDCl_3$) *δ* 178.7, 167.3, 159.8, 151.9, 138.3, 133.9, 132.5, 132.0, 130.5, 130.2, 128.8, 128.7, 128.4, 128.0, 127.8, 127.2, 127.2, 126.0, 125.6, 124.7, 67.6, 42.7, 39.3, 36.1, 29.8, 25.4, 23.9, 17.5.

IR (neat): *ν* (cm^{-1}): 3409, 2926, 1761, 1657, 1481, 1137, 971, 698.

HRMS (ESI-TOF) calcd for $C_{44}H_{36}N_2O_5S^+$ ([M]+H^+) = 705.2418, found 705.2418.

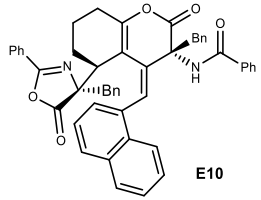


	Retention Time	Area	% Area
1	17.736	24471101	50.03
2	19.520	24442172	49.97



	Retention Time	Area	% Area
1	17.590	51168580	98.33
2	19.775	871117	1.67

***N*-((3*R*,5*S*,*E*)-3-benzyl-5-((*S*)-4-benzyl-5-oxo-2-phenyl-4,5-dihydrooxazol-4-yl)-4-(naphthalen-1-ylmethylene)-2-oxo-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)benzamide (E10)**



E10

74.2 mg, 99% yield; pale yellow solid, melting point: 208.5 – 212.4 °C, $[\alpha]^{22}_D$ = -228.9 (*c* = 1.26, CH_2Cl_2).

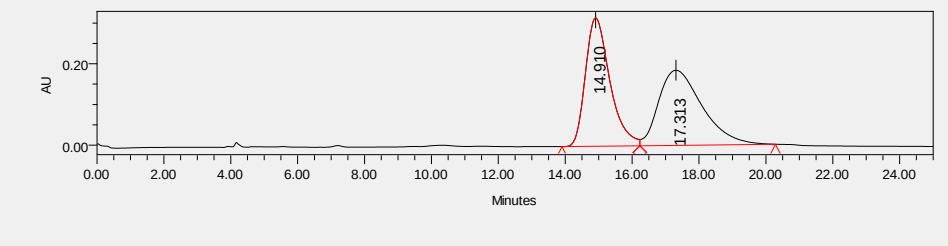
Dissolved in *i*PrOH for HPLC; HPLC (Chiralcel IC, hexane/*i*PrOH = 95/5, flow rate 0.8 mL/min, λ = 254 nm) retention time: t_{major} = 17.74 min, t_{minor} = 15.28 min. er = 99:1. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.21 – 8.07 (m, 1H), 7.94 – 7.76 (m, 4H), 7.64 – 7.60 (m, 2H), 7.56 – 7.25 (m, 15H), 7.23 (m, 1H), 7.06 – 6.75 (m, 6H), 4.73 – 4.57 (m, 1H), 3.72 – 3.55 (m, 1H), 3.14 – 3.01 (m, 1H), 2.69 (m, 1H), 2.58 – 2.36 (m, 2H), 1.90 – 1.55 (m, 4H), 1.28 – 1.25 (m, 1H).

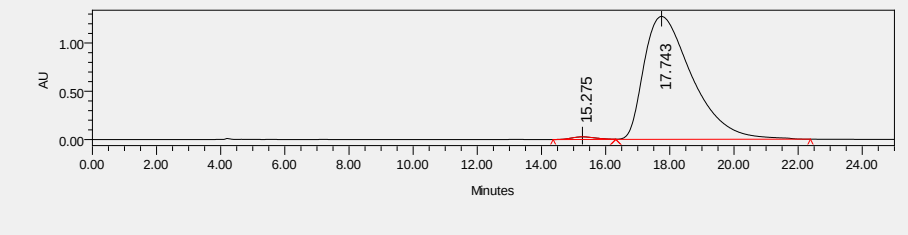
^{13}C NMR (101 MHz, $CDCl_3$) δ 178.8, 167.7, 159.7, 152.0, 136.1, 135.1, 134.9, 133.9, 133.7, 132.5, 132.0, 131.7, 130.4, 129.9, 129.0, 128.8, 128.7, 128.6, 128.0, 127.7, 127.5, 127.2, 126.6, 125.9, 125.5, 125.1, 68.1, 43.3, 40.2, 36.4, 29.8, 25.3, 23.7, 17.4.

IR (neat): ν (cm^{-1}): 3408, 2925, 1760, 1657, 1481, 1136, 969, 697.

HRMS (ESI-TOF) calcd for $C_{50}H_{40}N_2O_5^+$ ([M]+H^+) = 749.3010, found 749.3010.

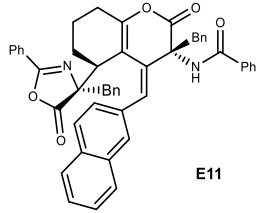


	Retention Time	Area	% Area
1	14.910	16064721	49.05
2	17.313	16689101	50.95



	Retention Time	Area	% Area
1	15.275	1436220	1.07
2	17.743	133314724	98.93

***N*-((3*R*,5*S*,*E*)-3-benzyl-5-((*S*)-4-benzyl-5-oxo-2-phenyl-4,5-dihydrooxazol-4-yl)-4-(naphthalen-2-ylmethylene)-2-oxo-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)benzamide (E11)**



E11

74.2 mg, 99% yield; pale yellow solid, melting point: 151.3 – 154.5 °C, $[\alpha]^{22}_D$ = -275.4 (*c* = 1.20, CH_2Cl_2).

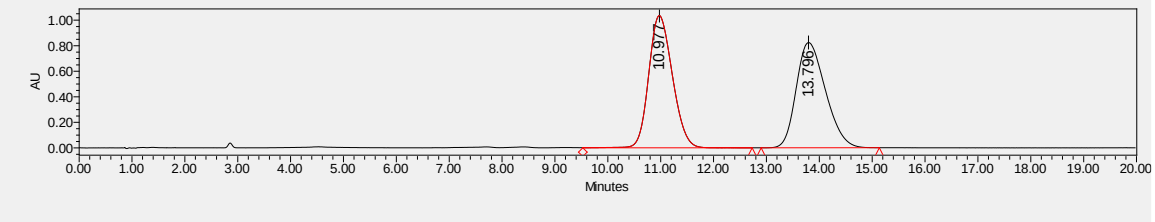
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IC-3, CO_2/MeOH = 80/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 10.94 min, t_{minor} = 13.98 min. er = 98:2. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 – 7.54 (m, 8H), 7.46 – 7.01 (m, 15H), 6.96 – 6.82 (m, 6H), 4.61 – 4.35 (m, 1H), 3.64 – 3.46 (m, 1H), 3.27 – 3.17 (m, 1H), 2.93 – 2.80 (m, 1H), 2.58 – 2.45 (m, 2H), 1.91 – 1.73 (m, 3H), 1.58 – 1.44 (m, 1H), 1.20 – 1.16 (m, 1H).

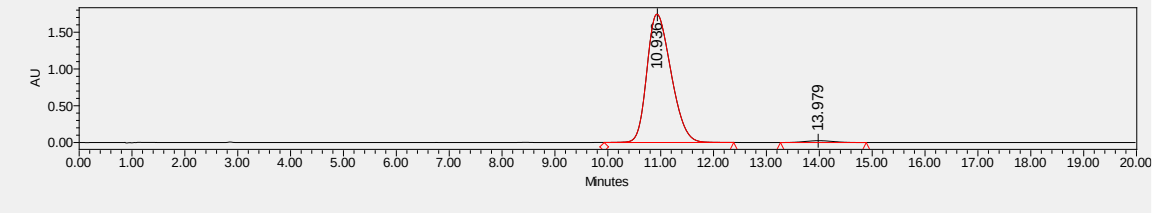
^{13}C NMR (101 MHz, $CDCl_3$) δ 178.7, 167.3, 159.8, 152.2, 135.0, 133.8, 133.3, 132.9, 132.5, 132.0, 130.5, 130.3, 128.8, 128.7, 128.5, 128.2, 128.1, 128.0, 127.9, 127.8, 127.5, 127.4, 127.2, 127.0, 126.6, 125.5, 67.9, 42.6, 39.7, 36.1, 29.8, 25.4, 23.8, 17.5.

IR (neat): ν (cm^{-1}): 3409, 2925, 1761, 1656, 1481, 1137, 970, 697.

HRMS (ESI-TOF) calcd for $C_{50}H_{40}N_2O_5^+$ ([M]+K^+) = 787.2569, found 787.2569.

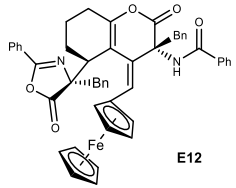


	Retention Time	Area	% Area
1	10.977	32173511	50.40
2	13.796	31662039	49.60



	Retention Time	Area	% Area
1	10.936	55233407	98.35
2	13.979	927239	1.65

***N*-((3*R*,5*S*)-3-benzyl-5-((*S*)-4-benzyl-5-oxo-2-phenyl-4,5-dihydrooxazol-4-yl)-4-((*E*)-ferrocenyl-ylmethylene)-2-oxo-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)benzamide (E12)**



E12

68.6 mg, 85% yield; orange solid, melting point: 149.6 – 153.1 °C, $[\alpha]^{21}_{D}$ = 437.3 (*c* = 1.29, CH_2Cl_2).

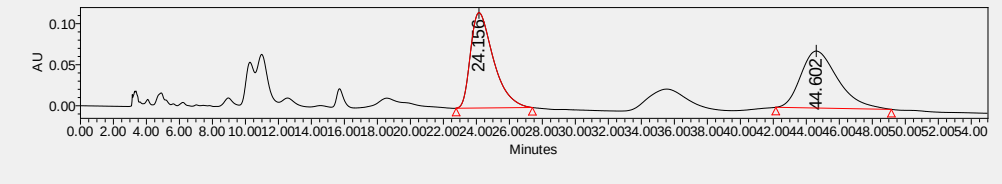
Dissolved in *i*PrOH for HPLC; HPLC (Chiralcel IC, hexane/*i*PrOH = 90/10, flow rate 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 44.84 min, t_{minor} = 24.87 min. er = 99:1. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.90 – 7.64 (m, 4H), 7.54 – 7.36 (m, 4H), 7.32 – 7.12 (m, 8H), 7.04 – 6.94 (m, 5H), 6.68 (s, 1H), 4.51 – 4.18 (m, 5H), 4.07 – 4.00 (m, 5H), 3.84 – 3.47 (m, 2H), 3.03 – 2.92 (m, 1H), 2.63 – 2.45 (m, 2H), 2.10 – 1.52 (m, 5H).

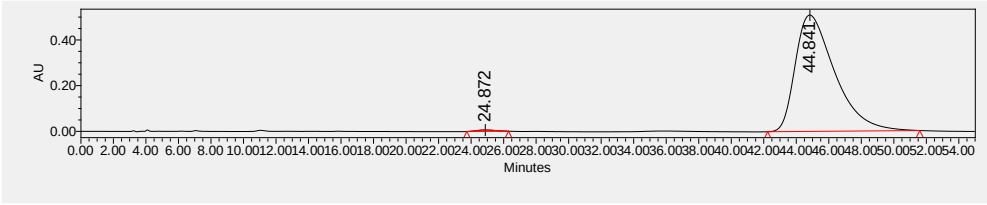
^{13}C NMR (101 MHz, $CDCl_3$) *δ* 178.7, 166.0, 159.7, 151.0, 134.0, 132.5, 132.0, 130.5, 130.2, 128.9, 128.7, 128.0, 127.7, 127.1, 127.0, 125.6, 71.4, 70.2, 70.0, 69.6, 69.0, 68.1, 42.6, 38.5, 35.8, 29.8, 25.4, 23.9, 17.5.

IR (neat): *ν* (cm^{-1}): 3408, 2926, 1762, 1656, 1452, 1141, 967, 697.

HRMS (ESI-TOF) calcd for $C_{50}H_{42}FeN_2O_5^+$ ([M]+H^+) = 807.2516, found 807.2515.

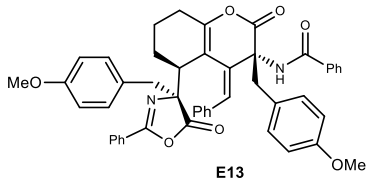


	Retention Time	Area	% Area
1	24.156	11252525	50.94
2	44.602	10836079	49.06



	Retention Time	Area	% Area
1	24.872	500331	0.58
2	44.841	85819965	99.42

***N*-((3*R*,5*S*)-4-((*E*)-benzylidene)-3-(4-methoxybenzyl)-5-((*S*)-4-(4-methoxybenzyl)-5-oxo-2-phenyl-4,5-dihydrooxazol-4-yl)-2-oxo-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)benzamide (E13)**



E13

75.0 mg, 99% yield; pale yellow solid, melting point: 141.2 – 144.7 °C, $[\alpha]^{21}_{D}$ = -198.4 (*c* = 1.32, CH_2Cl_2).

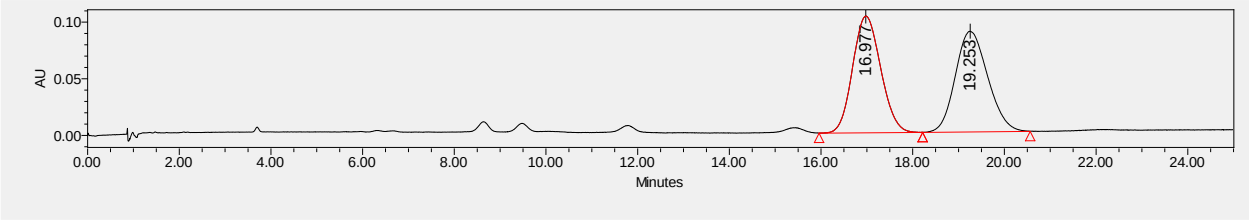
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IC-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 16.53 min, t_{minor} = 19.32 min. er = 99:1. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.83 – 7.66 (m, 4H), 7.57 – 7.28 (m, 10H), 7.27 – 7.20 (m, 2H), 7.11 – 7.06 (m, 2H), 6.96 – 6.72 (m, 5H), 6.60 – 6.54 (m, 2H), 4.56 – 4.30 (m, 1H), 3.77 – 3.72 (m, 3H), 3.63 – 3.60 (m, 3H), 3.55 – 3.26 (m, 1H), 3.23 – 3.14 (m, 1H), 2.98 – 2.85 (m, 1H), 2.64 – 2.48 (m, 2H), 2.07 – 1.74 (m, 4H), 1.63 – 1.47 (m, 1H).

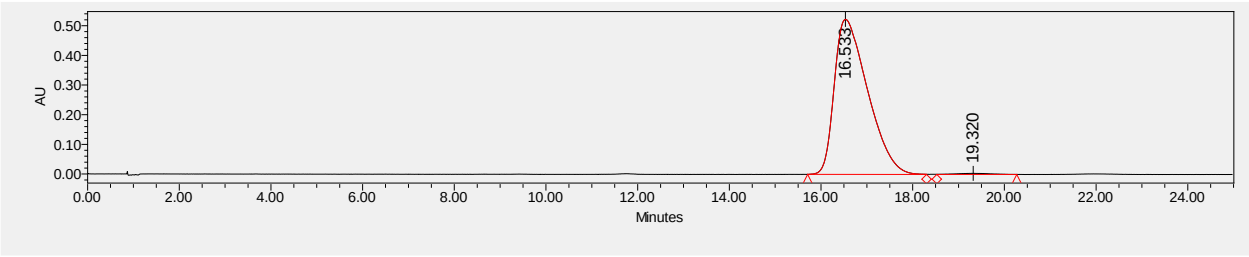
^{13}C NMR (101 MHz, $CDCl_3$) *δ* 178.7, 167.3, 159.8, 158.7, 152.0, 132.5, 132.0, 131.5, 131.2, 129.2, 128.8, 128.7, 128.4, 128.0, 127.8, 127.1, 125.9, 125.6, 113.8, 113.4, 68.0, 55.3, 55.1, 45.6, 41.6, 39.2, 35.1, 25.4, 23.6, 17.3.

IR (neat): *ν* (cm^{-1}): 3410, 2954, 1762, 1655, 1511, 1249, 1031, 696.

HRMS (ESI-TOF) calcd for $C_{48}H_{42}N_2O_7^+$ ([M]+K^+) = 797.2624, found 797.2625.

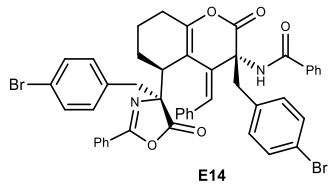


	Retention Time	Area	% Area
1	16.977	4387918	50.10
2	19.253	4370725	49.90



	Retention Time	Area	% Area
1	16.533	26363194	99.26
2	19.320	197004	0.74

_N_-((3_R_,5_S_)-4-((_E_)-benzylidene)-3-(4-bromobenzyl)-5-((_S_)-4-(4-bromobenzyl)-5-oxo-2-phenyl-4,5-dihydrooxazol-4-yl)-2-oxo-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)benzamide (E14)



E14

84.7 mg, 99% yield; white solid, melting point: 149.6 – 153.7 °C, $[\alpha]^{20}_{D}$ = -202.4 (*c* = 1.44, CH_2Cl_2).

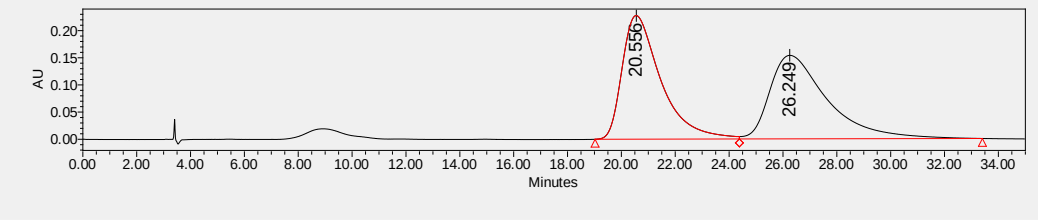
Dissolved in *i*PrOH for HPLC; HPLC (Chiralcel IC, hexane/*i*PrOH = 98/2, flow rate 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 20.77 min, t_{minor} = 26.72 min. er = 95:5. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 – 7.70 (m, 4H), 7.57 – 7.26 (m, 12H), 7.26 – 7.12 (m, 4H), 7.04 – 6.97 (m, 2H), 6.89 – 6.85 (m, 3H), 4.52 – 4.24 (m, 1H), 3.55 – 3.39 (m, 1H), 3.21 – 3.13 (m, 1H), 2.99 – 2.89 (m, 1H), 2.64 – 2.43 (m, 2H), 2.00 – 1.70 (m, 4H), 1.59 – 1.45 (m, 1H).

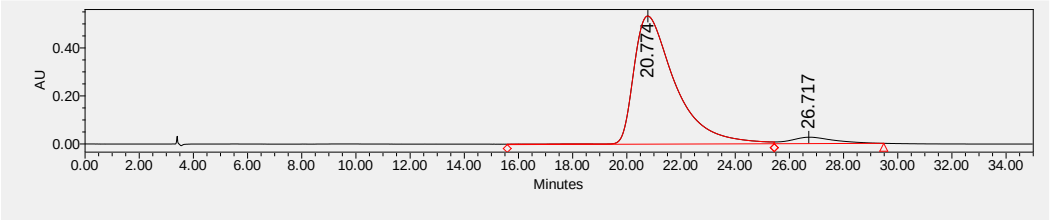
^{13}C NMR (101 MHz, $CDCl_3$) δ 178.5, 167.3, 160.1, 152.2, 137.4, 132.9, 132.8, 132.2, 132.1, 131.8, 131.6, 131.2, 129.2, 128.9, 128.8, 128.5, 127.8, 127.1, 125.3, 121.5, 67.3, 41.8, 39.3, 38.2, 35.3, 25.3, 23.6, 17.4.

IR (neat): ν (cm^{-1}): 3408, 2952, 1761, 1655, 1484, 1137, 973, 696.

HRMS (ESI-TOF) calcd for $C_{46}H_{36}Br_2N_2O_5^+$ ([M]+K^+) = 893.0623, 895.0602, found 893.0627, 895.0610.

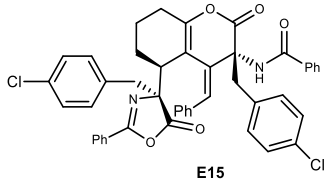


	Retention Time	Area	% Area
1	20.556	22747678	49.93
2	26.249	22809372	50.07



	Retention Time	Area	% Area
1	20.774	56675227	95.05
2	26.717	2954270	4.95

_N_-((3_R_,5_S_)-4-((_E_)-benzylidene)-3-(4-chlorobenzyl)-5-((_S_)-4-(4-chlorobenzyl)-5-oxo-2-phenyl-4,5-dihydrooxazol-4-yl)-2-oxo-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)benzamide (E15)



E15

72.9 mg, 95% yield; white solid, melting point: 142.8 – 146.5 °C, $[\alpha]^{19}_{D}$ = -225.4 (*c* = 1.20, CH_2Cl_2).

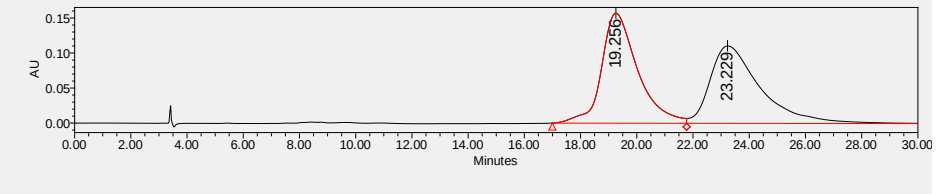
Dissolved in *i*PrOH for HPLC; HPLC (Chiralcel IC, hexane/*i*PrOH = 98/2, flow rate 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 19.38 min, t_{minor} = - min. er >99:1. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 – 7.69 (m, 4H), 7.58 – 7.15 (m, 14H), 7.10 – 6.98 (m, 4H), 6.96 – 6.84 (m, 3H), 4.52 – 4.27 (m, 1H), 3.57 – 3.45 (m, 1H), 3.23 – 3.14 (m, 1H), 3.00 – 2.92 (m, 1H), 2.64 – 2.43 (m, 2H), 1.94 – 1.73 (m, 4H), 1.61 – 1.45 (m, 1H).

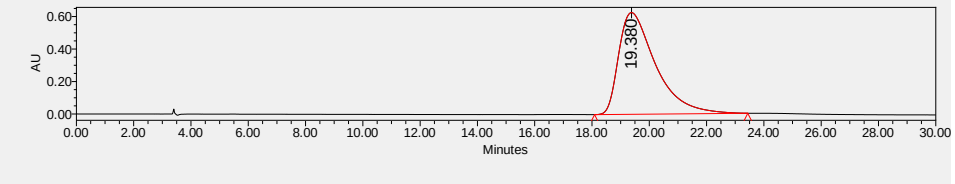
^{13}C NMR (101 MHz, $CDCl_3$) δ 178.6, 167.3, 160.1, 152.2, 137.4, 133.3, 132.8, 132.4, 132.2, 131.8, 131.4, 129.2, 128.9, 128.8, 128.7, 128.6, 128.3, 127.8, 127.1, 125.3, 67.5, 41.8, 39.3, 35.5, 29.8, 25.3, 23.6, 17.4.

IR (neat): ν (cm^{-1}): 3409, 2926, 1762, 1655, 1487, 1093, 973, 696.

HRMS (ESI-TOF) calcd for $C_{46}H_{36}Cl_2N_2O_5^+$ ([M]+H^+) = 767.2074, 769.2045, found 767.2071, 769.2045.

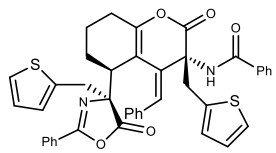


	Retention Time	Area	% Area
1	19.256	13989975	50.48
2	23.229	13724717	49.52



	Retention Time	Area	% Area
1	19.380	55946804	100.00

***N*-((3*R*,5*S*)-4-((*E*)-benzylidene)-2-oxo-5-((*S*)-5-oxo-2-phenyl-4-(thiophen-2-ylmethyl)-4,5-dihydrooxazol-4-yl)-3-(thiophen-2-ylmethyl)-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)benzamide (E16)**



E16

70.3 mg, 99% yield; white solid, melting point: 143.2 – 145.1 °C, $[\alpha]^{20}_D$ = -259.1 (*c* = 1.27, CH_2Cl_2).

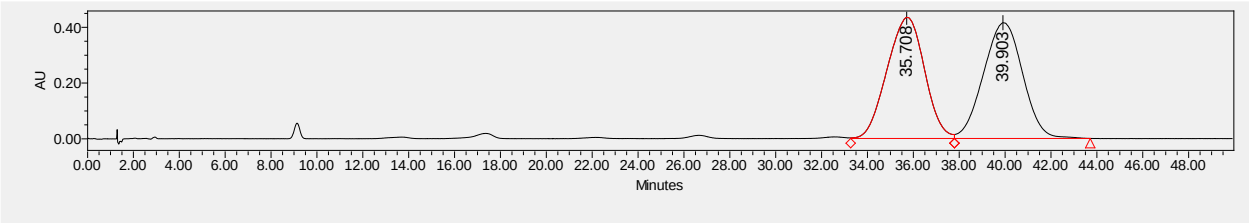
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IC-3, CO_2/IPROH = 85/15, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 39.78 min, t_{minor} = 36.13 min. er = 99:1. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 – 7.76 (m, 4H), 7.55 – 7.25 (m, 10H), 7.24 – 7.07 (m, 3H), 7.00 – 6.69 (m, 6H), 4.79 – 4.66 (m, 1H), 3.95 – 3.82 (m, 1H), 3.26 – 3.06 (m, 2H), 2.56 – 2.45 (m, 2H), 1.95 – 1.73 (m, 4H), 1.59 – 1.45 (m, 1H).

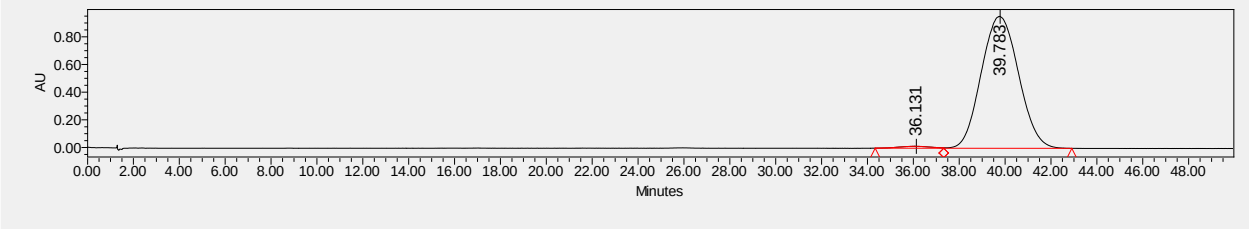
^{13}C NMR (101 MHz, $CDCl_3$) δ 178.4, 167.1, 161.0, 152.4, 137.2, 135.0, 132.8, 132.1, 130.7, 129.2, 128.8, 128.6, 128.2, 128.1, 127.8, 127.3, 126.7, 125.7, 125.6, 125.3, 67.5, 39.2, 36.7, 30.5, 29.8, 25.2, 23.5, 17.3.

IR (neat): ν (cm^{-1}): 3408, 2922, 1762, 1654, 1480, 1134, 969, 694.

HRMS (ESI-TOF) calcd for $C_{42}H_{34}N_2O_5S_2^+$ ([M]+Na^+) = 733.1801, found 733.1801.

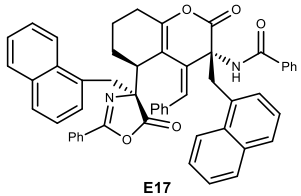


	Retention Time	Area	% Area
1	35.708	49362276	49.94
2	39.903	49483487	50.06



	Retention Time	Area	% Area
1	36.131	1335484	1.22
2	39.783	108038629	98.78

_N_-((3_R_,5_S_)-4-((_E_)-benzylidene)-3-(naphthalen-1-ylmethyl)-5-((_S_)-4-(naphthalen-1-ylmethyl)-5-oxo-2-phenyl-4,5-dihydrooxazol-4-yl)-2-oxo-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)benzamide (E17)



E17

79.0 mg, 99% yield; white solid, melting point: 154.8 – 158.2 °C, $[\alpha]^{20}_{D}$ = -104.1 (*c* = 2.86, CH_2Cl_2).

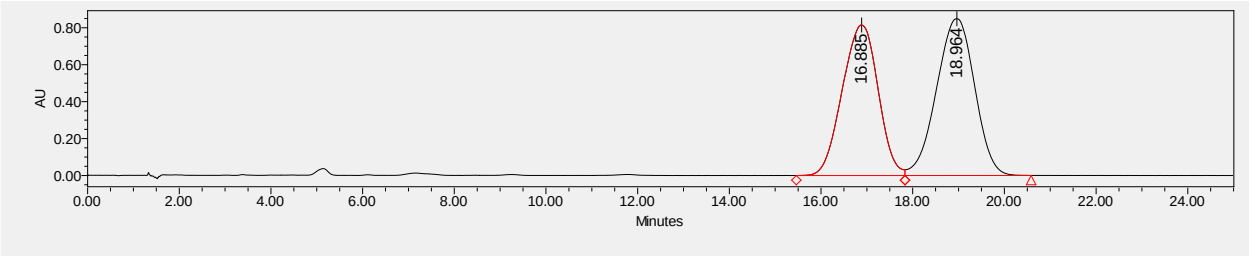
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IC-3, CO_2/MeOH = 70/30, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 17.15 min, t_{minor} = 19.31 min. er = 99:1. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.32 – 8.15 (m, 1H), 8.02 – 7.69 (m, 4H), 7.58 – 6.83 (m, 26H), 5.43 – 4.80 (m, 1H), 4.31 – 4.16 (m, 1H), 3.98 – 3.76 (m, 2H), 3.60 – 3.27 (m, 2H), 2.73 – 2.50 (m, 2H), 2.37 – 2.02 (m, 2H), 1.77 – 1.55 (m, 1H).

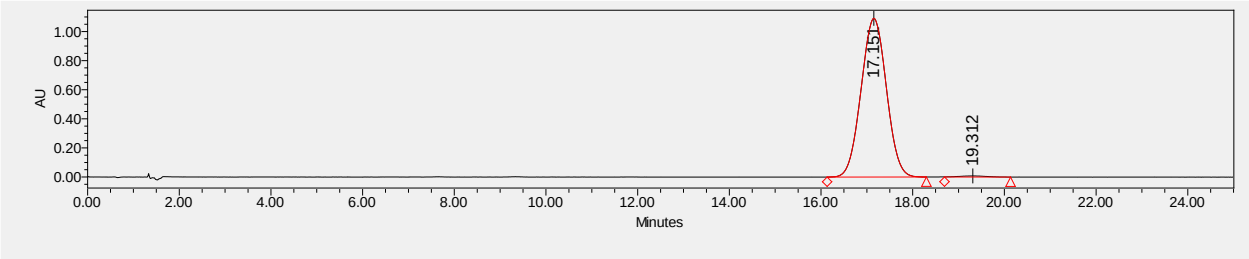
^{13}C NMR (101 MHz, $CDCl_3$) *δ* 178.9, 166.3, 159.3, 152.3, 138.7, 134.1, 133.6, 132.8, 132.2, 131.8, 130.6, 129.6, 129.2, 128.3, 128.2, 127.7, 127.4, 127.0, 126.2, 125.9, 125.5, 125.4, 125.2, 125.1, 125.0, 122.7, 64.8, 39.7, 38.9, 29.7, 25.7, 23.8, 17.4, 14.2.

IR (neat): *ν* (cm^{-1}): 3415, 3055, 1770, 1655, 1478, 1141, 967, 696.

HRMS (ESI-TOF) calcd for $C_{54}H_{42}N_2O_5^+$ ([M]+H^+) = 799.3166, found 799.3174.

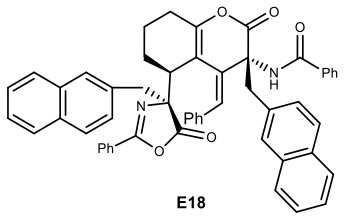


	Retention Time	Area	% Area
1	16.885	44205011	47.41
2	18.964	49038777	52.59



	Retention Time	Area	% Area
1	17.151	41761836	99.27
2	19.312	308641	0.73

_N_-((3_R_,5_S_)-4-((_E_)-benzylidene)-3-(naphthalen-2-ylmethyl)-5-((_S_)-4-(naphthalen-2-ylmethyl)-5-oxo-2-phenyl-4,5-dihydrooxazol-4-yl)-2-oxo-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)benzamide (E18)



E18

79.0 mg, 99% yield; white solid, melting point: 152.6 – 154.8 °C, $[\alpha]^{20}_D$ = -216.9 (*c* = 1.30, CH_2Cl_2).

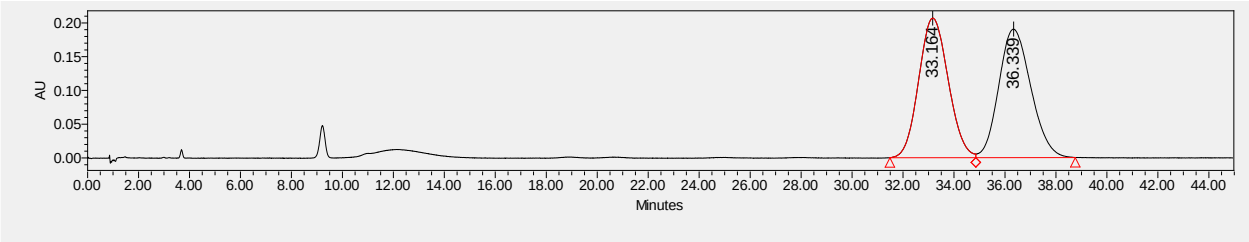
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IC-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 33.18 min, t_{minor} = 36.72 min. er = 99:1. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 – 7.52 (m, 10H), 7.53 – 7.24 (m, 16H), 7.24 – 7.11 (m, 4H), 6.95 (s, 1H), 4.84 – 4.51 (m, 1H), 3.88 – 3.70 (m, 1H), 3.36 – 3.17 (m, 2H), 2.74 – 2.48 (m, 2H), 2.26 – 1.73 (m, 4H), 1.66 – 1.48 (m, 1H).

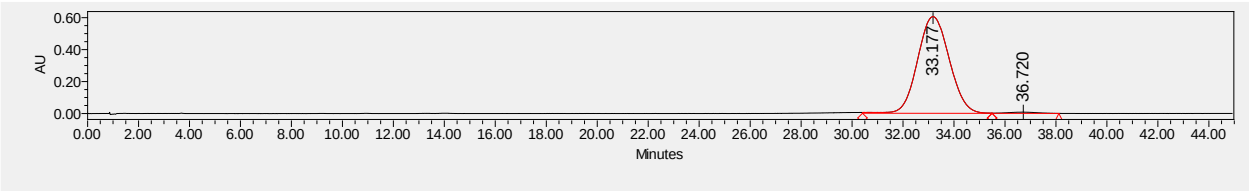
^{13}C NMR (101 MHz, $CDCl_3$) δ 178.7, 167.5, 159.9, 152.2, 137.6, 133.5, 133.1, 132.7, 132.5, 132.5, 132.0, 131.6, 129.4, 129.3, 128.8, 128.6, 128.5, 128.1, 127.9, 127.8, 127.7, 127.5, 127.1, 125.8, 125.7, 125.5, 67.8, 42.7, 39.4, 36.2, 29.8, 25.4, 23.7, 17.5.

IR (neat): ν (cm^{-1}): 3408, 3055, 1761, 1655, 1480, 1136, 972, 696.

HRMS (ESI-TOF) calcd for $C_{54}H_{42}N_2O_5^+$ ([M]+Na^+) = 821.2986, found 821.2986.

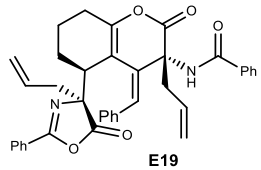


	Retention Time	Area	% Area
1	33.164	16663381	49.98
2	36.339	16674859	50.02



	Retention Time	Area	% Area
1	33.177	52416997	98.79
2	36.720	644596	1.21

_N_-((3_R_,5_S_)-3-allyl-5-((_S_)-4-allyl-5-oxo-2-phenyl-4,5-dihydrooxazol-4-yl)-4-((_E_)-benzylidene)-2-oxo-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)benzamide (E19)



E19

59.2 mg, 99% yield; pale yellow solid, melting point: 178.1 – 180.9 °C, $[\alpha]^{19}_{D}$ = -218.6 (*c* = 0.61, CH_2Cl_2).

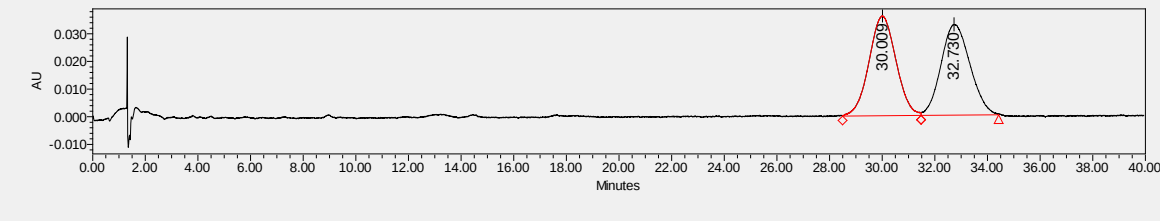
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IC-3, CO_2/IPROH = 85/15, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 29.04 min, t_{minor} = 32.77 min. er = 99:1. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.93 – 7.74 (m, 4H), 7.59 – 7.37 (m, 6H), 7.36 – 7.19 (m, 6H), 6.61 (s, 1H), 6.06 – 5.82 (m, 1H), 5.42 – 5.27 (m, 3H), 5.07 – 4.93 (m, 2H), 3.09 – 3.01 (m, 1H), 2.82 – 2.67 (m, 1H), 2.50 – 2.32 (m, 3H), 2.23 – 2.11 (m, 1H), 1.90 – 1.82 (m, 1H).

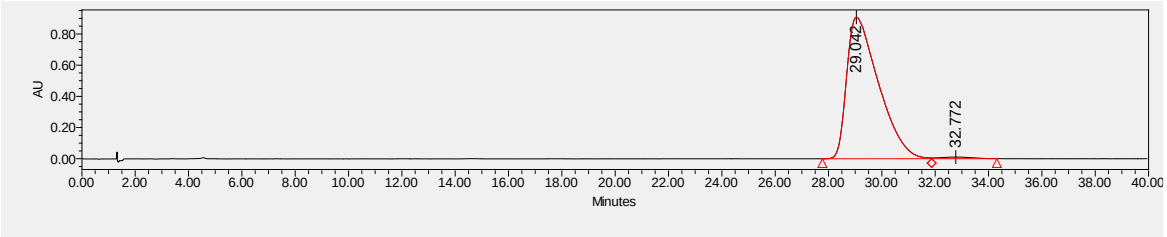
^{13}C NMR (101 MHz, $CDCl_3$) *δ* 178.5, 166.0, 159.7, 152.4, 138.2, 132.9, 132.1, 131.5, 130.0, 129.2, 129.0, 128.8, 128.2, 127.9, 127.6, 127.2, 125.7, 121.1, 75.8, 40.1, 37.8, 25.4, 23.1, 17.2.

IR (neat): *ν* (cm^{-1}): 3414, 2924, 1768, 1654, 1480, 1152, 929, 698.

HRMS (ESI-TOF) calcd for $C_{38}H_{34}N_2O_5^+$ ([M]+H^+) = 599.2540, found 599.2540.

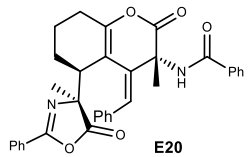


	Retention Time	Area	% Area
1	30.009	2562004	50.45
2	32.730	2515810	49.55



	Retention Time	Area	% Area
1	29.042	75240821	98.83
2	32.772	890407	1.17

_N_-((3_R_,5_S_)-4-((_E_)-benzylidene)-3-methyl-5-((_S_)-4-methyl-5-oxo-2-phenyl-4,5-dihydrooxazol-4-yl)-2-oxo-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)benzamide (E20)



E20

45.3 mg, 83% yield; white solid, melting point: 199.3 – 201.5 °C, $[\alpha]^{20}_D$ = -315.8 (*c* = 0.79, CH_2Cl_2).

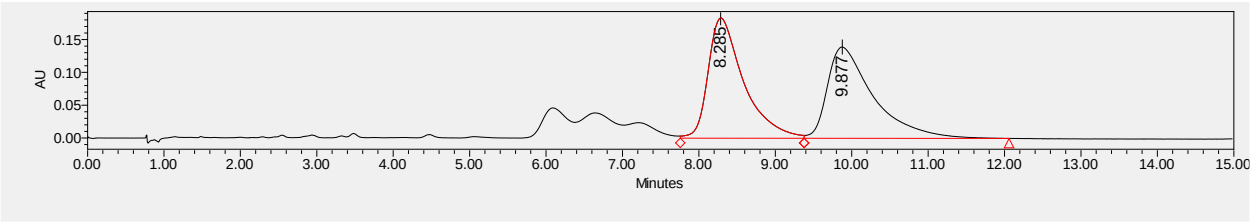
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 7.71 min, t_{minor} = 9.68 min. er = 98:2. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.79 (m, 4H), 7.60 – 7.37 (m, 6H), 7.34 – 7.15 (m, 6H), 6.68 (s, 1H), 3.07 – 2.92 (m, 1H), 2.52 – 2.31 (m, 2H), 2.04 – 1.90 (m, 4H), 1.84 – 1.73 (m, 3H), 1.35 (s, 3H).

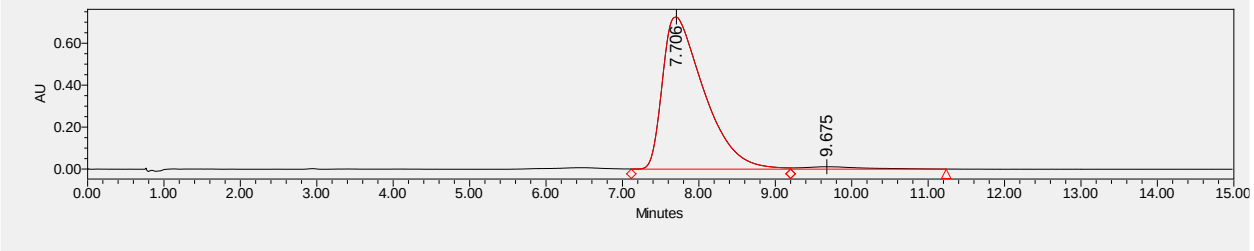
^{13}C NMR (101 MHz, $CDCl_3$) δ 180.0, 166.4, 159.5, 152.0, 138.1, 133.8, 132.9, 132.1, 129.1, 129.0, 128.7, 128.3, 127.9, 127.6, 127.3, 126.0, 71.4, 61.5, 38.6, 25.4, 24.0, 23.1, 17.2.

IR (neat): ν (cm^{-1}): 3326, 2929, 1771, 1652, 1522, 1190, 1003, 696.

HRMS (ESI-TOF) calcd for $C_{34}H_{30}N_2O_5^+$ ([M]+K^+) = 585.1786, found 585.1786.

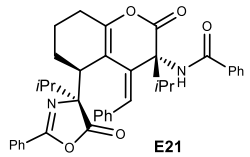


	Retention Time	Area	% Area
1	8.285	5918096	50.51
2	9.877	5797628	49.49



	Retention Time	Area	% Area
1	7.706	27395395	97.74
2	9.675	632160	2.26

_N_-((3_R_,5_S_)-4-((_E_)-benzylidene)-3-isopropyl-5-((_S_)-4-isopropyl-5-oxo-2-phenyl-4,5-dihydrooxazol-4-yl)-2-oxo-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)benzamide (E21)



E21

52.4 mg, 87% yield; white solid, melting point: 240.2 – 243.4 °C, $[\alpha]^{20}_{D}$ = -187.8 (*c* = 0.91, CH_2Cl_2).

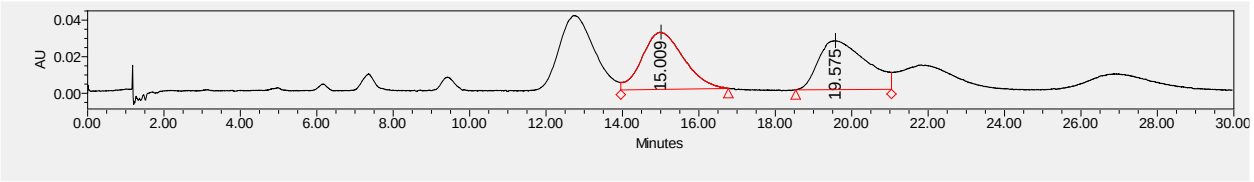
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/MeOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 20.37 min, t_{minor} = 14.78 min. er = 98:2. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.93 – 7.86 (m, 2H), 7.81 – 7.69 (m, 2H), 7.61 – 7.25 (m, 10H), 7.25 – 7.18 (m, 1H), 6.51 (s, 1H), 6.34 (s, 1H), 3.22 – 3.13 (m, 1H), 2.58 – 2.30 (m, 3H), 2.15 – 2.06 (m, 1H), 1.96 – 1.68 (m, 4H), 1.25 – 1.20 (m, 3H), 0.74 – 0.51 (m, 9H).

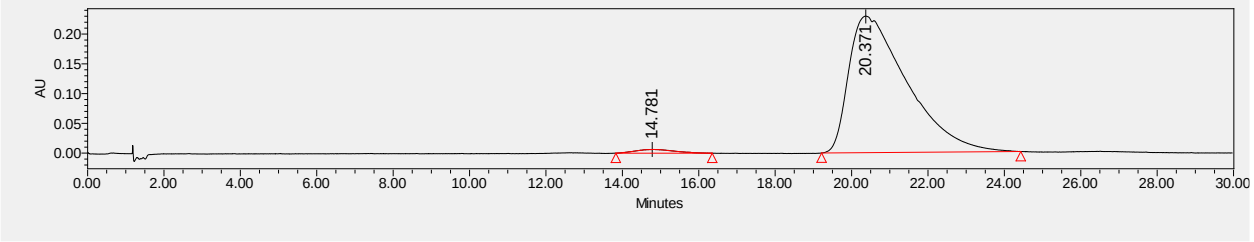
^{13}C NMR (101 MHz, $CDCl_3$) δ 177.7, 166.7, 159.4, 152.0, 138.8, 134.2, 132.8, 132.0, 129.3, 129.1, 128.9, 128.7, 128.2, 127.9, 127.8, 127.4, 127.1, 126.7, 125.9, 108.8, 78.5, 67.5, 35.0, 32.2, 31.3, 25.4, 23.2, 17.8, 17.2, 17.2, 16.7, 14.1.

IR (neat): ν (cm^{-1}): 3345, 2970, 1773, 1654, 1482, 1165, 1020, 694.

HRMS (ESI-TOF) calcd for $C_{38}H_{38}N_2O_5^+$ ([M]+K^+) = 641.2412, found 641.2412.

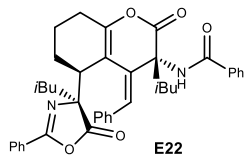


	Retention Time	Area	% Area
1	15.009	2356495	50.12
2	19.575	2345363	49.88



	Retention Time	Area	% Area
1	14.781	437069	1.77
2	20.371	24277643	98.23

***N*-((3*R*,5*S*)-4-((*E*)-benzylidene)-3-isobutyl-5-((*S*)-4-isobutyl-5-oxo-2-phenyl-4,5-dihydrooxazol-4-yl)-2-oxo-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)benzamide (E22)**



E22

57.3 mg, 91% yield; yellow solid, melting point: 186.7 – 188.4 °C, $[\alpha]^{20}_D$ = -313.7 (*c* = 0.84, CH_2Cl_2).

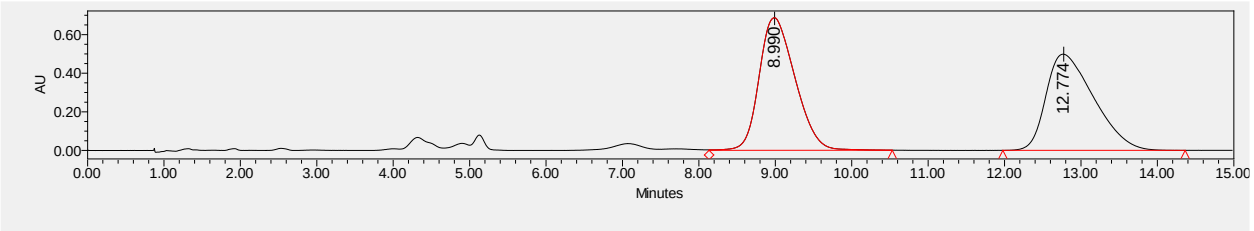
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IC-3, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 12.81 min, t_{minor} = 9.43 min. er = 98:2. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 – 7.87 (m, 4H), 7.62 – 6.93 (m, 12H), 6.68 (s, 1H), 3.29 – 2.82 (m, 1H), 2.73 – 2.63 (m, 1H), 2.48 – 2.36 (m, 2H), 2.17 – 1.59 (m, 7H), 1.46 – 1.29 (m, 2H), 1.08 – 0.75 (m, 12H).

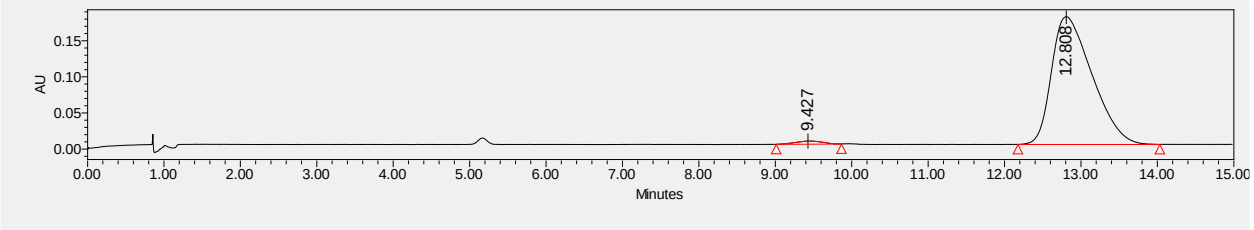
^{13}C NMR (101 MHz, $CDCl_3$) δ 180.1, 166.4, 159.2, 151.8, 138.0, 134.9, 132.7, 131.9, 129.1, 129.0, 128.8, 128.5, 128.3, 127.7, 127.2, 126.1, 75.2, 65.8, 44.6, 39.8, 29.8, 25.1, 25.0, 24.9, 24.5, 24.3, 23.5, 23.3, 22.8, 17.5.

IR (neat): ν (cm^{-1}): 3411, 2957, 1760, 1656, 1483, 1157, 957, 699.

HRMS (ESI-TOF) calcd for $C_{40}H_{42}N_2O_5^+$ ([M]+H^+) = 631.3166, found 631.3165.

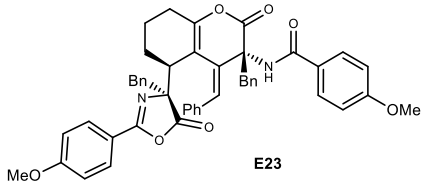


	Retention Time	Area	% Area
1	8.990	22363336	50.90
2	12.774	21571120	49.10



	Retention Time	Area	% Area
1	9.427	106689	1.61
2	12.808	6522254	98.39

***N*-((3*R*,5*S*)-3-benzyl-5-((*S*)-4-benzyl-2-(4-methoxyphenyl)-5-oxo-4,5-dihydrooxazol-4-yl)-4-((*E*)-benzylidene)-2-oxo-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)-4-methoxybenzamide (E23)**



E23

75.1 mg, 99% yield; pale yellow solid, melting point: 147.2 – 148.8 °C, $[\alpha]^{19}_{D}$ = -225.3 (*c* = 1.37, CH_2Cl_2).

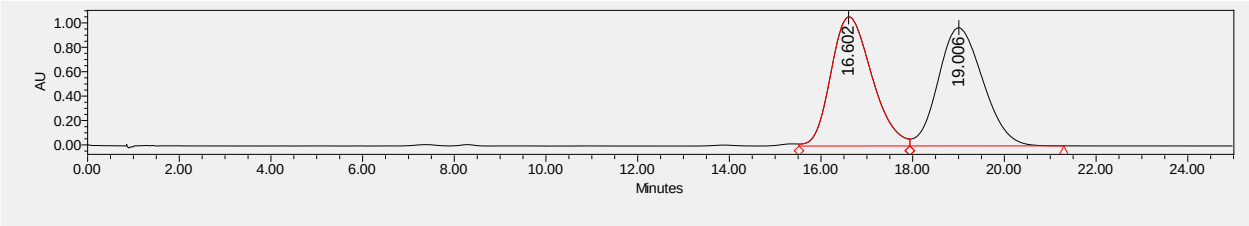
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IC-3, CO_2/IPROH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 18.82 min, t_{minor} = 16.65 min. er = 99:1. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 – 7.62 (m, 4H), 7.39 – 7.25 (m, 4H), 7.26 – 7.14 (m, 6H), 7.07 – 6.73 (m, 11H), 4.61 – 4.36 (m, 1H), 3.81 (s, 3H), 3.75 (s, 3H), 3.63 – 3.46 (m, 1H), 3.24 – 3.16 (m, 1H), 3.01 – 2.94 (m, 1H), 2.61 – 2.44 (m, 2H), 1.97 – 1.78 (m, 4H), 1.58 – 1.47 (m, 1H).

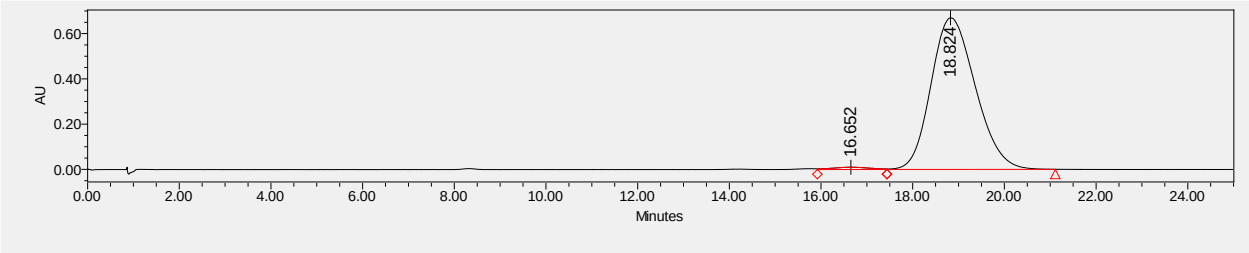
^{13}C NMR (101 MHz, $CDCl_3$) δ 178.8, 166.7, 163.0, 162.6, 159.4, 152.0, 137.7, 134.1, 130.5, 130.3, 129.6, 129.2, 129.0, 128.4, 127.9, 127.3, 127.1, 117.9, 114.1, 113.9, 110.1, 67.7, 55.5, 55.5, 42.6, 39.4, 36.0, 29.8, 25.3, 23.6, 17.4.

IR (neat): ν (cm^{-1}): 3413, 2931, 1762, 1653, 1491, 1257, 1028, 699.

HRMS (ESI-TOF) calcd for $C_{48}H_{42}N_2O_7^+$ ([M]+K^+) = 797.2624, found 797.2625.

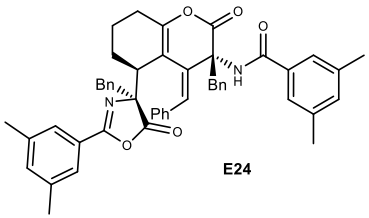


	Retention Time	Area	% Area
1	16.602	65650707	50.01
2	19.006	65626346	49.99



	Retention Time	Area	% Area
1	16.652	564602	1.24
2	18.824	45018366	98.76

_N_-((3_R_,5_S_)-3-benzyl-5-((_S_)-4-benzyl-2-(3,5-dimethylphenyl)-5-oxo-4,5-dihydrooxazol-4-yl)-4-((_E_)-benzylidene)-2-oxo-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)-3,5-dimethylbenzamide (E24)



E24

74.7 mg, 99% yield; white solid, melting point: 136.5 – 139.2 °C, $[\alpha]^{20}_D$ = -226.1 (*c* = 1.26, CH_2Cl_2).

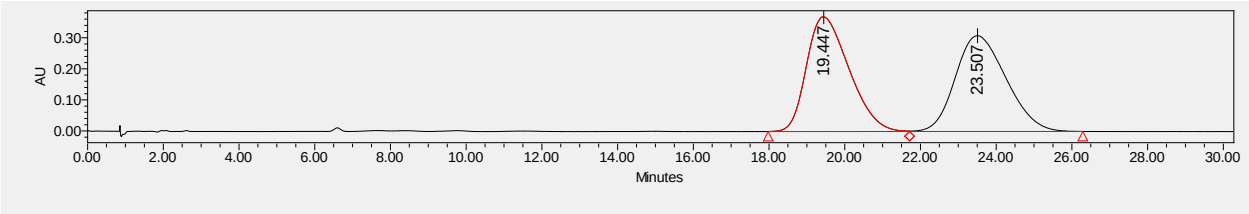
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IC-3, CO_2/IPROH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 22.64 min, t_{minor} = 19.38 min. er = 99:1. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.43 – 7.10 (m, 16H), 7.07 – 6.98 (m, 6H), 6.86 (s, 1H), 4.69 – 4.42 (m, 1H), 3.66 – 3.51 (m, 1H), 3.23 – 3.19 (m, 1H), 3.01 – 2.94 (m, 1H), 2.63 – 2.43 (m, 2H), 2.38 – 2.08 (m, 12H), 1.93 – 1.74 (m, 3H), 1.59 – 1.48 (m, 1H), 1.33 – 1.22 (m, 1H).

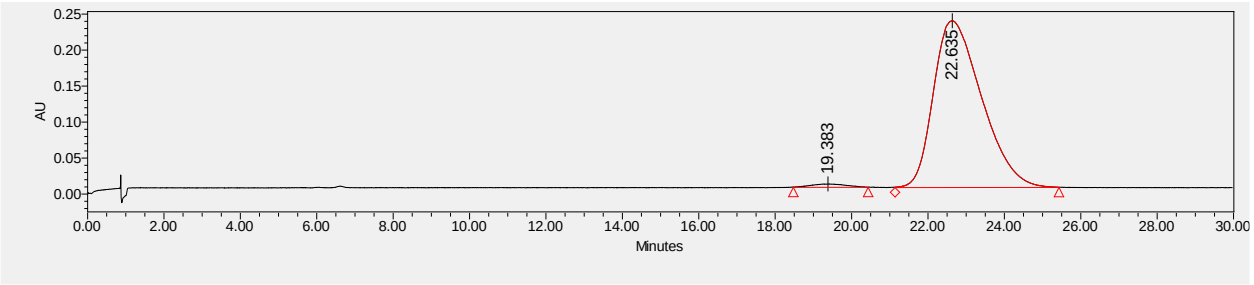
^{13}C NMR (101 MHz, $CDCl_3$) *δ* 178.7, 167.5, 160.1, 152.1, 138.5, 136.1, 134.8, 134.3, 134.0, 133.6, 130.5, 130.3, 129.3, 128.5, 128.0, 127.3, 127.2, 125.5, 125.4, 124.9, 67.8, 42.6, 39.5, 36.1, 29.8, 25.3, 23.7, 21.3, 21.1, 17.4.

IR (neat): *ν* (cm^{-1}): 3411, 2921, 1763, 1653, 1494, 1137, 908, 699.

HRMS (ESI-TOF) calcd for $C_{50}H_{46}N_2O_5^+$ ([M]+K^+) = 793.3038, found 793.3045.

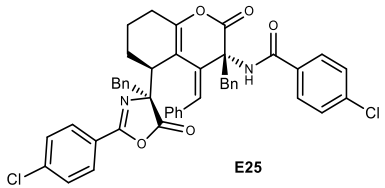


	Retention Time	Area	% Area
1	19.447	28796261	50.03
2	23.507	28759470	49.97



	Retention Time	Area	% Area
1	19.383	301442	1.47
2	22.635	20272957	98.53

_N_-((3_R_,5_S_)-3-benzyl-5-((_S_)-4-benzyl-2-(4-chlorophenyl)-5-oxo-4,5-dihydrooxazol-4-yl)-4-((_E_)-benzylidene)-2-oxo-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)-4-chlorobenzamide (E25)



E25

76.0 mg, 99% yield; white solid, melting point: 150.8 – 154.6 °C, $[\alpha]^{19}_{D}$ = -211.9 (*c* = 2.87, CH_2Cl_2).

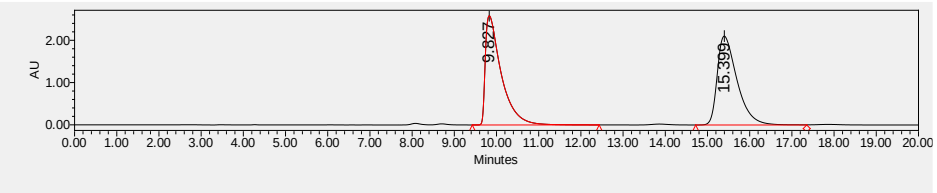
Dissolved in *i*PrOH for HPLC; HPLC (Chiralcel IA, hexane/*i*PrOH = 80/20, flow rate 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 15.61 min, t_{minor} = 10.32 min. er = 99:1. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.71 – 7.61 (m, 4H), 7.40 – 7.25 (m, 7H), 7.26 – 7.10 (m, 7H), 7.06 – 6.93 (m, 6H), 6.83 (s, 1H), 4.57 – 4.22 (m, 1H), 3.61 – 3.43 (m, 1H), 3.22 – 3.15 (m, 1H), 3.04 – 2.96 (m, 1H), 2.58 – 2.47 (m, 2H), 2.00 – 1.82 (m, 4H), 1.60 – 1.48 (m, 1H).

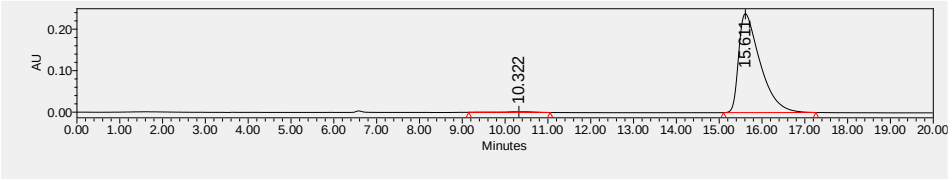
^{13}C NMR (101 MHz, $CDCl_3$) *δ* 178.3, 166.1, 158.9, 152.1, 138.9, 138.2, 133.7, 131.8, 130.4, 130.1, 129.1, 129.1, 129.0, 128.5, 128.5, 128.3, 128.1, 128.0, 127.3, 124.0, 67.6, 42.4, 39.0, 36.0, 29.8, 25.3, 23.5, 17.4.

IR (neat): *ν* (cm^{-1}): 3407, 2951, 1761, 1654, 1479, 1089, 964, 699.

HRMS (ESI-TOF) calcd for $C_{46}H_{36}Cl_2N_2O_5^+$ ([M]+H^+) = 767.2074, 769.2045, found 767.2079, 769.2046.

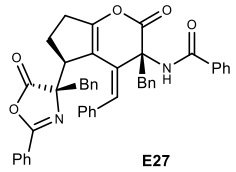


	Retention Time	Area	% Area
1	9.827	67508564	49.70
2	15.399	68320111	50.30



	Retention Time	Area	% Area
1	10.322	84637	1.01
2	15.611	8304589	98.99

_N_-((3_R_,5_S_)-3-benzyl-5-((_S_)-4-benzyl-5-oxo-2-phenyl-4,5-dihydrooxazol-4-yl)-4-((_E_)-benzylidene)-2-oxo-2,3,4,5,6,7-hexahydrocyclopenta[b]pyran-3-yl)benzamide (E27)



E27

28.8 mg, 42% yield; pale yellow solid, melting point: 134.3 – 137.8 °C, $[\alpha]^{20}_{D}$ = -118.5 (*c* = 0.44, CH_2Cl_2).

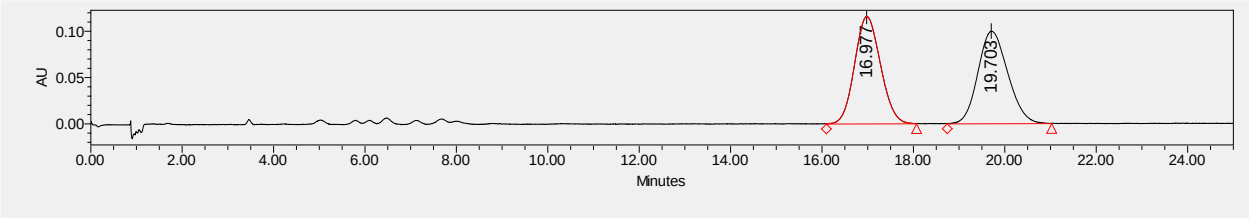
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IC-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 16.99 min, t_{minor} = 19.94 min. er = 97:3. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.73 – 7.60 (m, 4H), 7.52 – 7.31 (m, 11H), 7.23 – 7.10 (m, 5H), 7.10 – 6.85 (m, 6H), 6.48 (s, 1H), 3.92 – 3.77 (m, 1H), 3.59 – 3.47 (m, 1H), 3.21 – 3.10 (m, 1H), 2.96 – 2.82 (m, 2H), 2.60 – 2.48 (m, 1H), 2.30 – 2.10 (m, 2H), 1.27 – 1.22 (m, 1H).

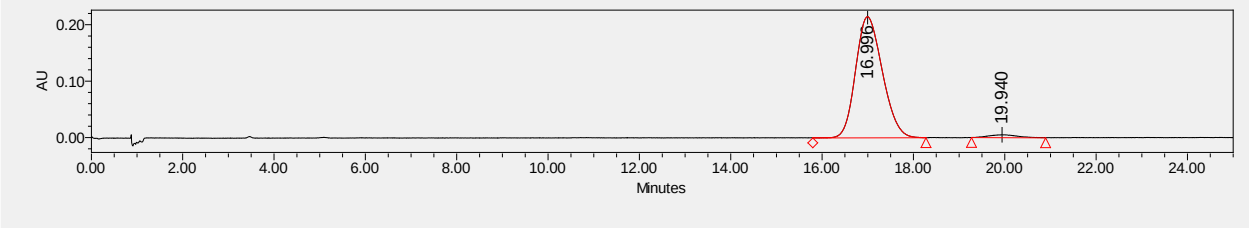
^{13}C NMR (101 MHz, $CDCl_3$) *δ* 178.5, 168.3, 159.9, 156.4, 137.6, 134.1, 132.6, 132.1, 130.9, 130.3, 129.6, 129.1, 128.8, 128.7, 128.1, 128.0, 127.9, 127.2, 127.1, 125.7, 77.6, 47.6, 40.4, 29.8, 29.6, 24.1.

IR (neat): *ν* (cm^{-1}): 3428, 2926, 1781, 1656, 1479, 1289, 971, 698.

HRMS (ESI-TOF) calcd for $C_{45}H_{36}N_2O_5^+$ ([M]+Na^+) = 707.2516, found 707.2516.

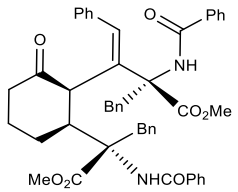


	Retention Time	Area	% Area
1	16.977	4572549	50.17
2	19.703	4540778	49.83



	Retention Time	Area	% Area
1	16.996	8735853	97.45
2	19.940	228815	2.55

Methyl (*R*,*E*)-2-benzamido-3-((1*R*,2*S*)-2-((*S*)-2-benzamido-1-methoxy-1-oxo-3-phenylpropan-2-yl)-6-oxocyclohexyl)-2-benzyl-4-phenylbut-3-enoate (F1)



F1

137.3 mg, 90% yield; white solid, melting point: 63.4 – 65.9 °C, $[\alpha]^{23}_D$ = -34.9 (*c* = 1.25, CH_2Cl_2).

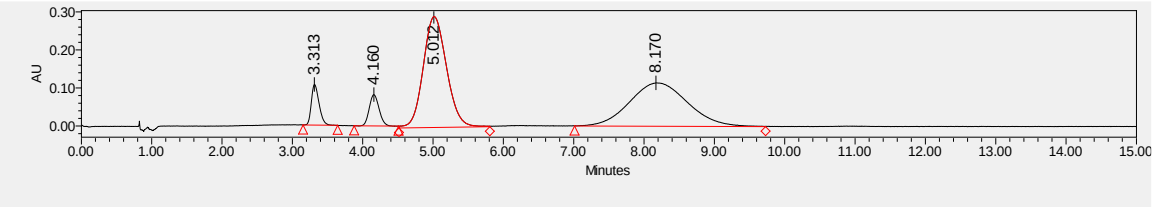
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel AD-3, CO_2/MeOH = 85/15, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 3.58 min. er >99:1. dr >19:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.35 (m, 2H), 7.36 – 7.24 (m, 12H), 7.23 – 7.14 (m, 6H), 7.15 – 7.08 (m, 4H), 7.09 – 7.05 (m, 4H), 4.35 – 4.29 (m, 2H), 4.01 – 3.93 (m, 4H), 3.69 – 3.60 (m, 2H), 3.45 – 3.39 (m, 2H), 3.36 (s, 6H), 2.44 – 2.33 (m, 2H).

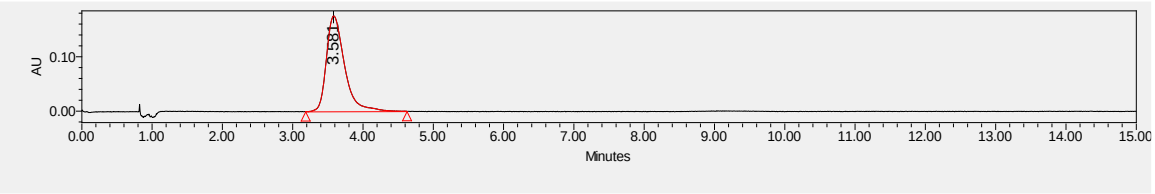
^{13}C NMR (101 MHz, $CDCl_3$) δ 199.4, 170.4, 168.4, 141.6, 138.2, 136.7, 136.5, 136.2, 130.5, 129.2, 128.8, 128.7, 128.5, 128.3, 127.1, 126.9, 126.6, 79.3, 66.9, 52.6, 41.5, 36.2, 31.7, 30.9, 20.7.

IR (neat): ν (cm^{-1}): 3030, 2949, 2360, 1741, 1632, 1398, 1232, 702, 489.

HRMS (ESI-TOF) calcd for $C_{48}H_{46}N_2O_7^+$ ([M]+Na^+) = 785.3197, found 785.3198.

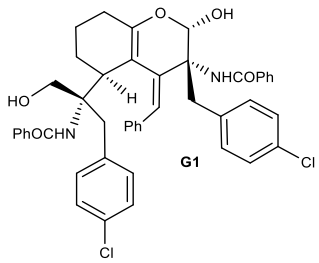


	Retention Time	Area	% Area
1	3.313	814683	5.47
2	4.160	800975	5.38
3	5.012	6717973	45.12
4	8.170	6554836	44.03



	Retention Time	Area	% Area
1	3.581	3184177	100.00

_N_-((2_S_,3_R_,5_S_)-5-((_S_)-2-benzamido-1-(4-chlorophenyl)-3-hydroxypropan-2-yl)-4-((_E_)-benzylidene)-3-(4-chlorobenzyl)-2-hydroxy-3,4,5,6,7,8-hexahydro-2H-chromen-3-yl)benzamide (G1)



G1

146.8 mg, 95% yield; white solid, melting point: 138.7 – 141.0 °C, $[\alpha]^{22}_{D}$ = -170.7 (*c* = 1.31, CH_2Cl_2).

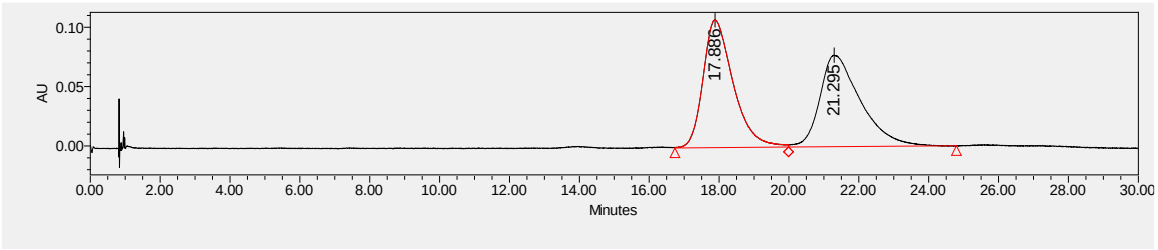
Dissolved in *i*PrOH for SFC; SFC (Daicel chiralcel IA-3, CO_2/EtOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm) retention time: t_{major} = 21.63 min, t_{minor} = - min. er >99:1. dr >19:1.

^{1}H NMR (400 MHz, Acetone-d_6) δ 7.88 – 7.79 (m, 4H), 7.59 – 7.44 (m, 6H), 7.29 – 7.05 (m, 12H), 7.01 – 6.97 (m, 2H), 6.92 – 6.80 (m, 2H), 6.43 (s, 1H), 6.39 – 6.35 (m, 1H), 5.14 – 5.11 (m, 1H), 4.95 – 4.90 (m, 1H), 4.65 – 4.59 (m, 1H), 4.13 – 4.07 (m, 1H), 3.71 – 3.66 (m, 1H), 3.59 – 3.51 (m, 1H), 3.40 – 3.35 (m, 1H), 3.08 – 2.98 (m, 2H), 2.94 – 2.88 (m, 3H), 2.14 – 2.08 (m, 2H).

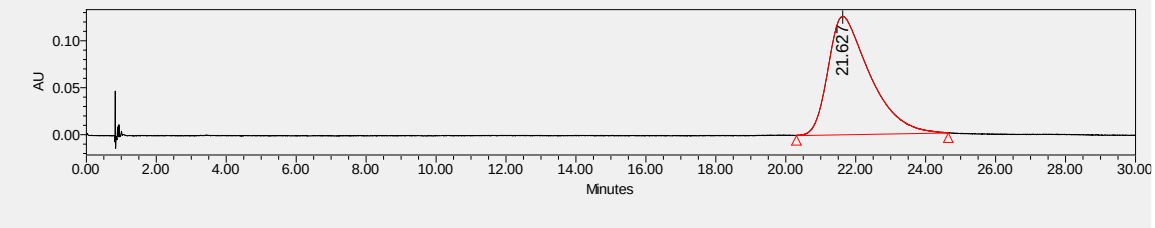
^{13}C NMR (101 MHz, Acetone-d_6) δ 170.0, 169.1, 153.3, 140.4, 138.0, 137.7, 137.6, 137.6, 134.3, 134.2, 133.9, 133.4, 133.3, 130.7, 130.7, 130.5, 129.9, 129.8, 129.6, 129.0, 128.8, 128.7, 126.0, 107.8, 94.9, 69.1, 67.3, 64.5, 40.1, 38.8, 37.2, 28.5, 25.6, 20.7.

IR (neat): ν (cm^{-1}): 3408, 3059, 2940, 2859, 1647, 1519, 1299, 1067, 835, 703.

HRMS (ESI-TOF) calcd for $C_{46}H_{42}Cl_2N_2O_5^+$ ([M]+H^+) = 773.2544, 775.2514, found 773.2534, 775.2524.



	Retention Time	Area	% Area
1	17.886	6433856	50.91
2	21.295	6204618	49.09



	Retention Time	Area	% Area
1	21.627	10473834	100.00

12. References

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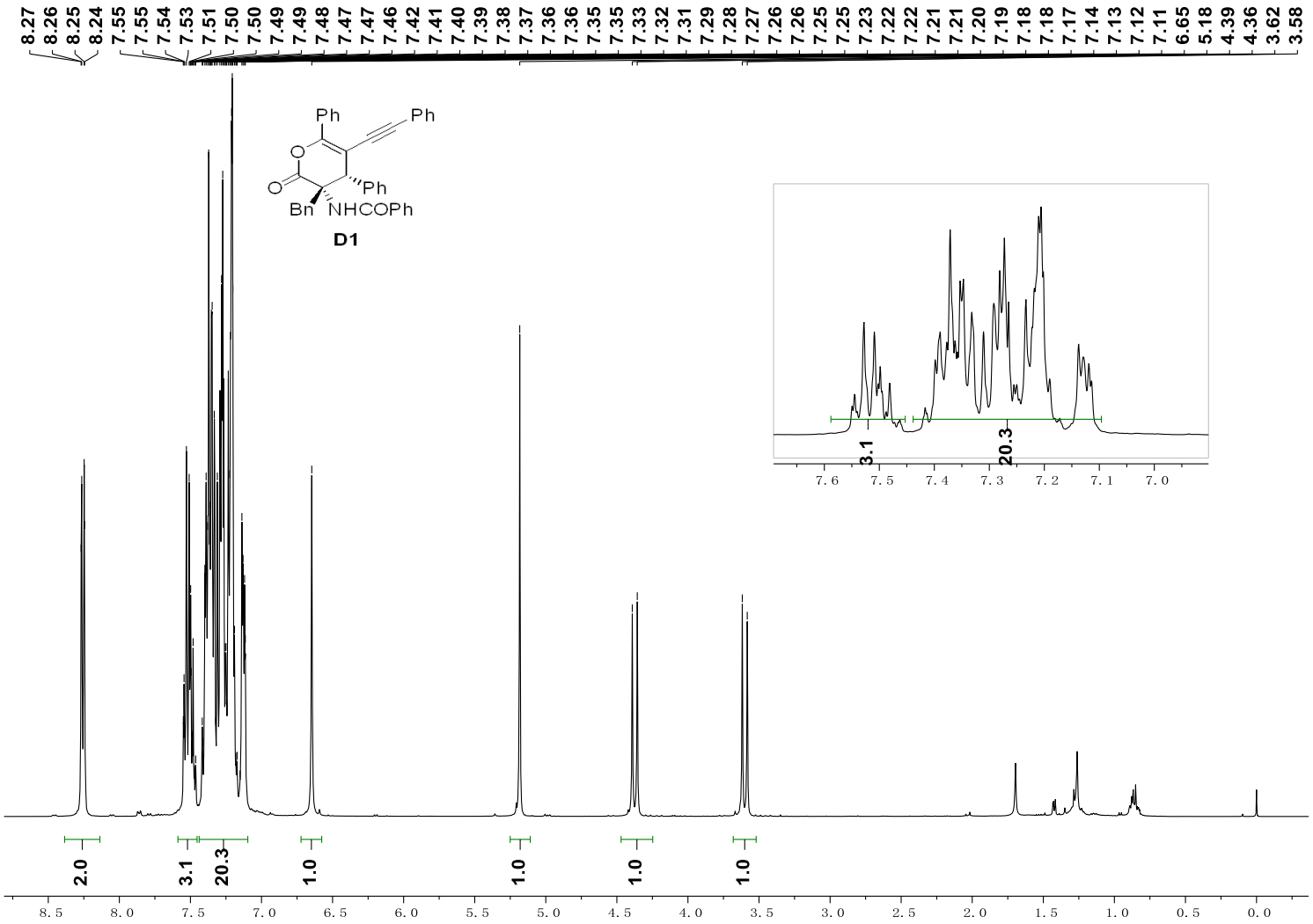
13. Copies of NMR spectra for products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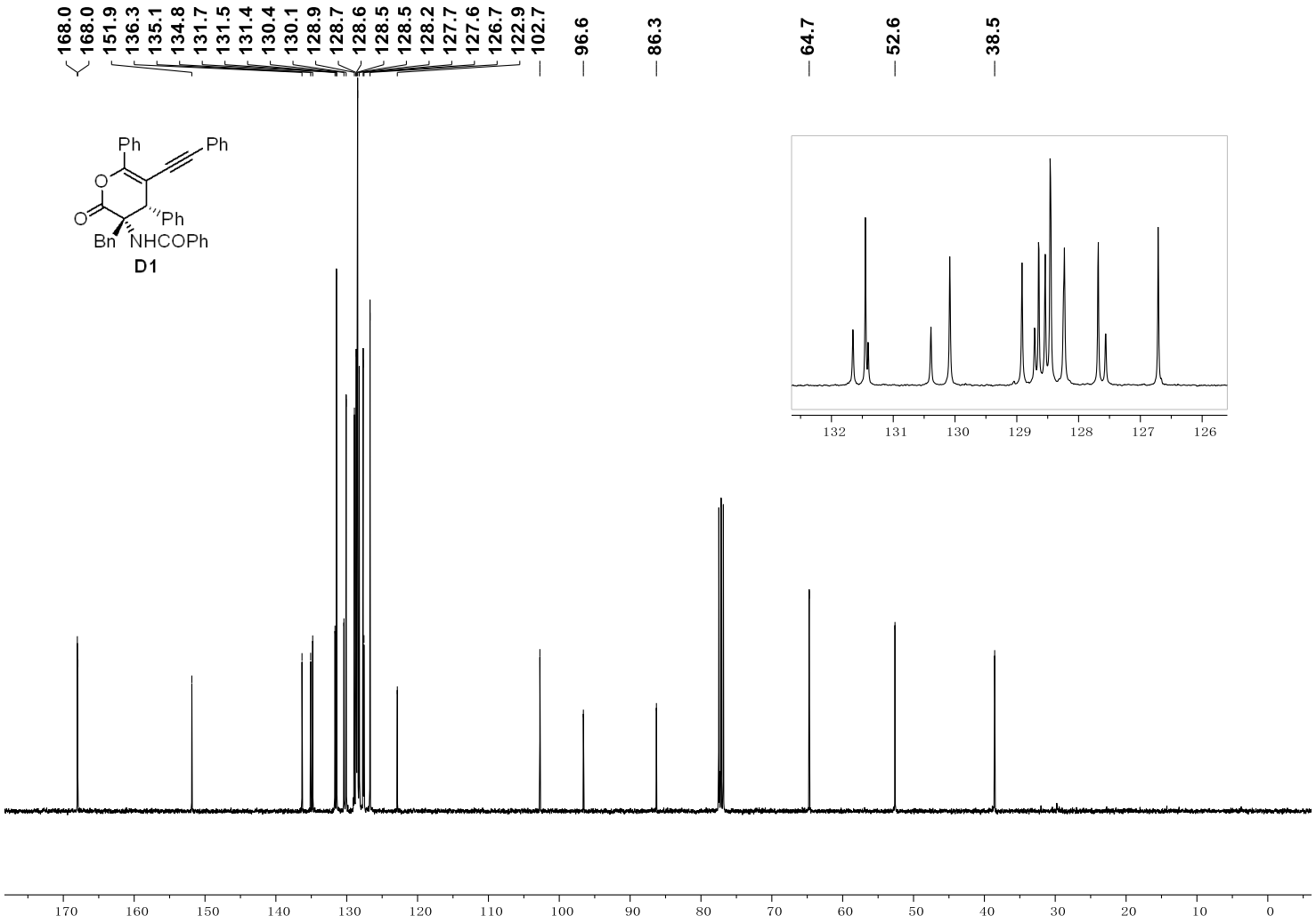
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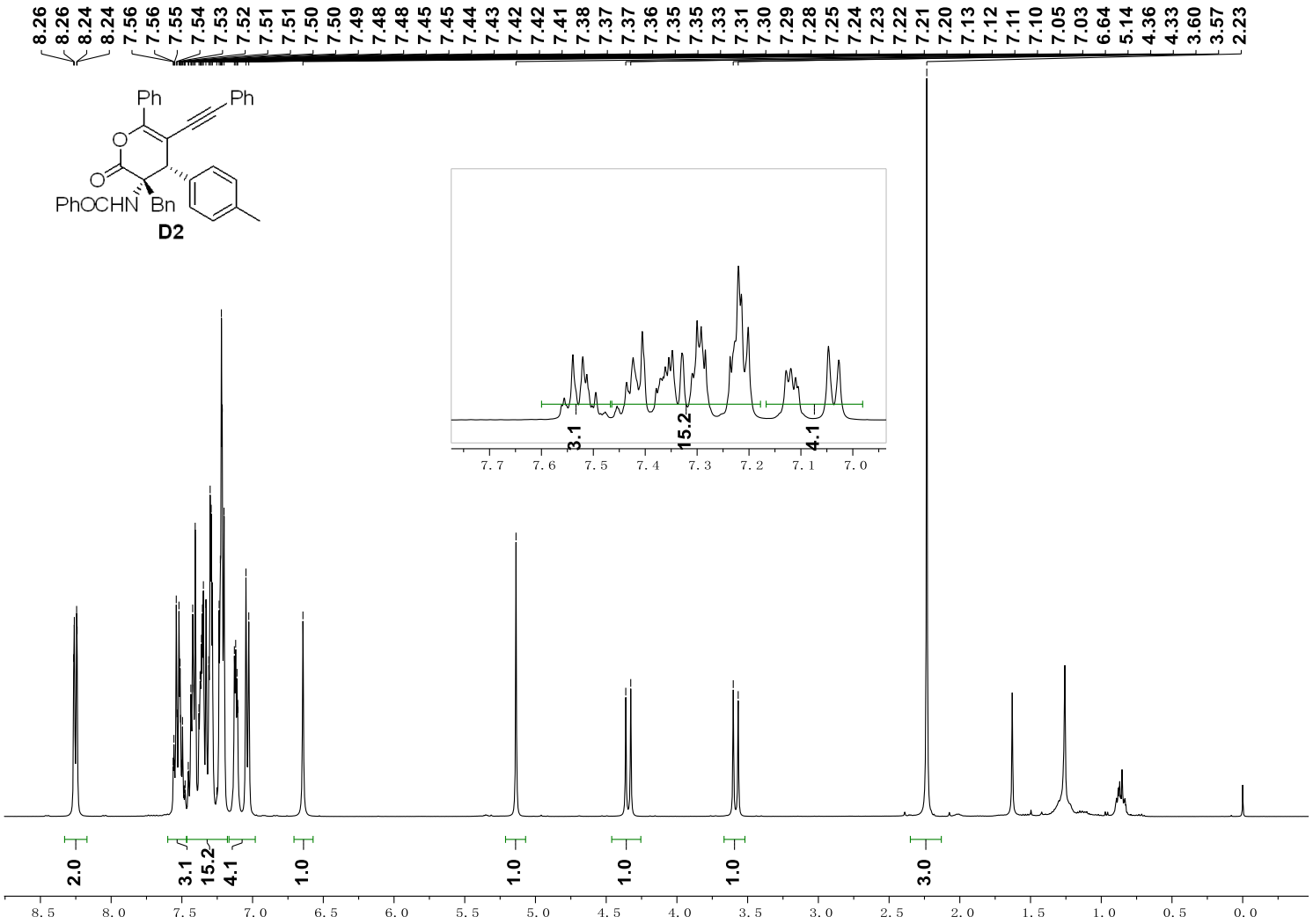
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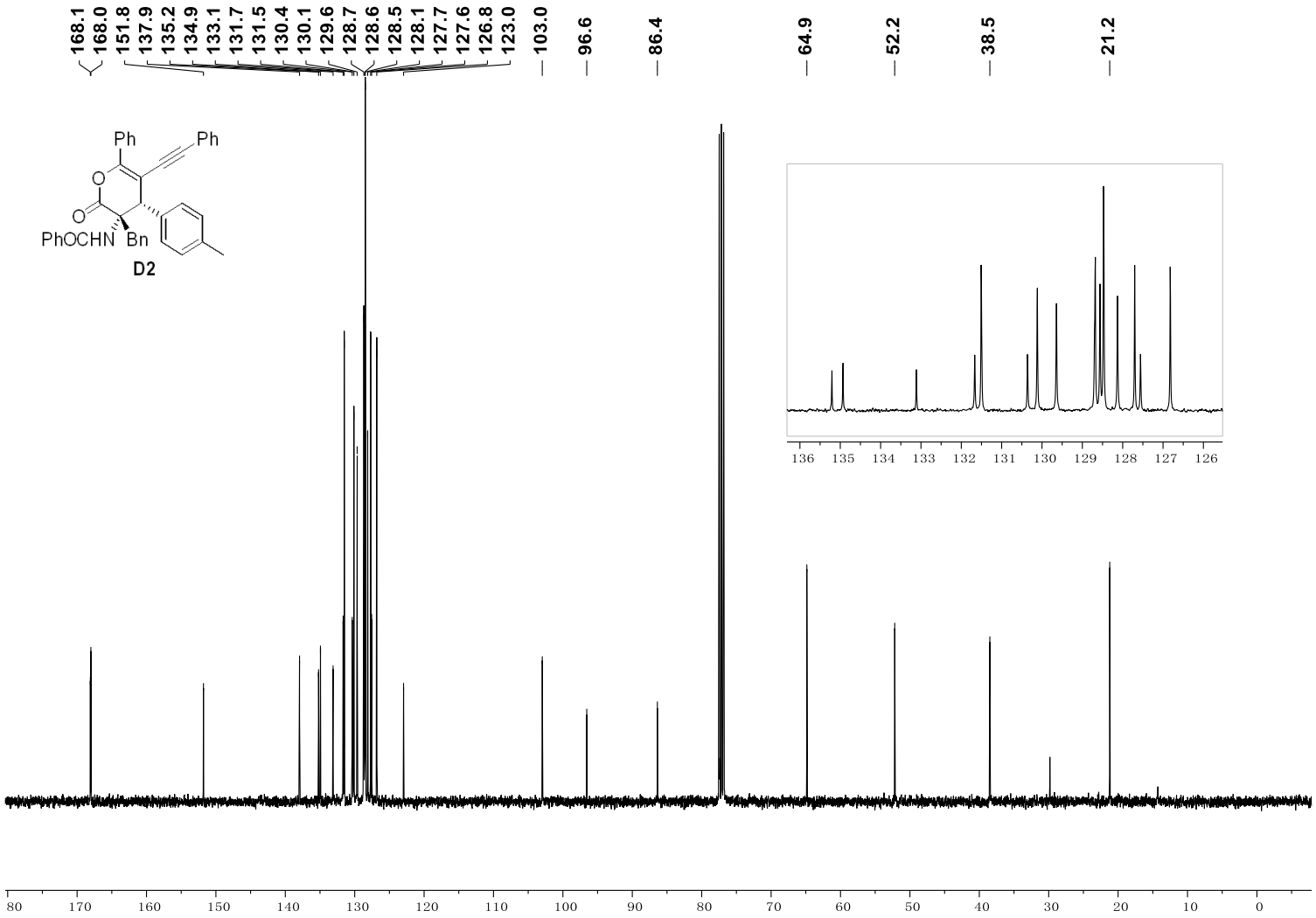
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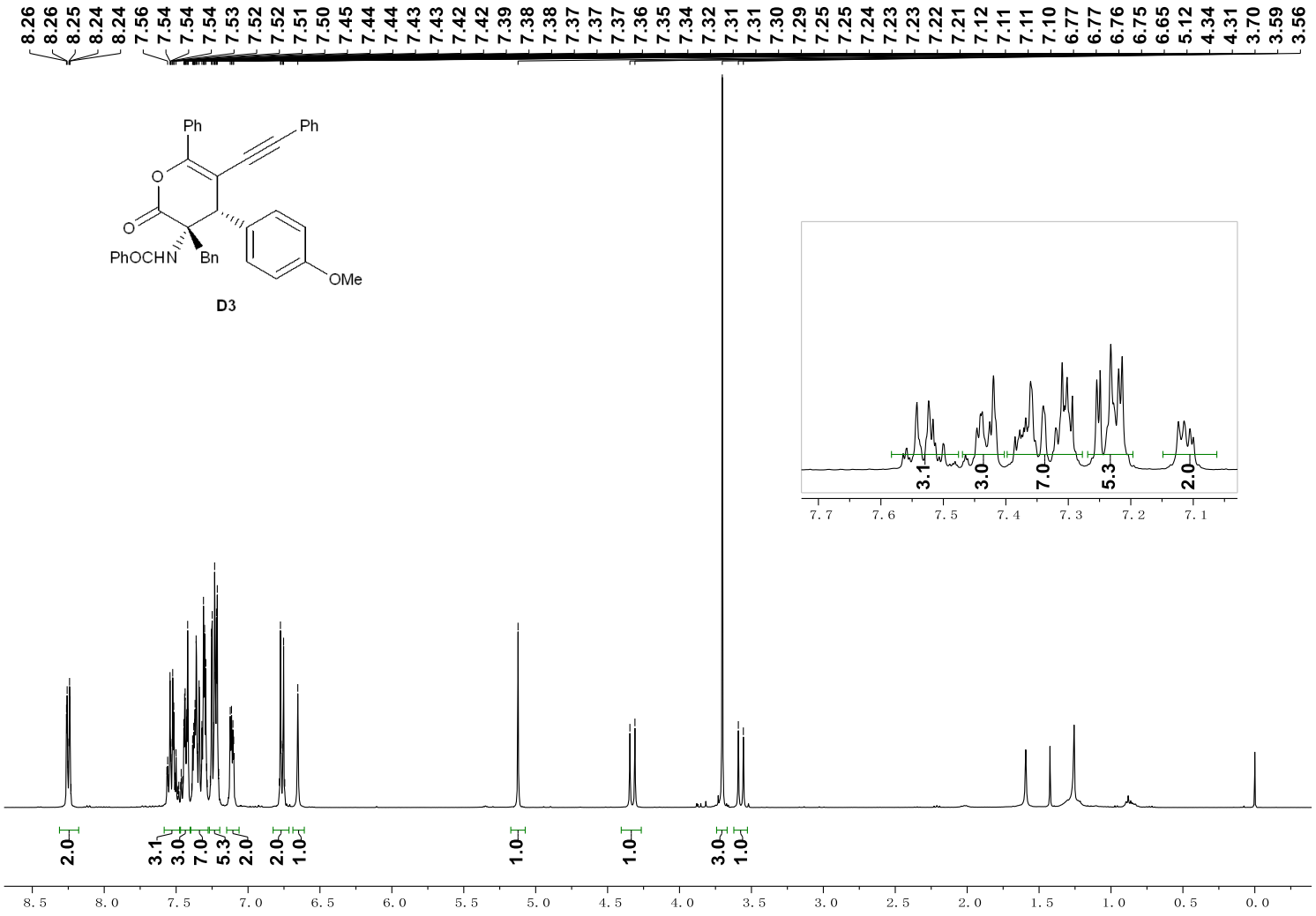
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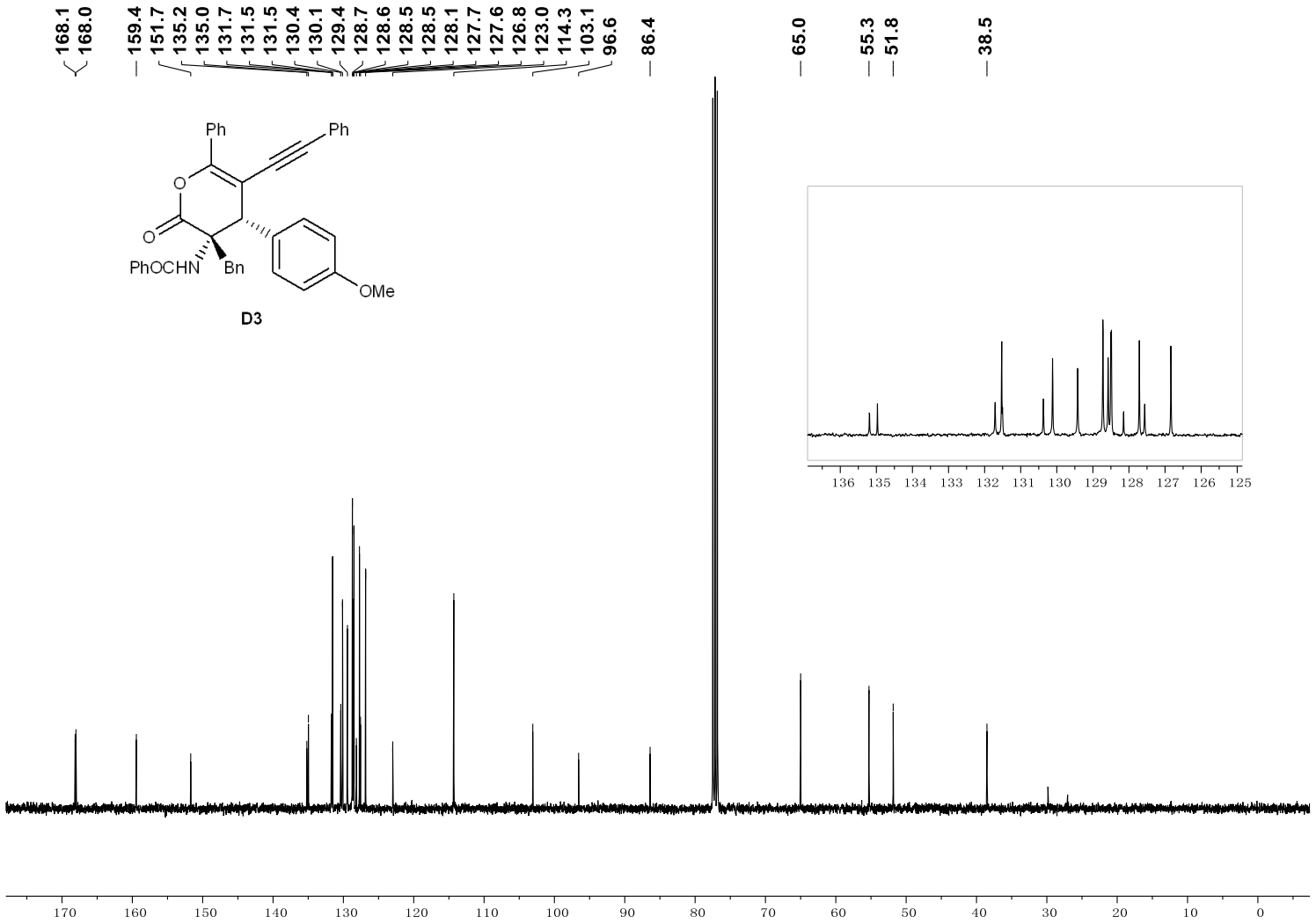
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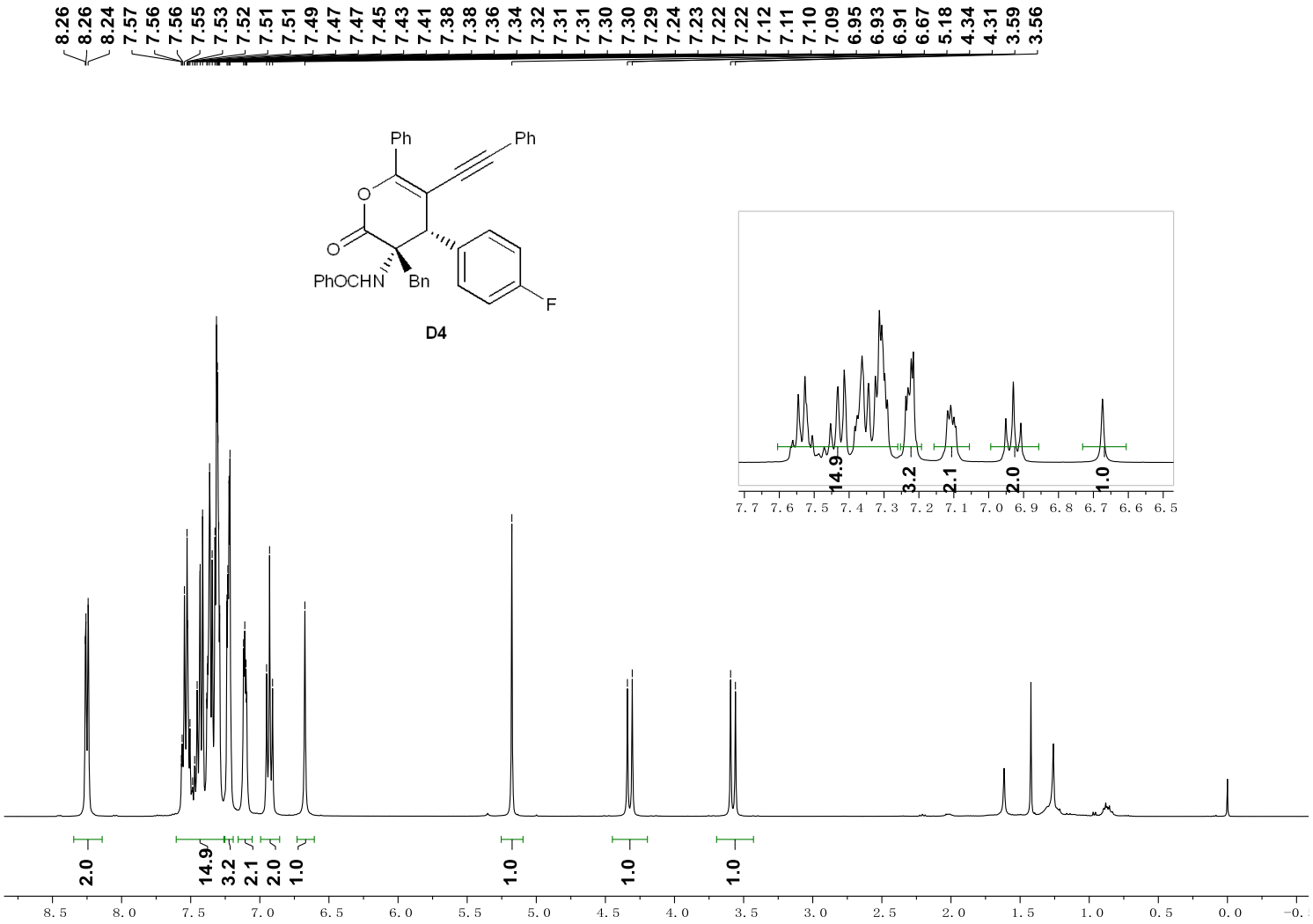
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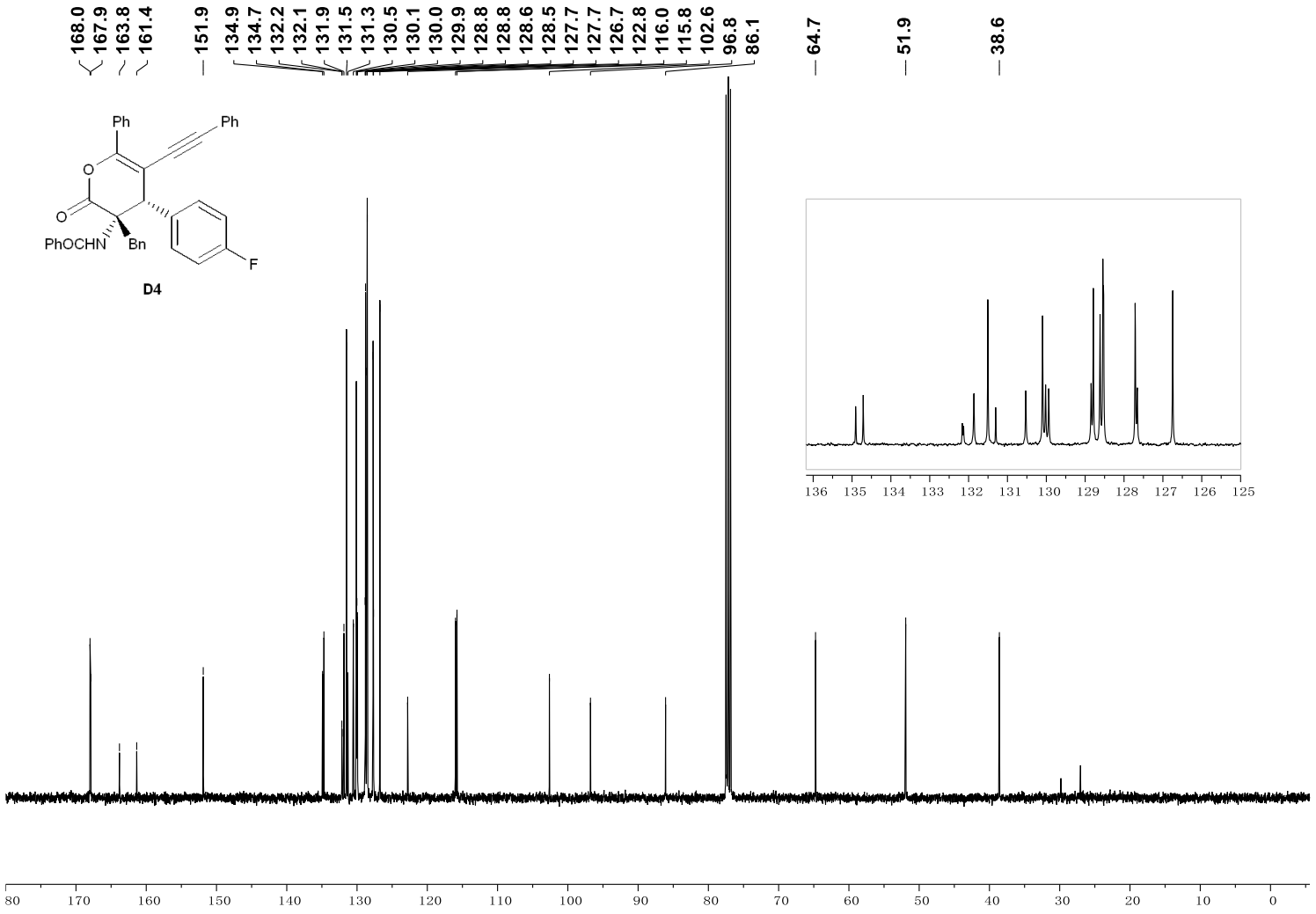
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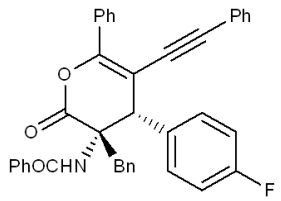
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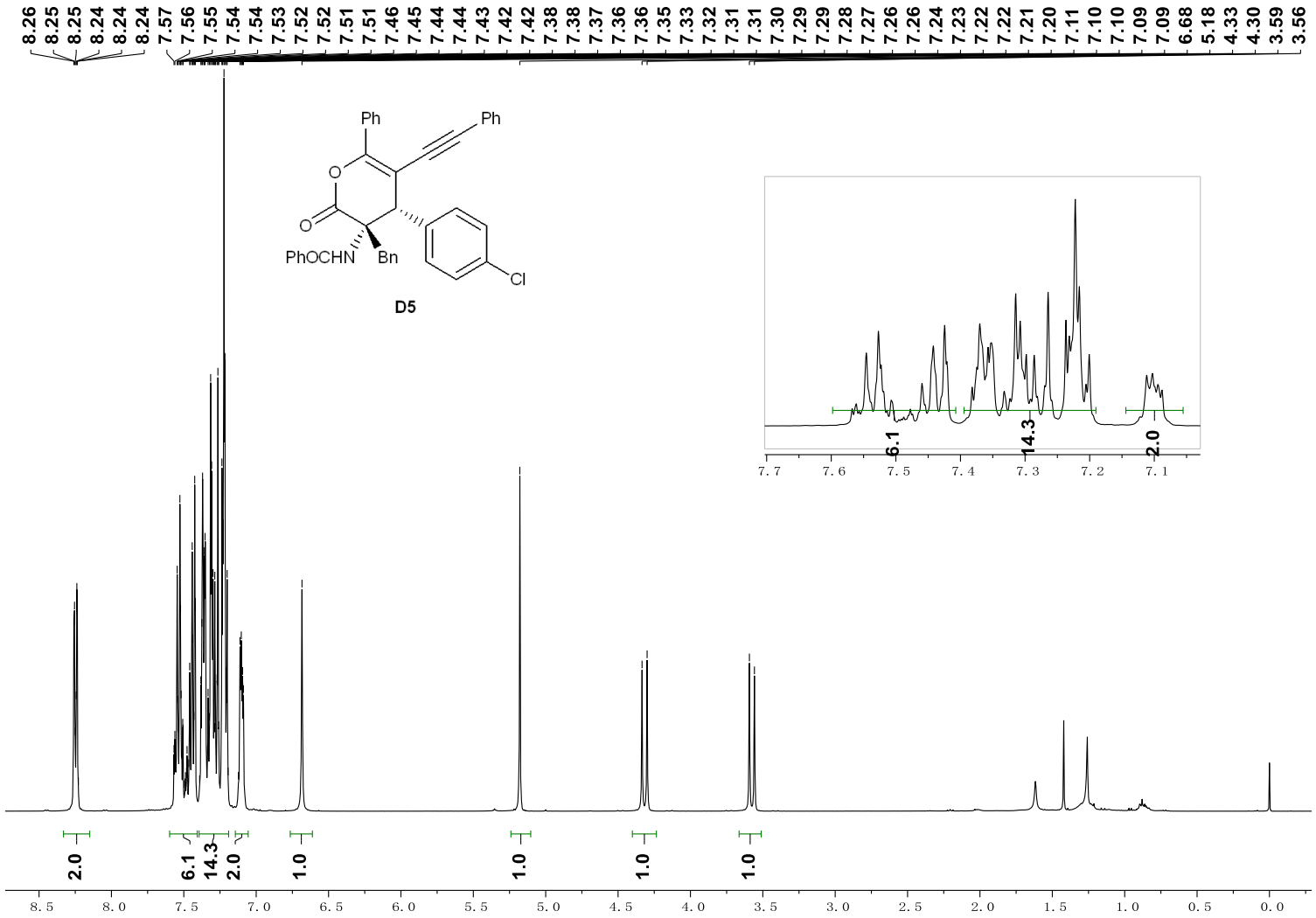
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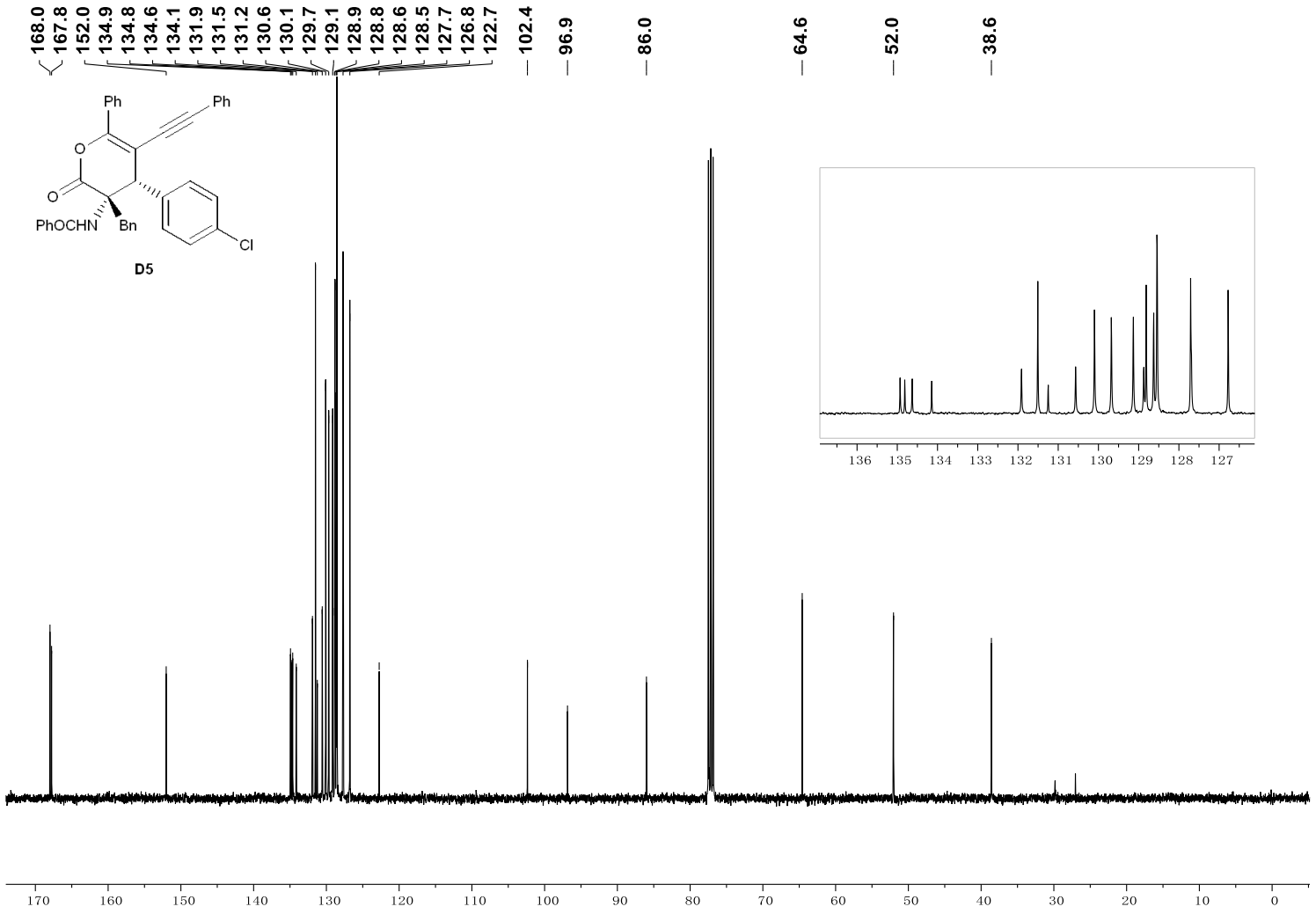
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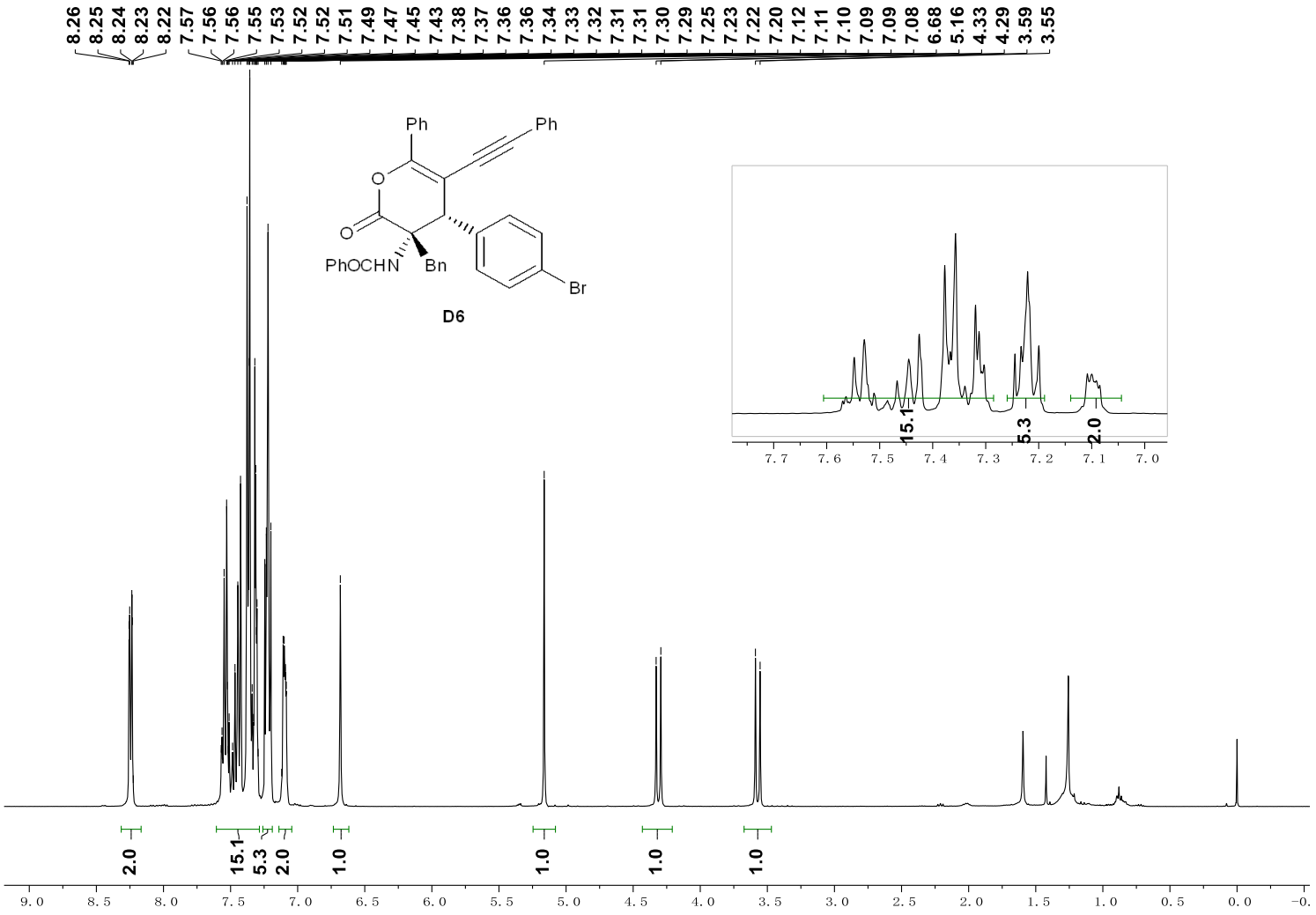
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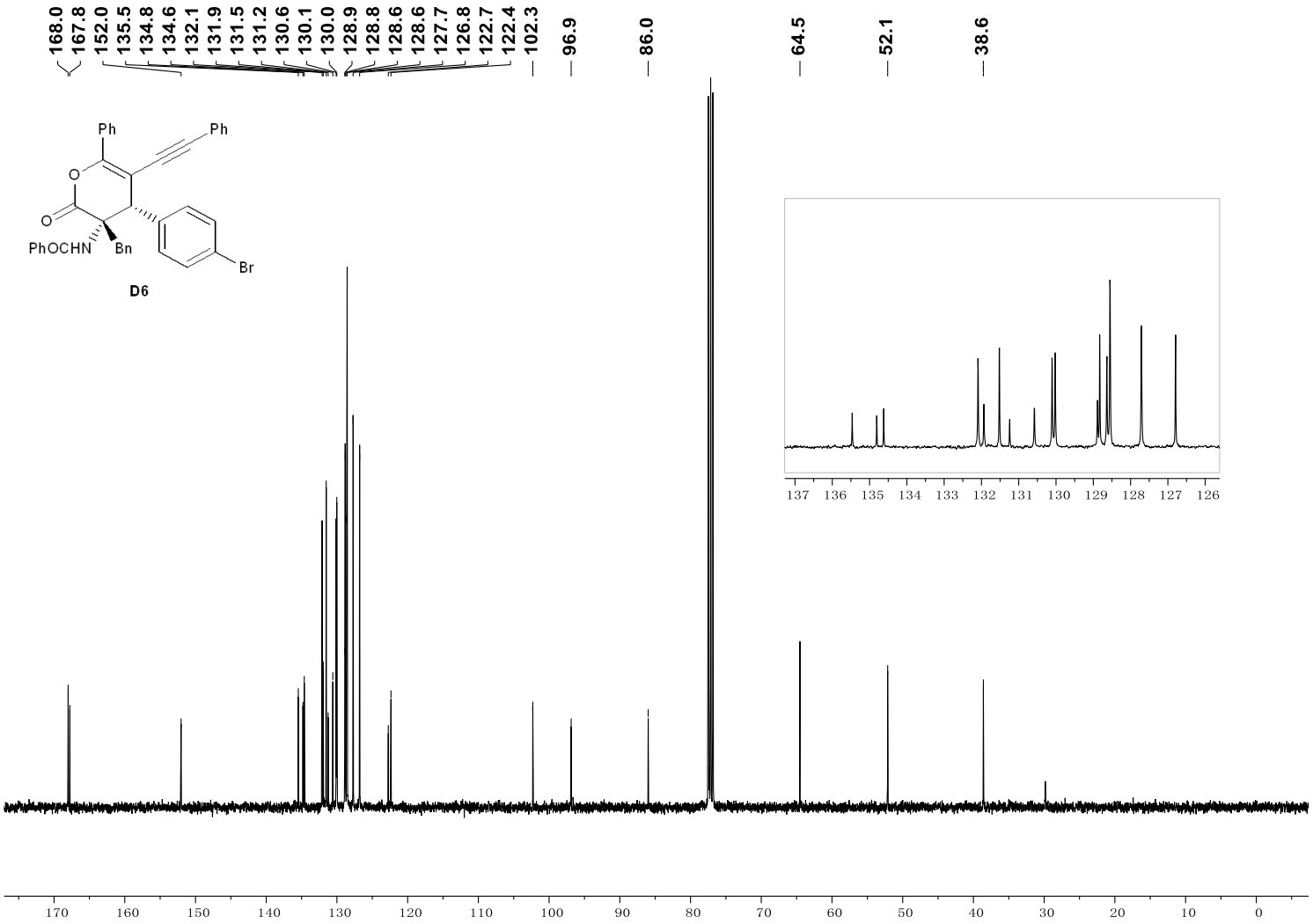
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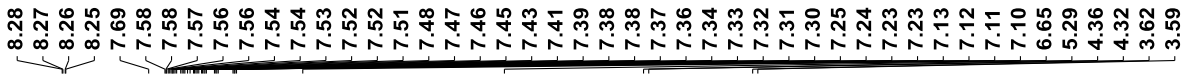
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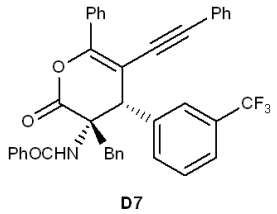
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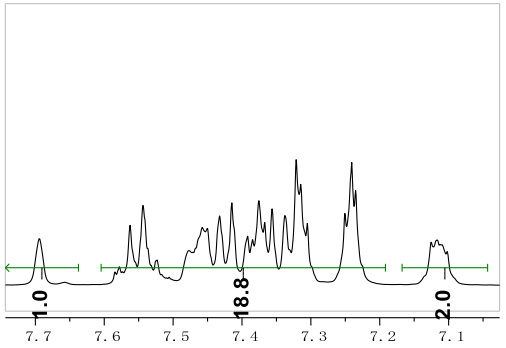
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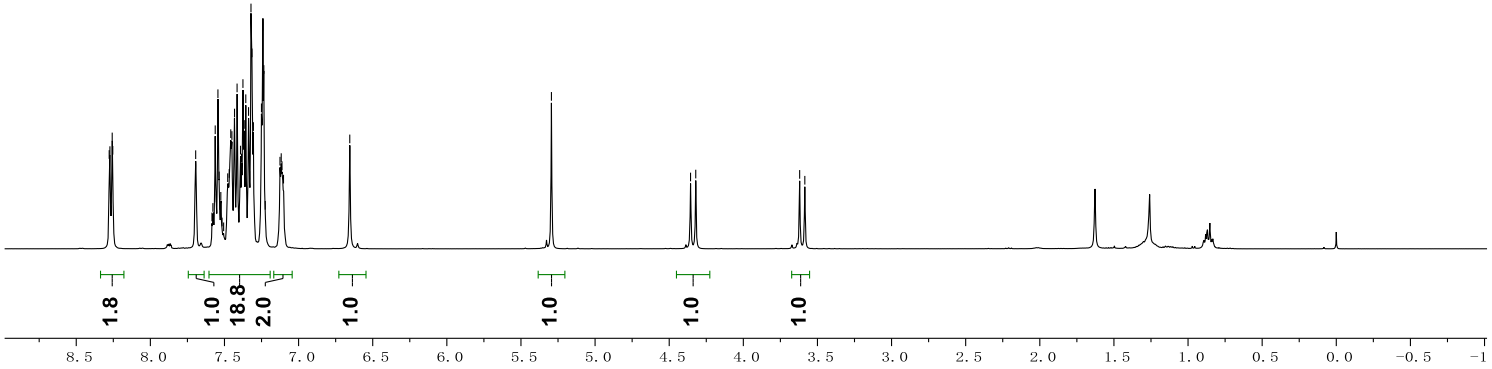
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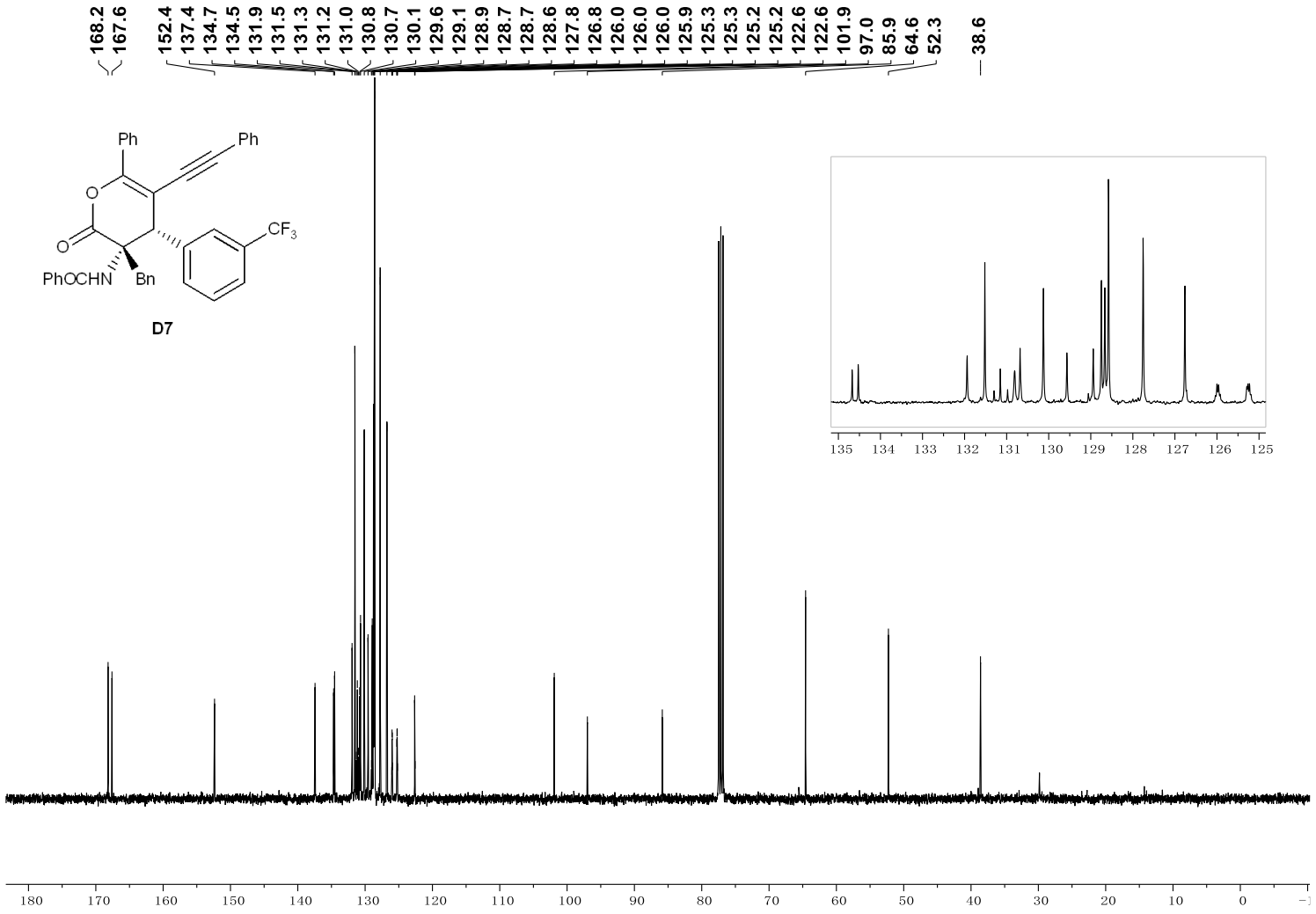
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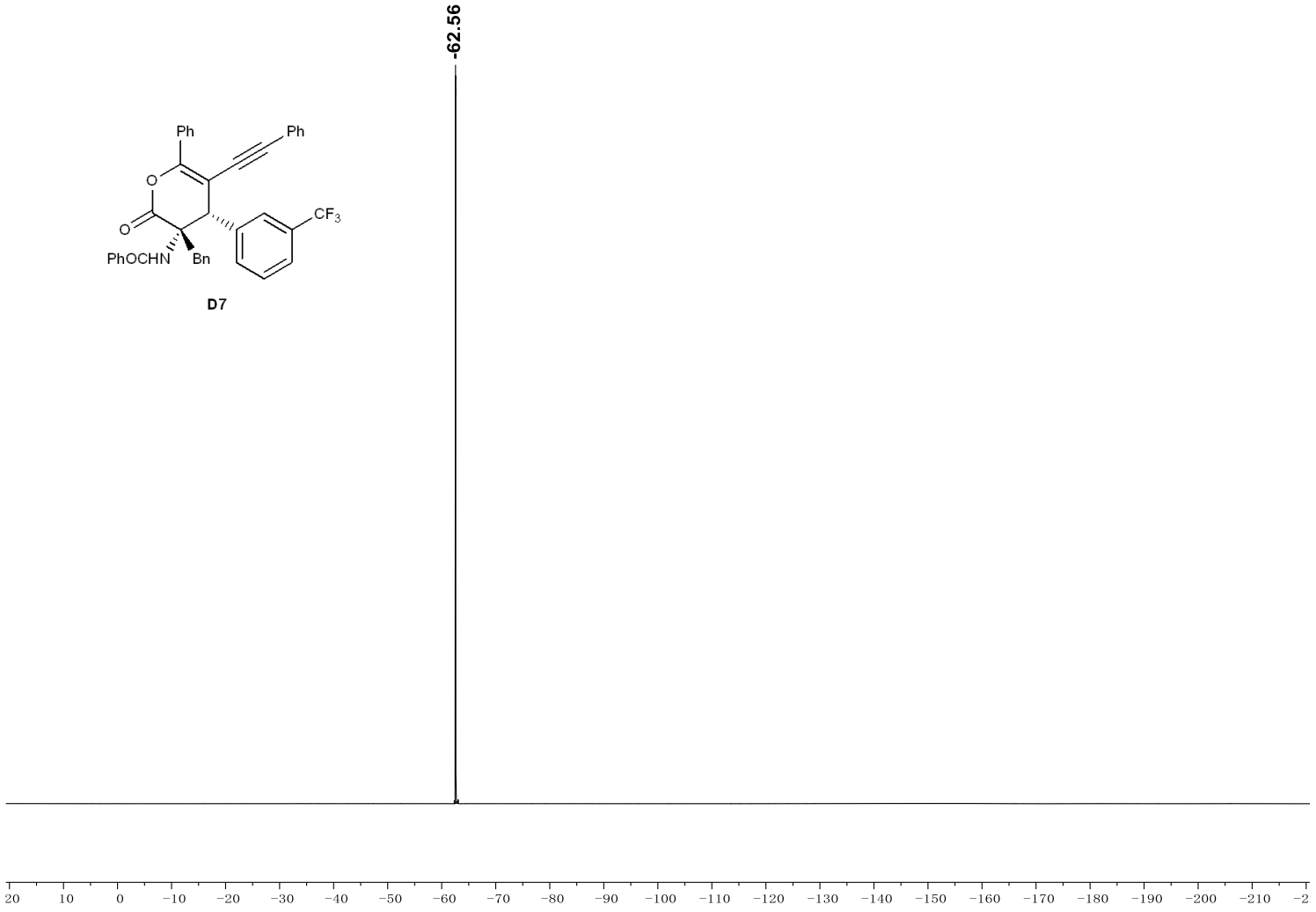
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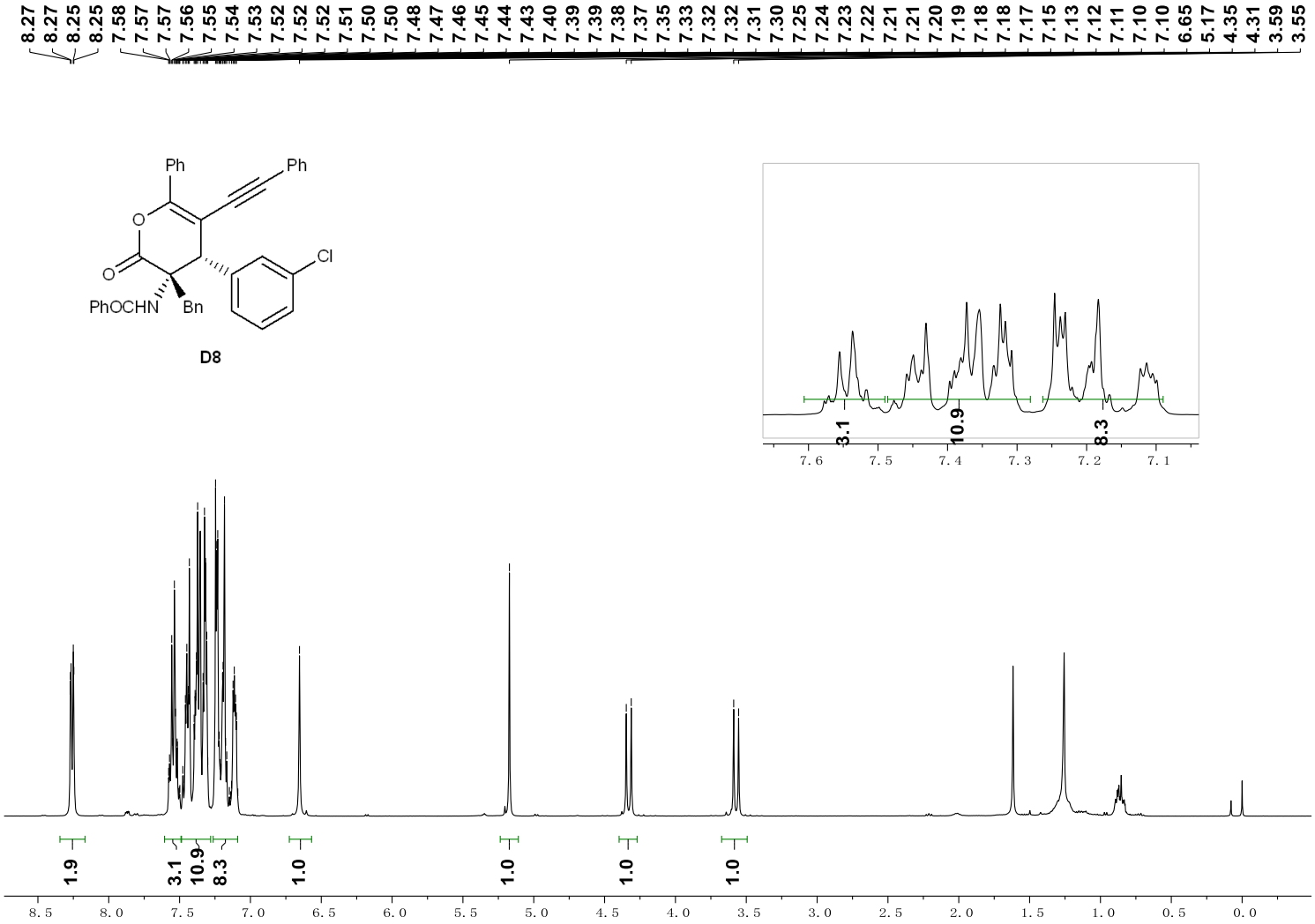
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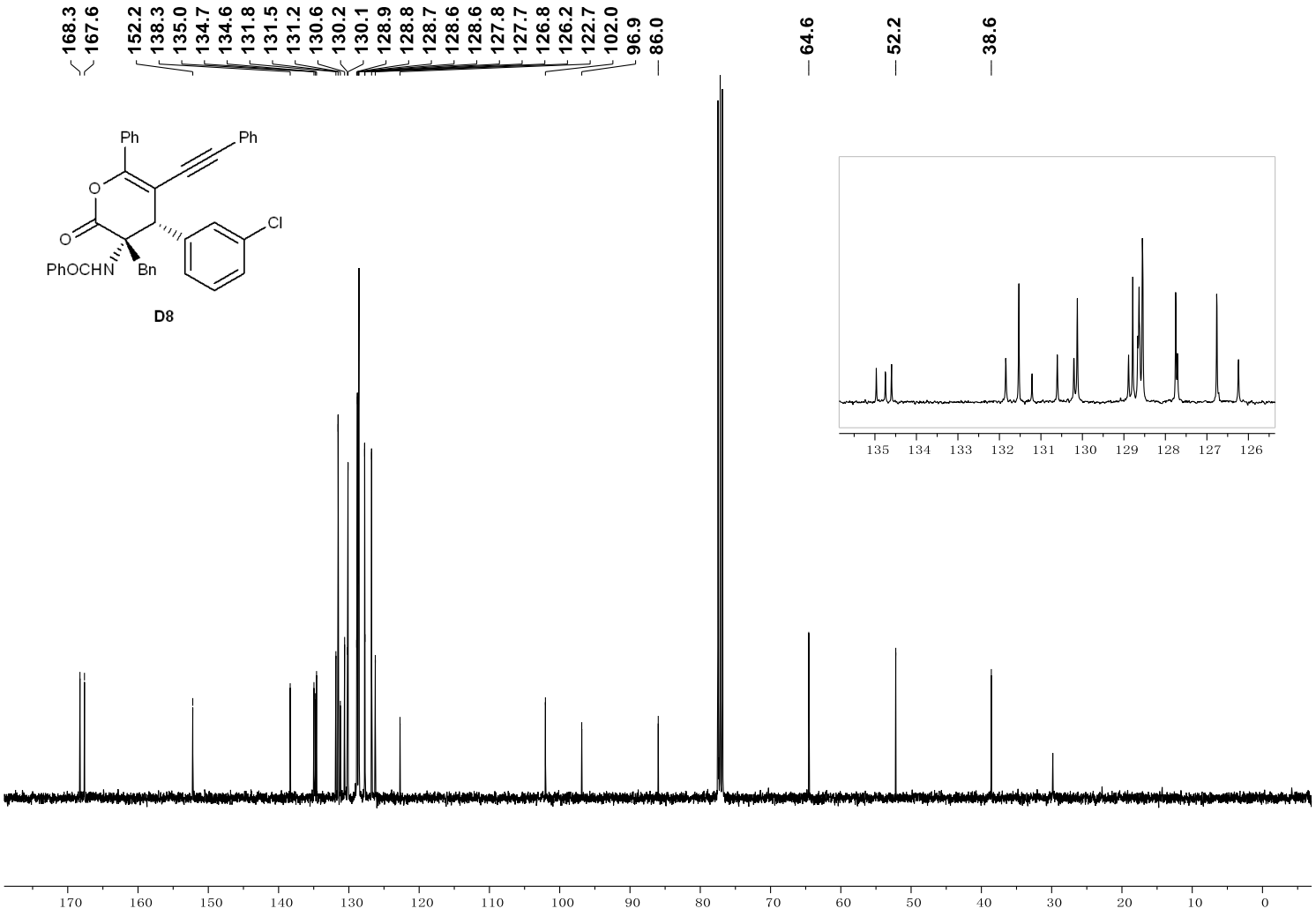
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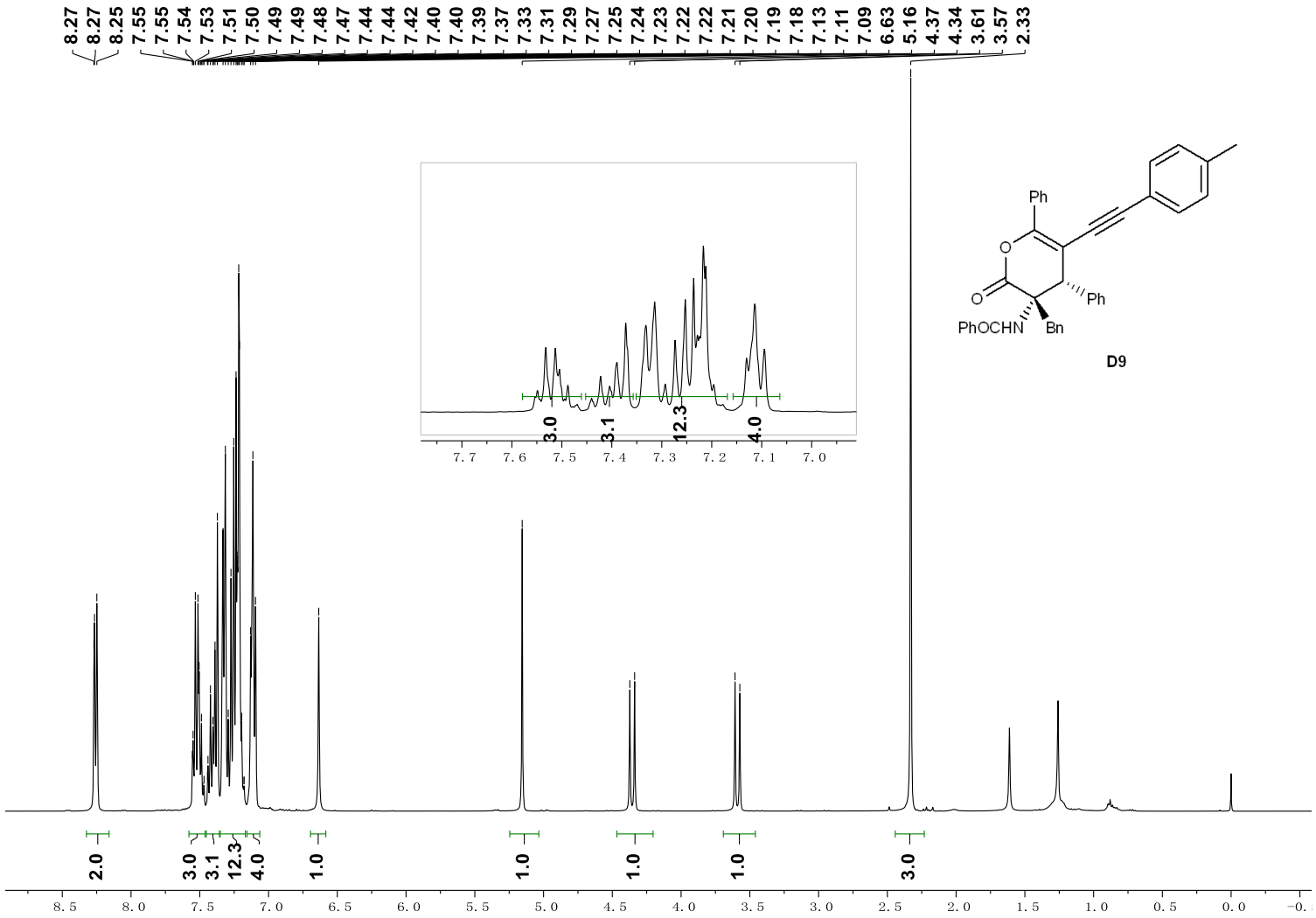
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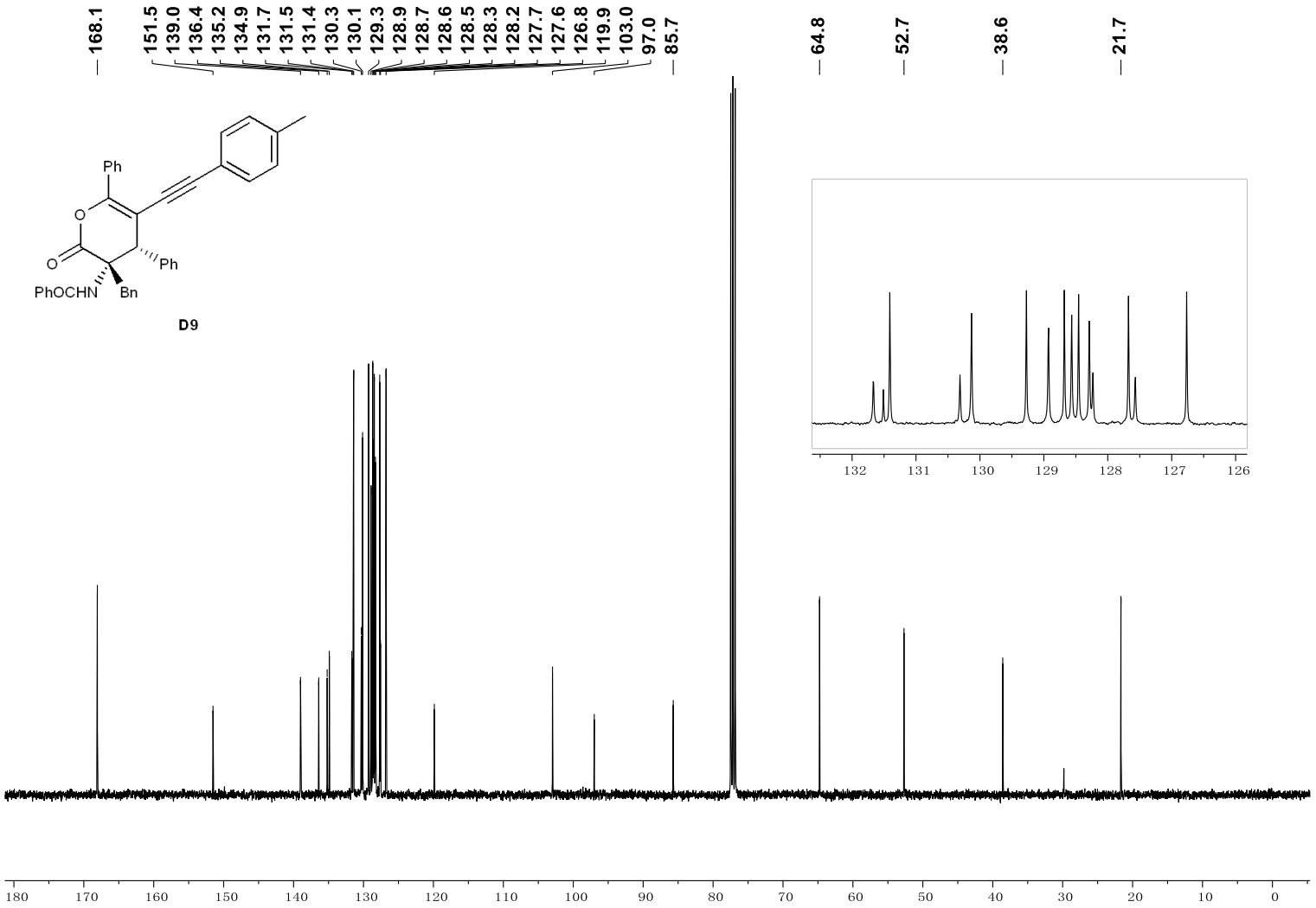
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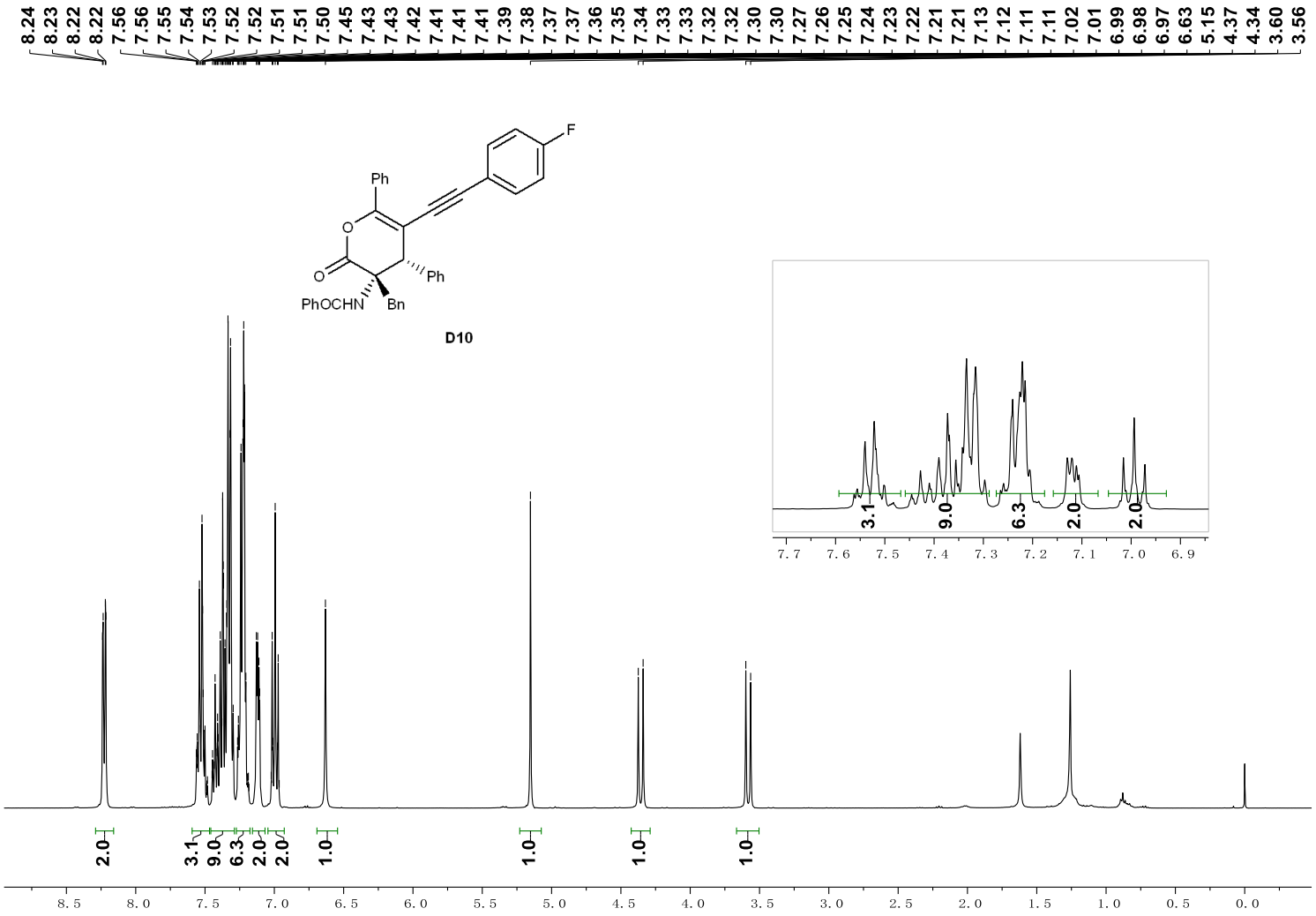
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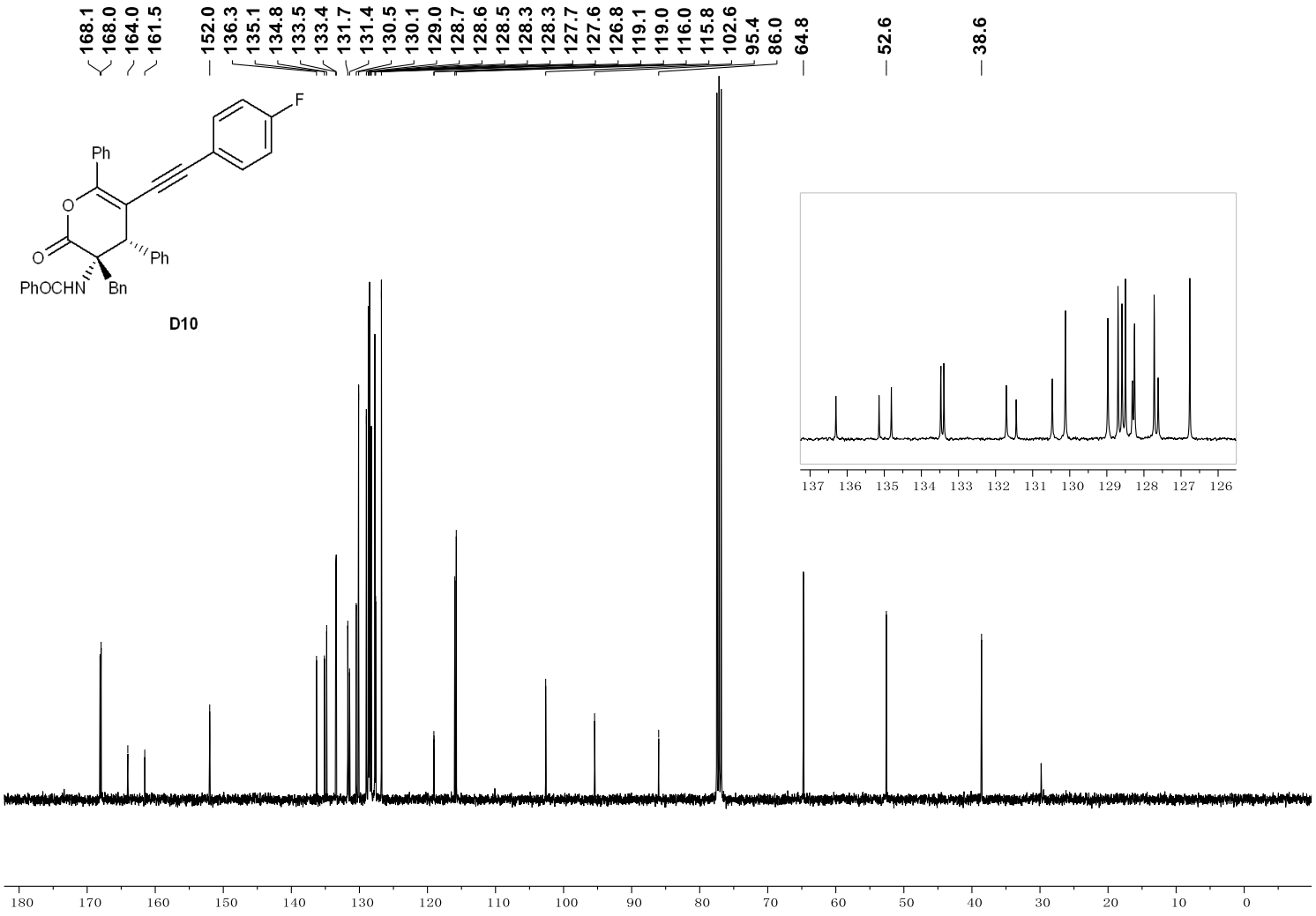
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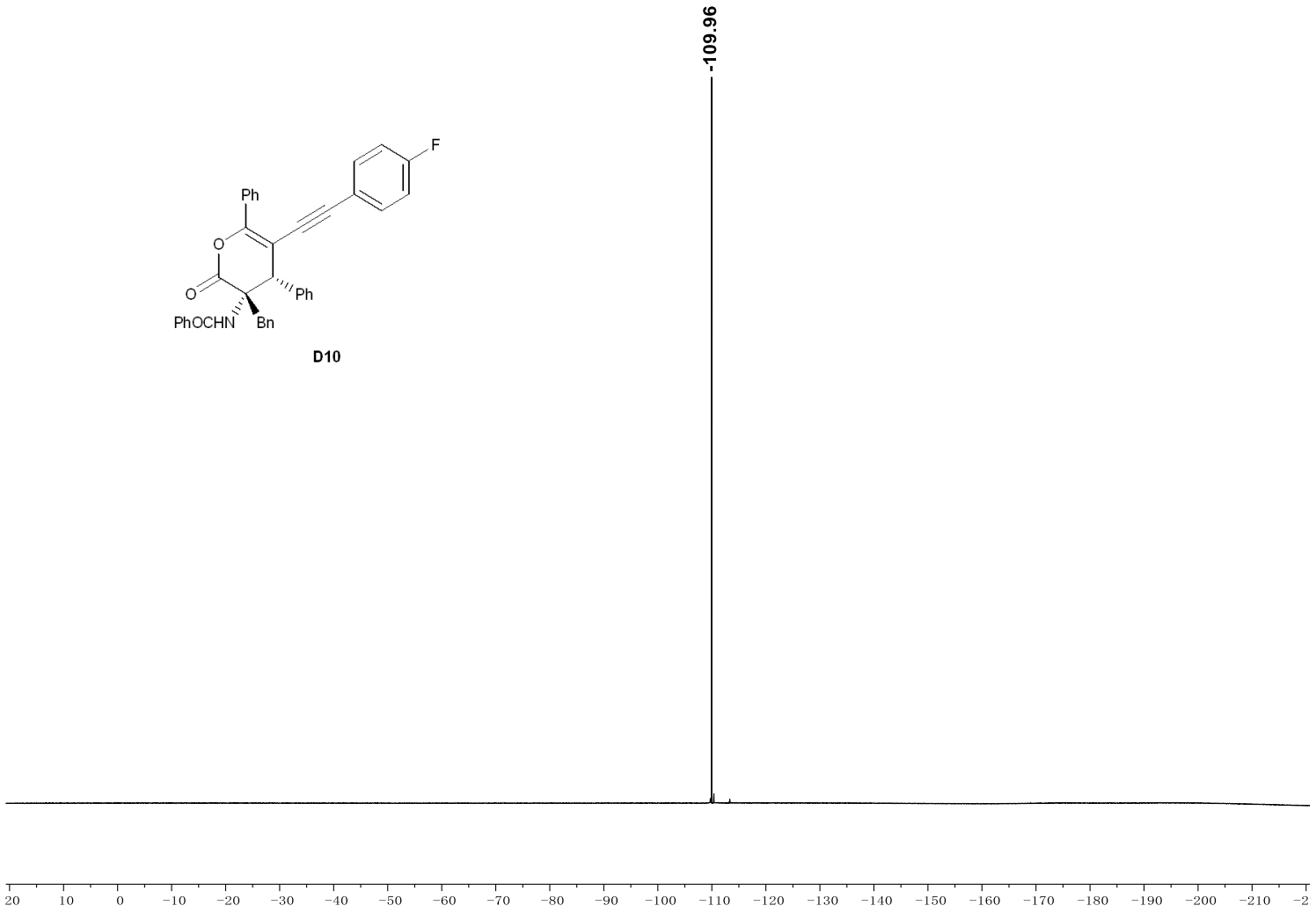
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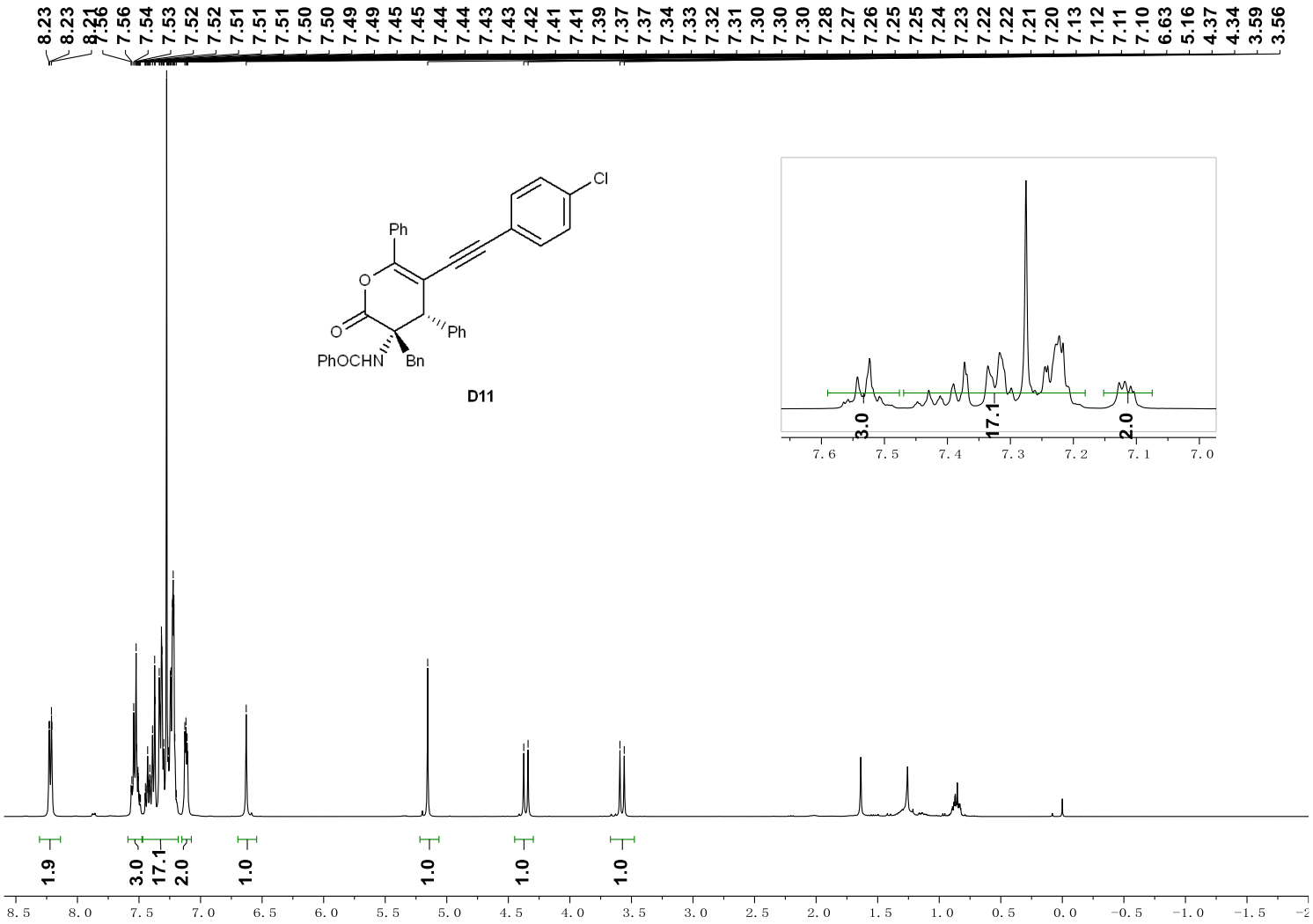
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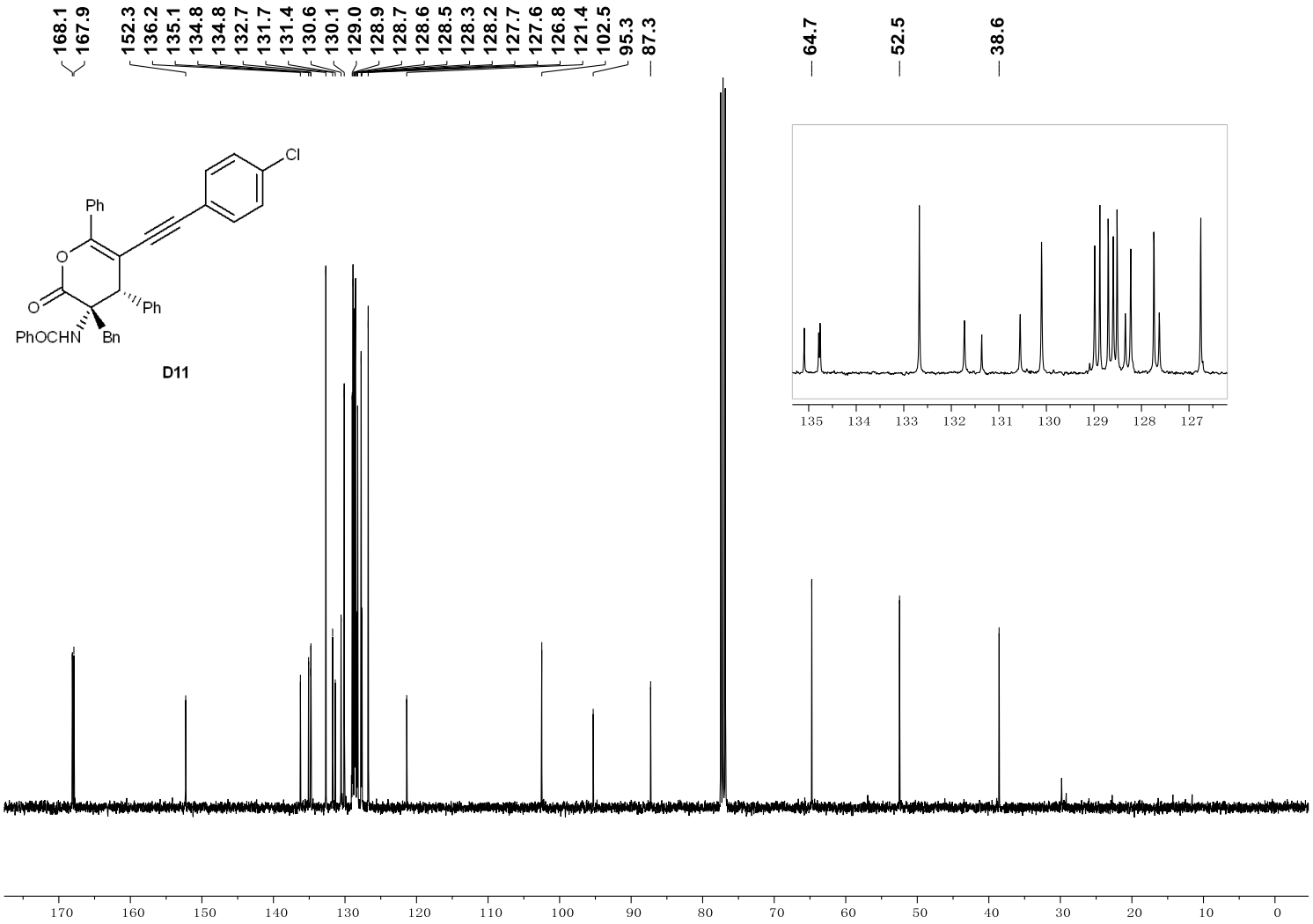
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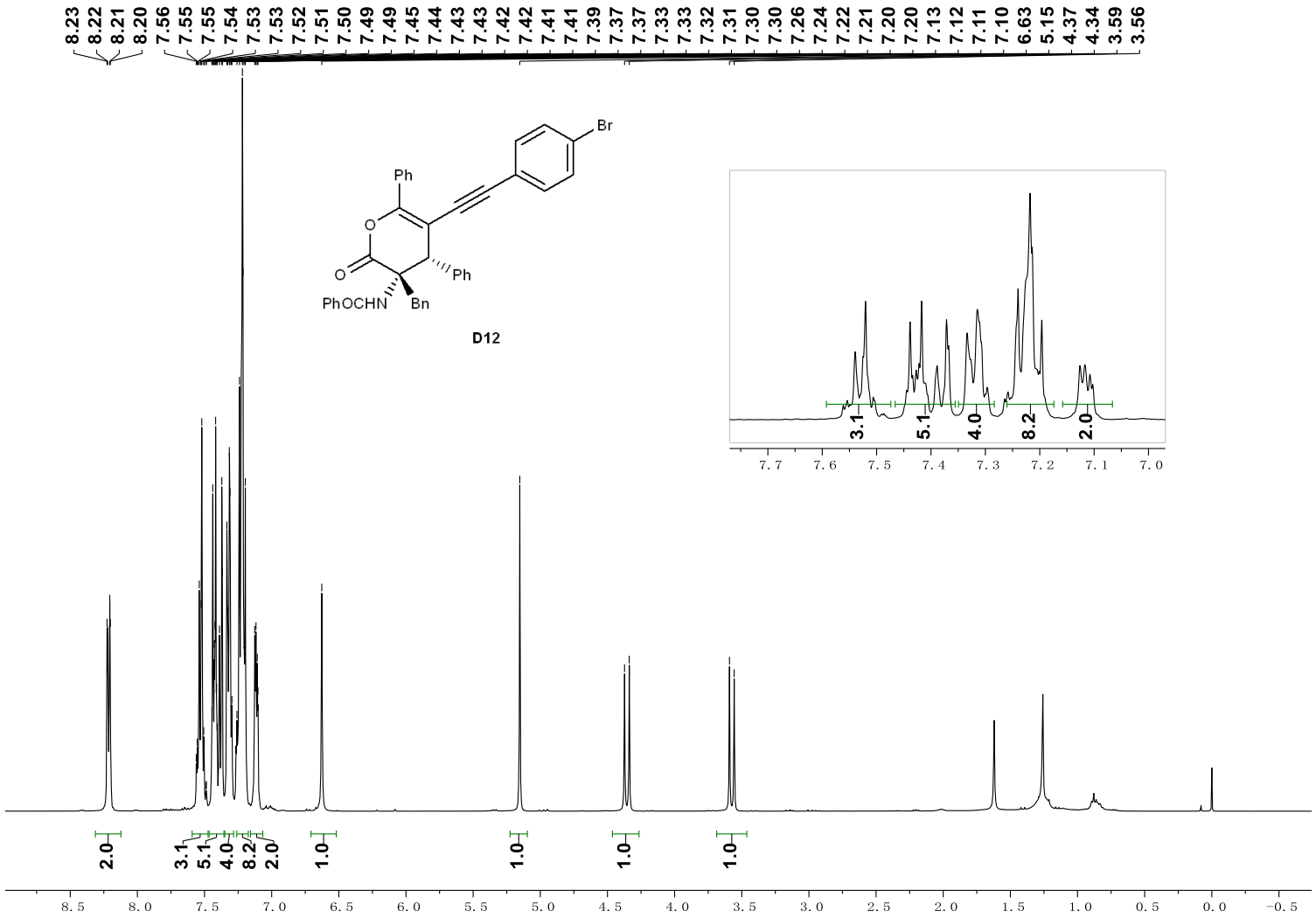
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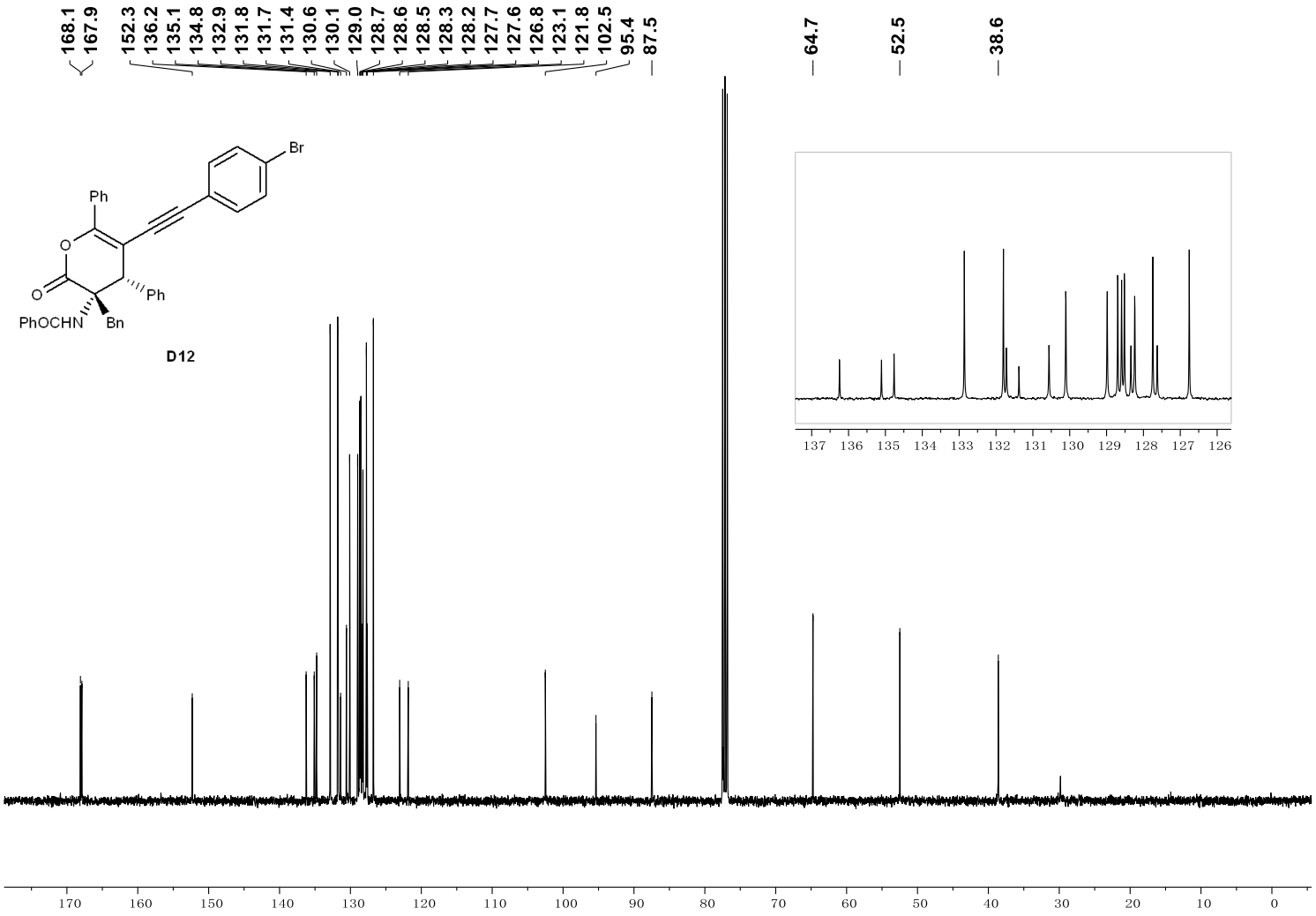
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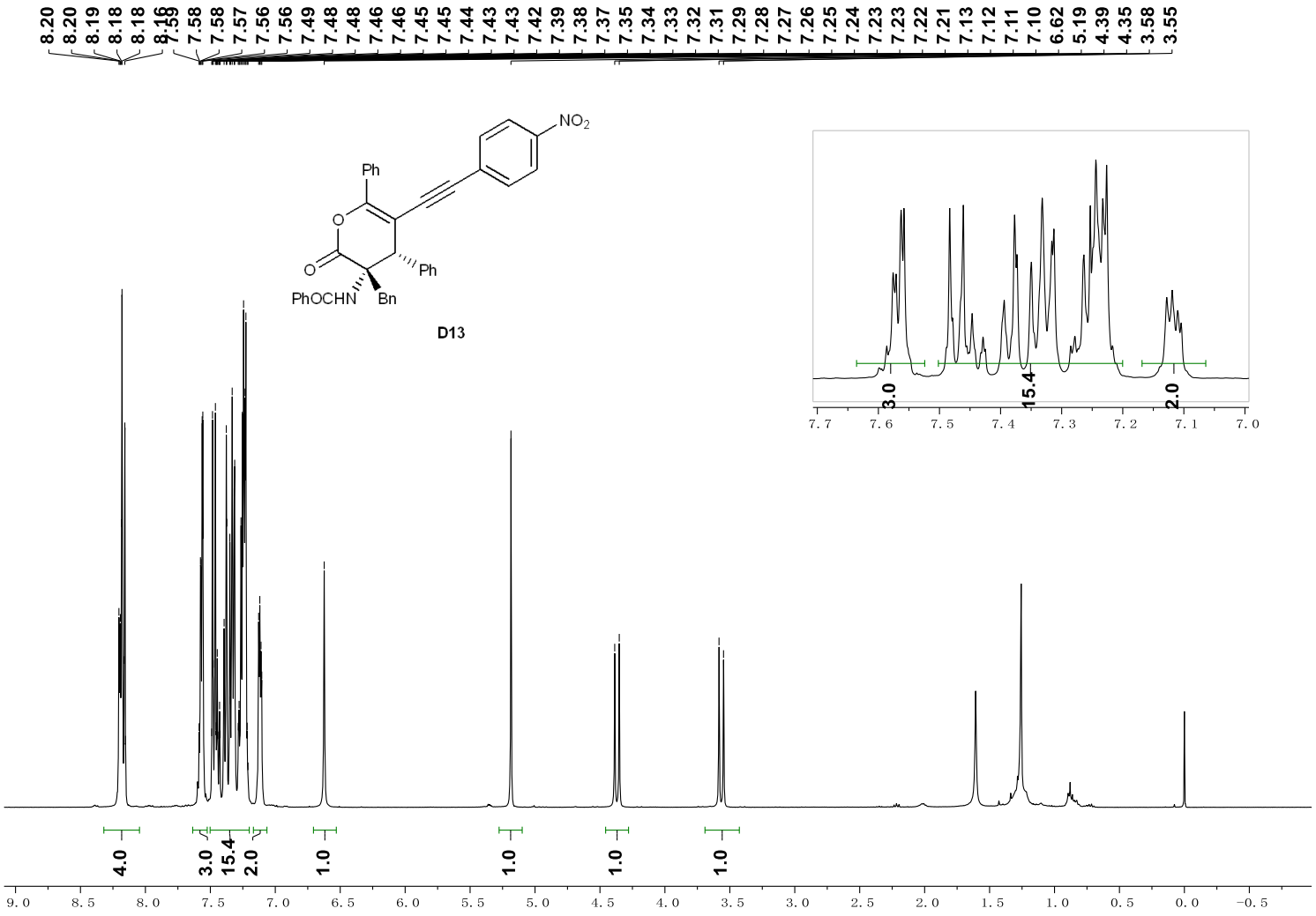
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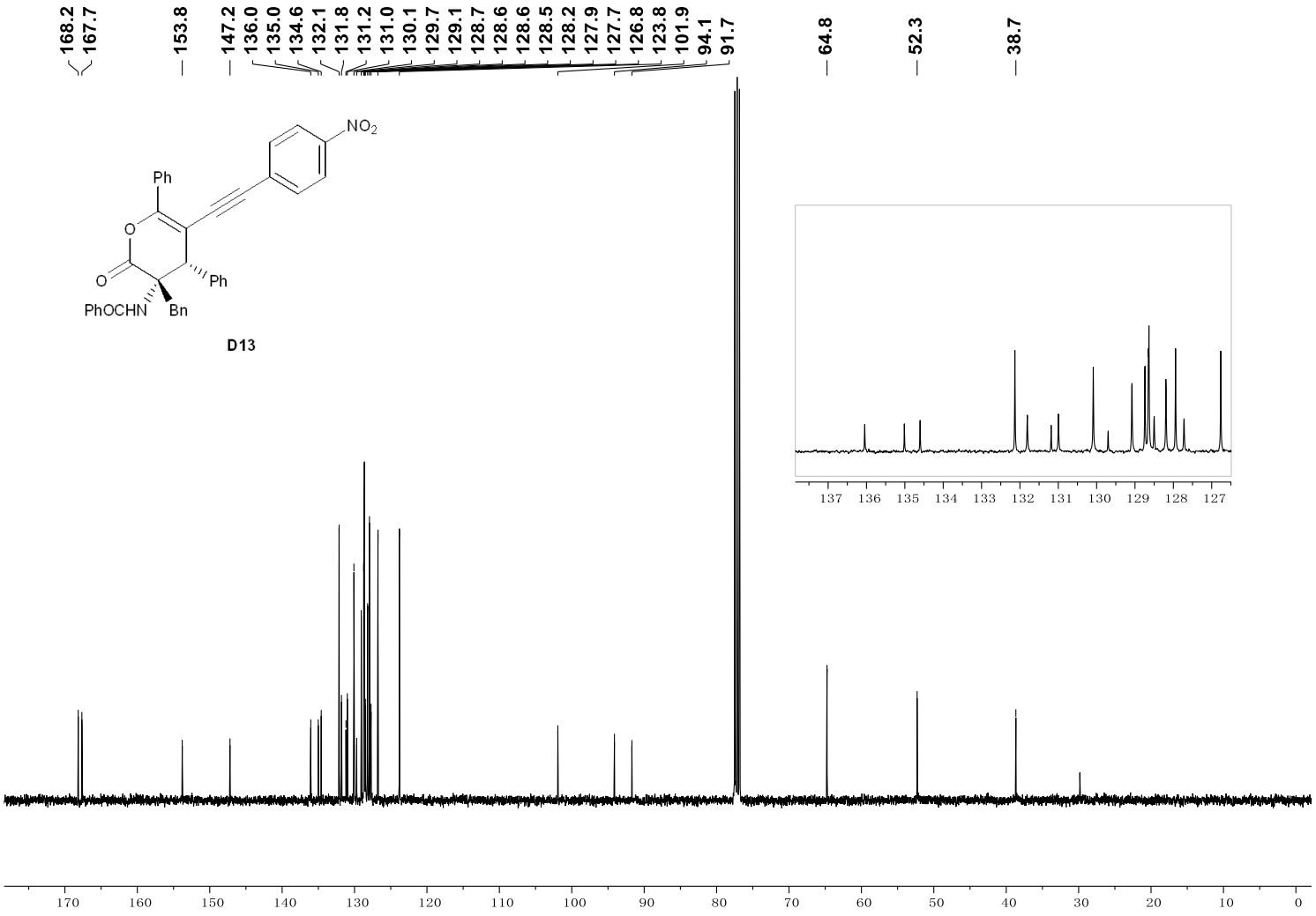
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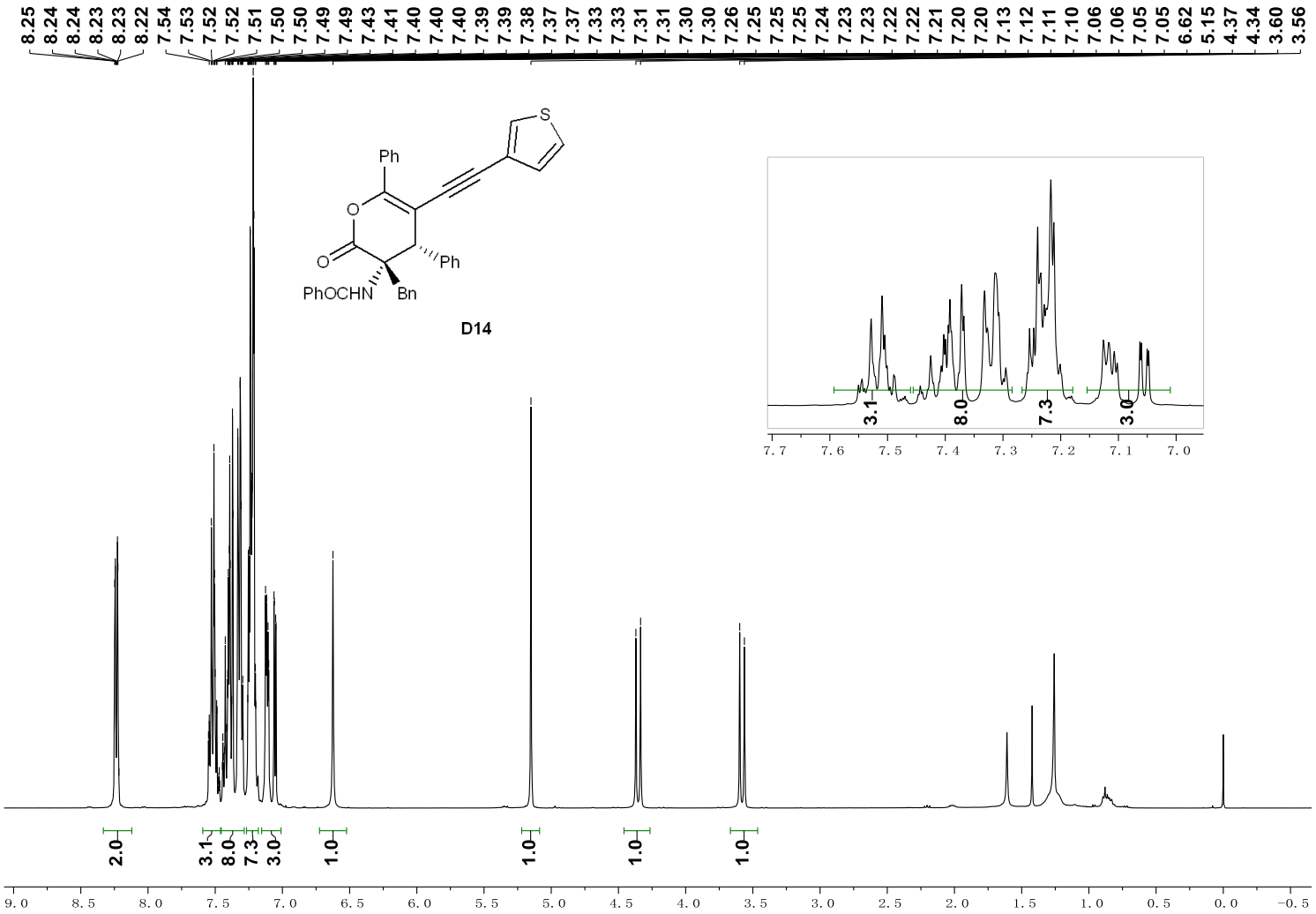
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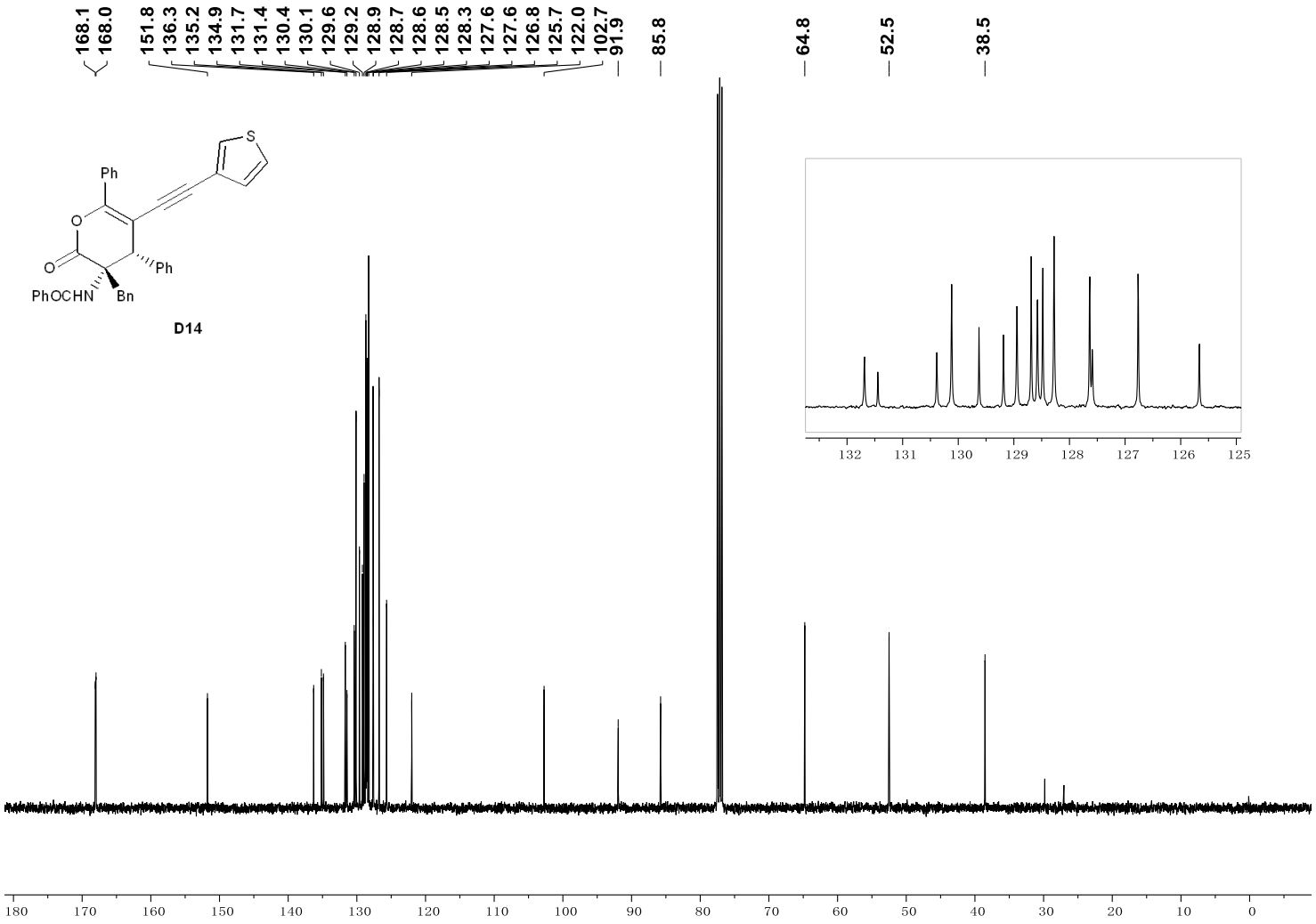
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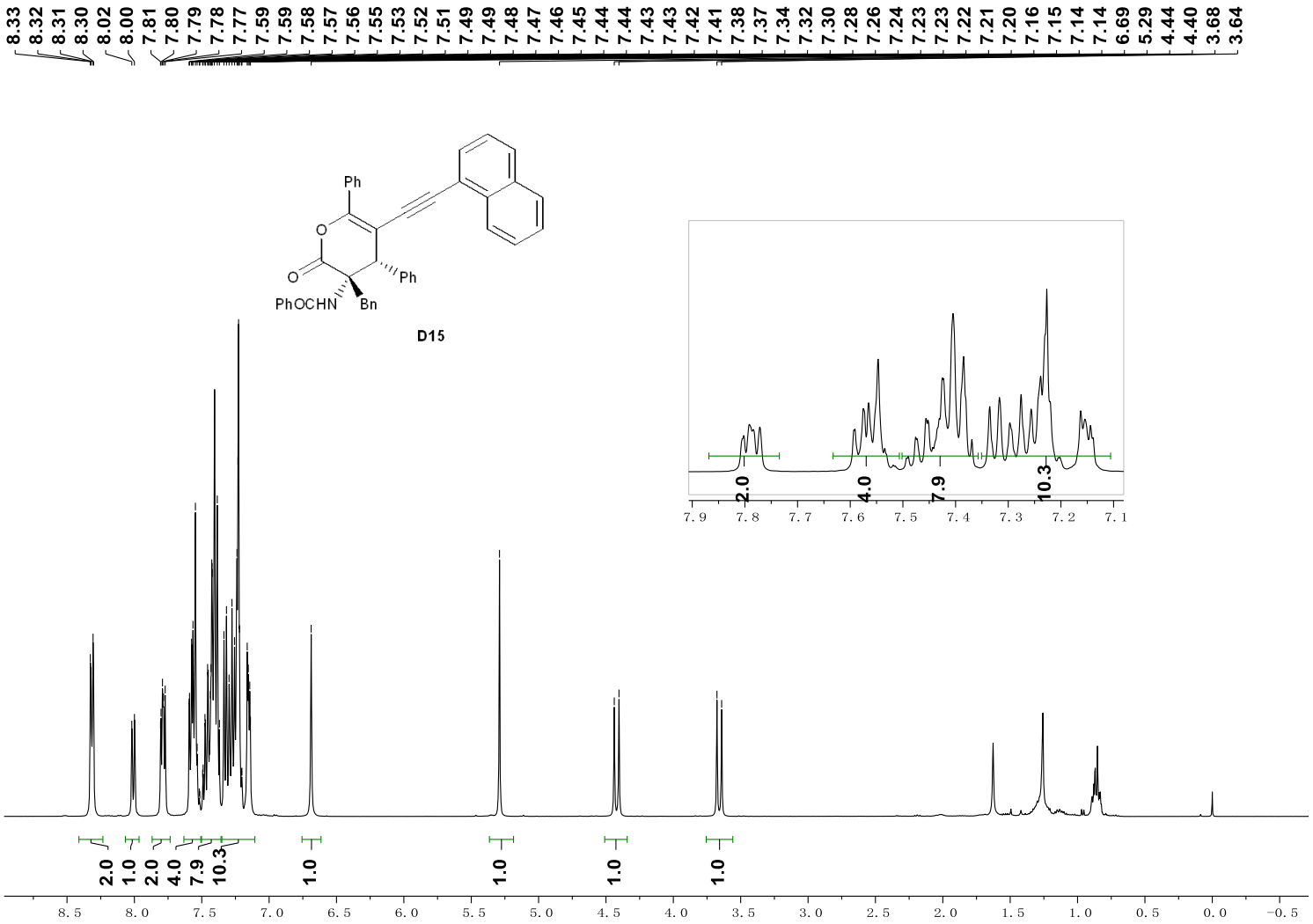
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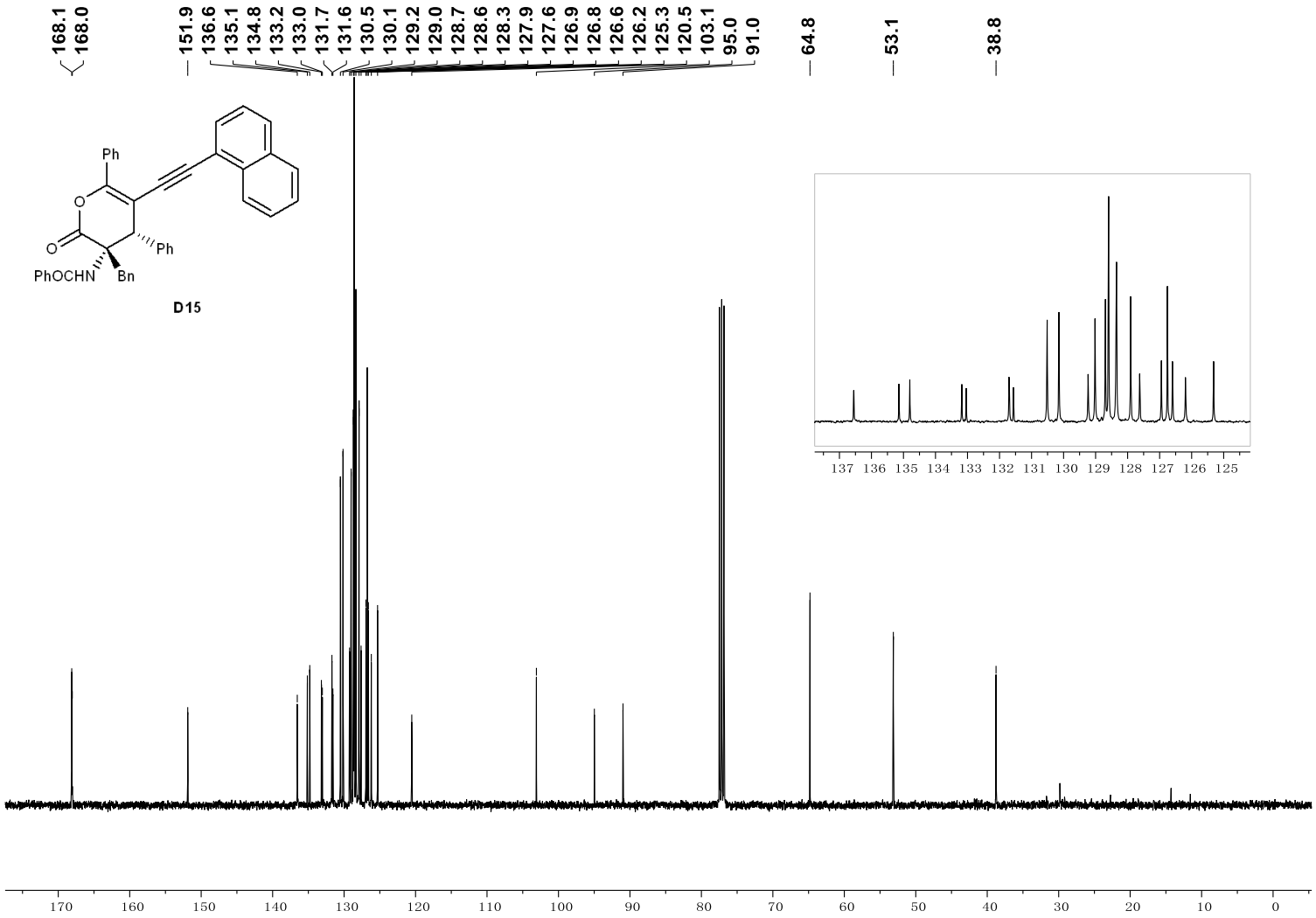
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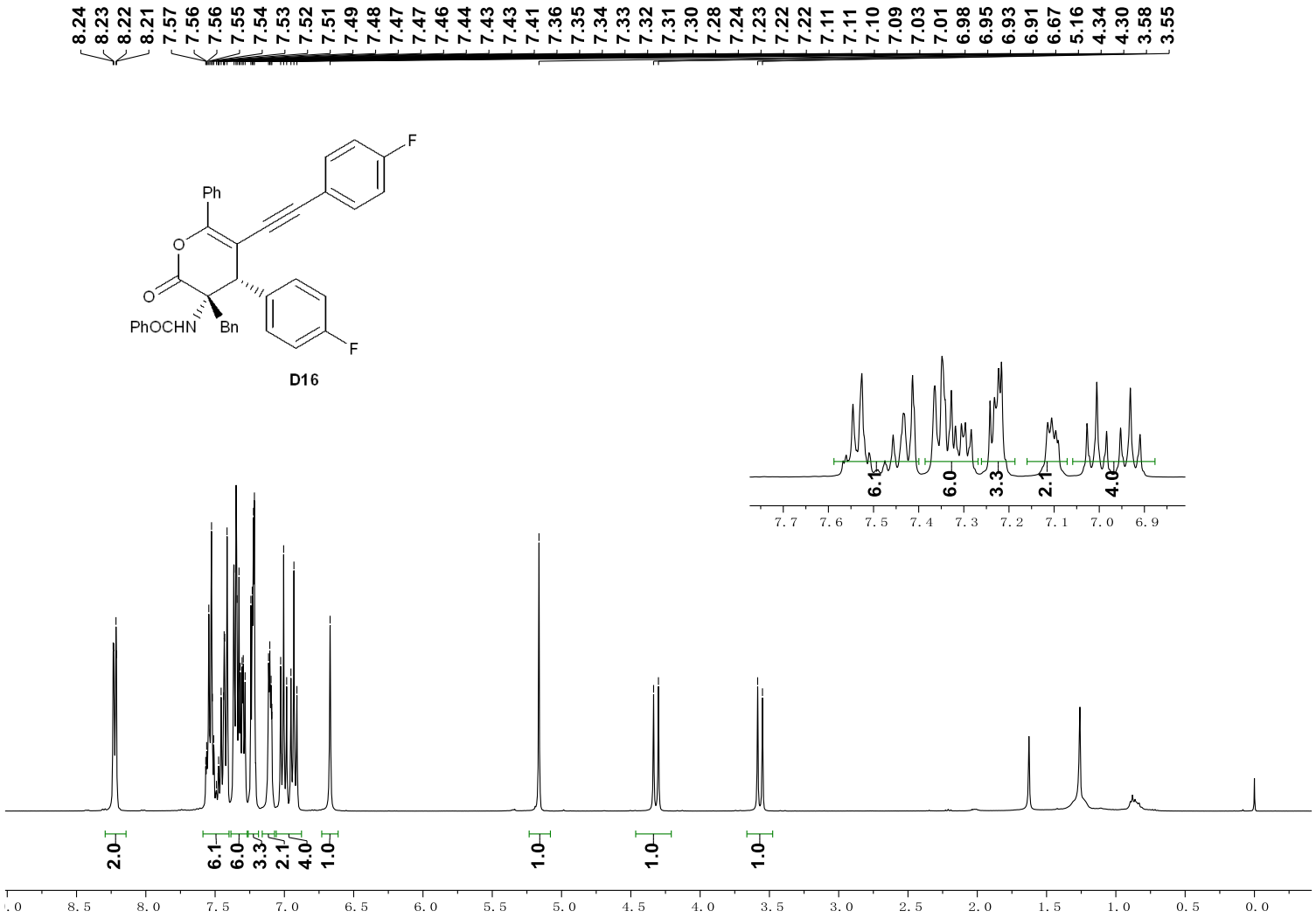
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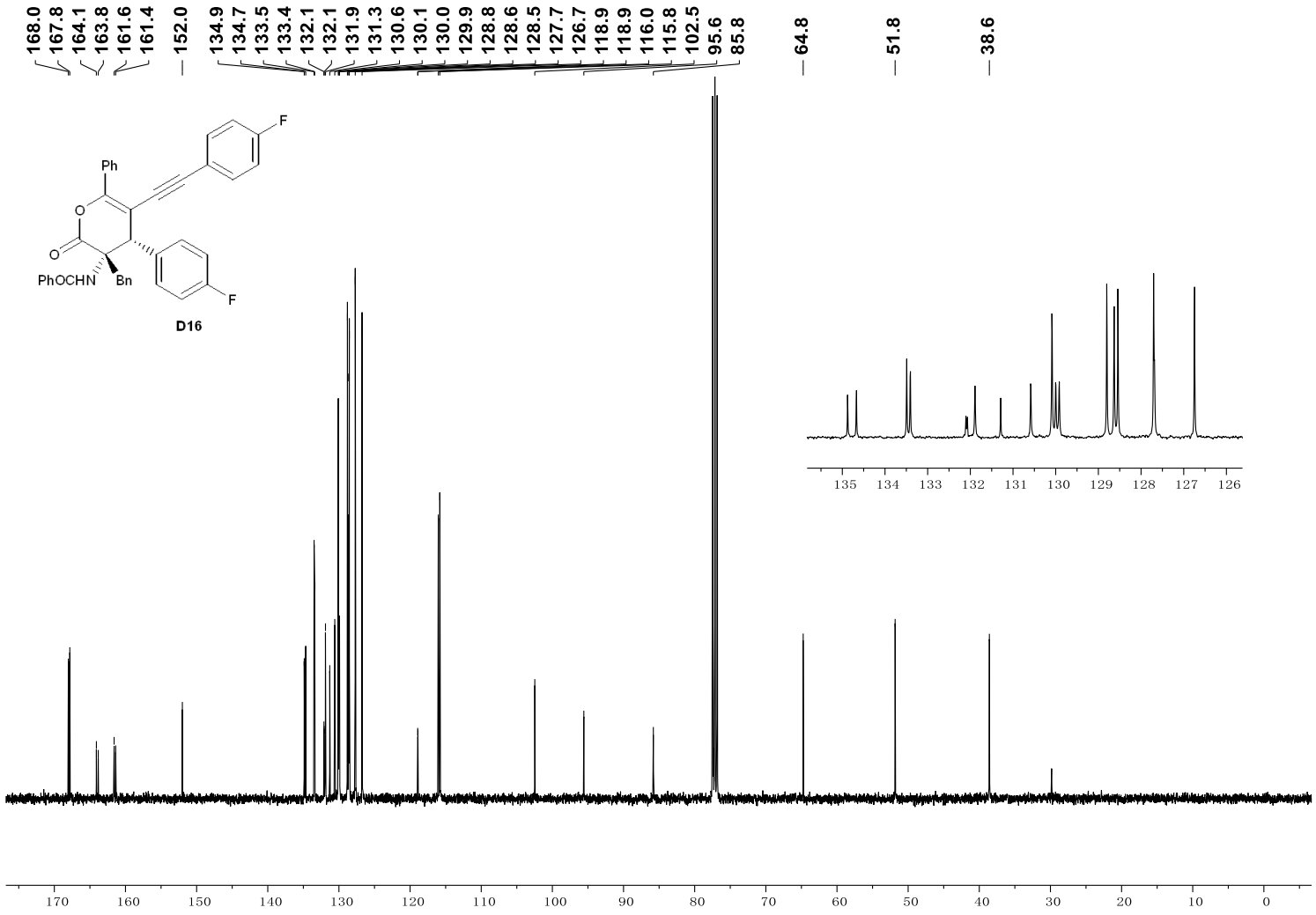
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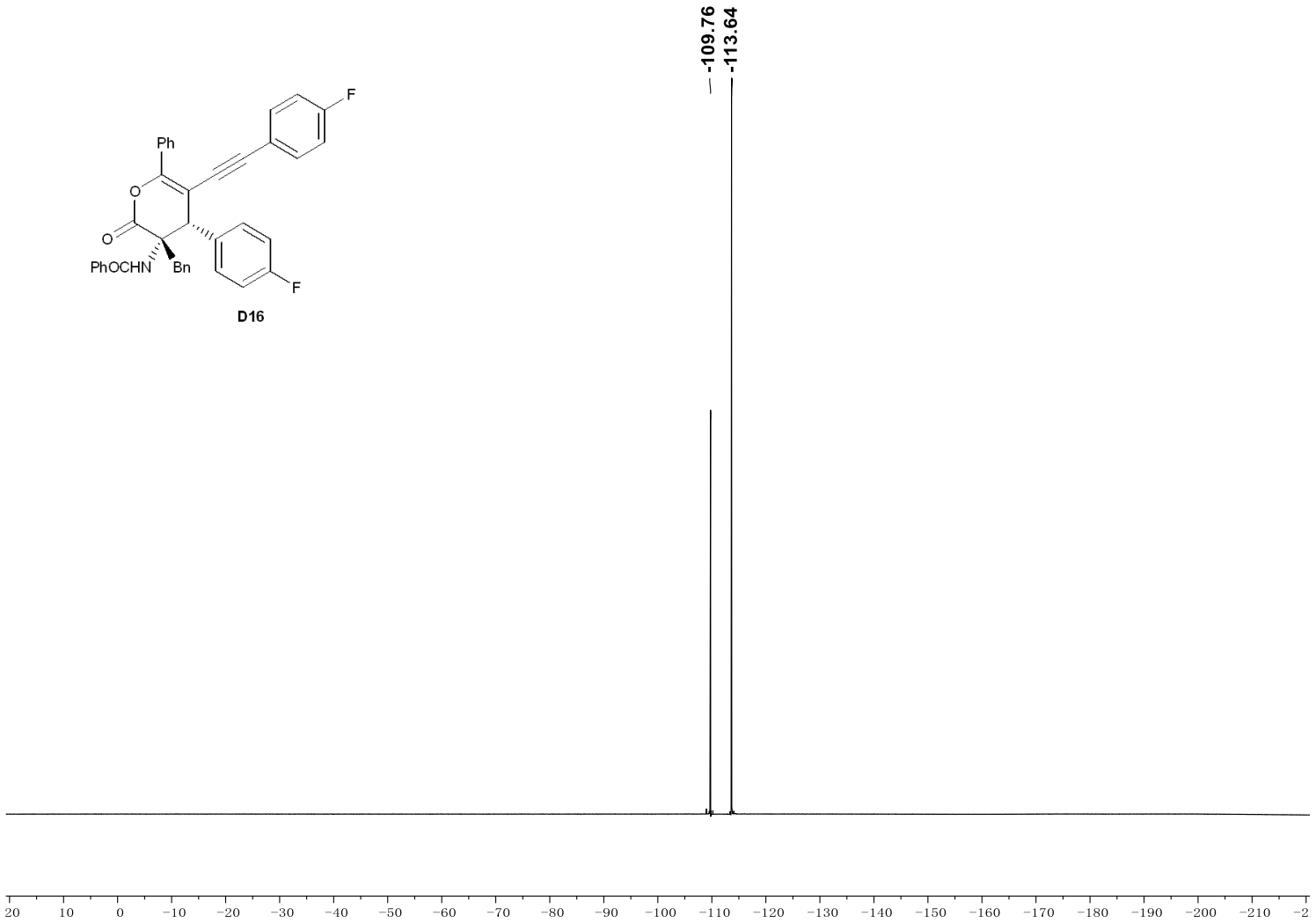
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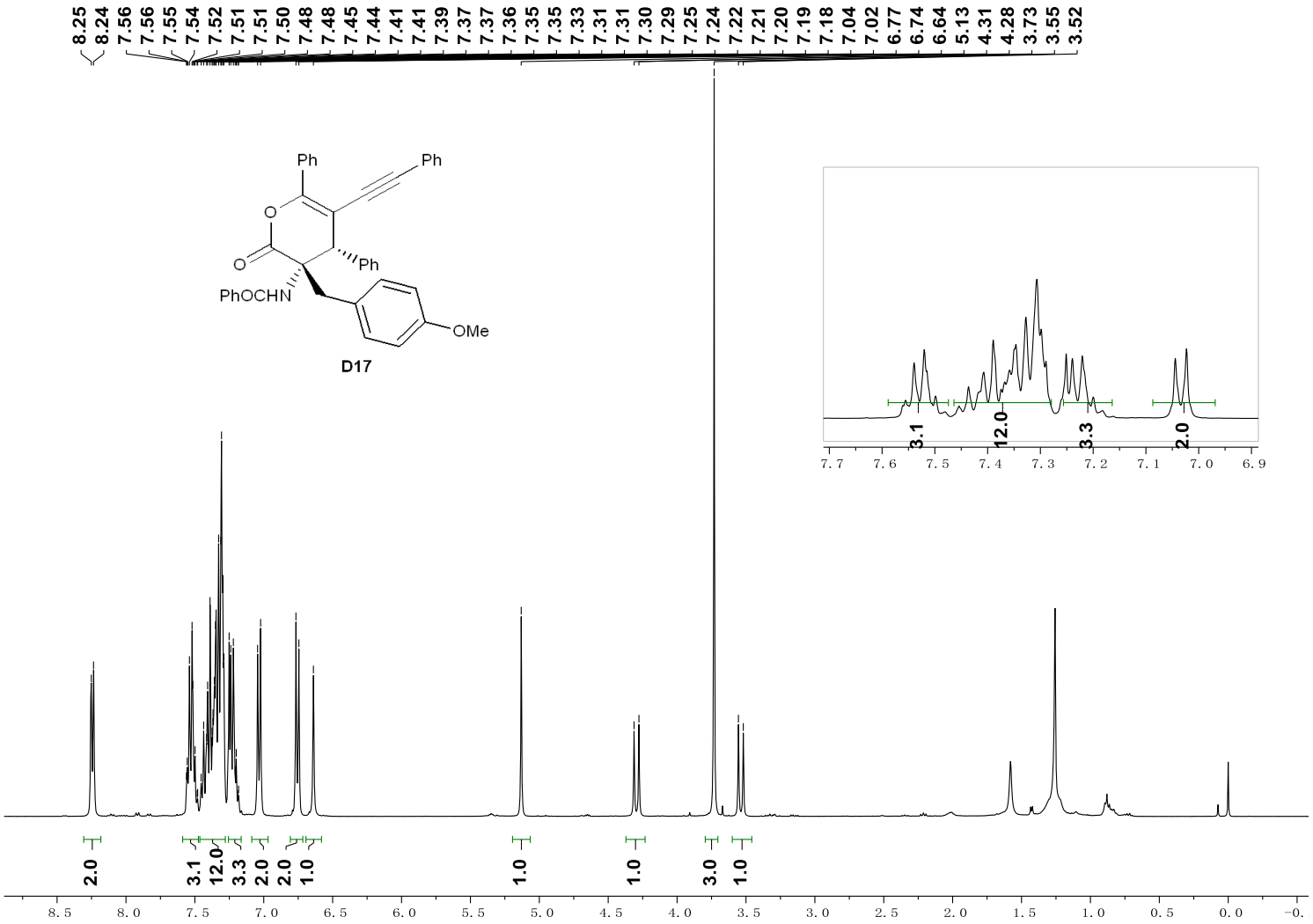
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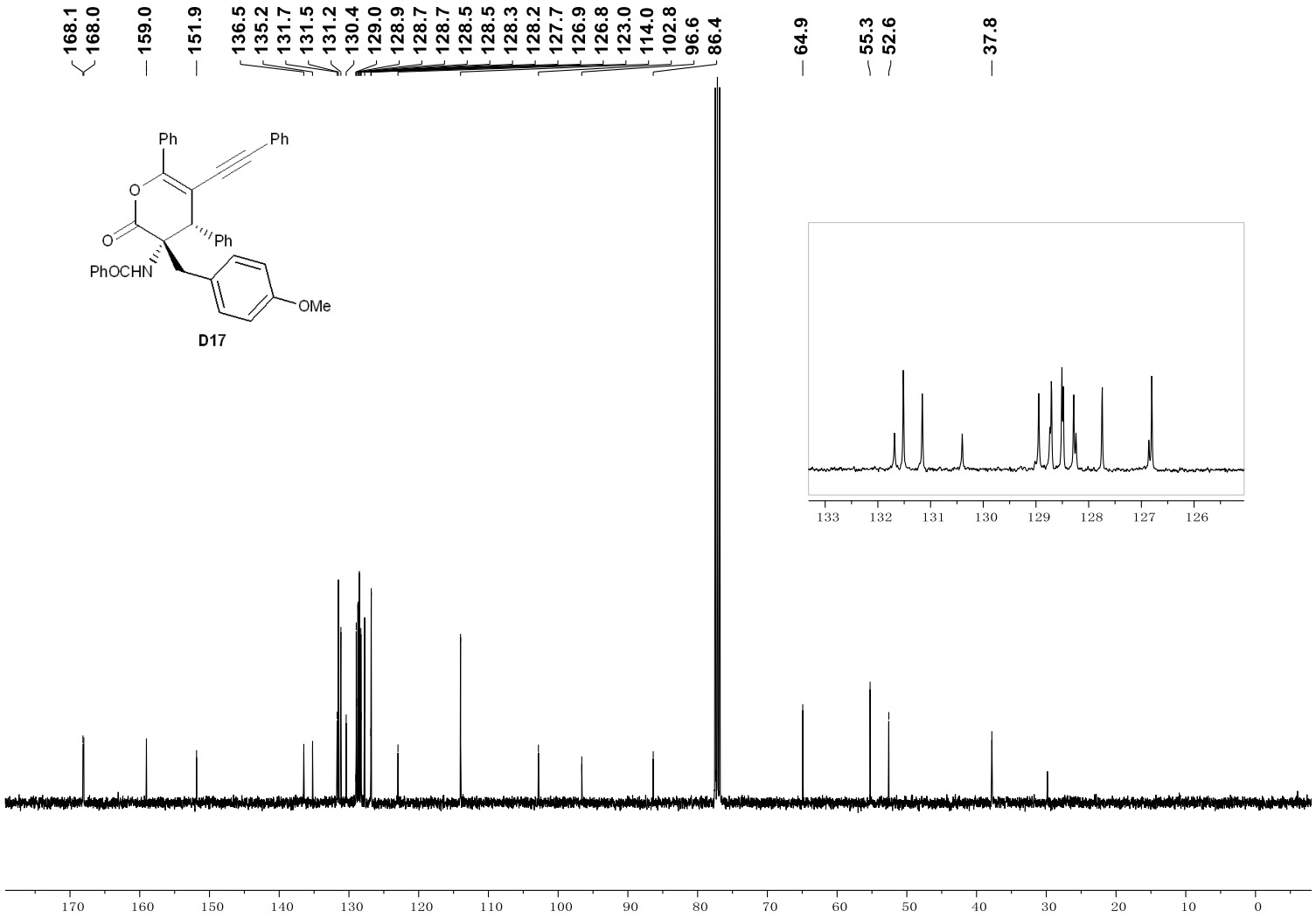
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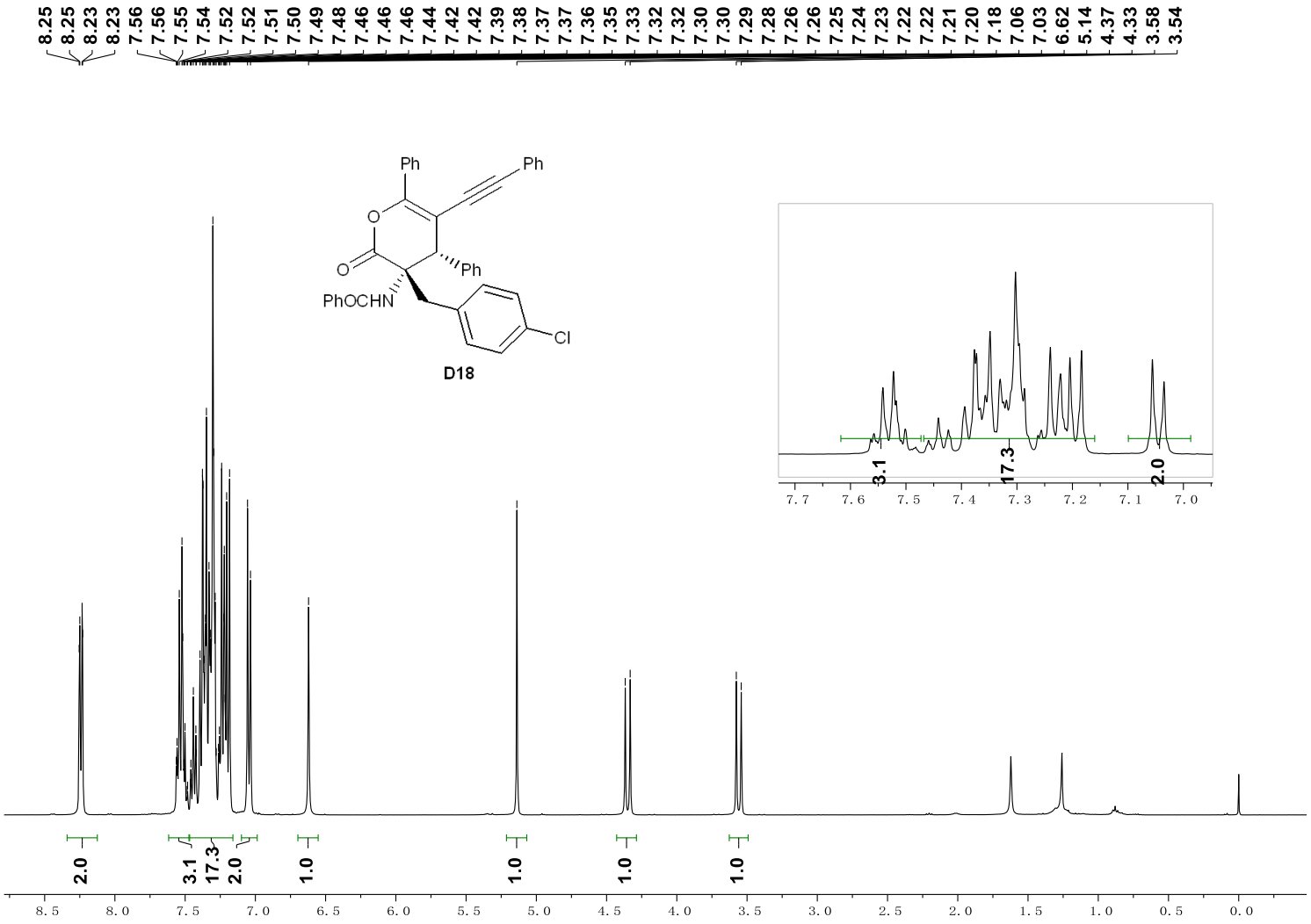
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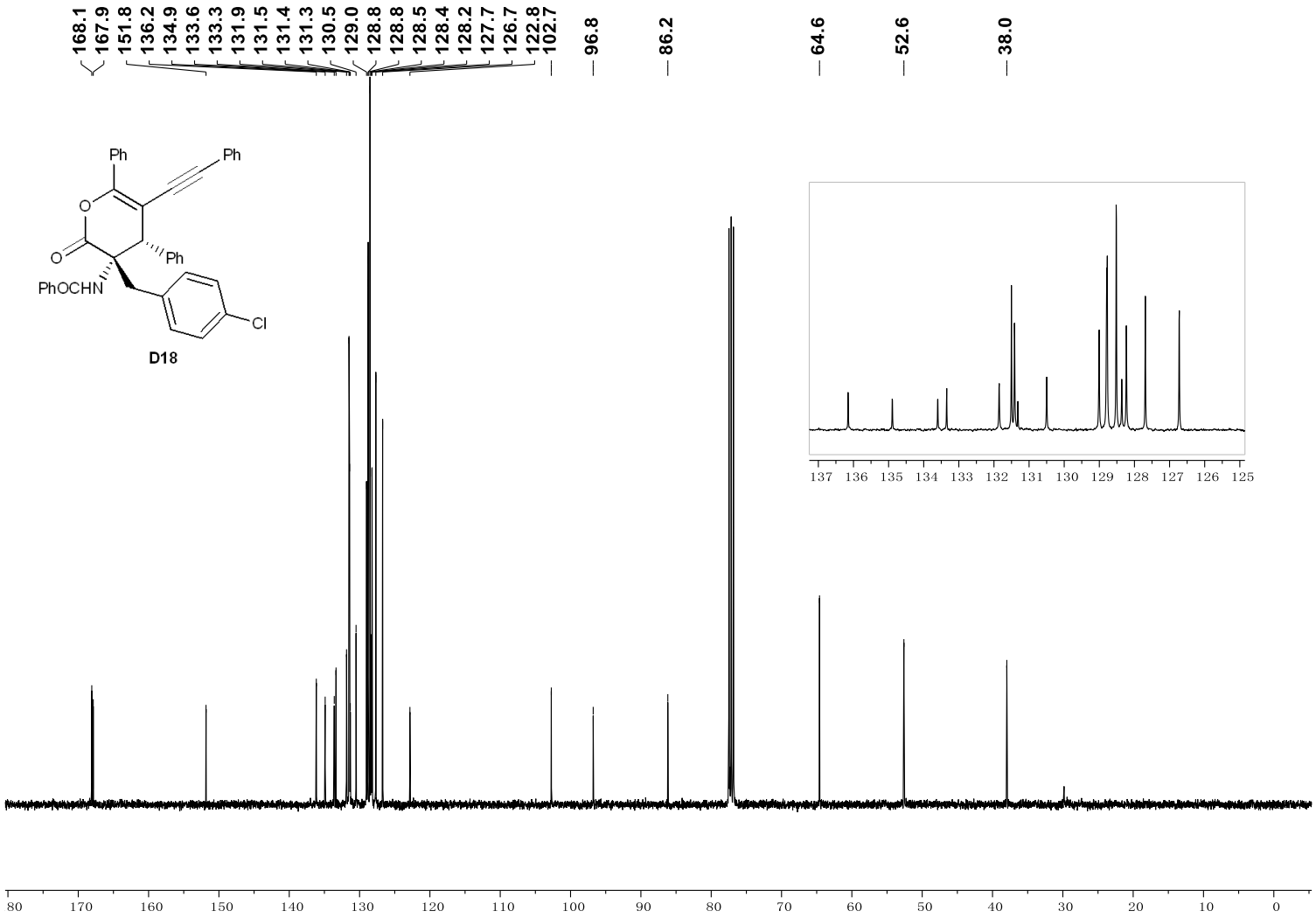
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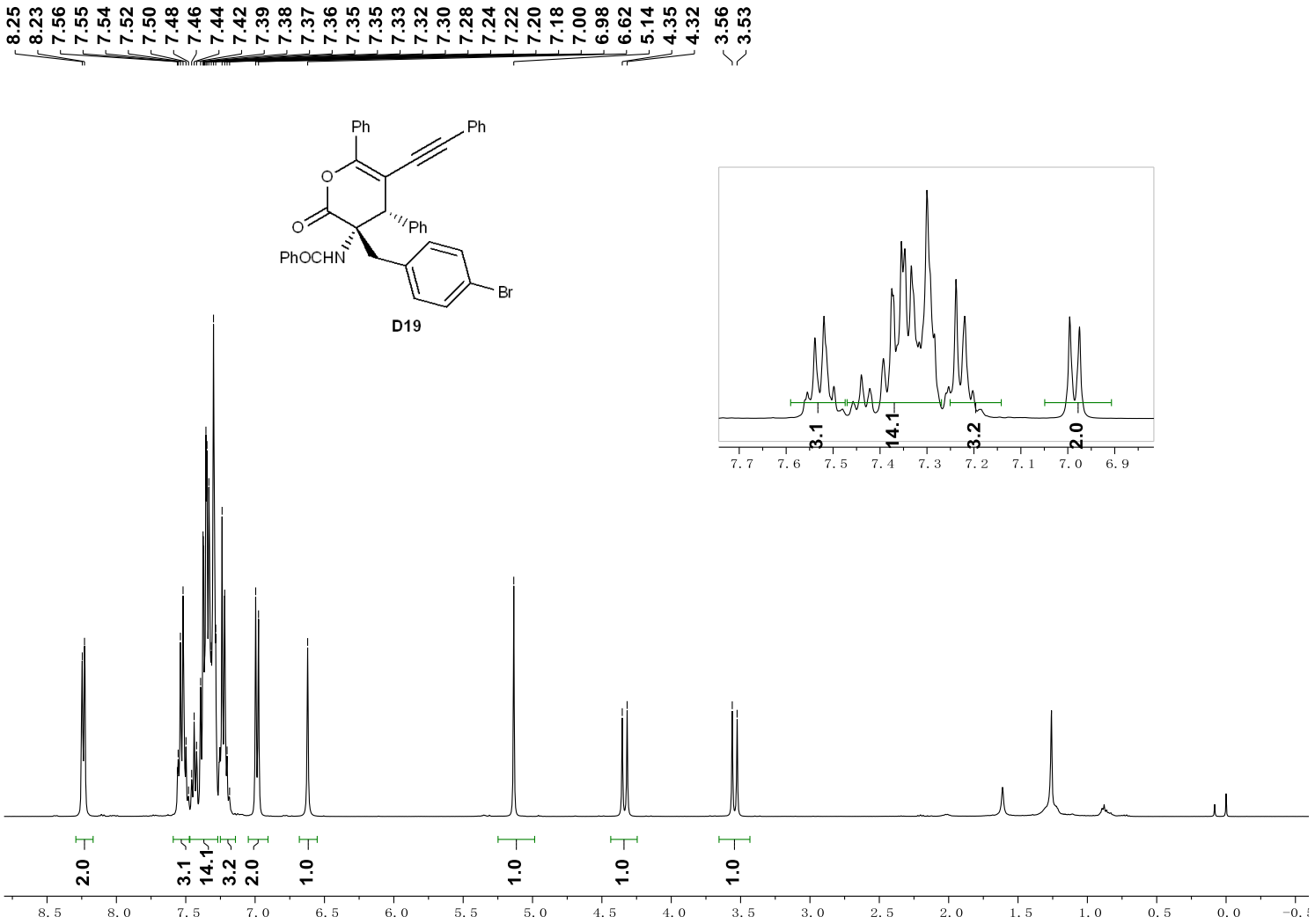
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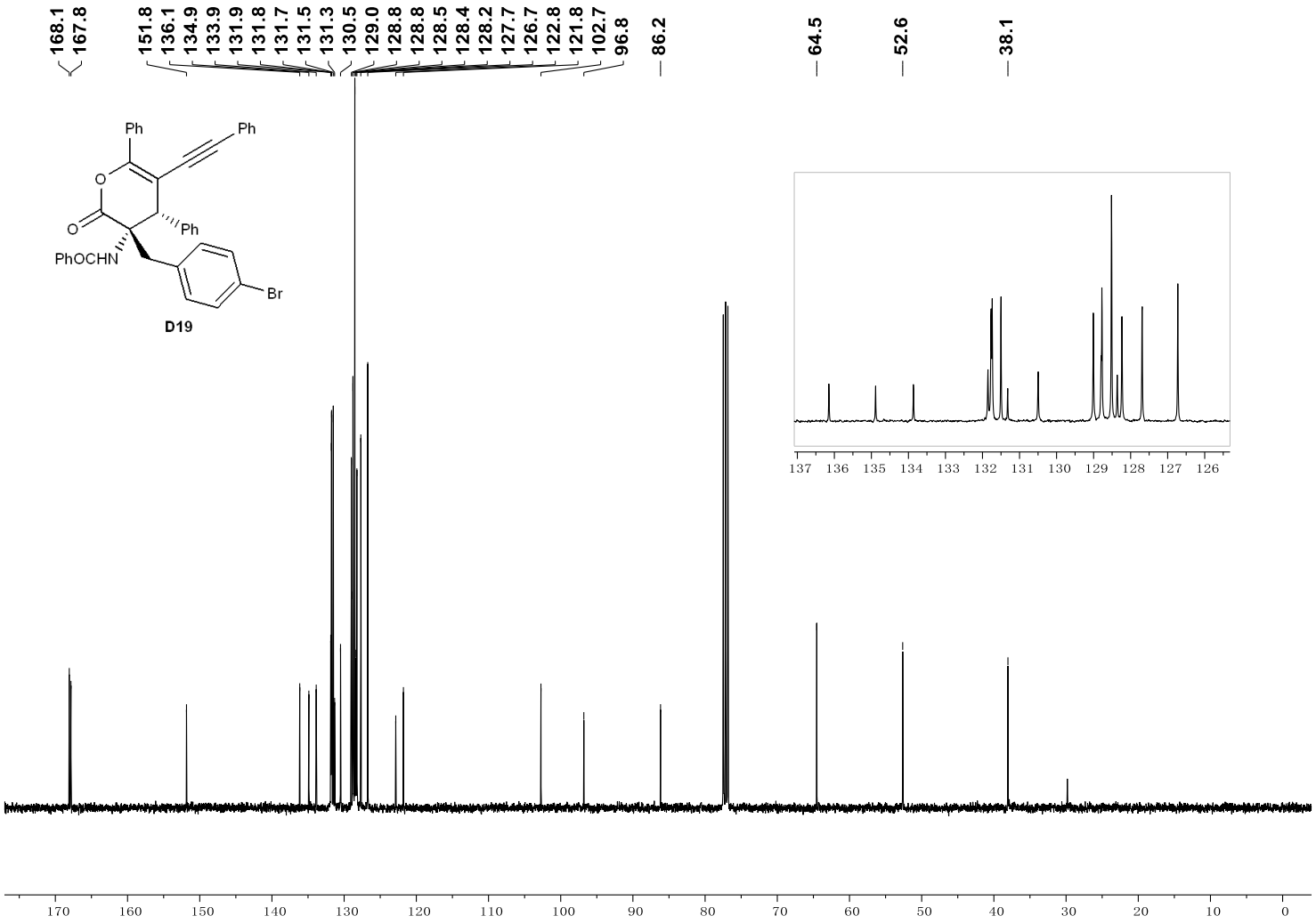
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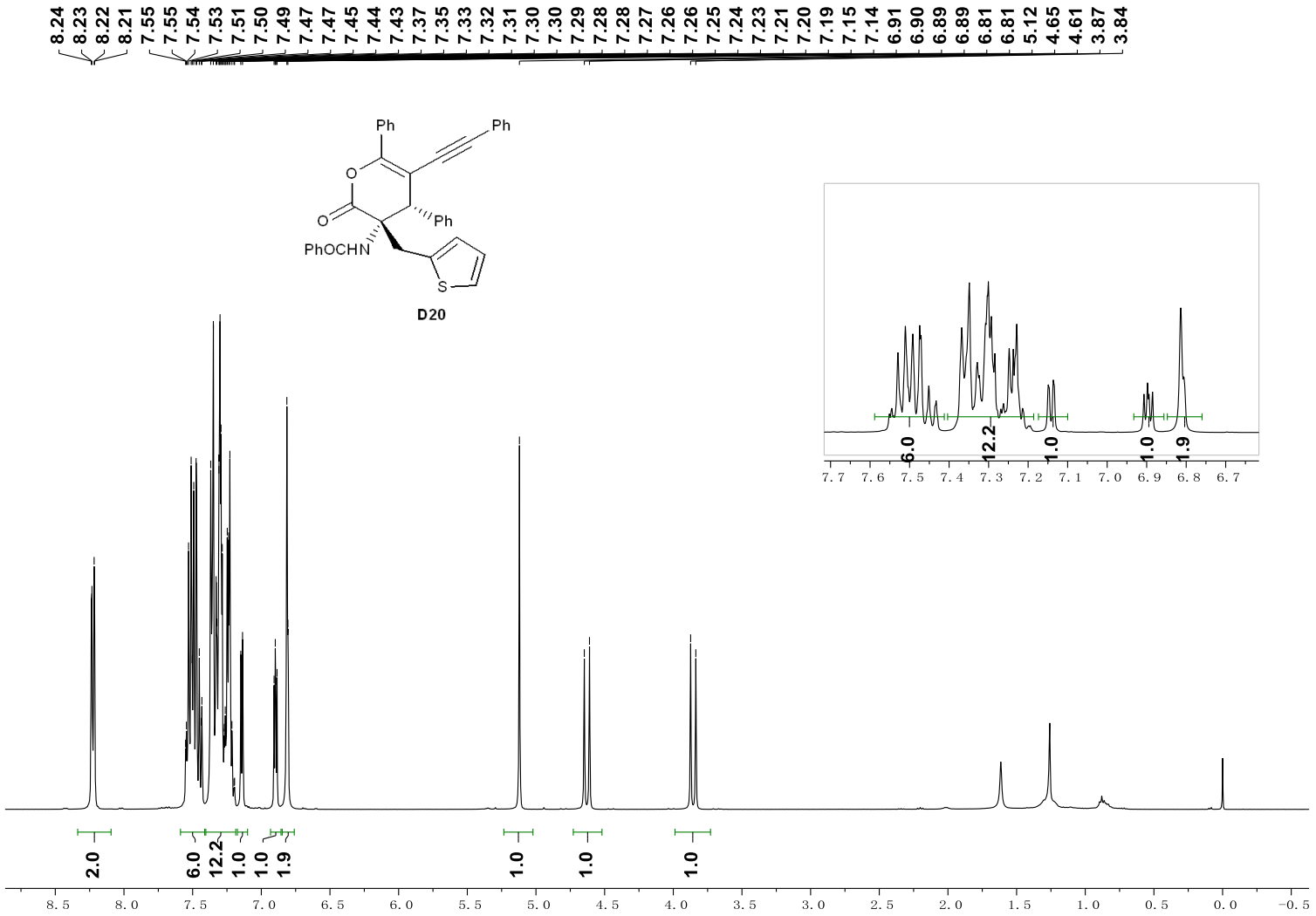
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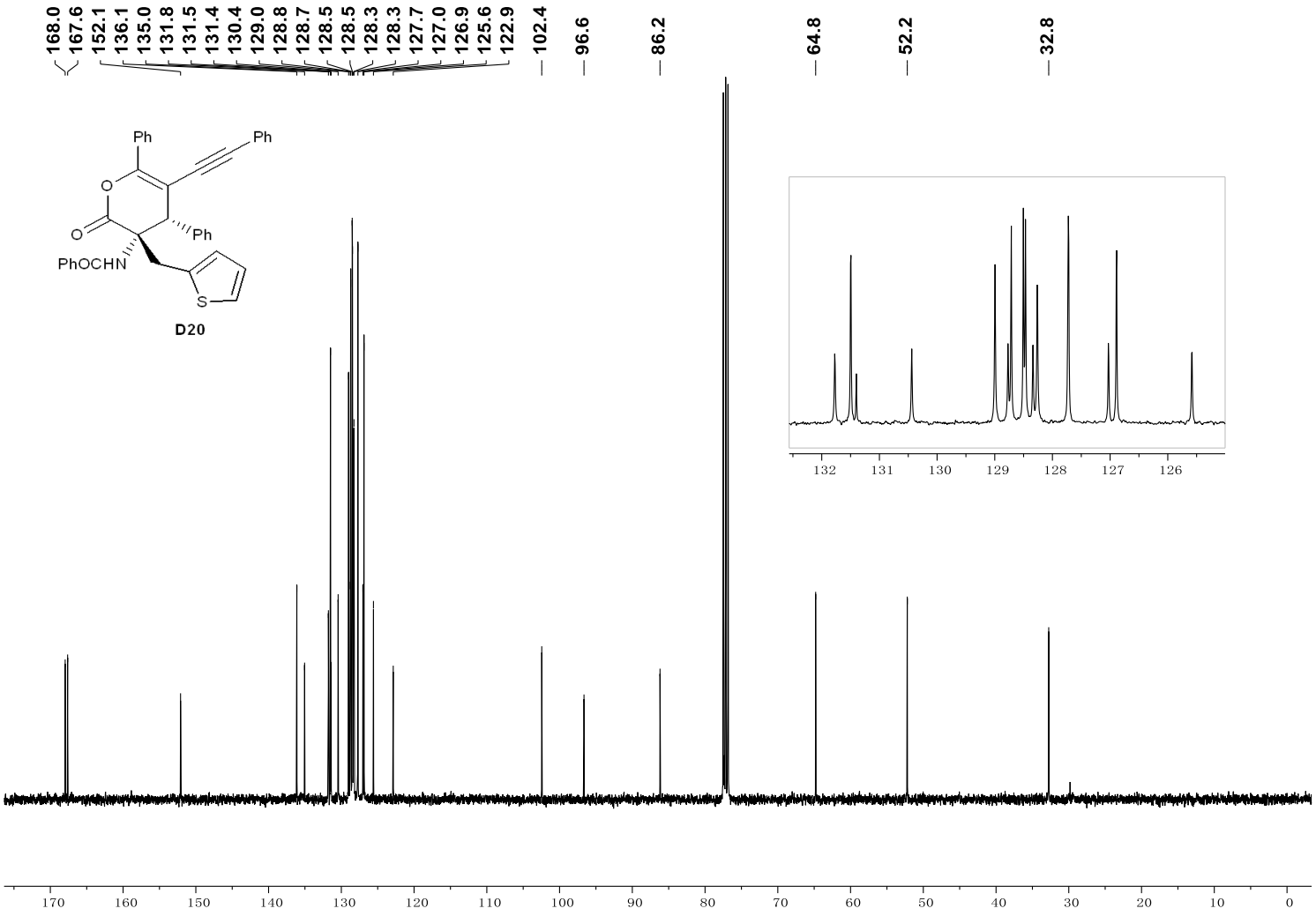
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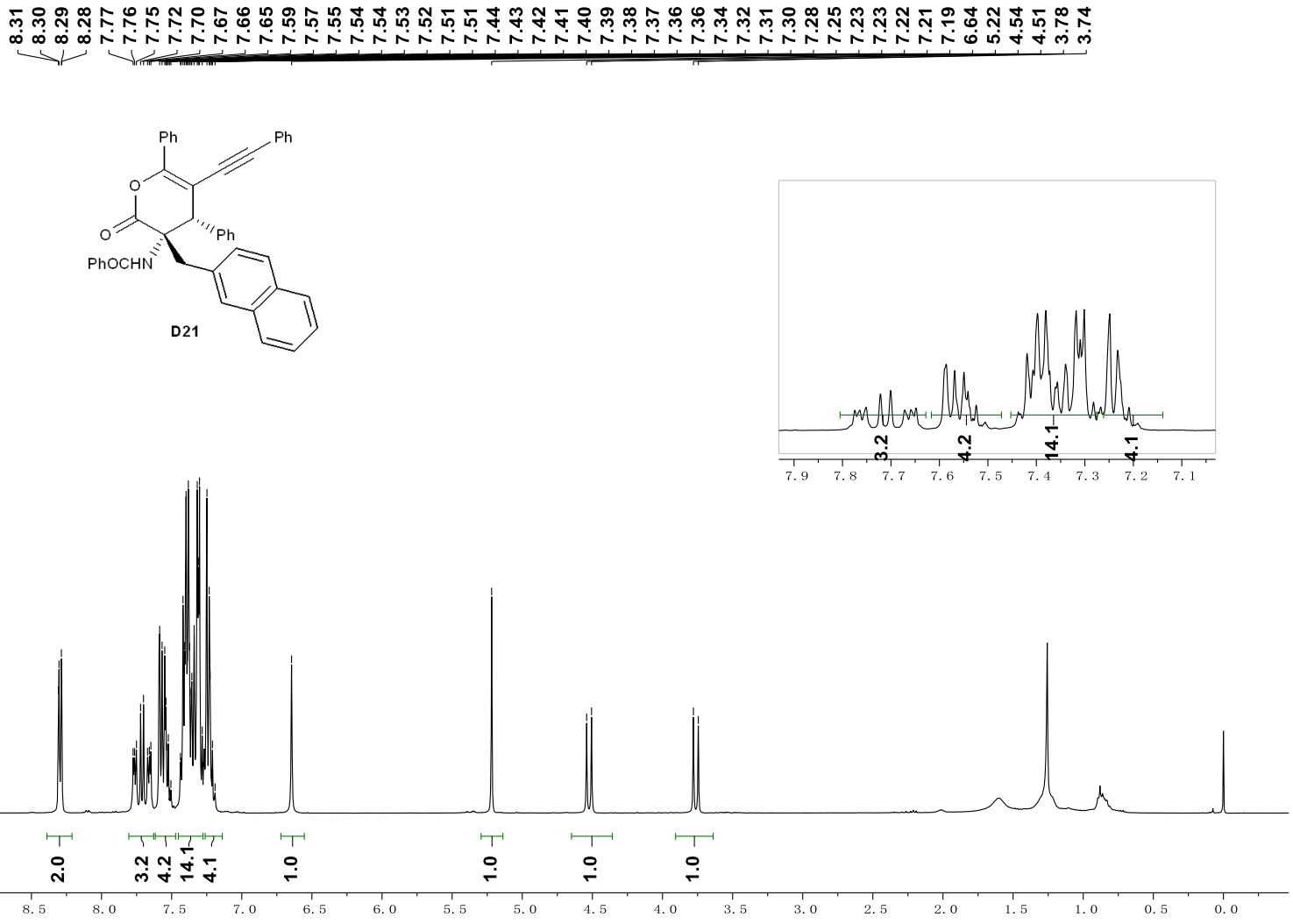
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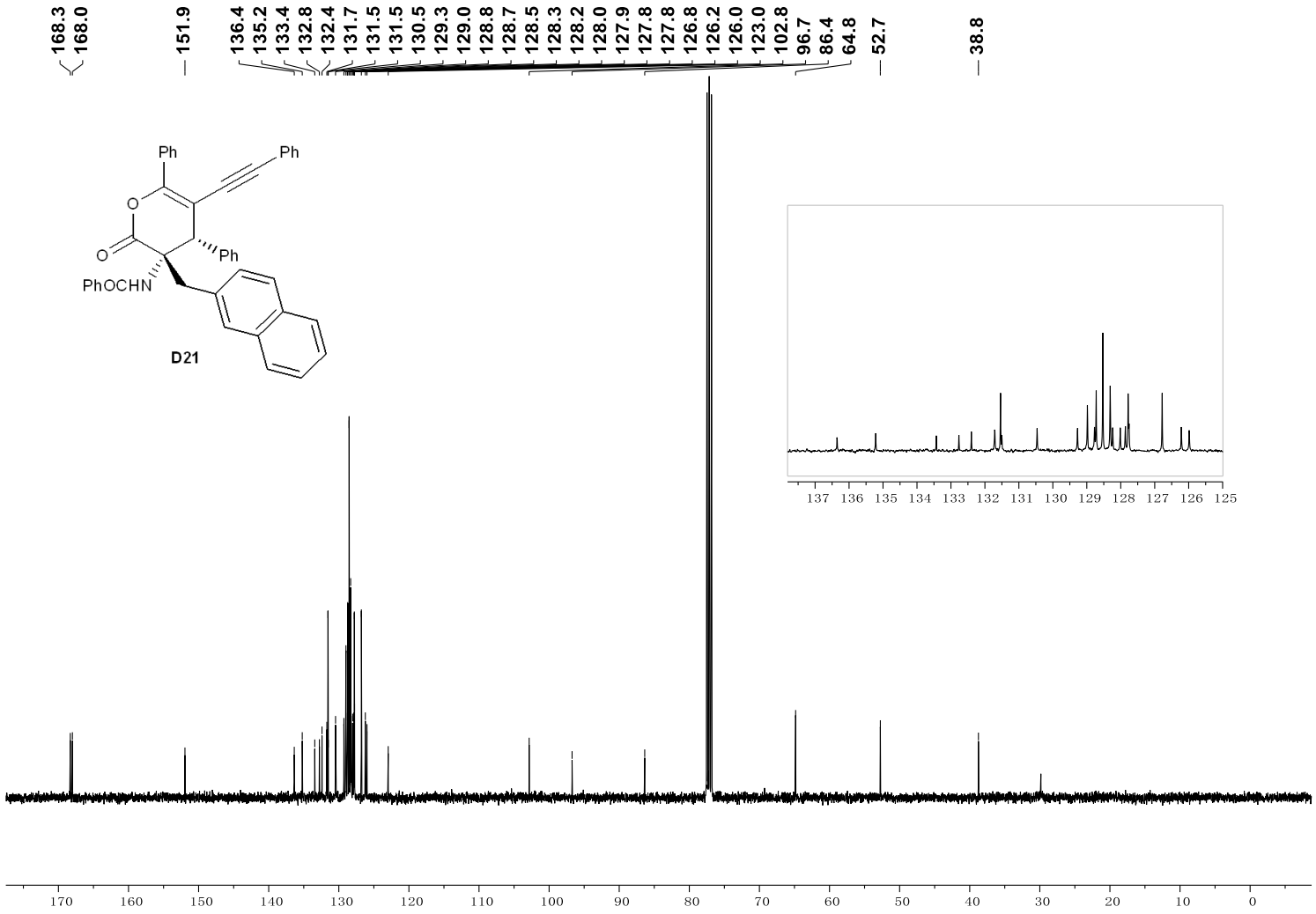
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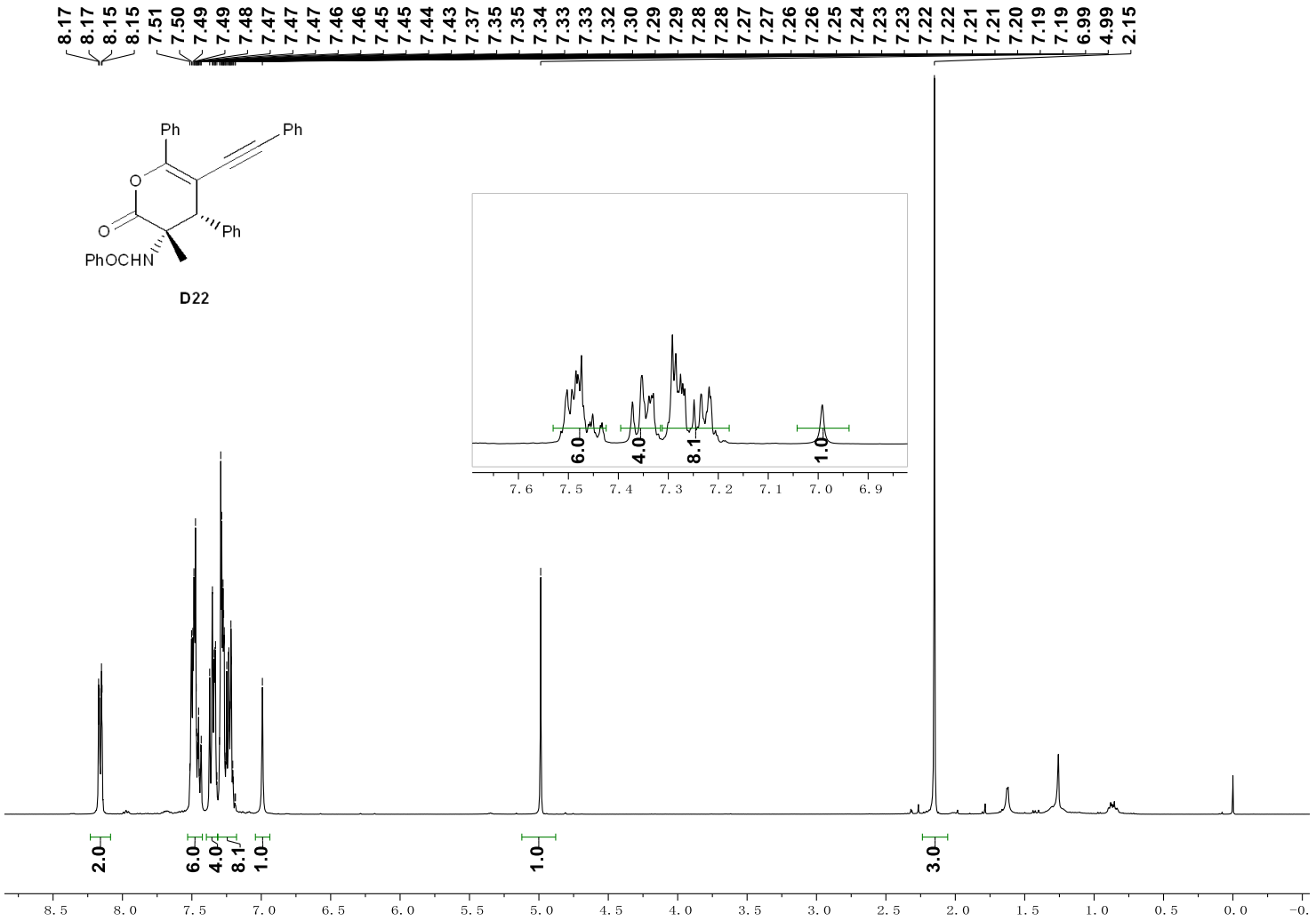
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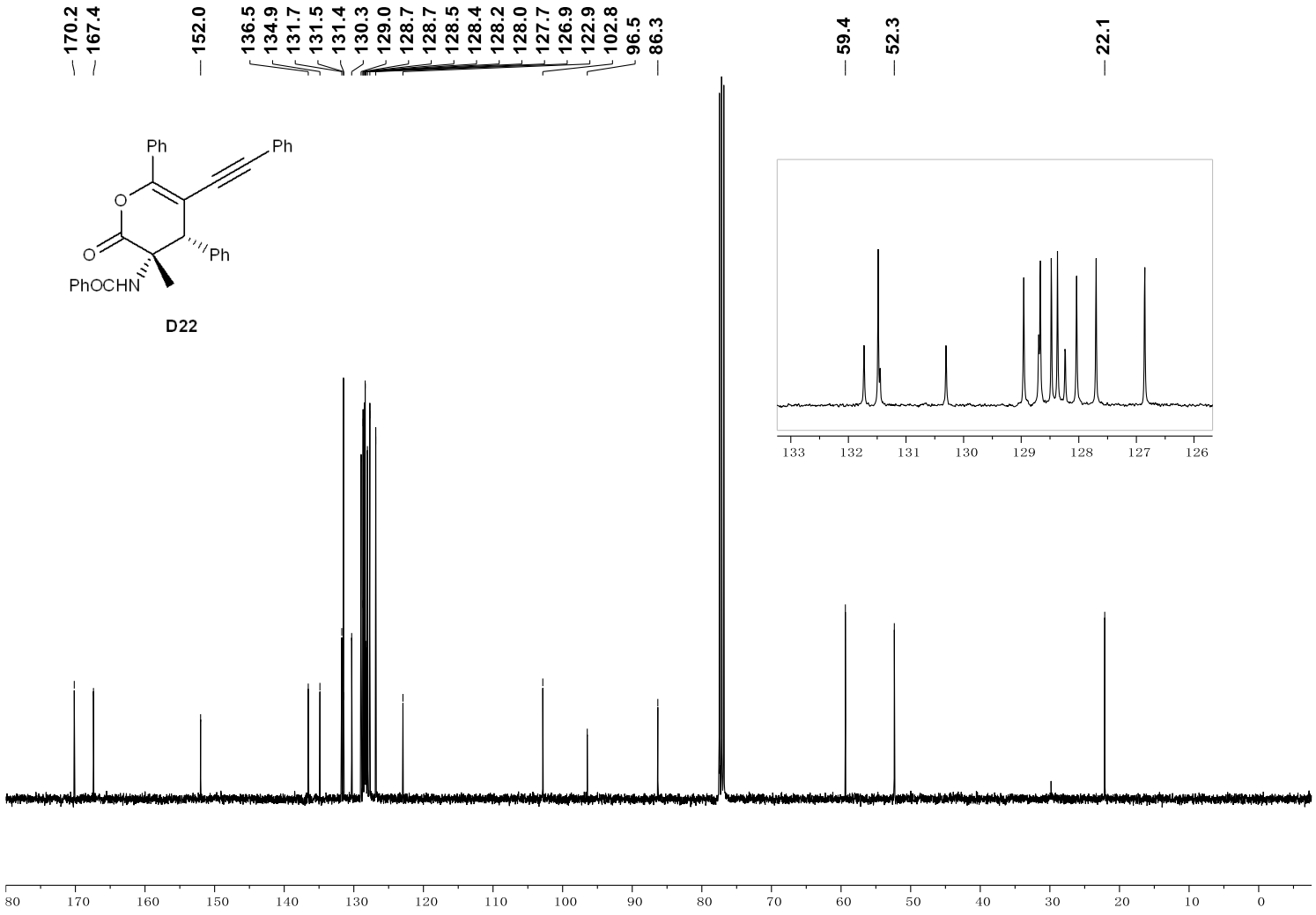
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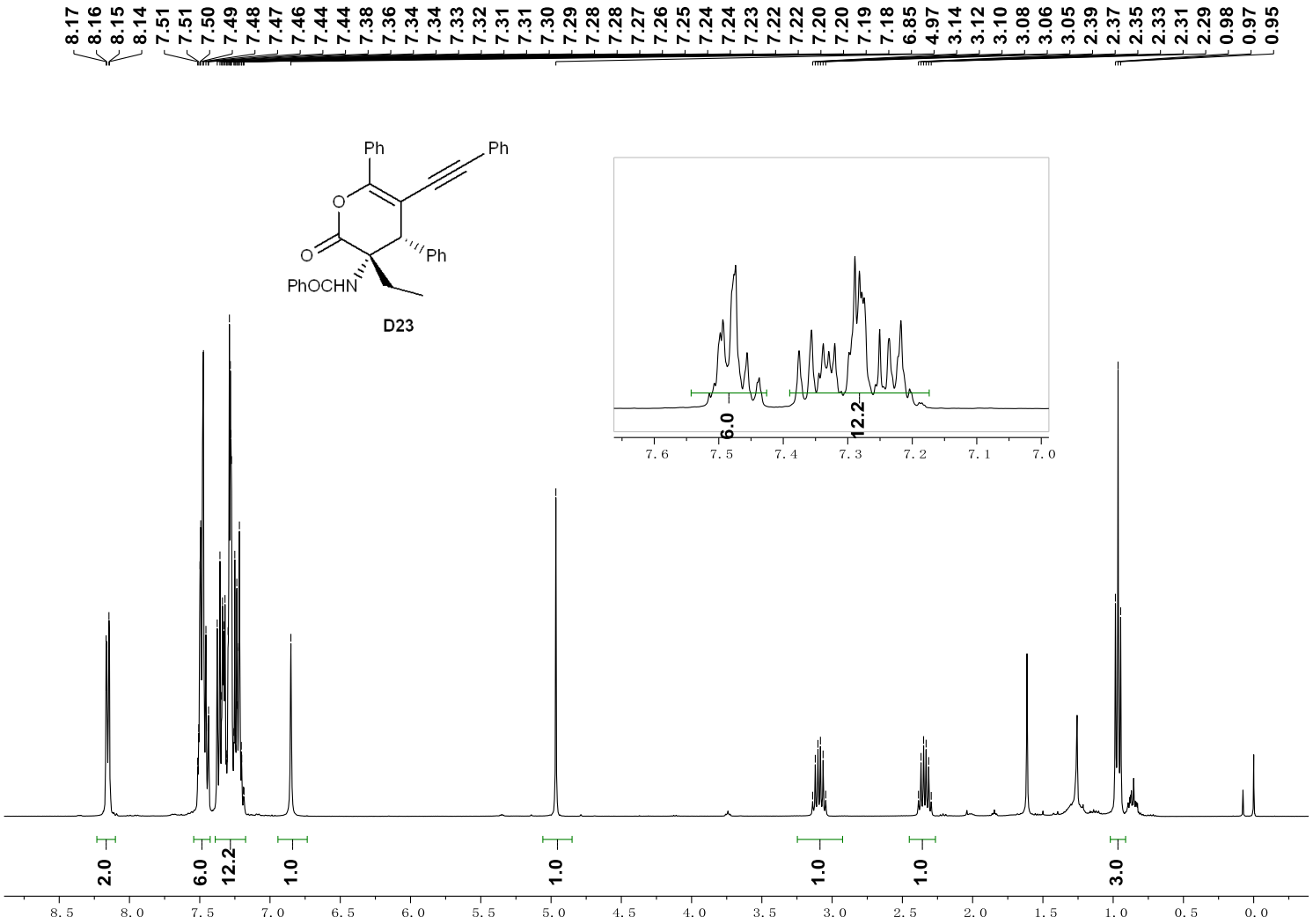
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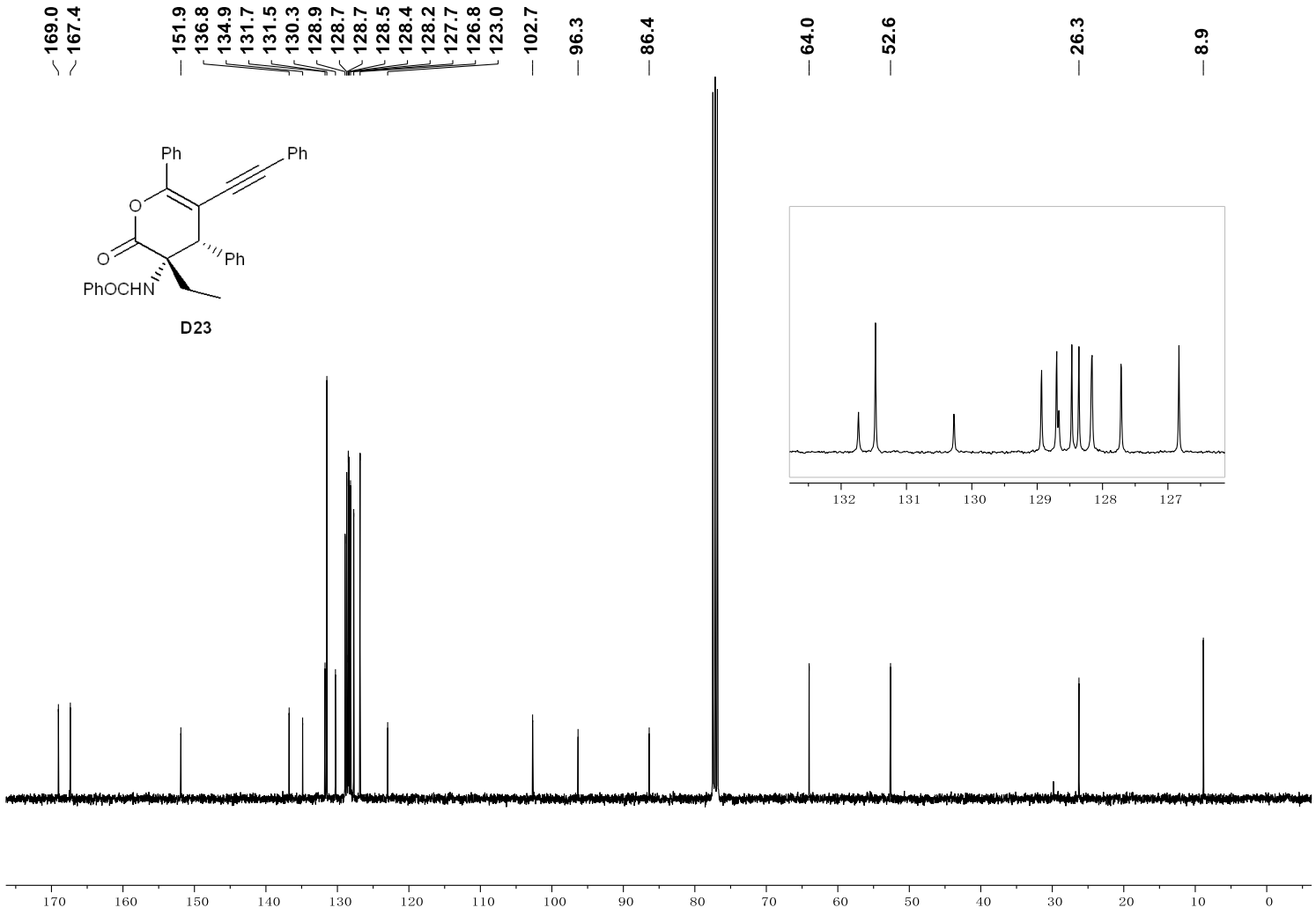
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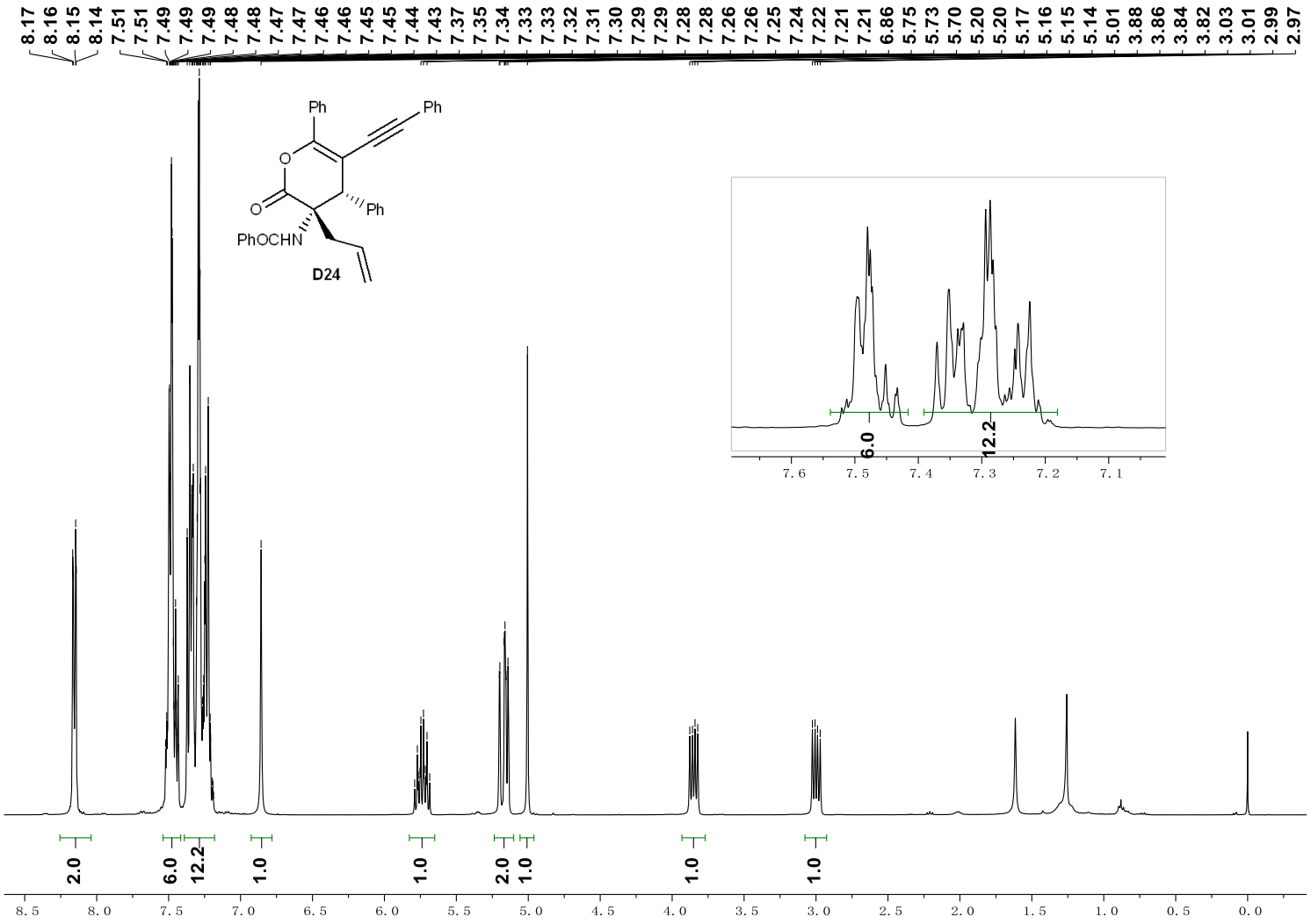
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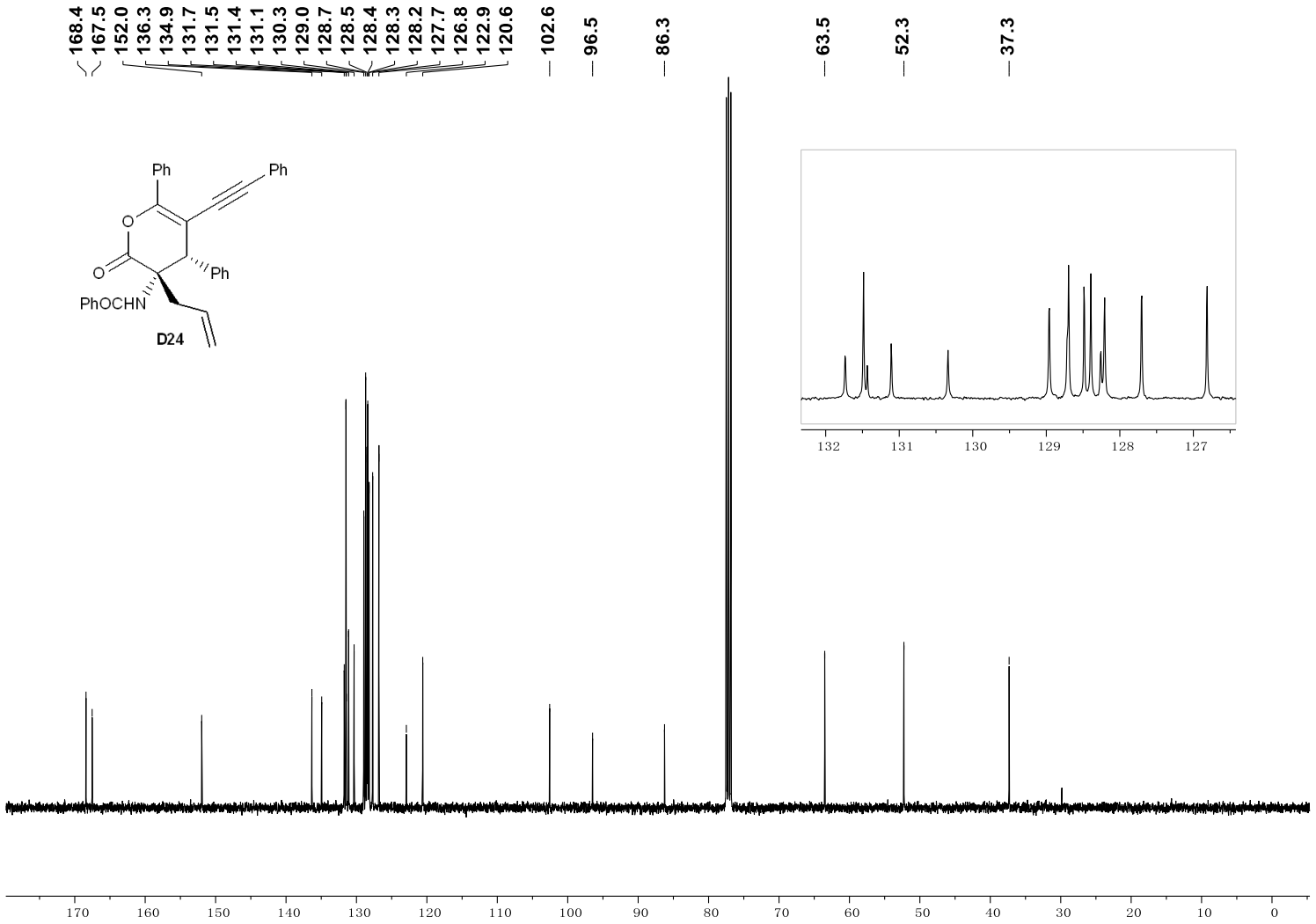
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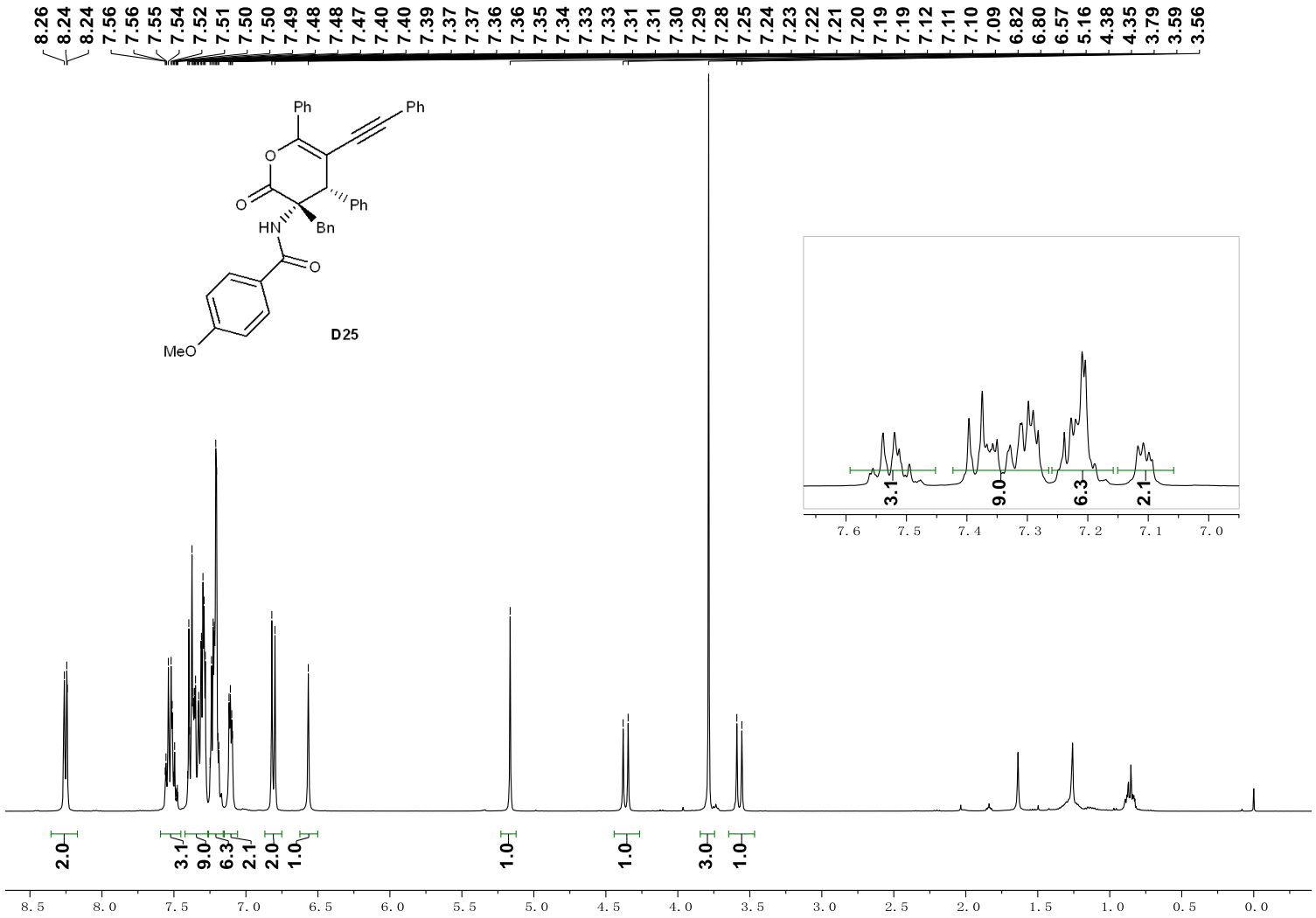
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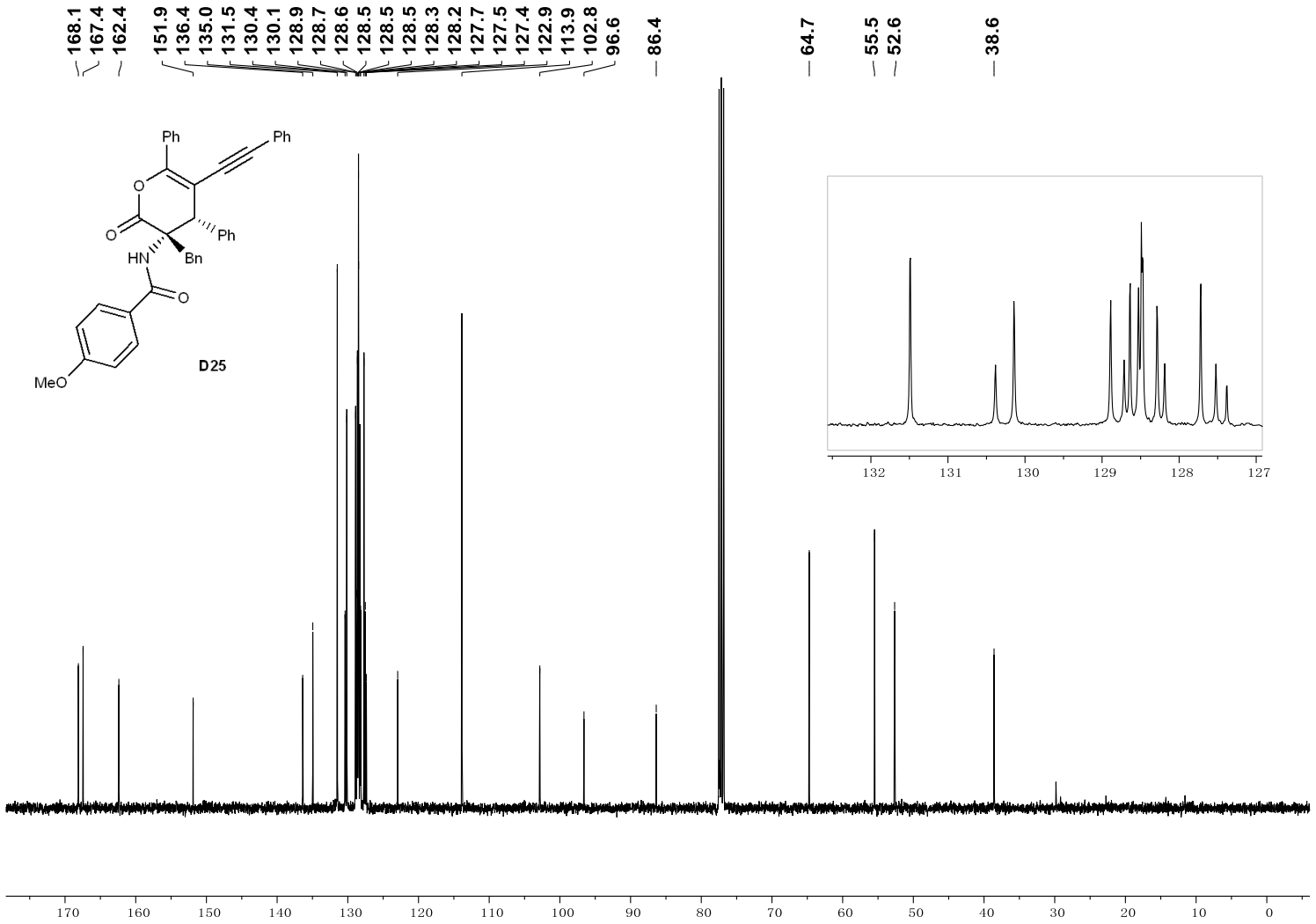
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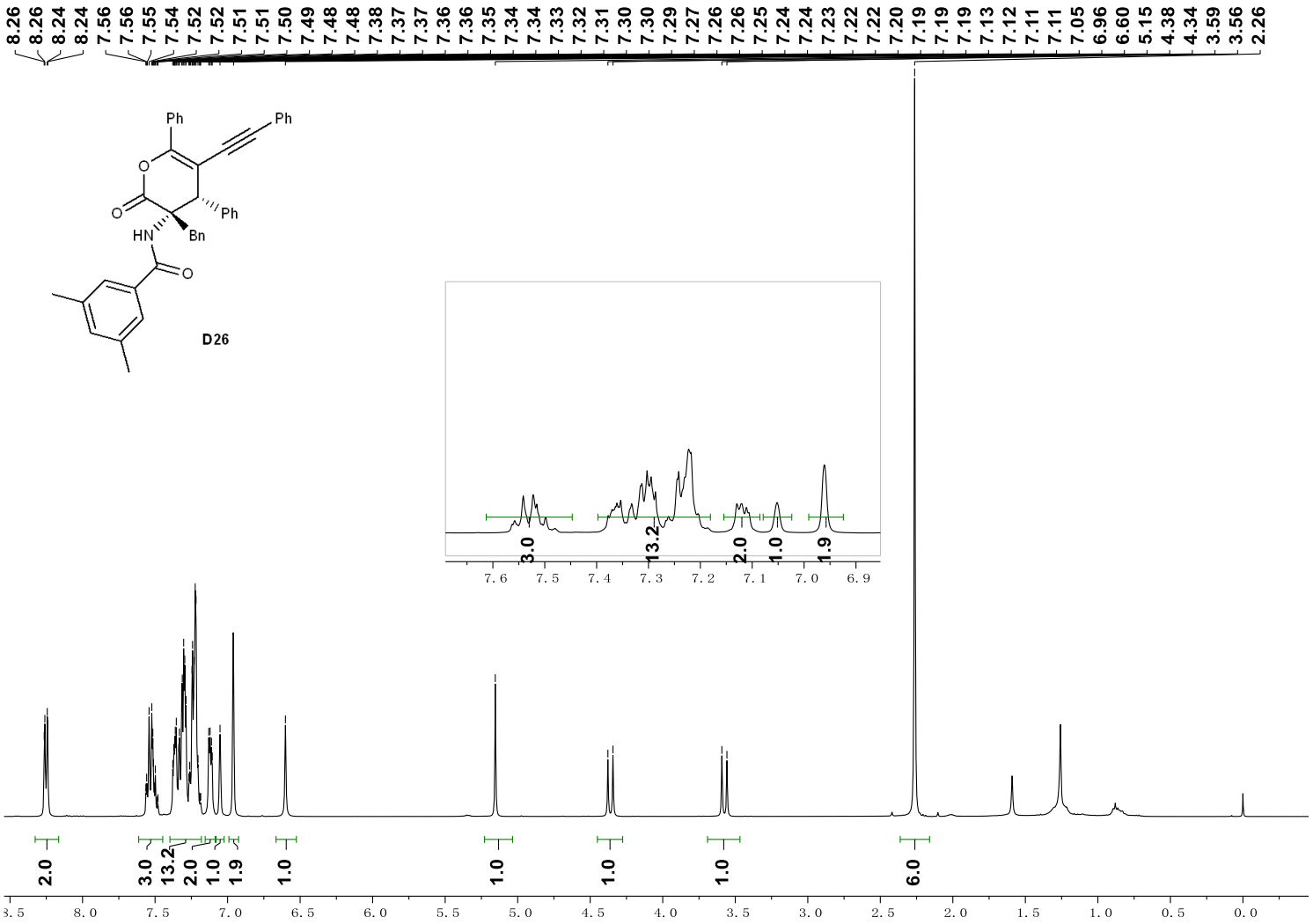
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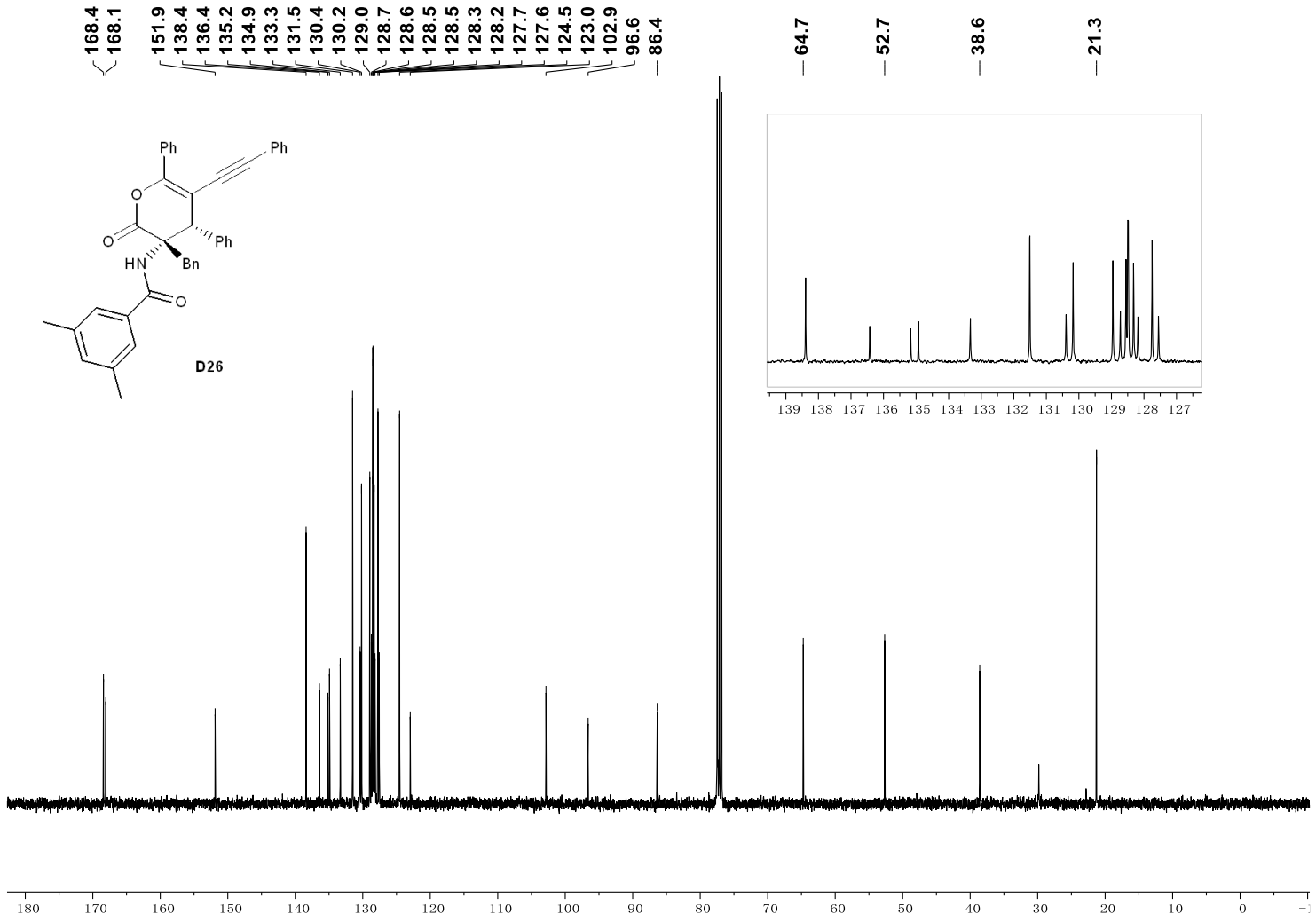
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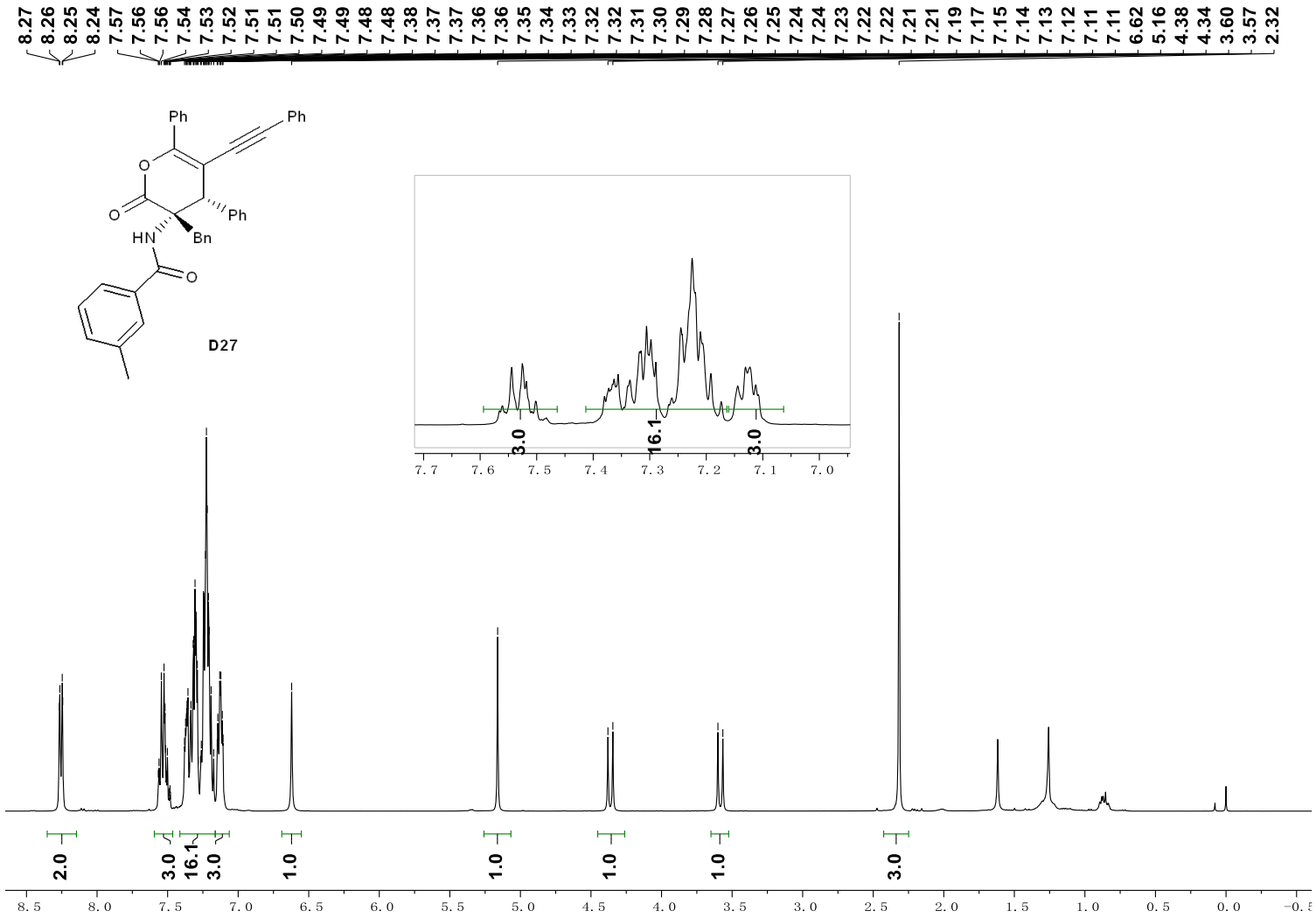
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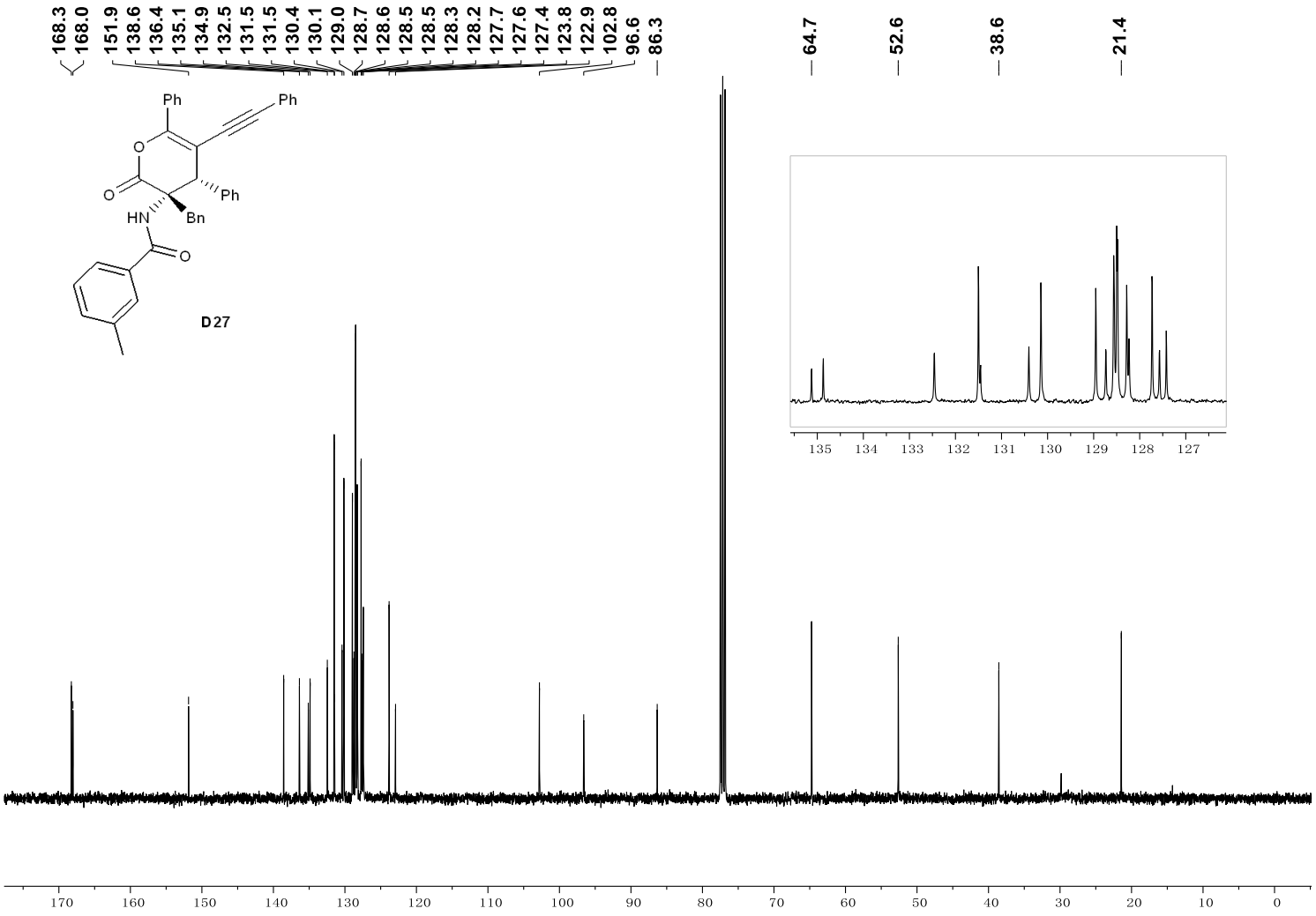
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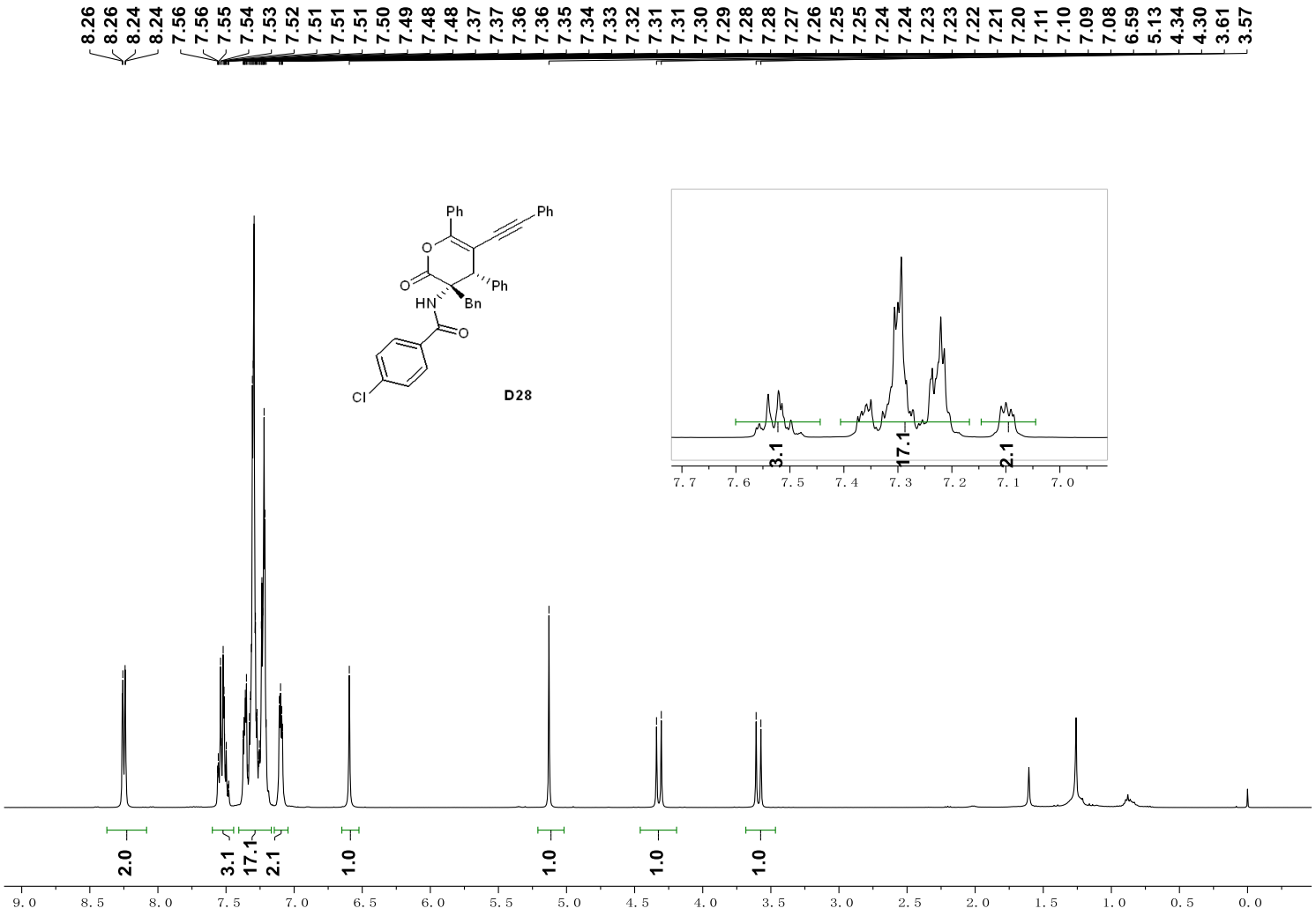
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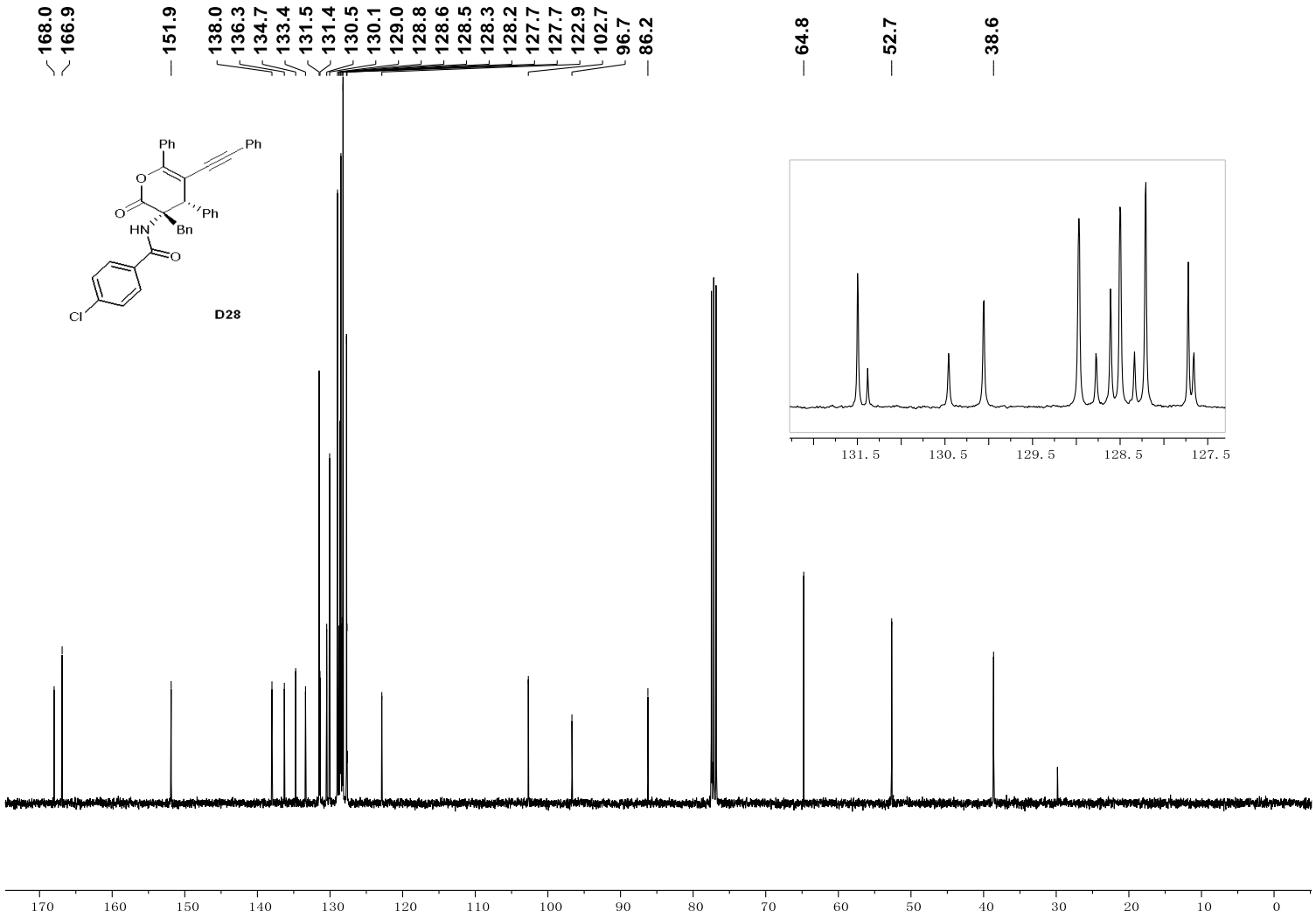
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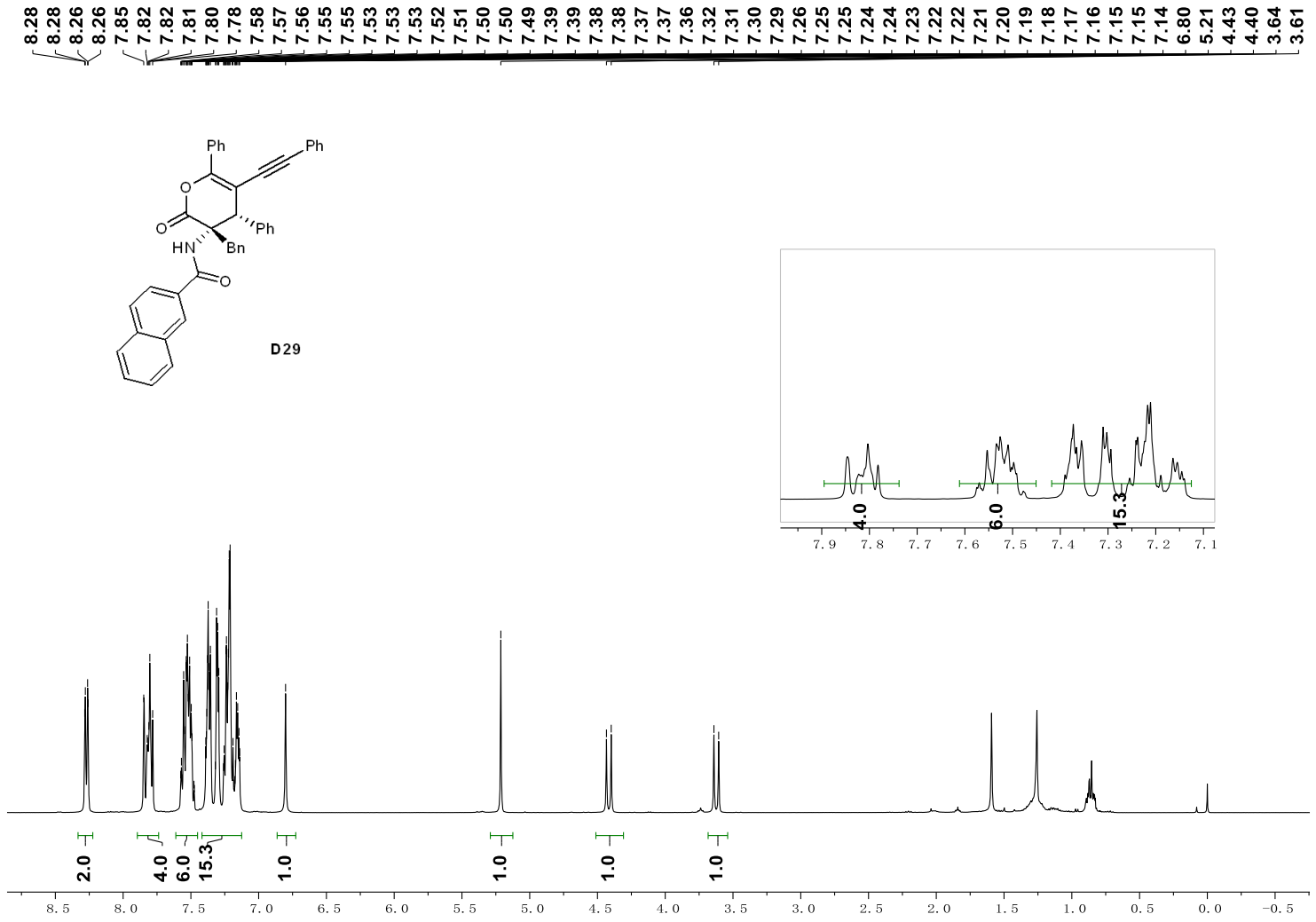
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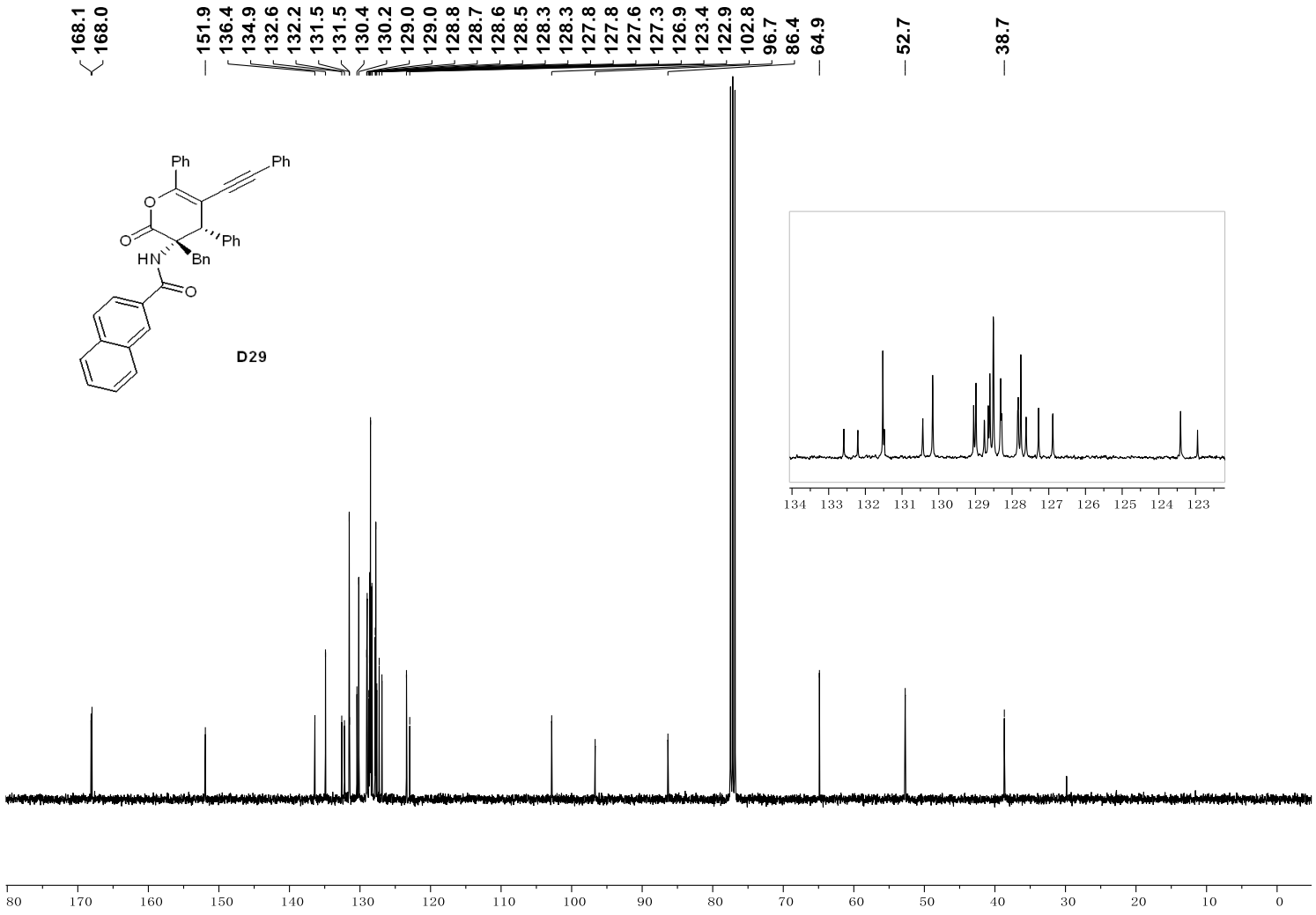
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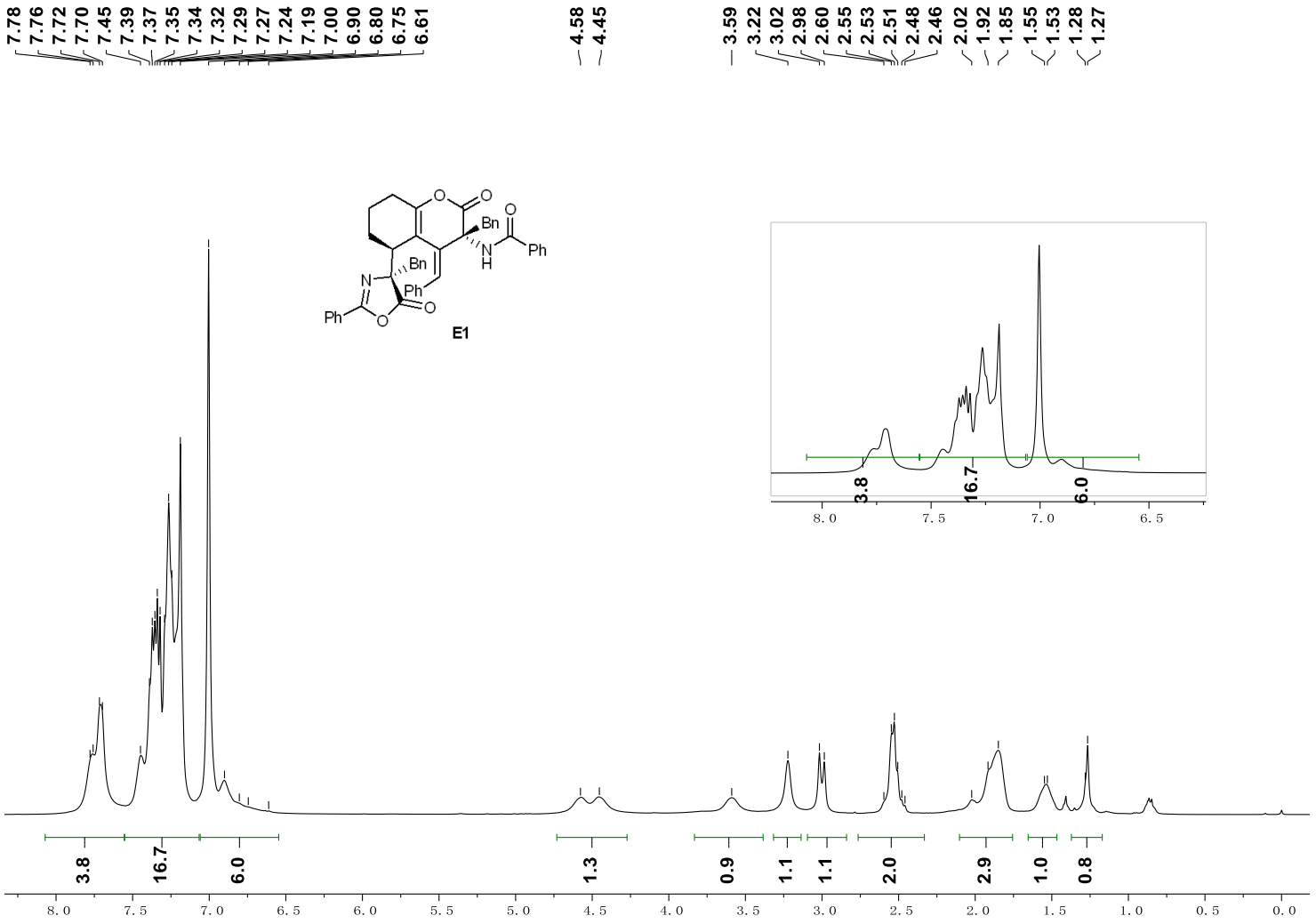
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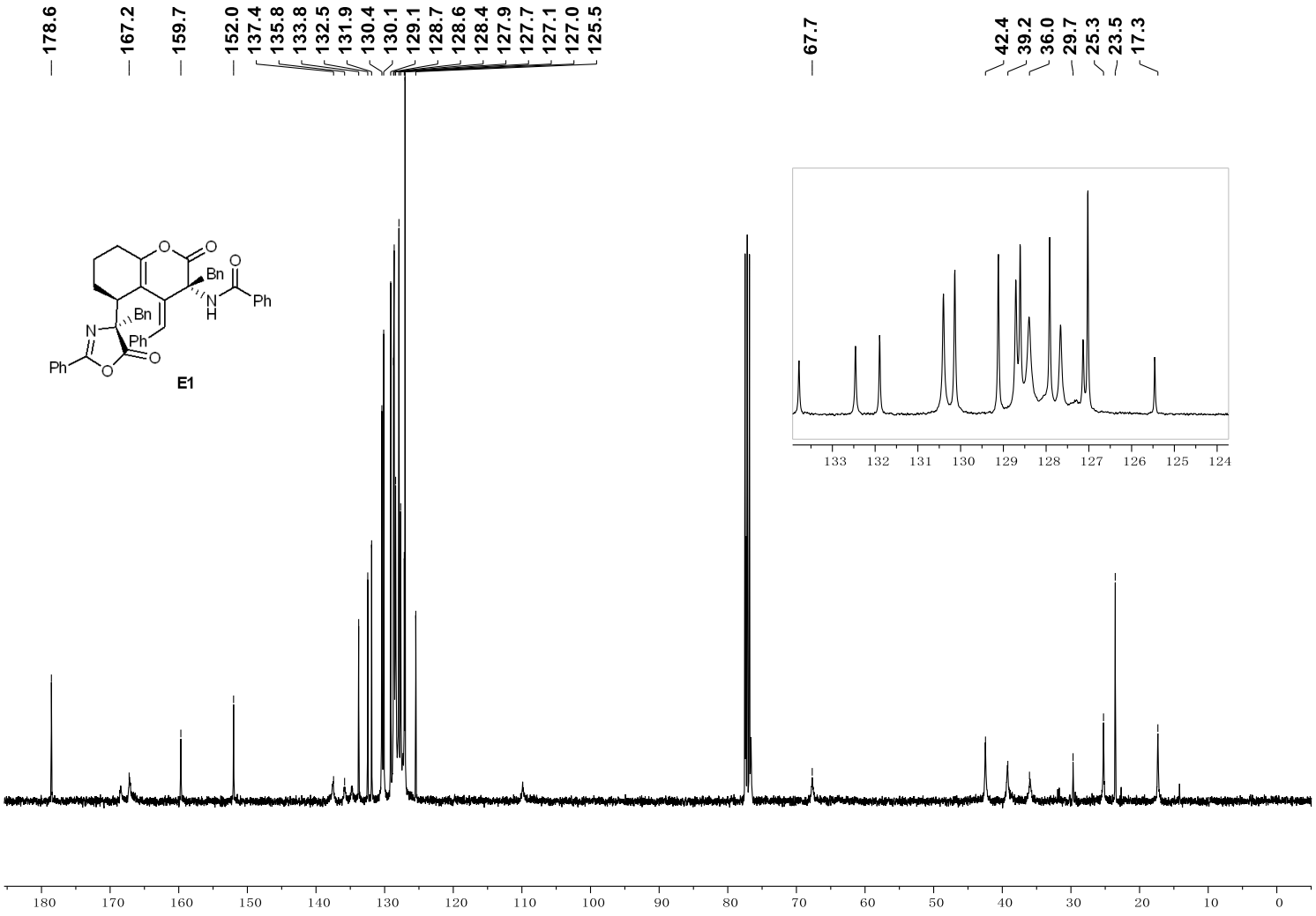
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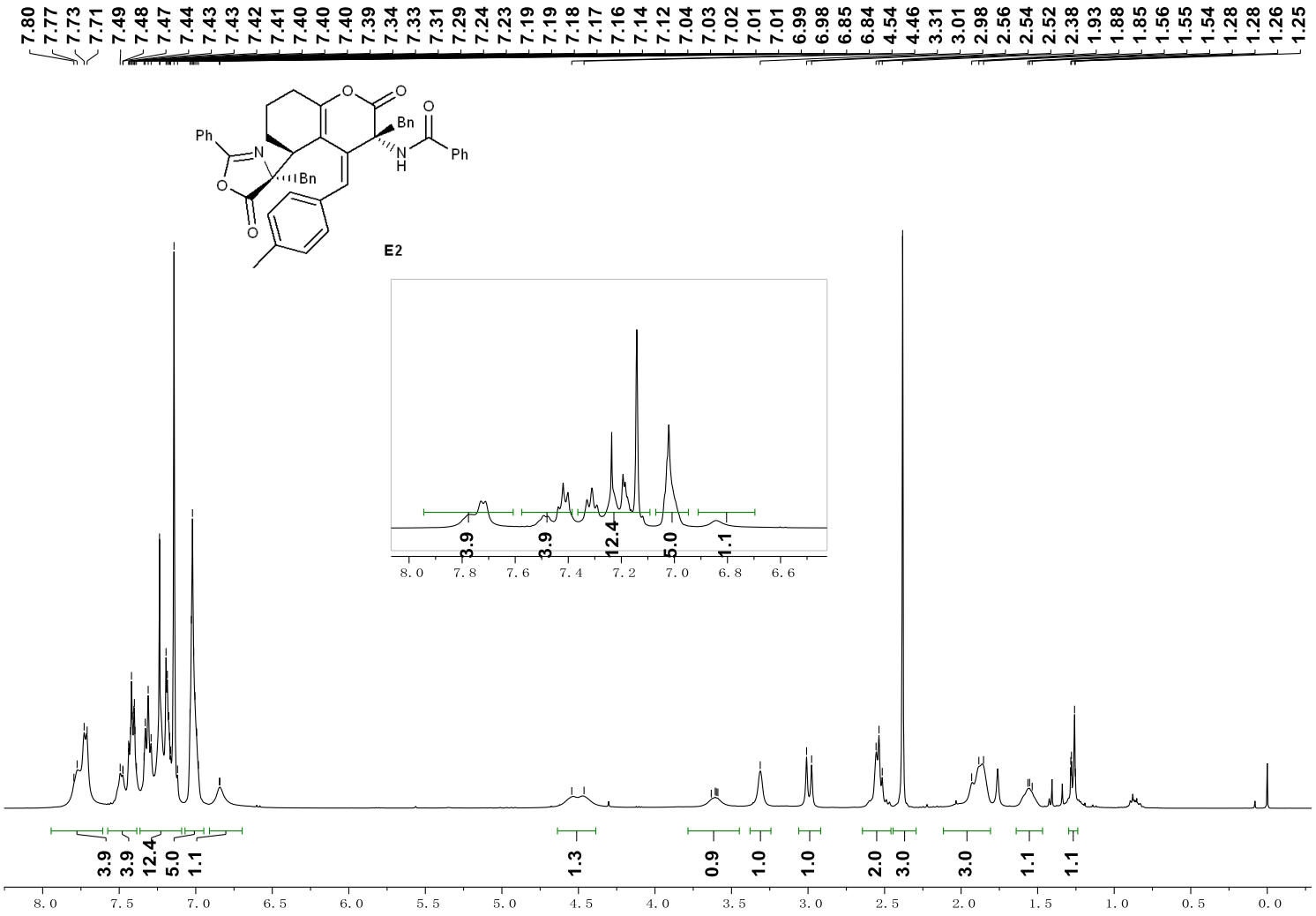
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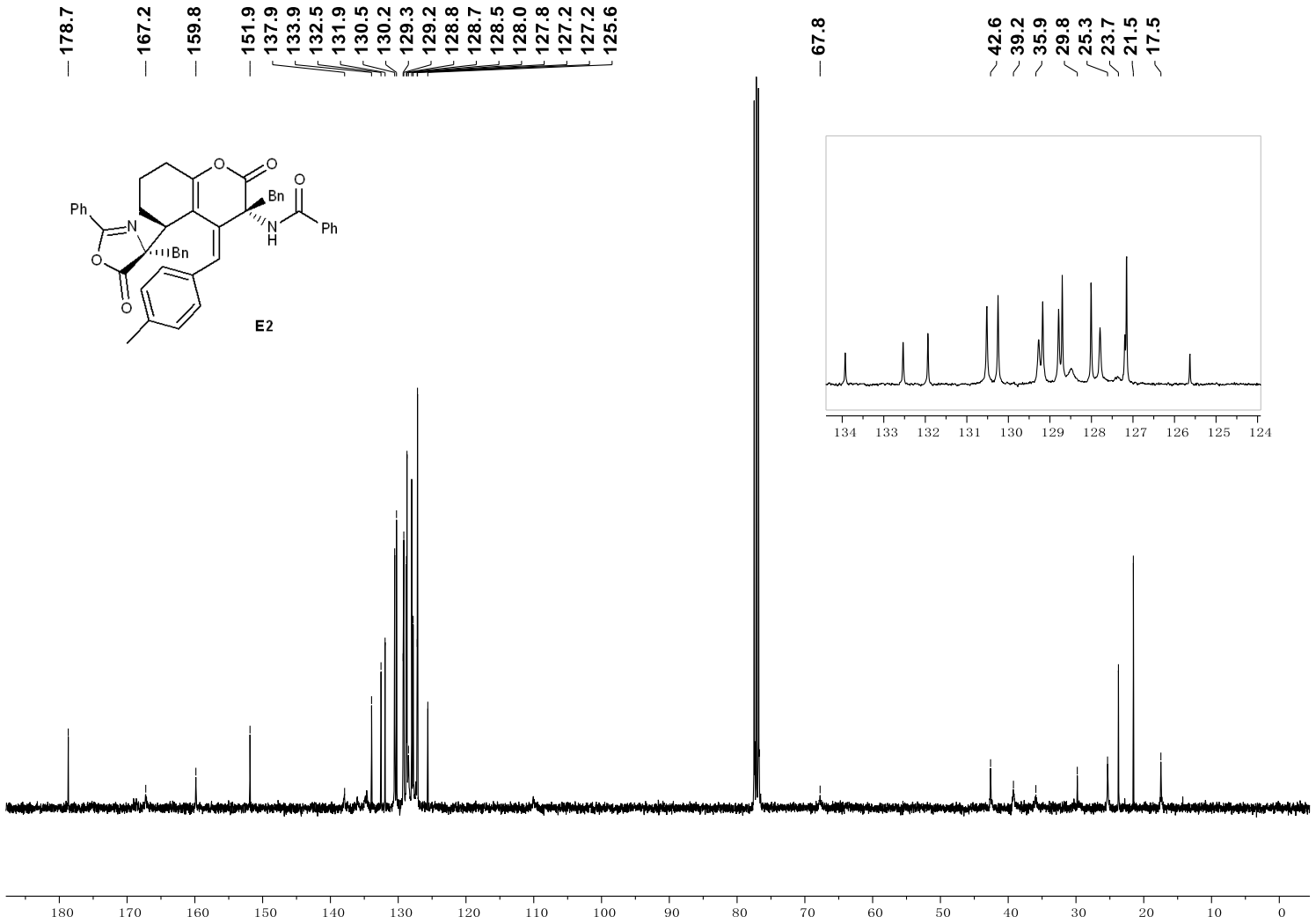
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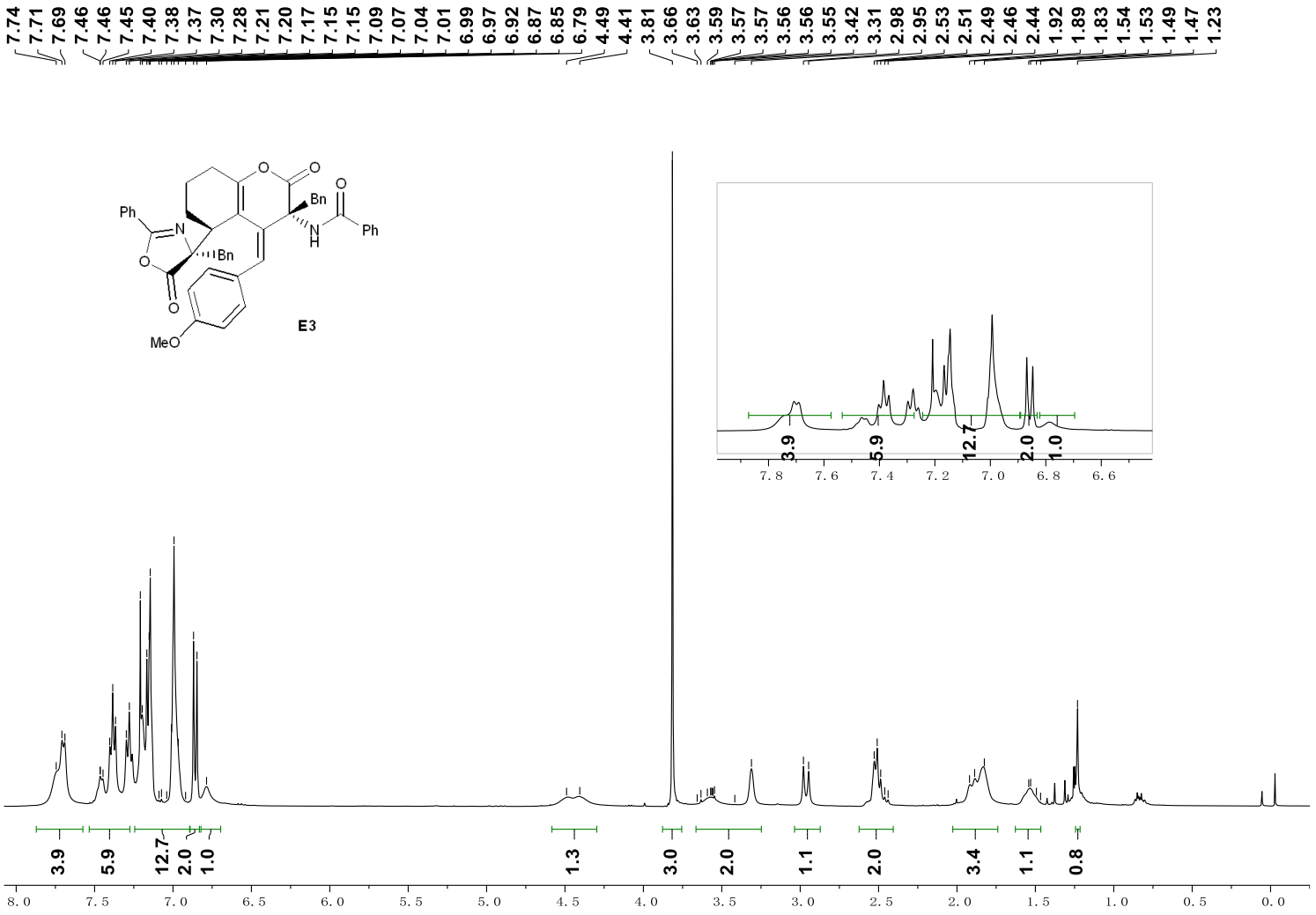
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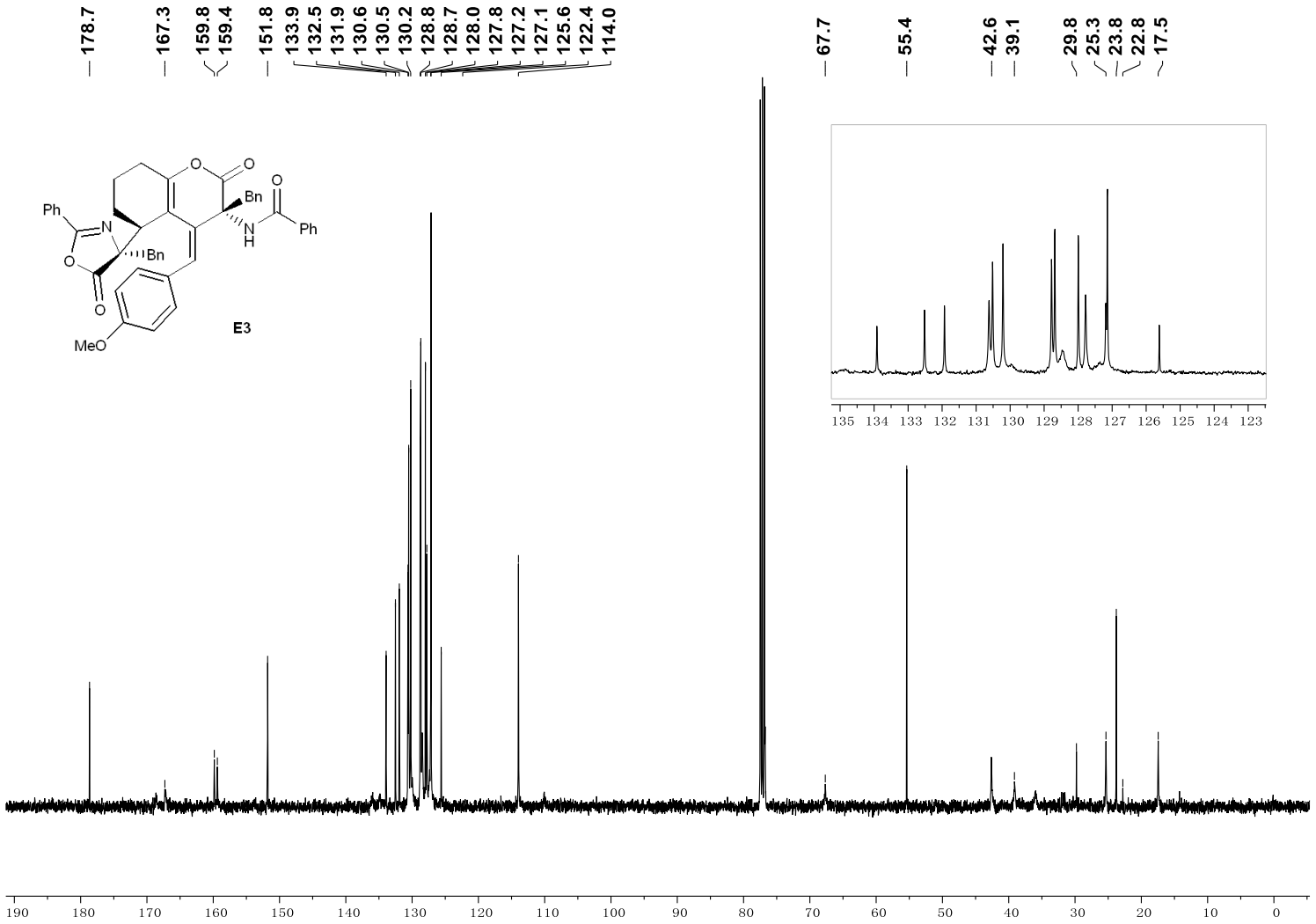
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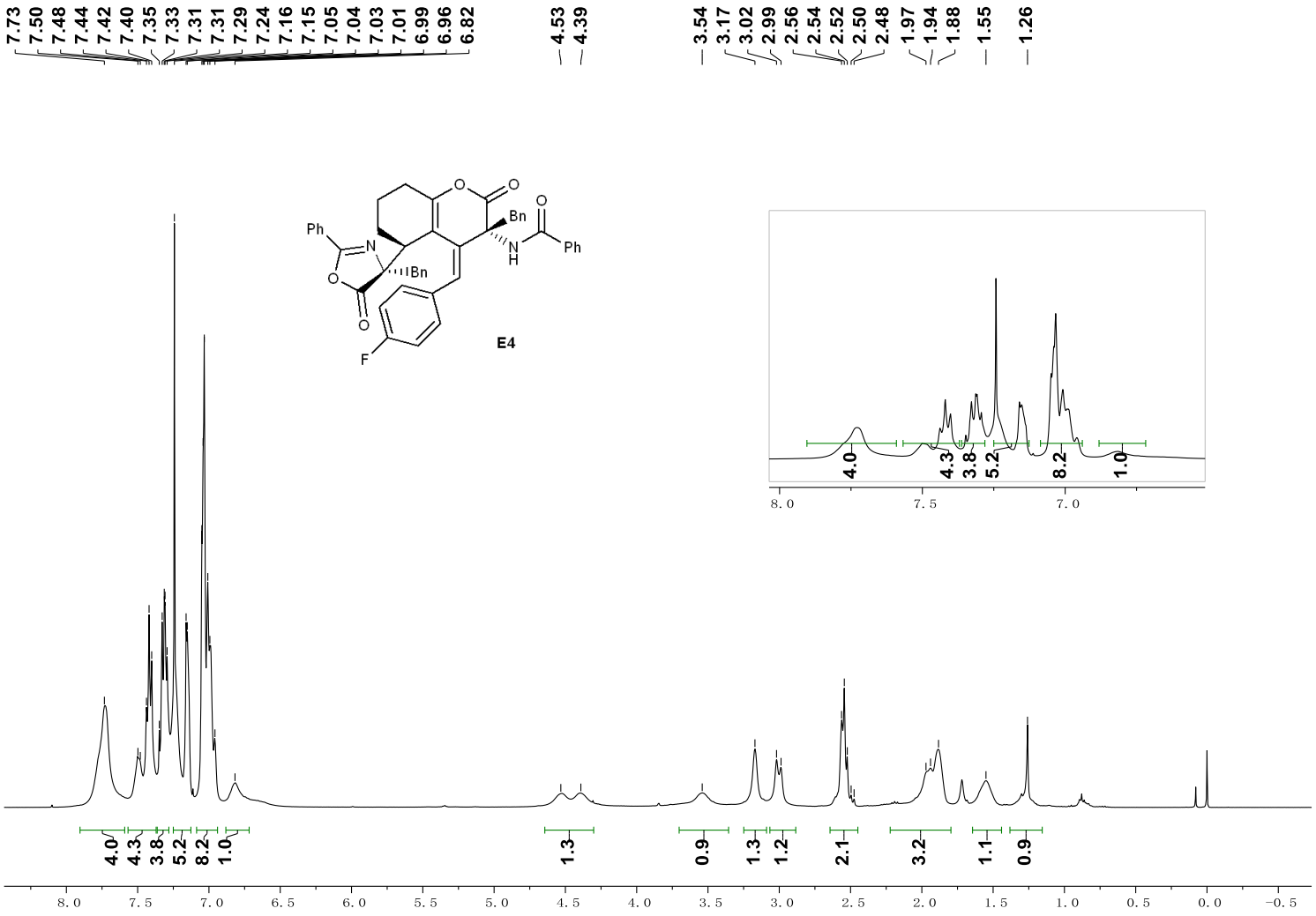
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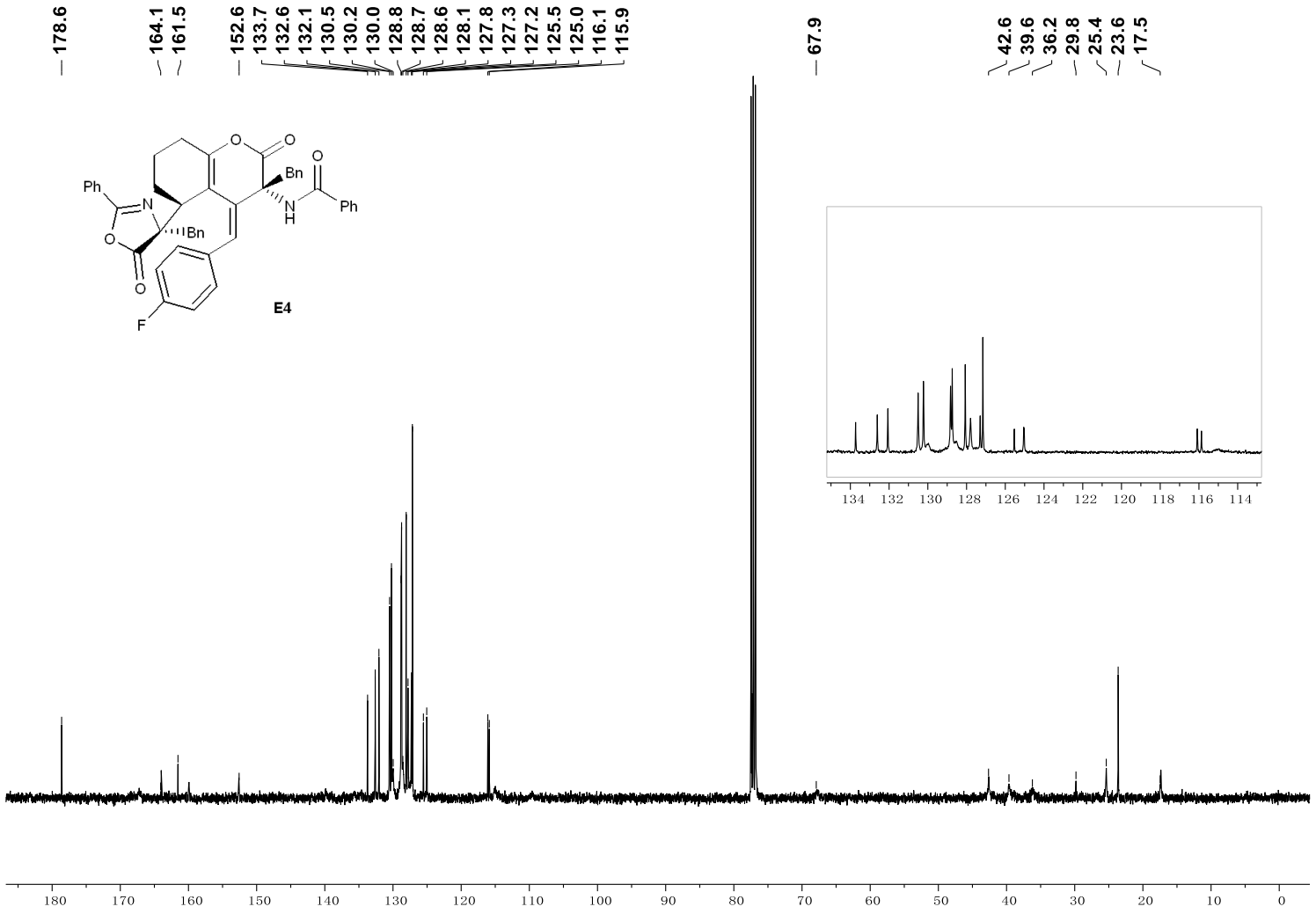
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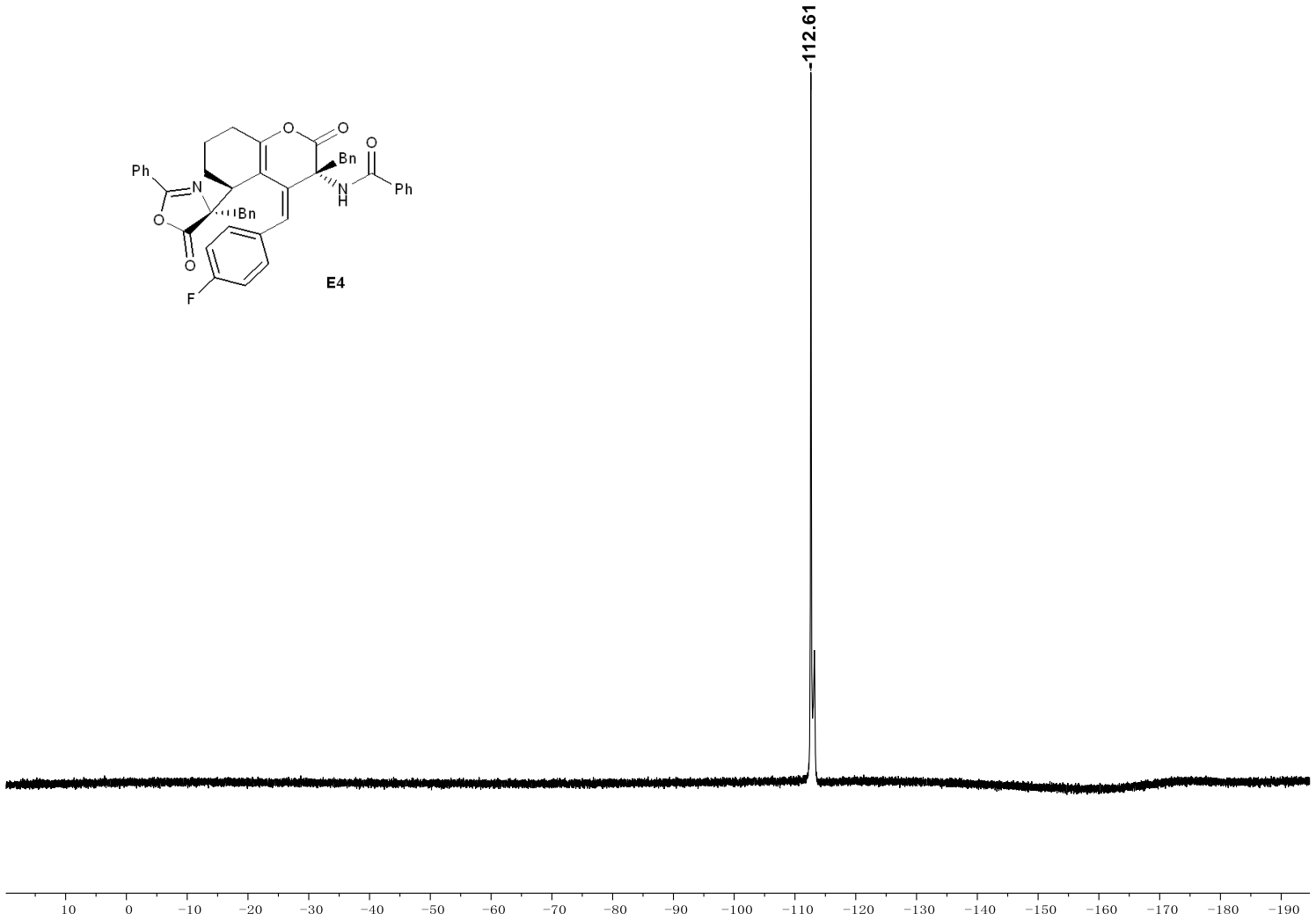
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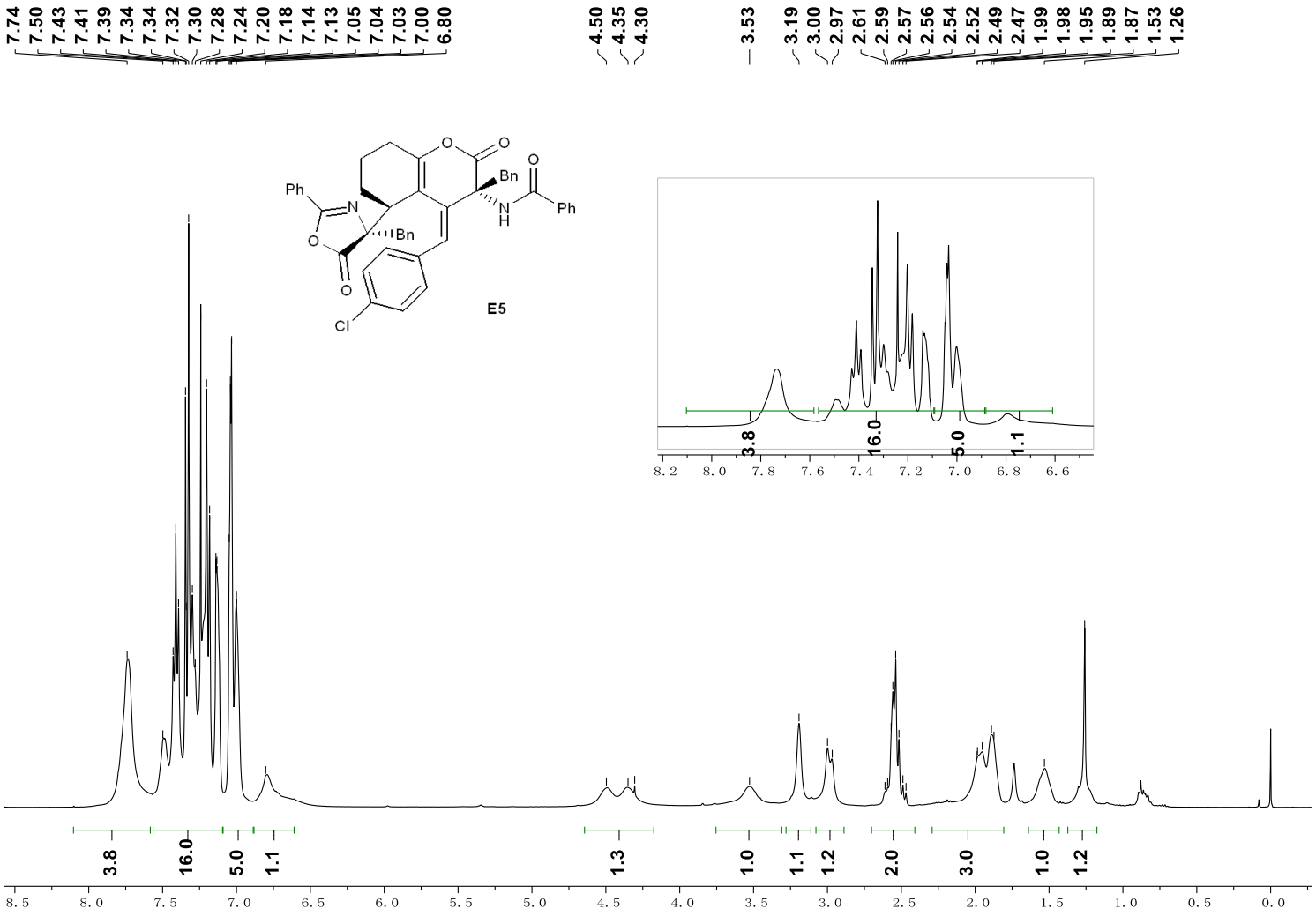
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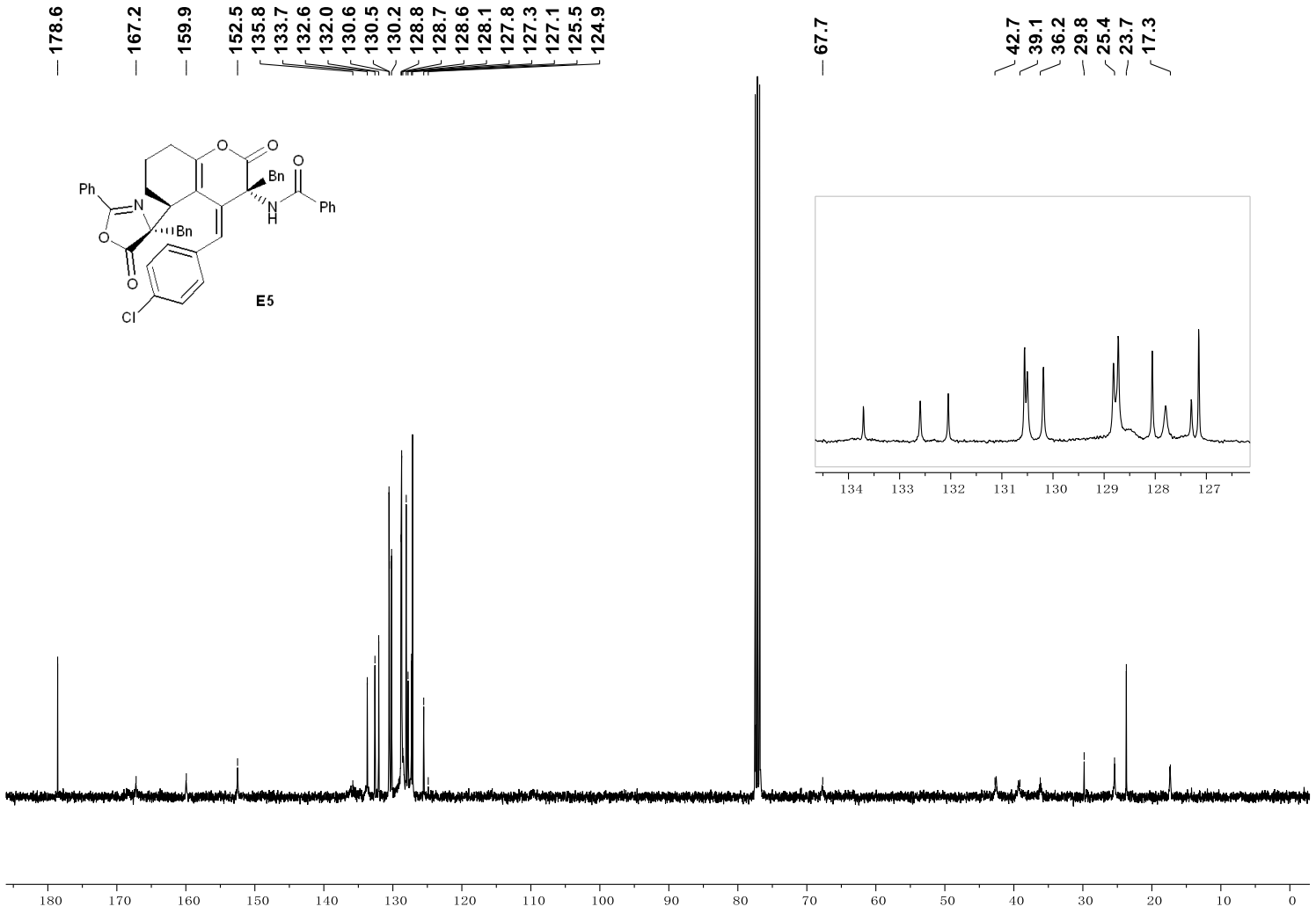
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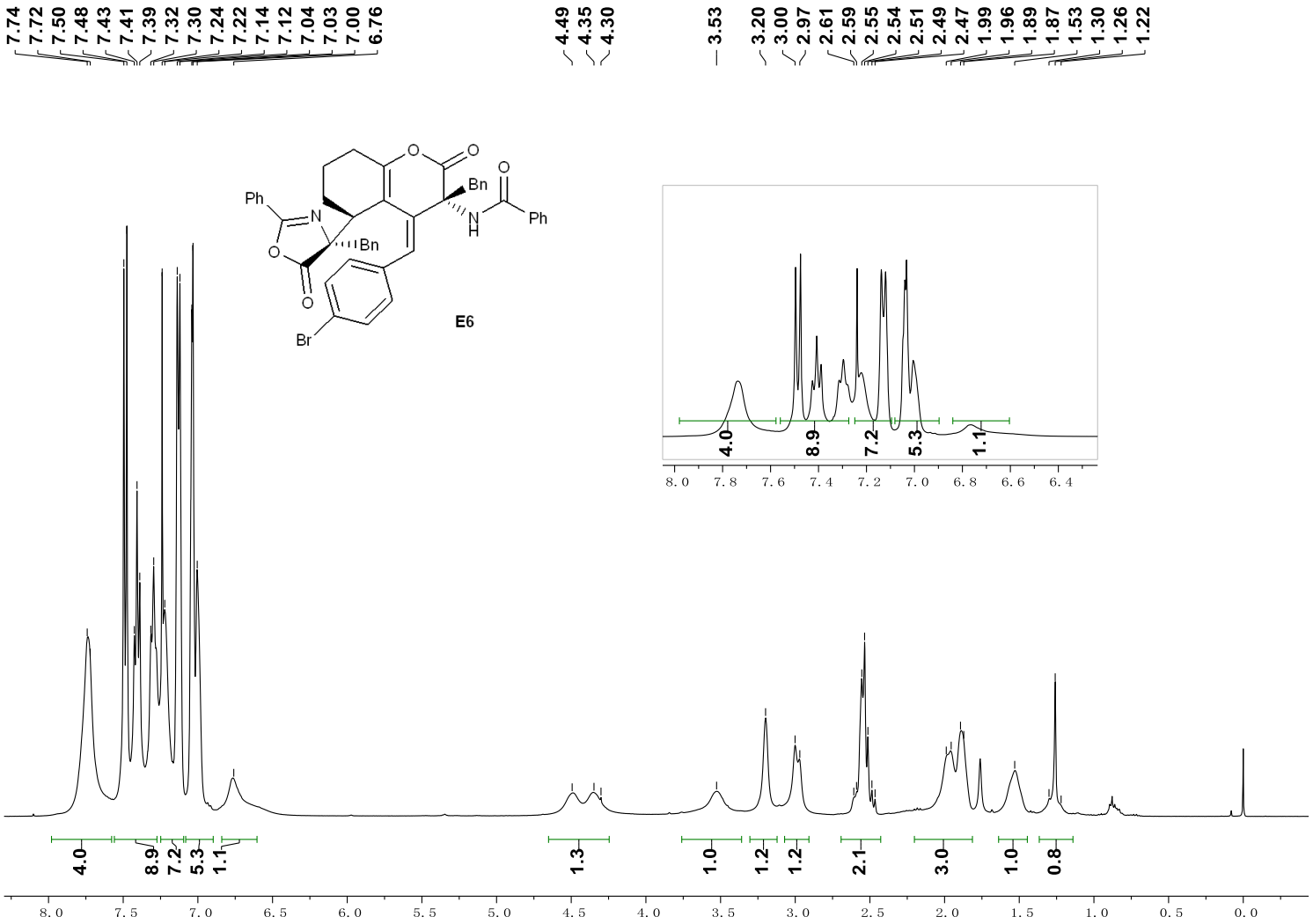
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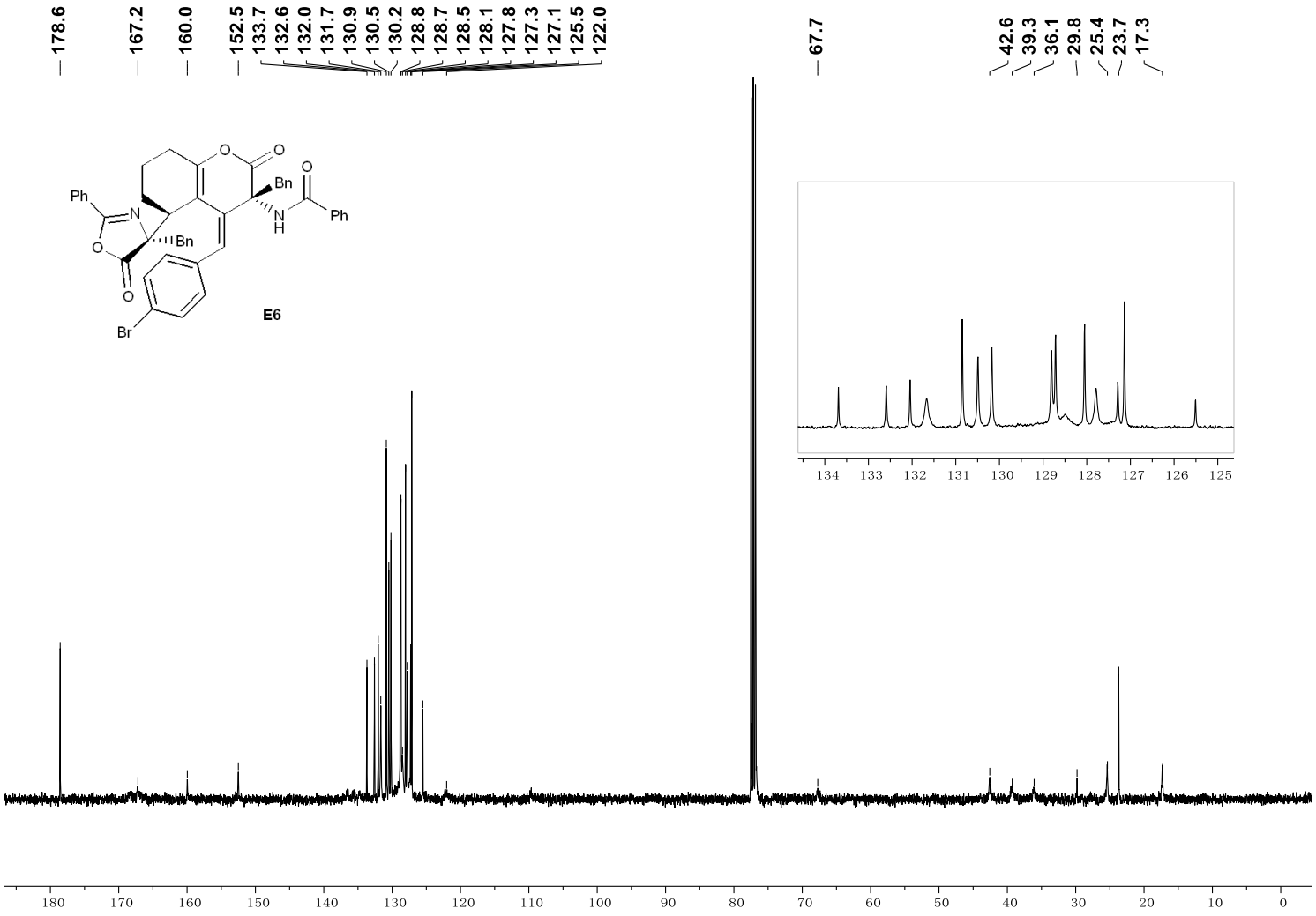
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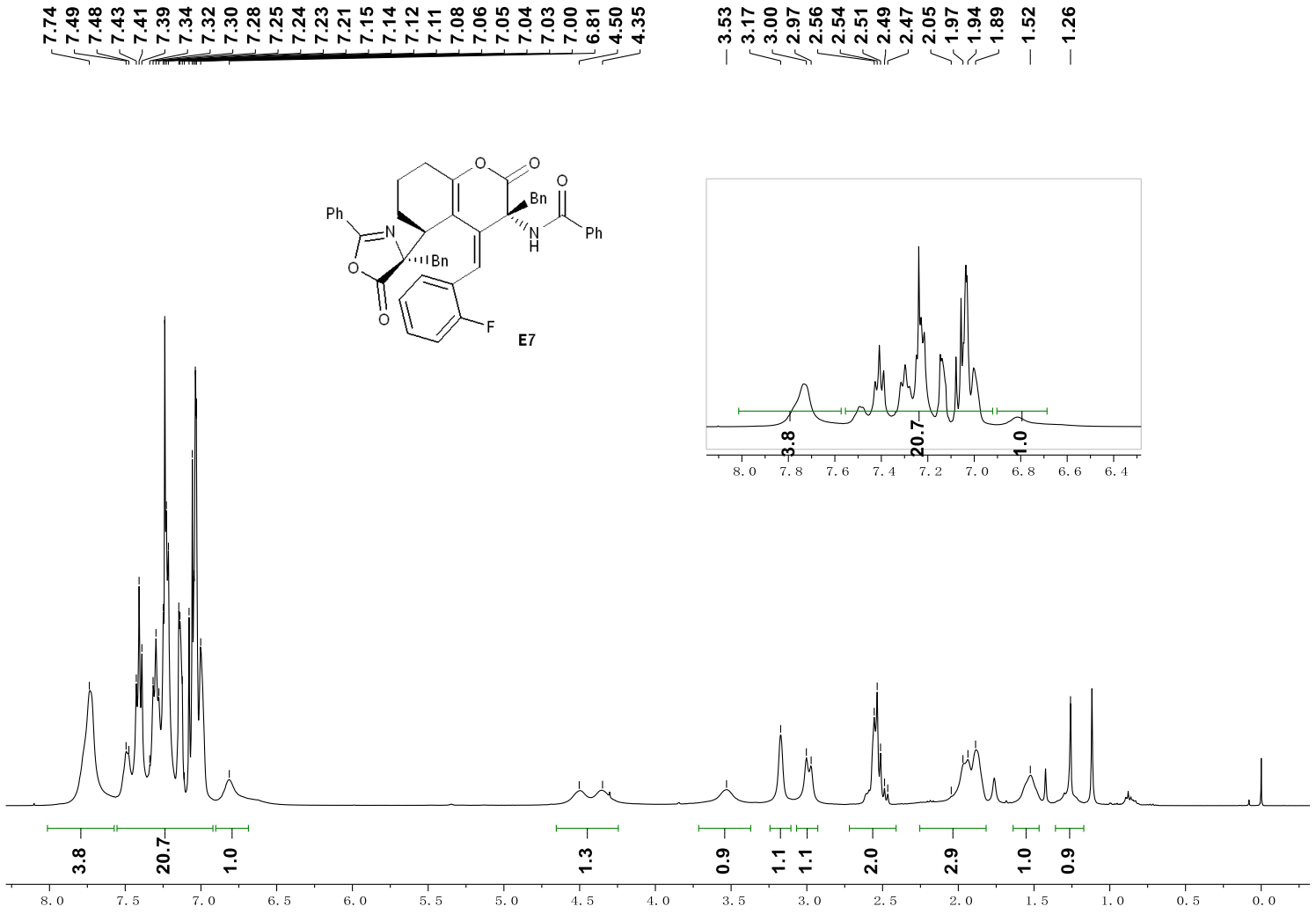
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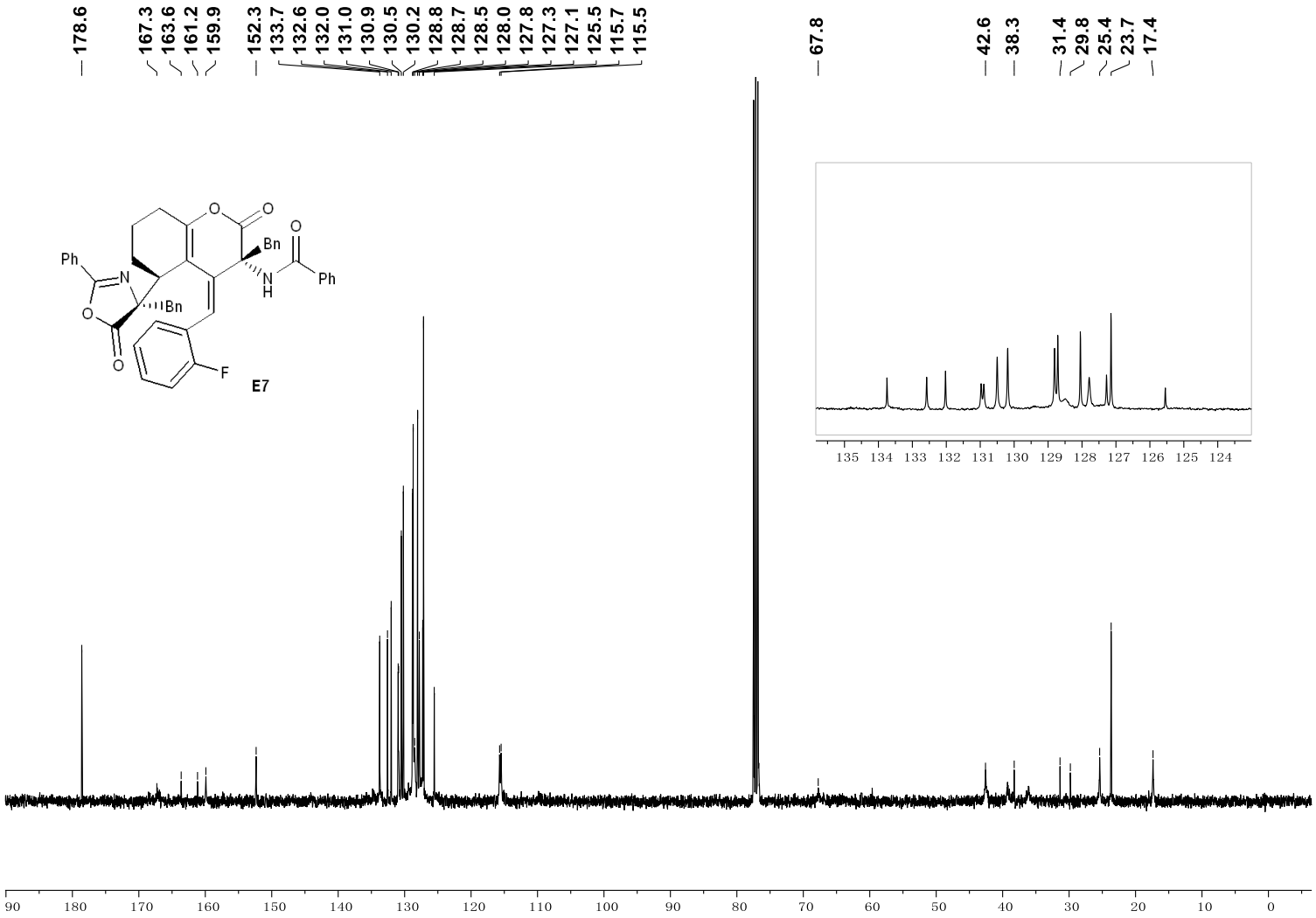
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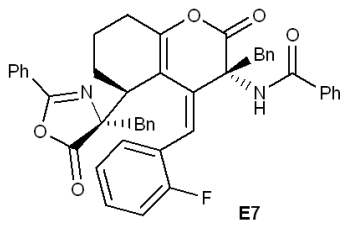
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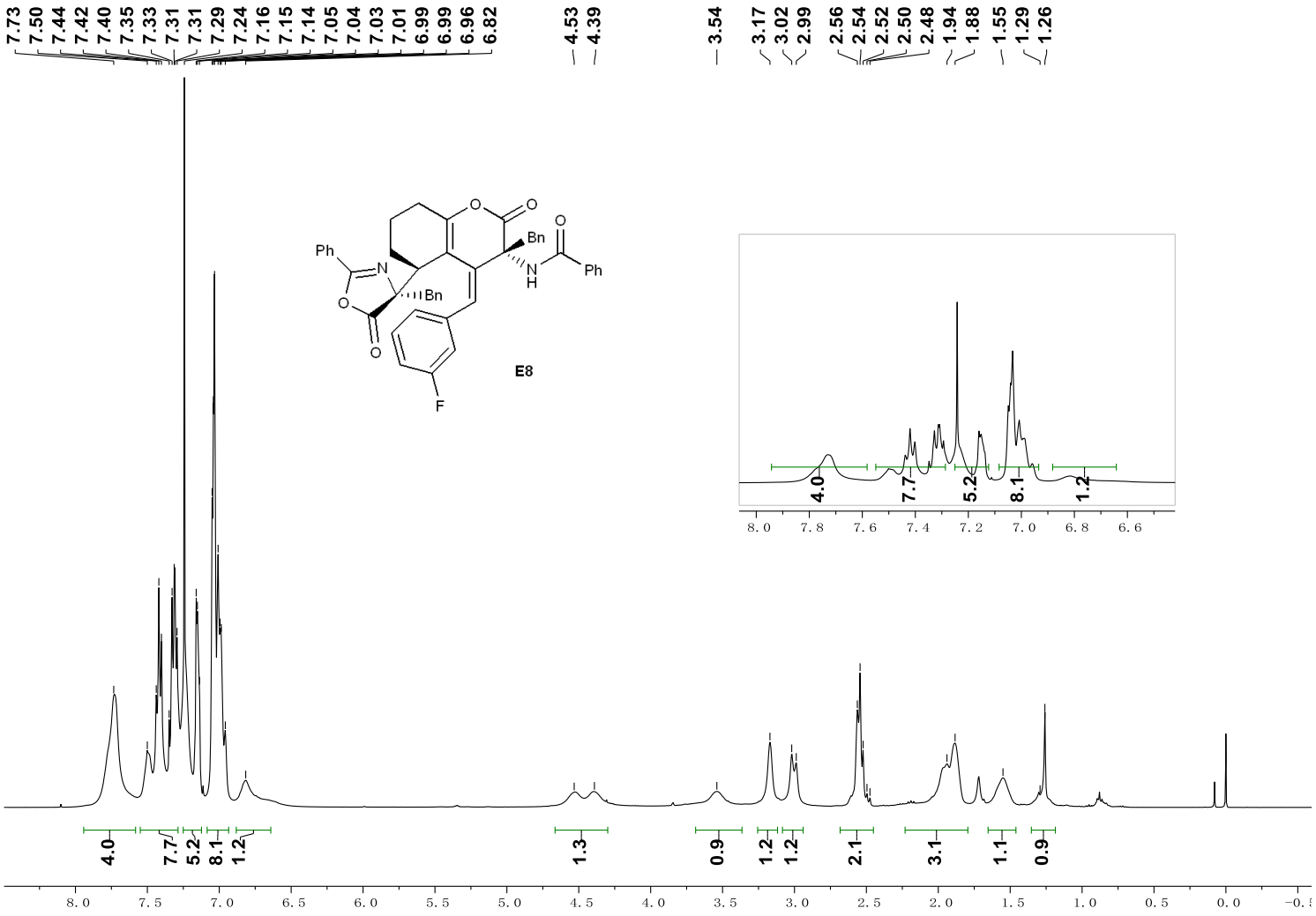
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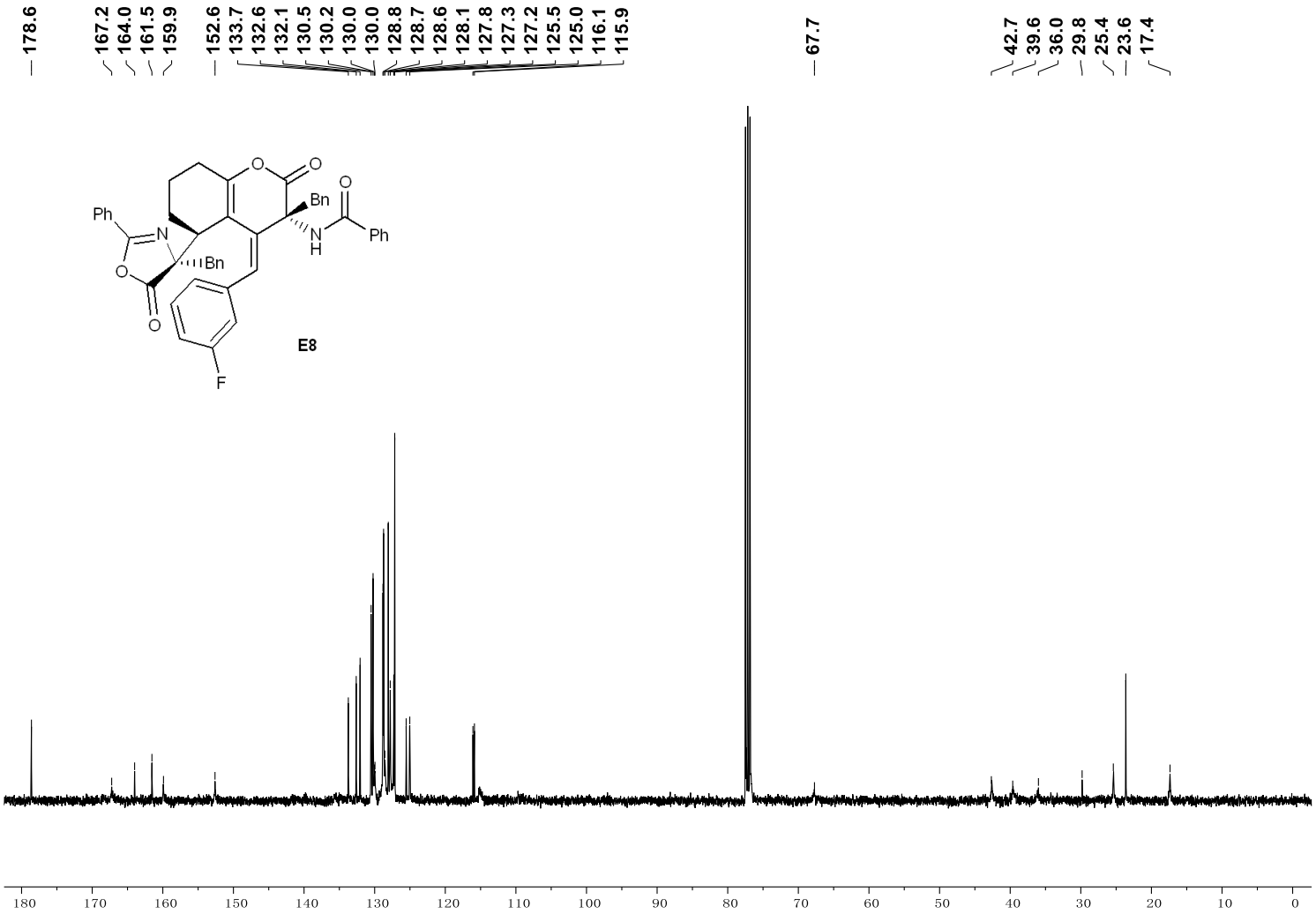
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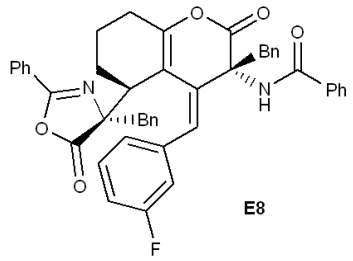
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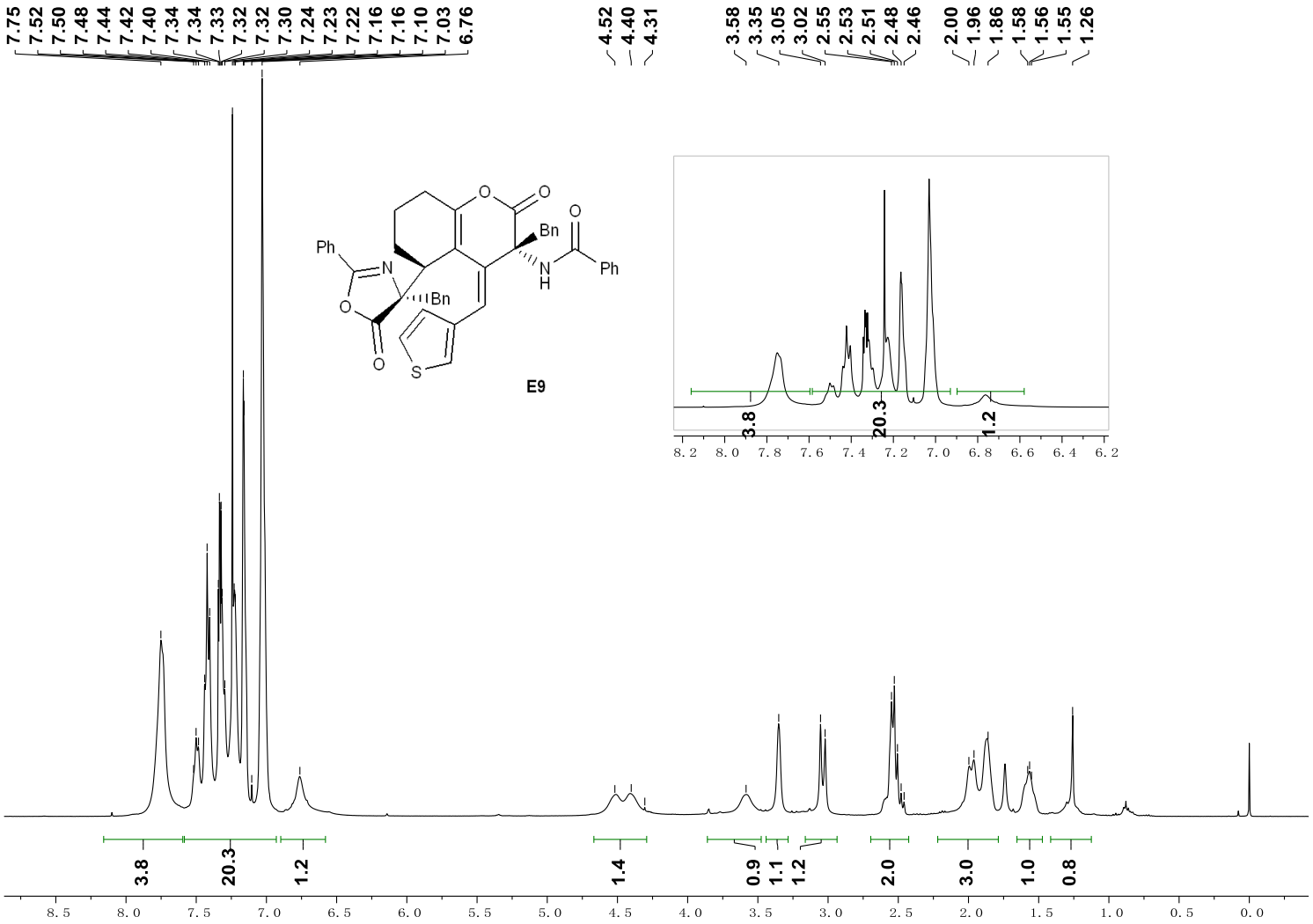
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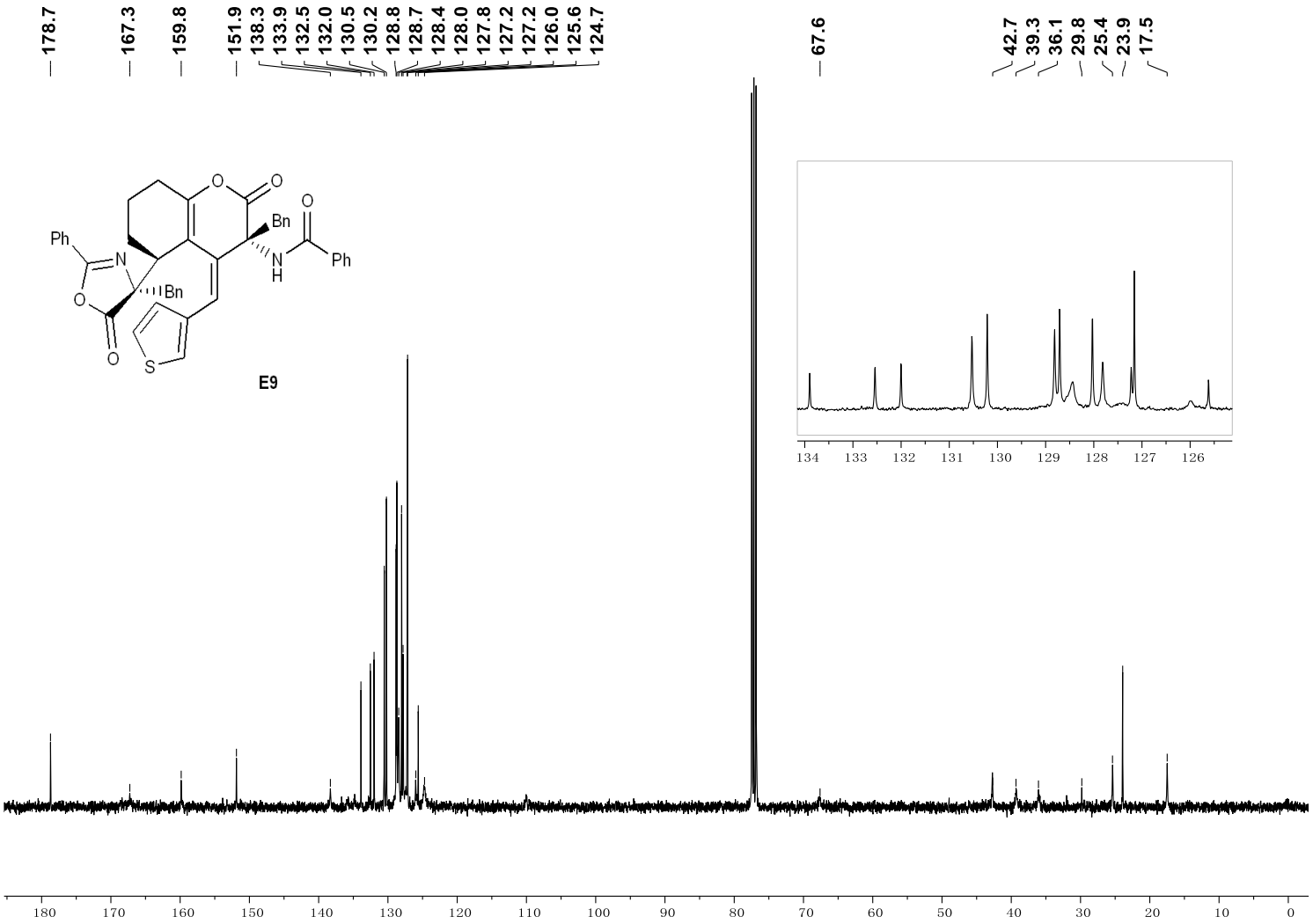
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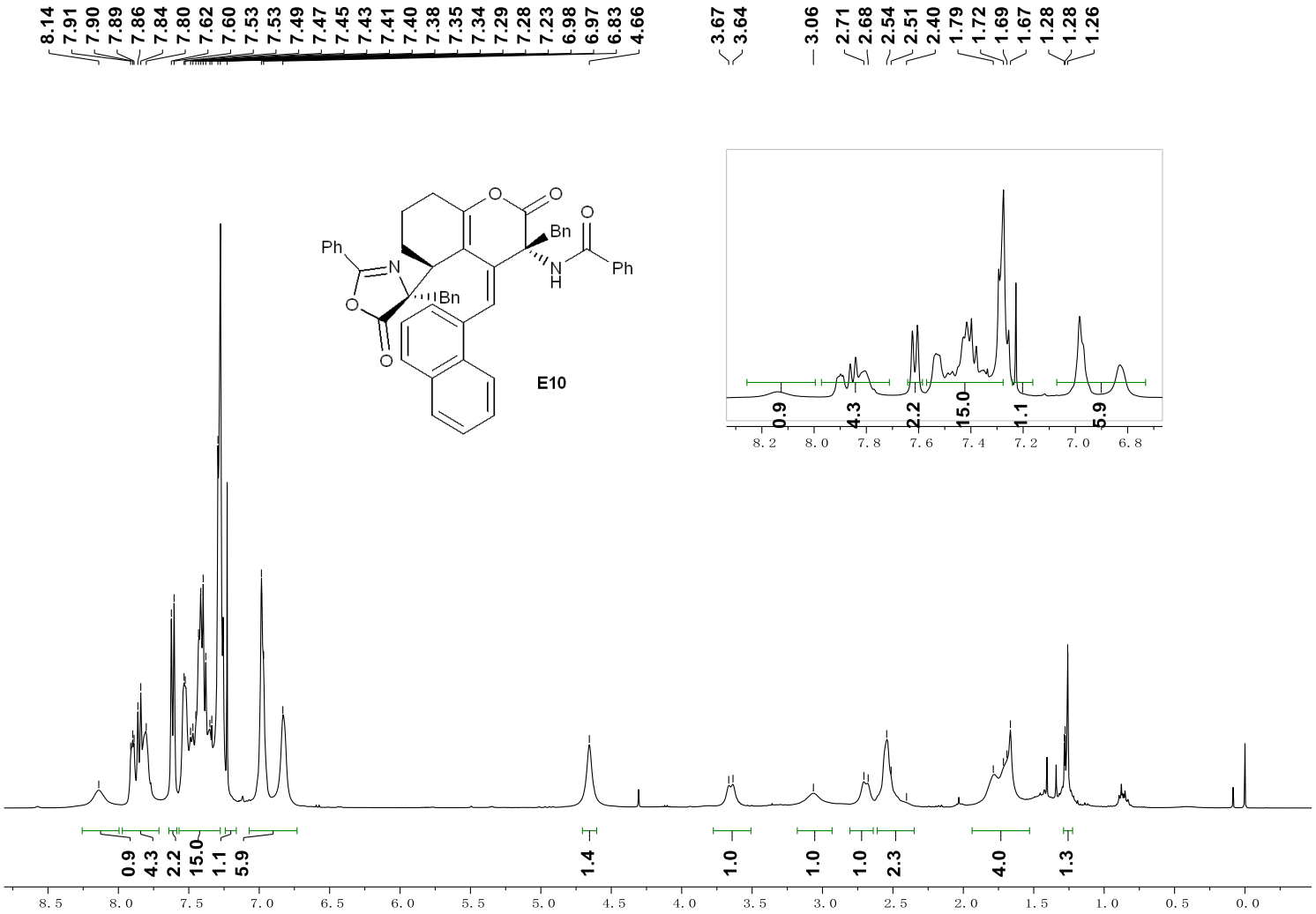
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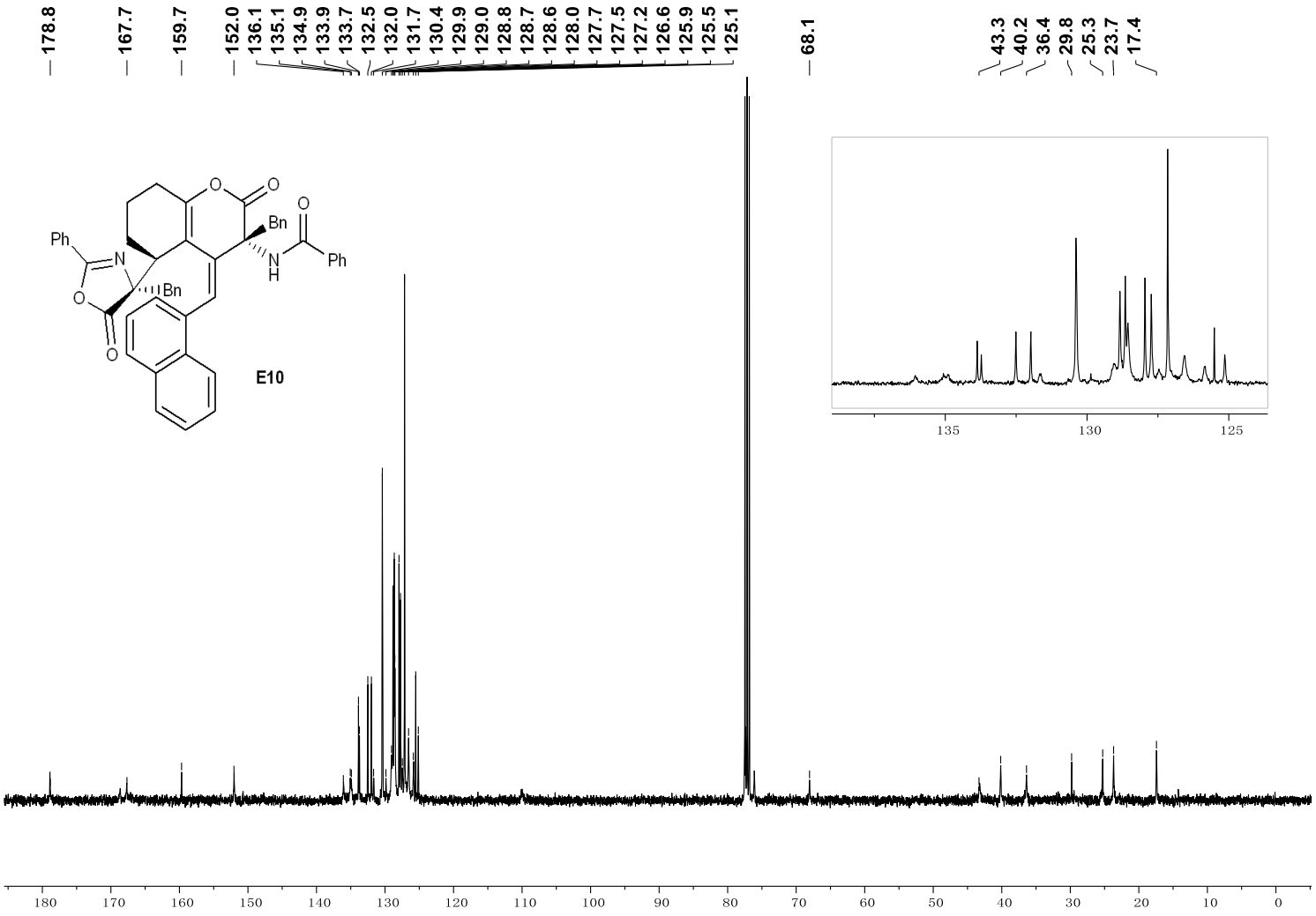
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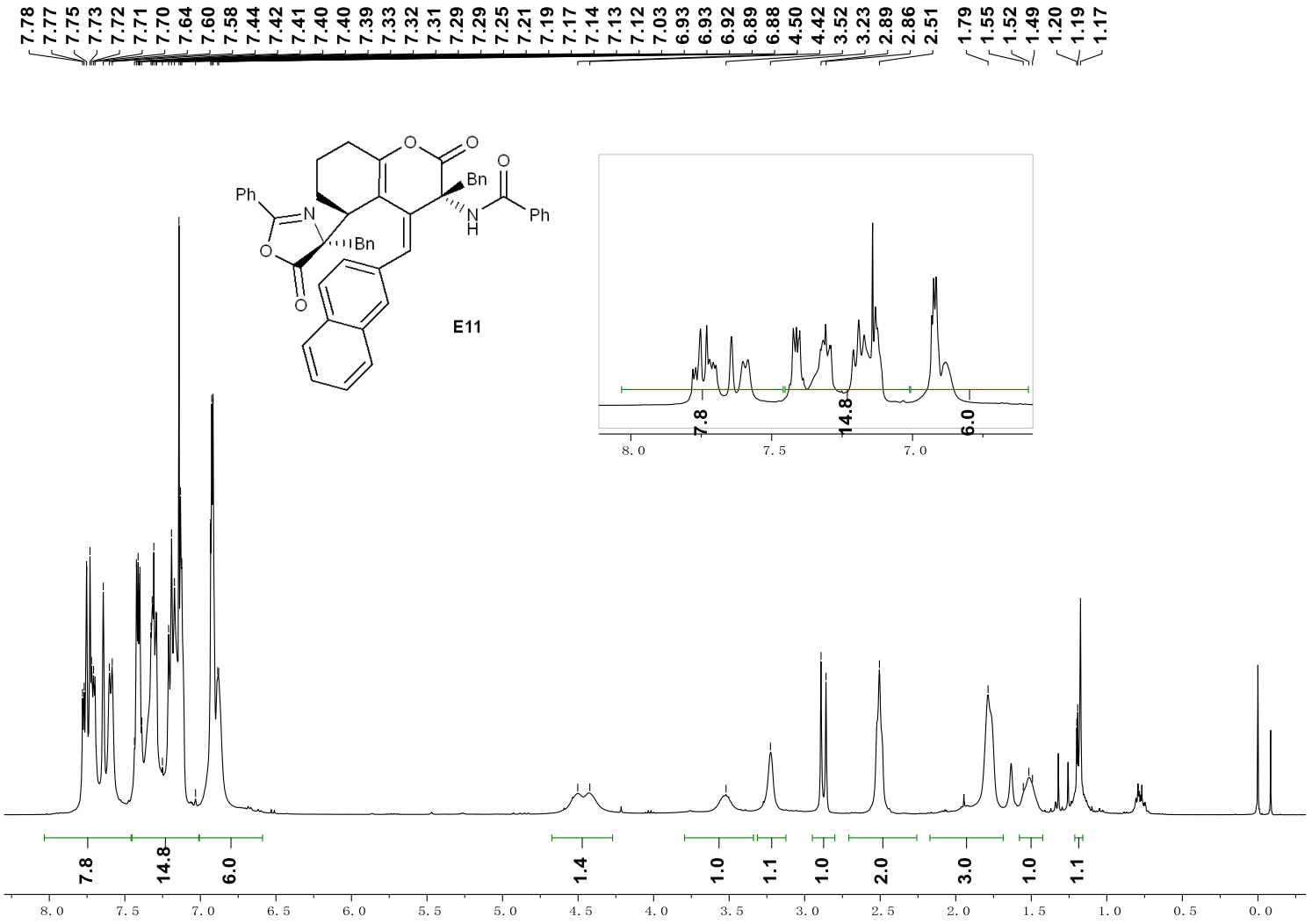
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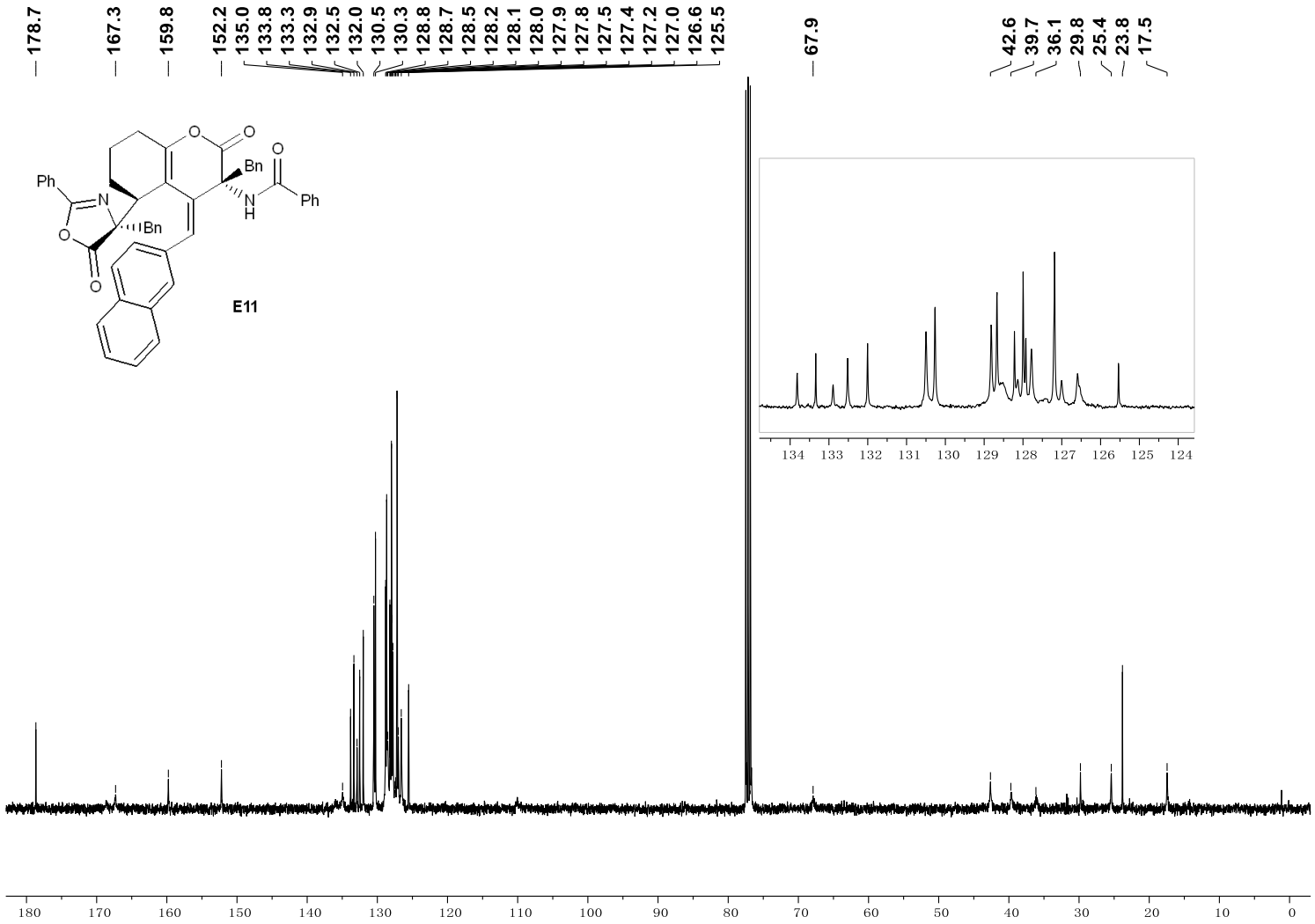
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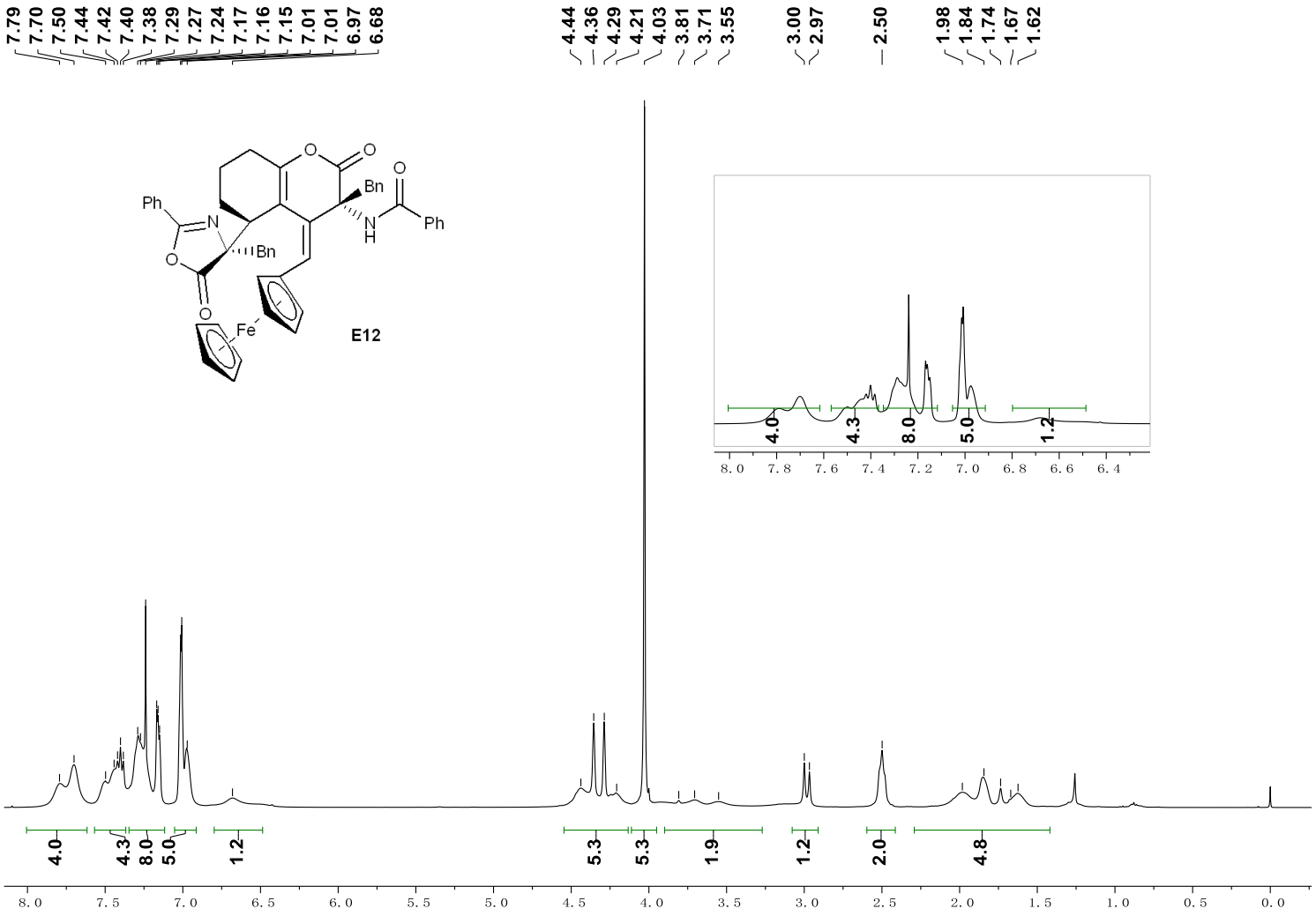
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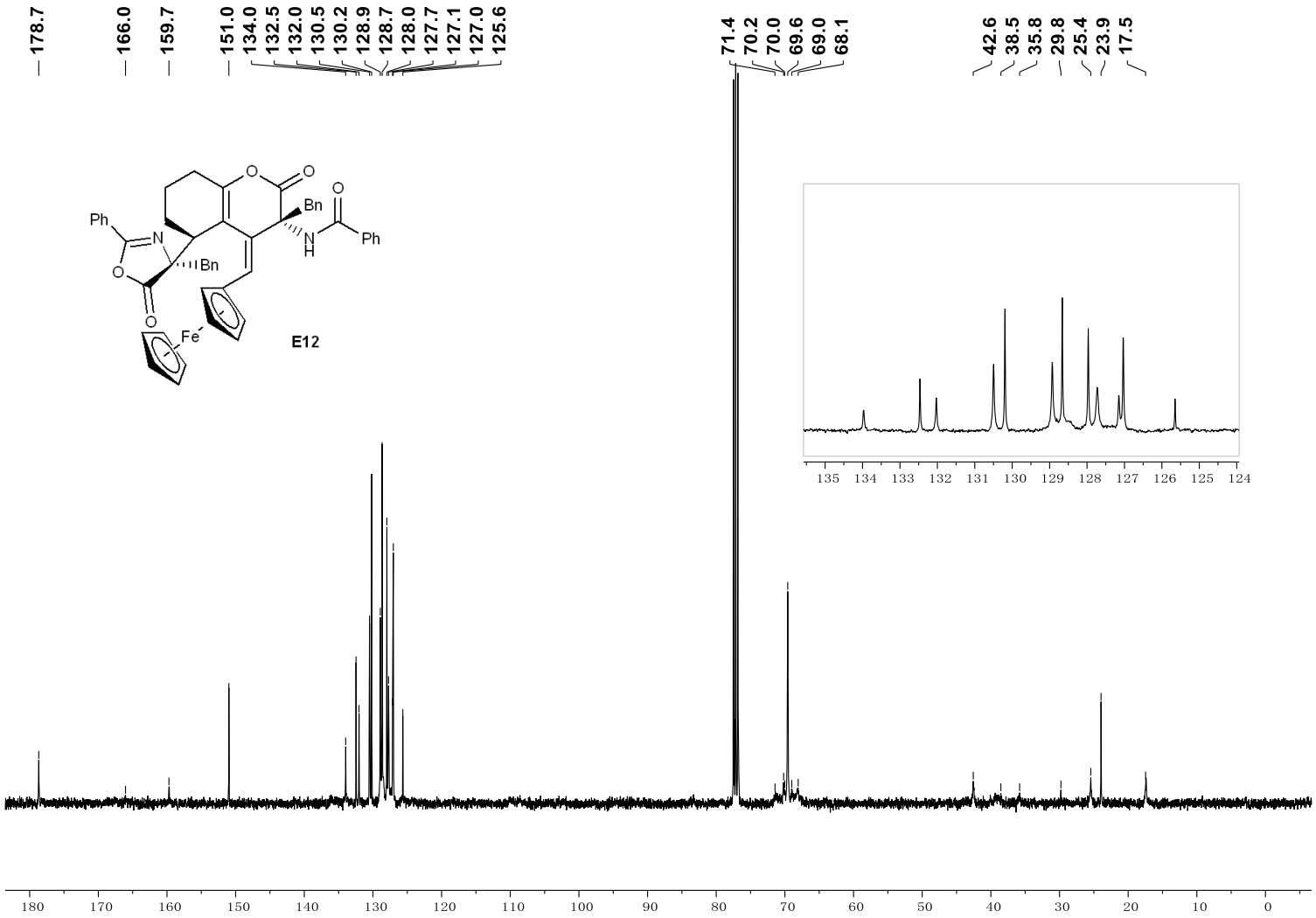
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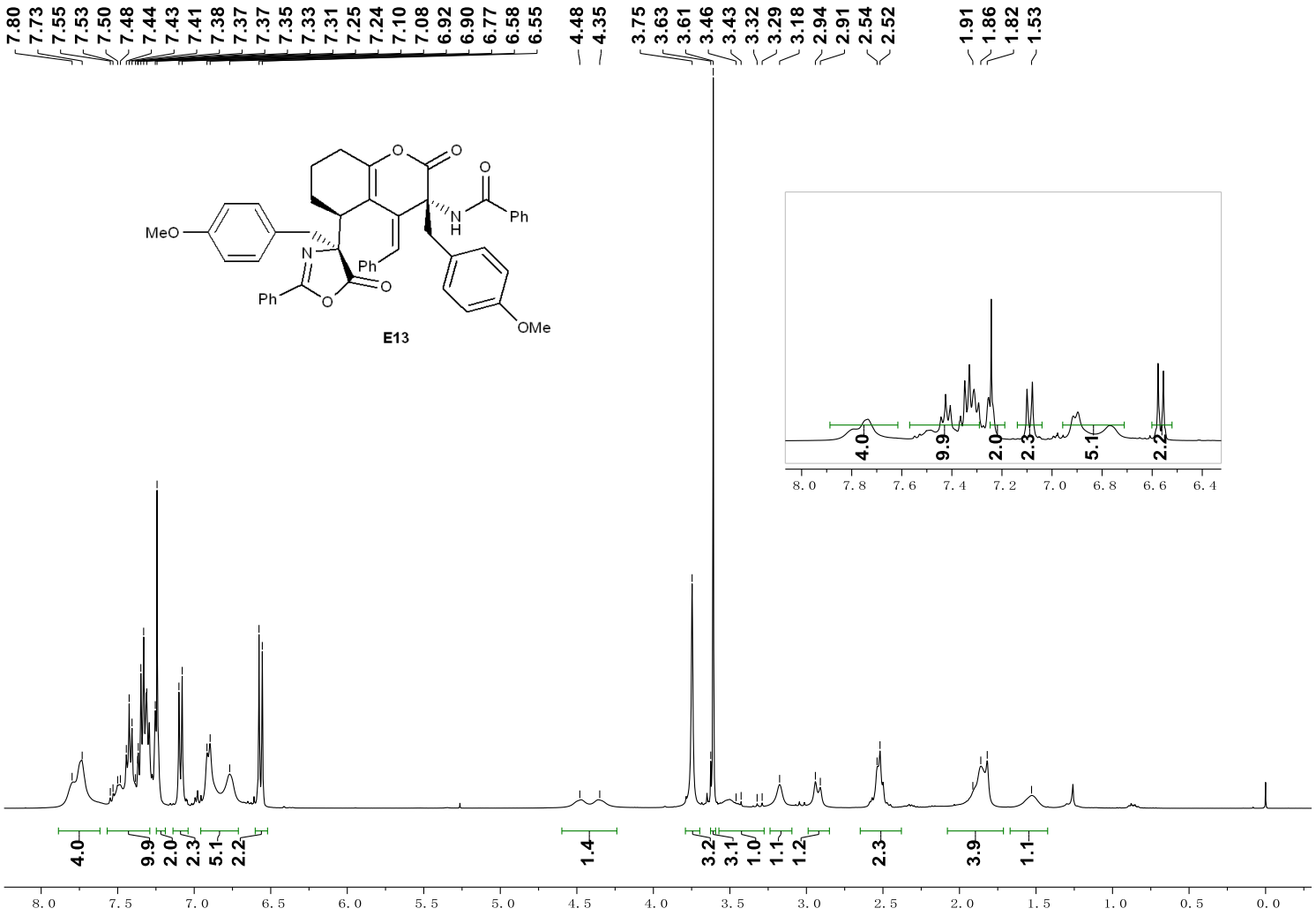
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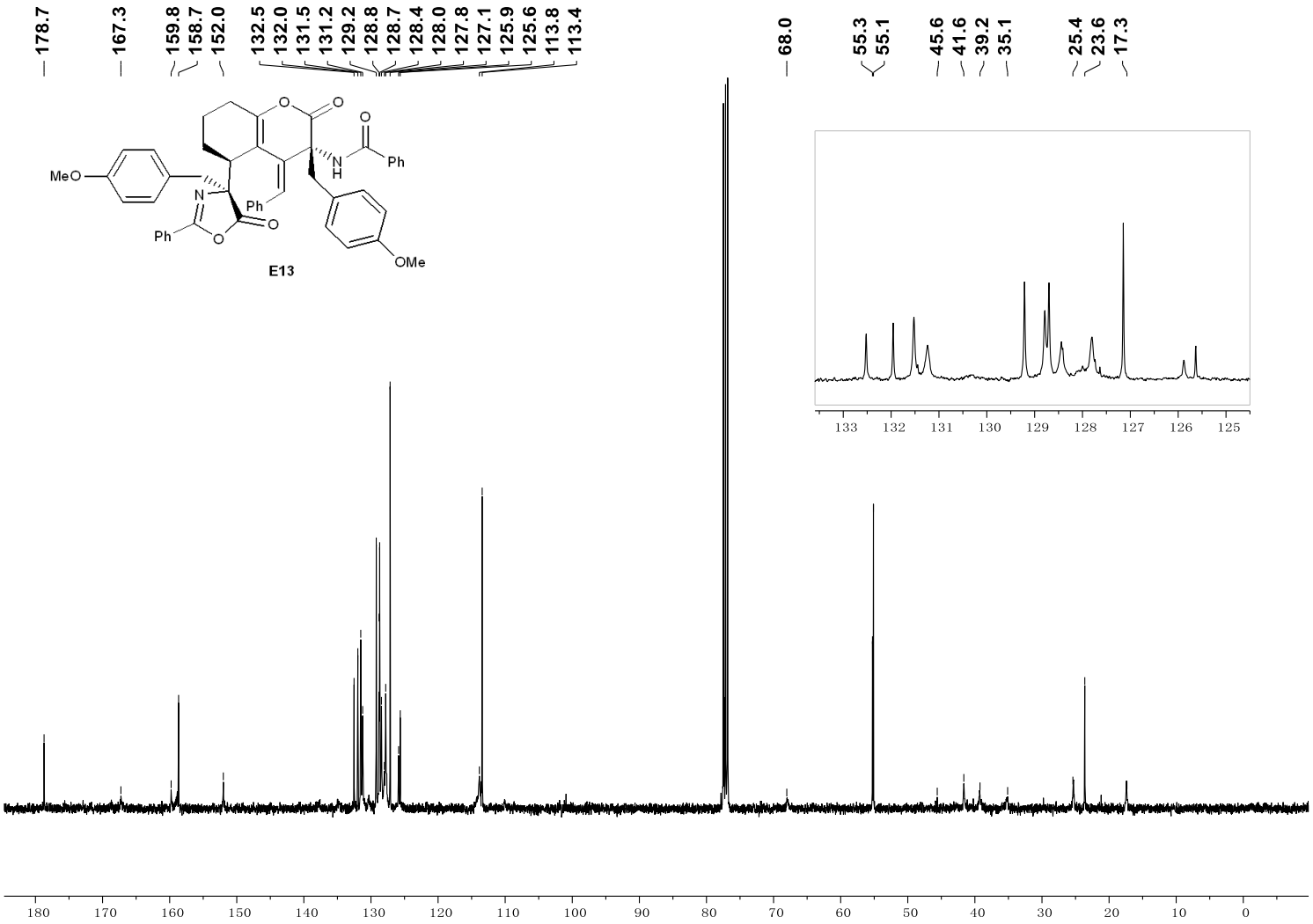
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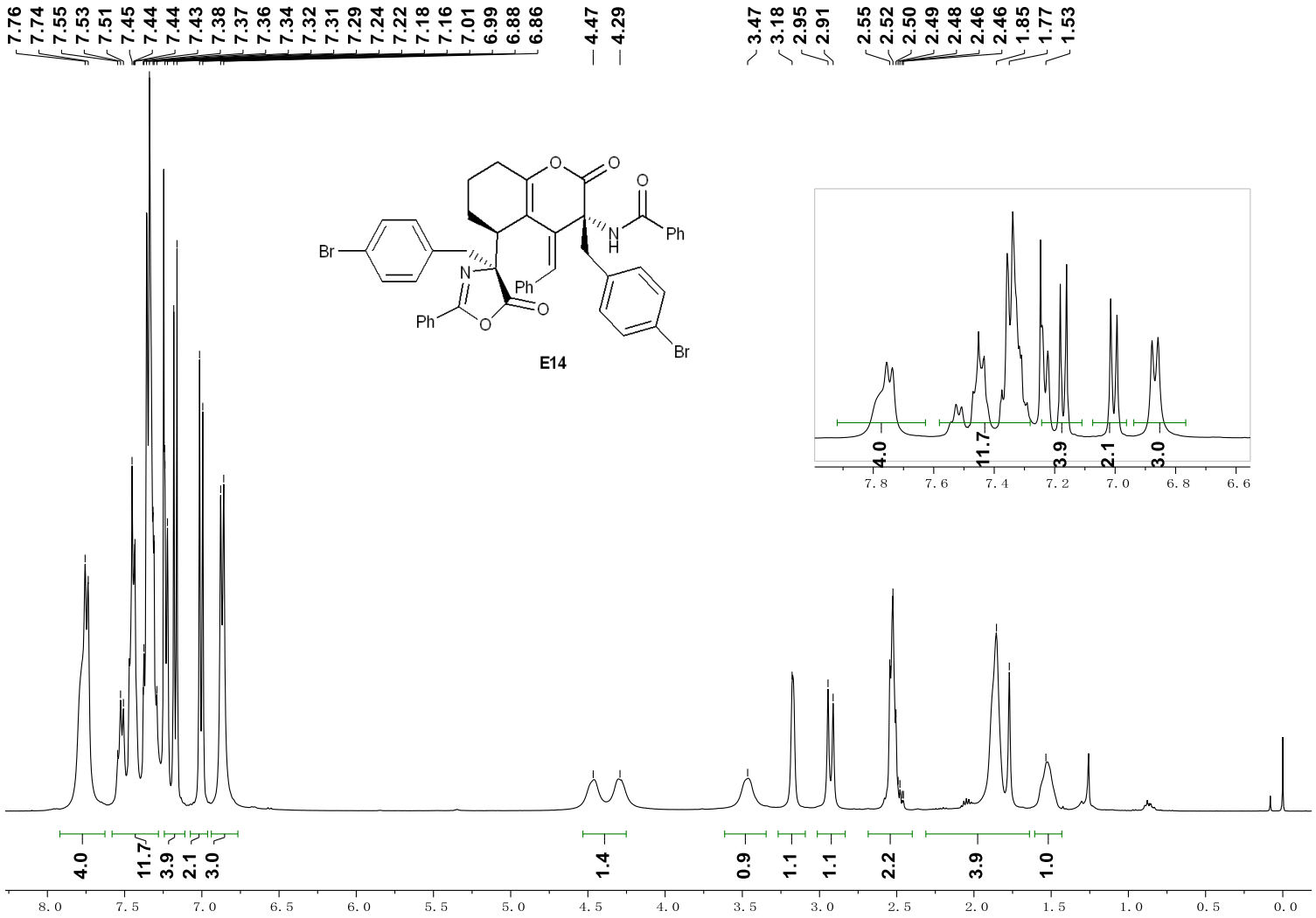
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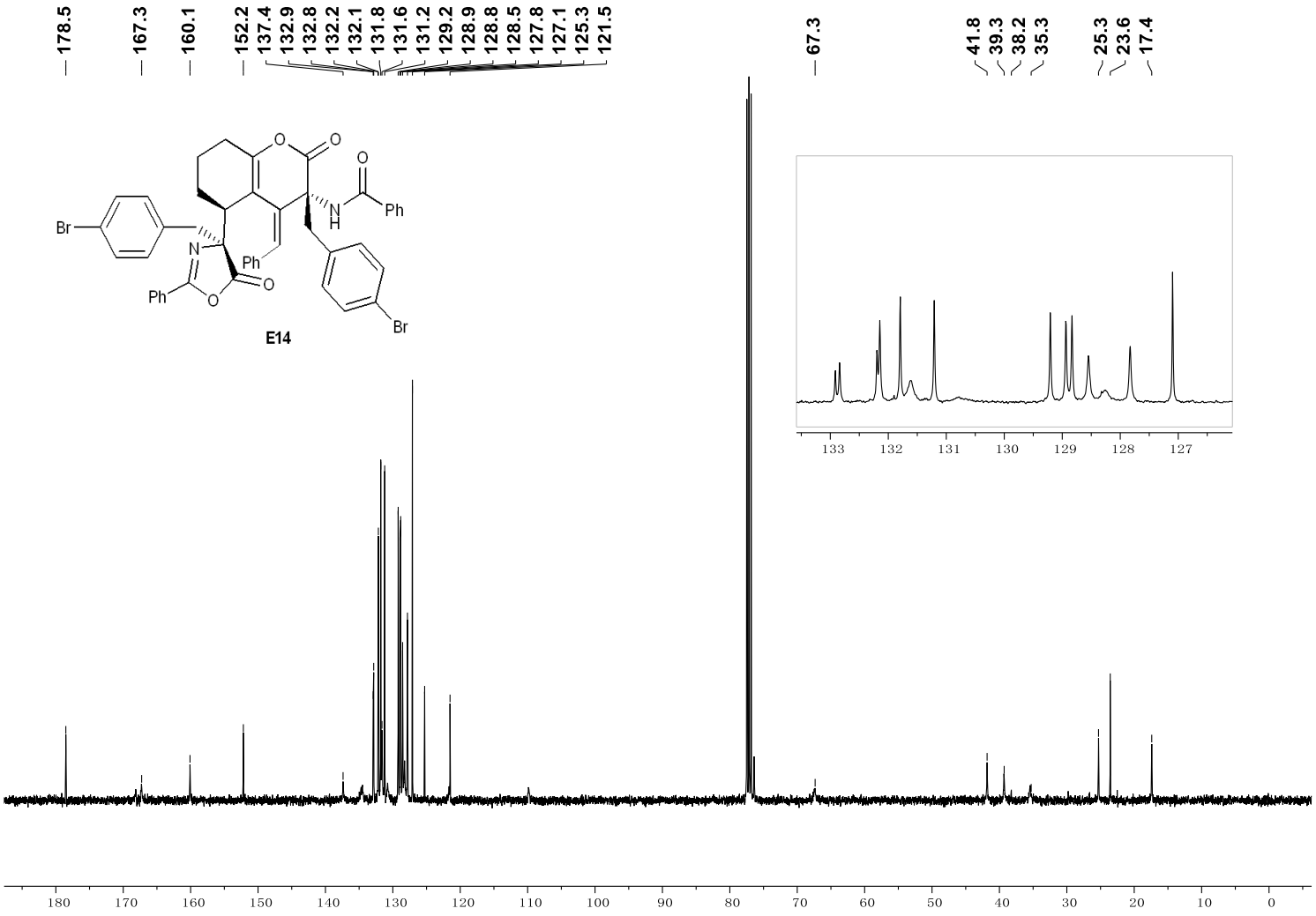
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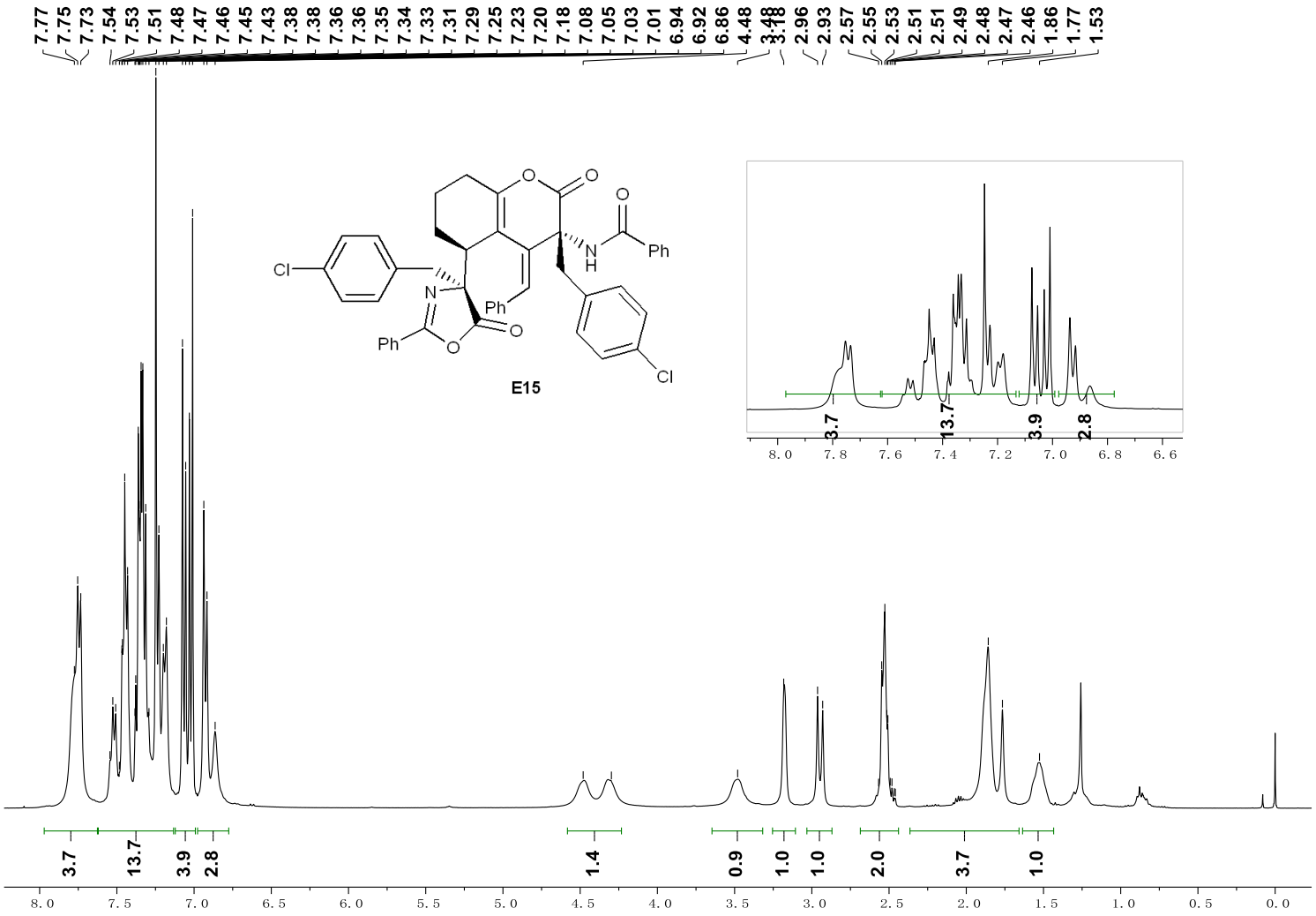
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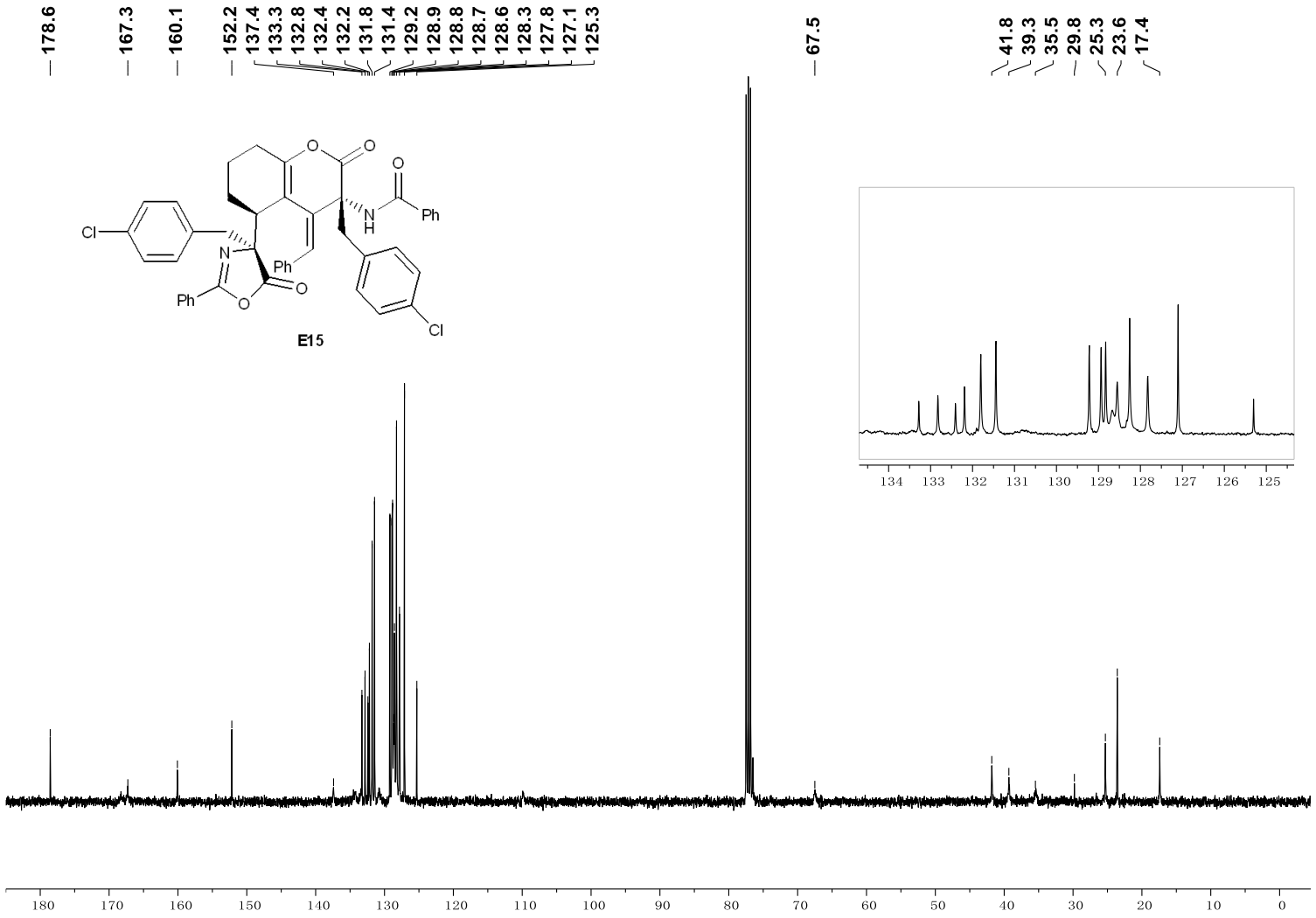
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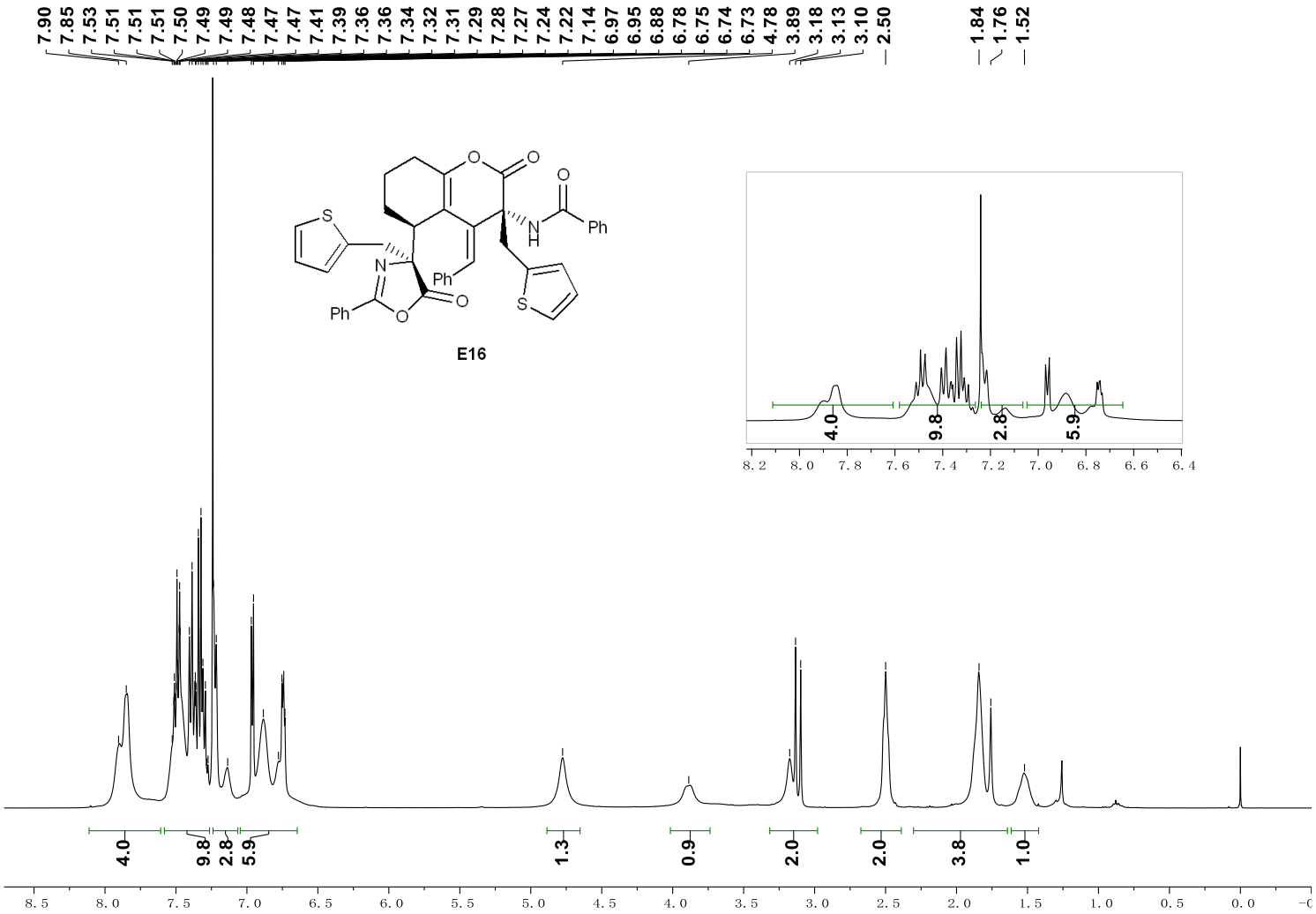
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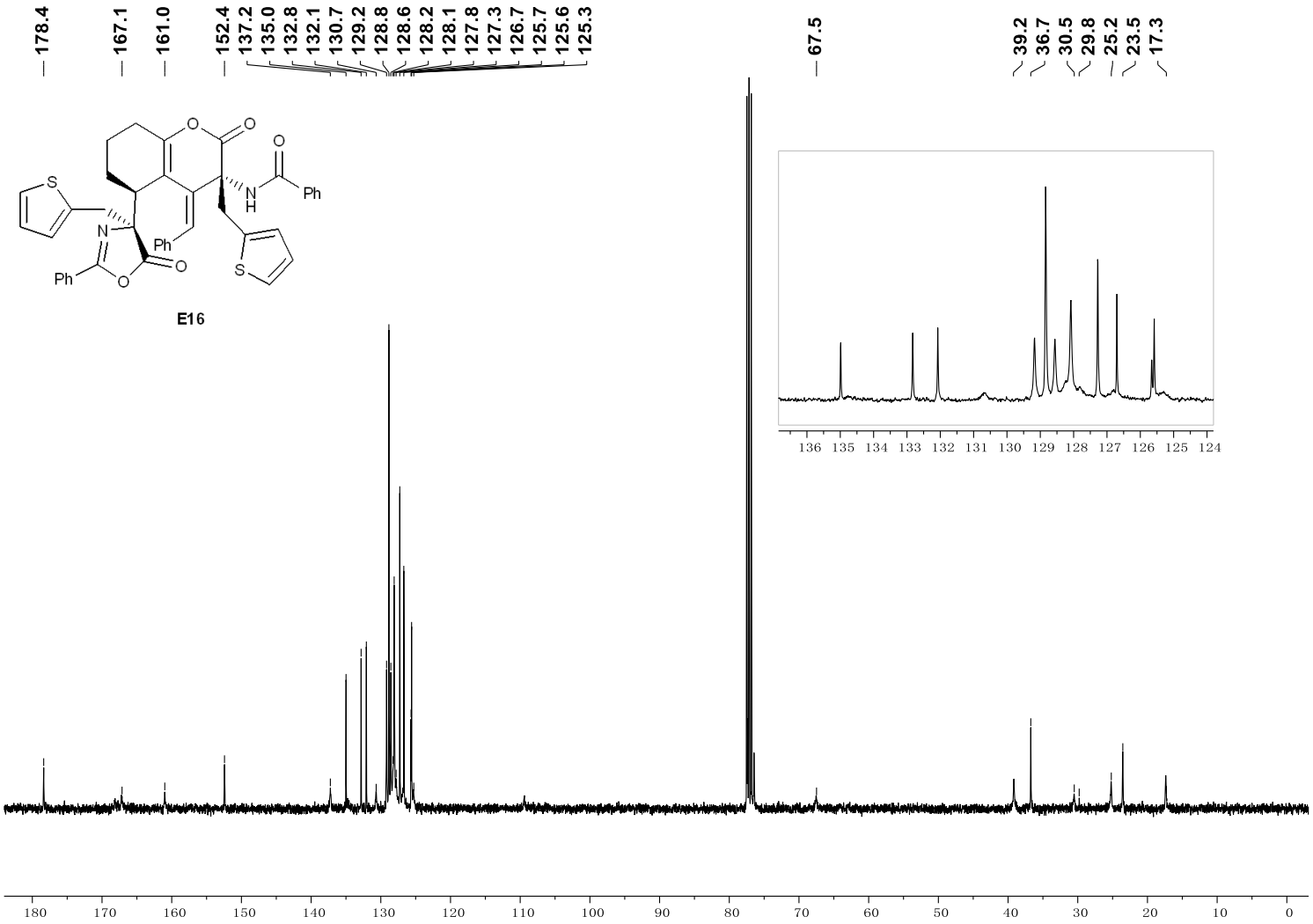
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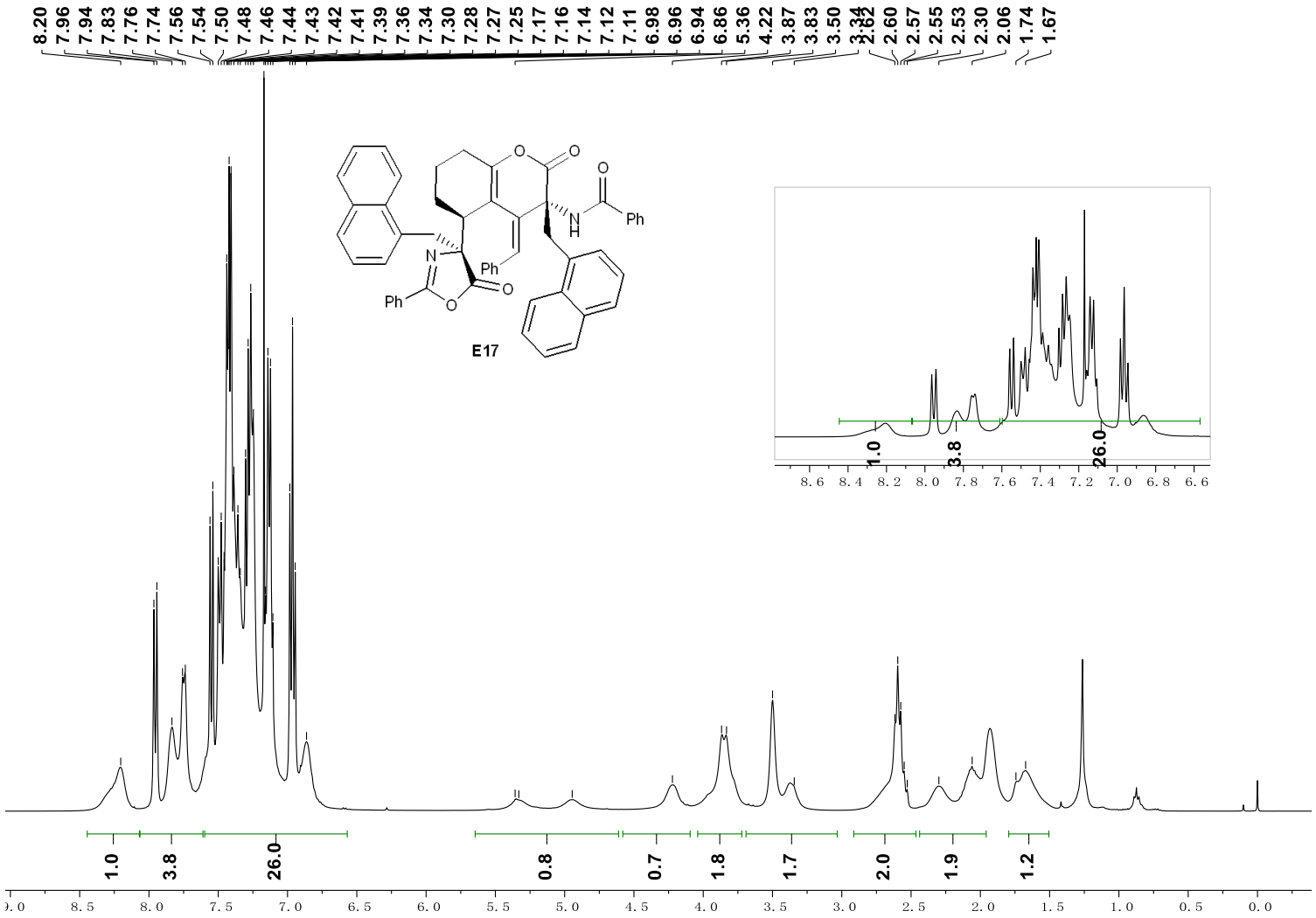
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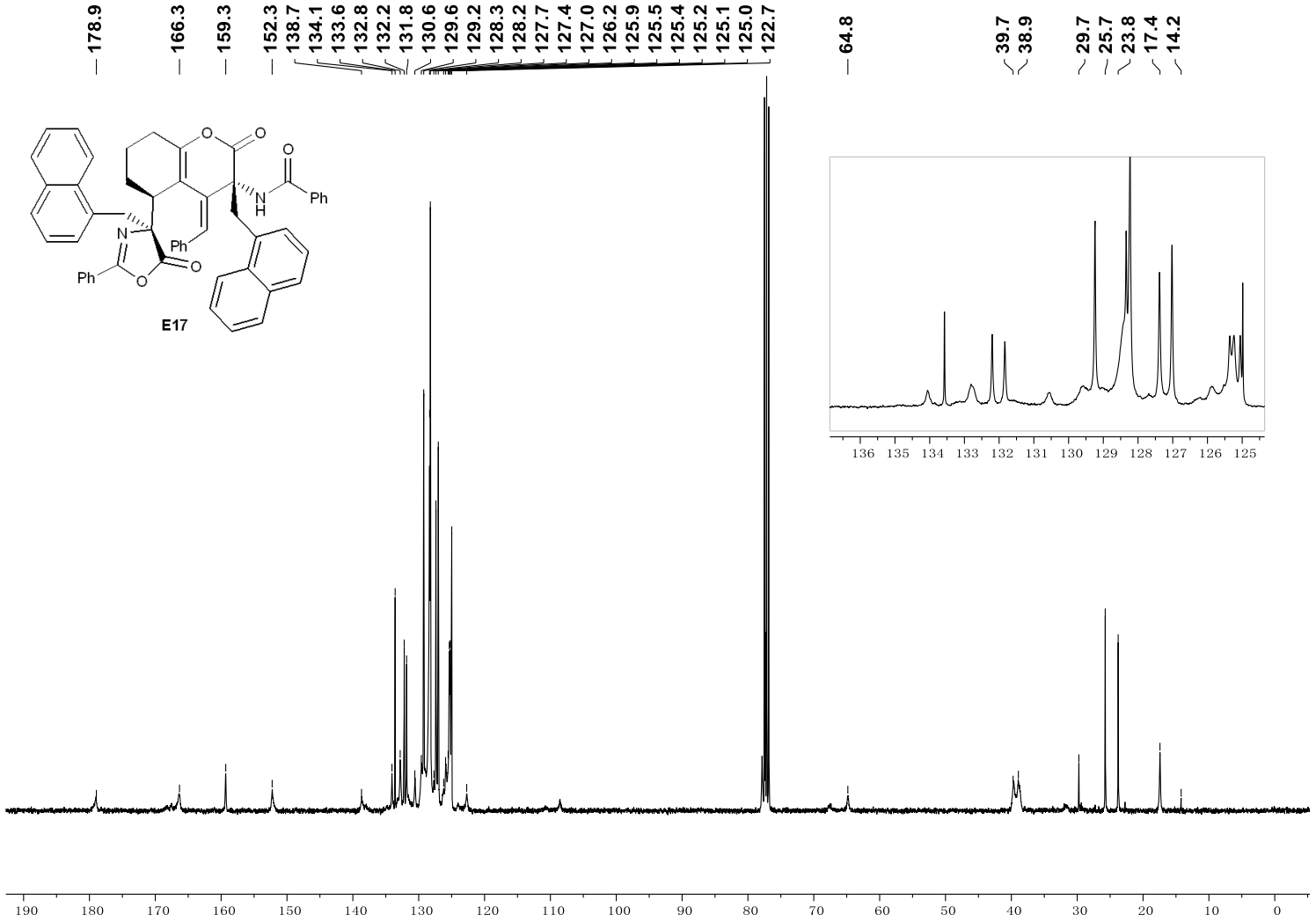
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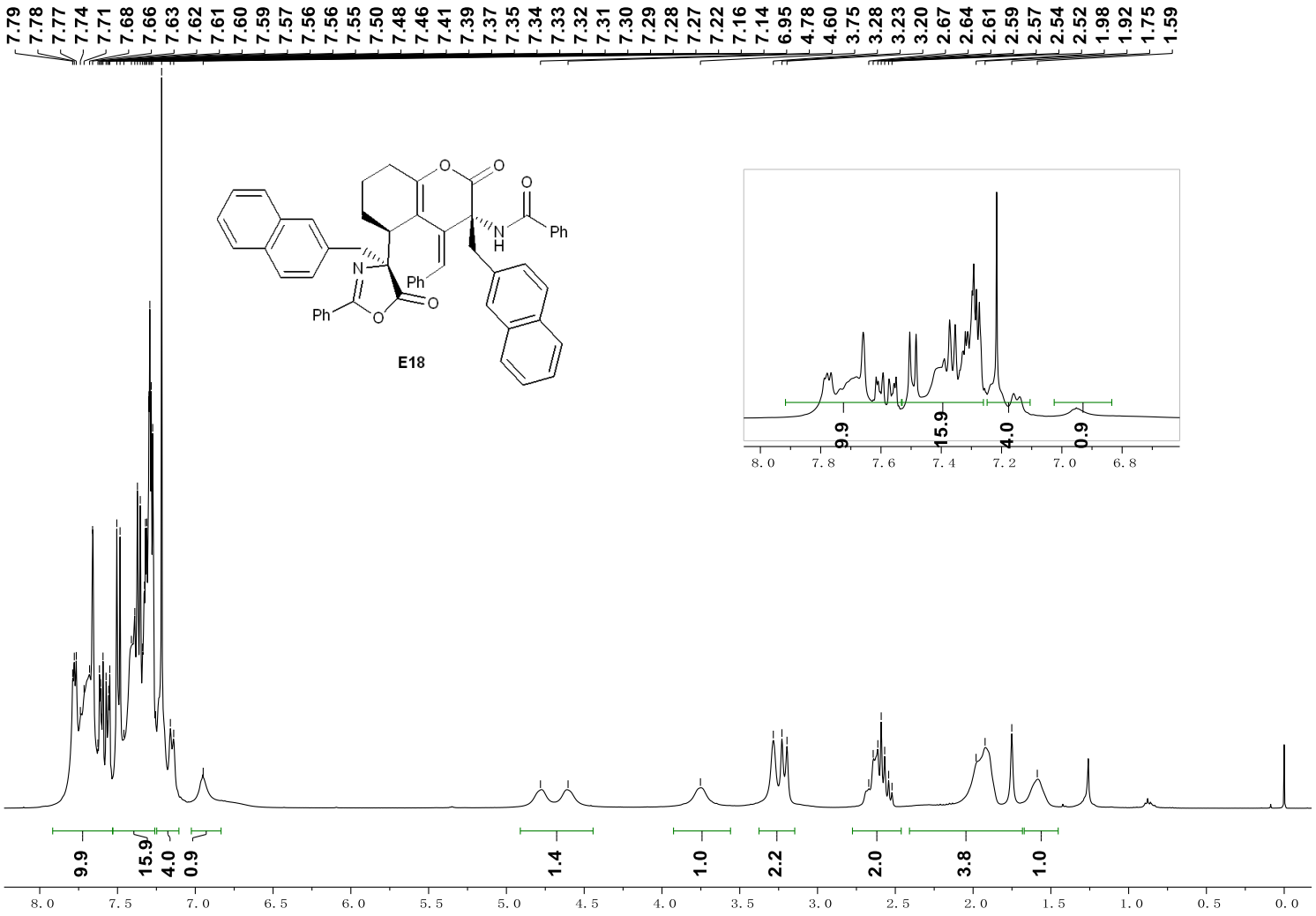
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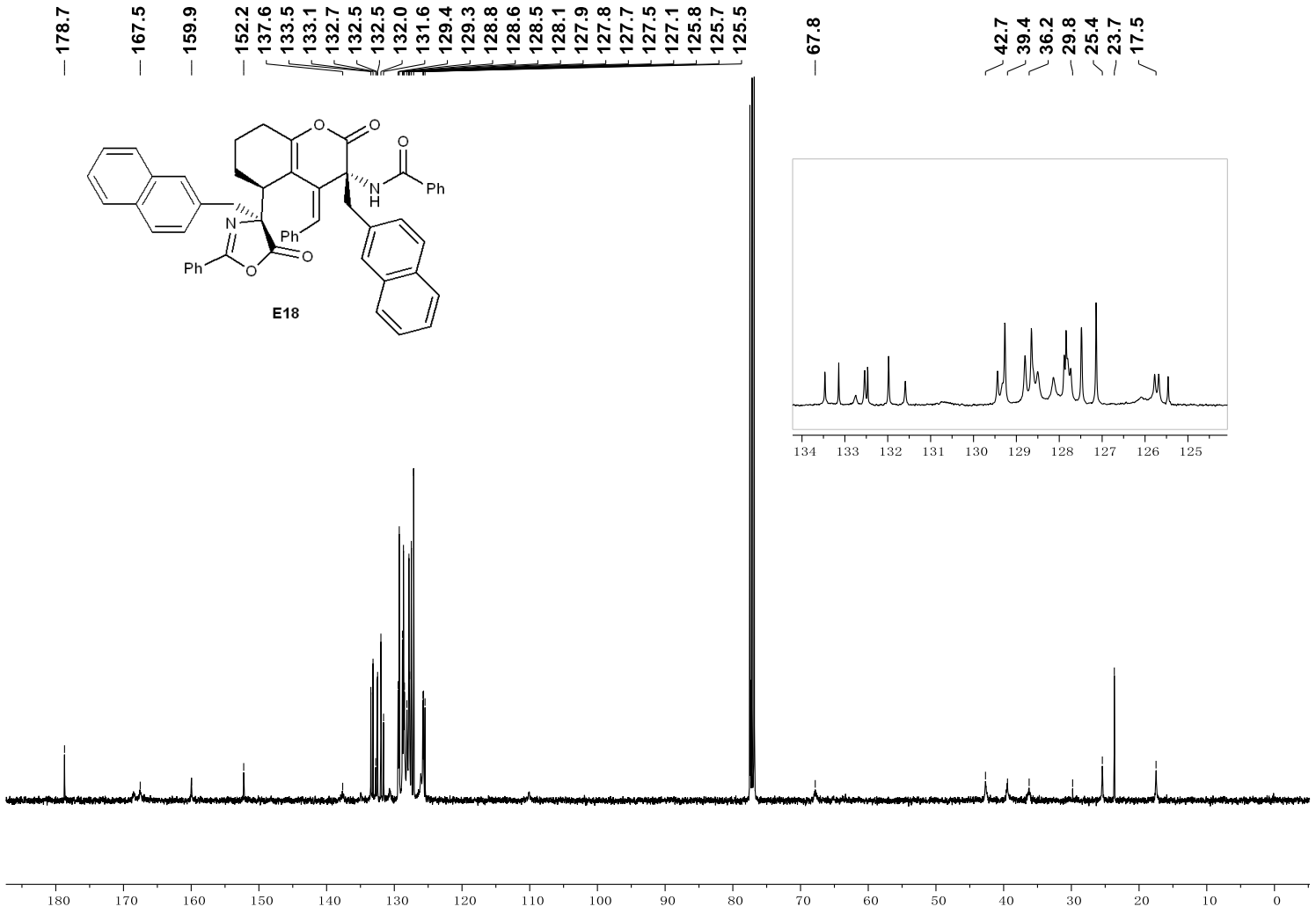
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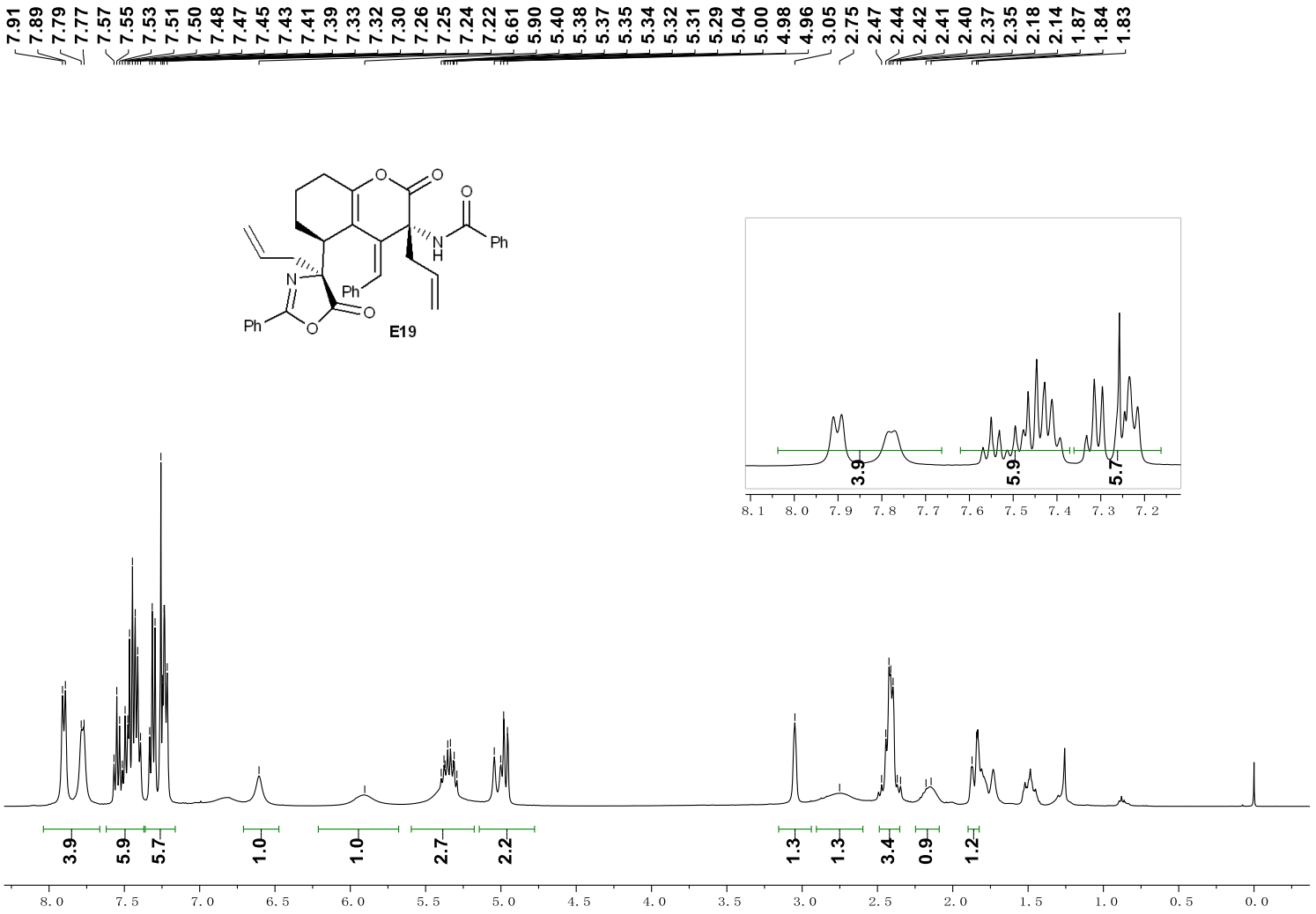
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E19
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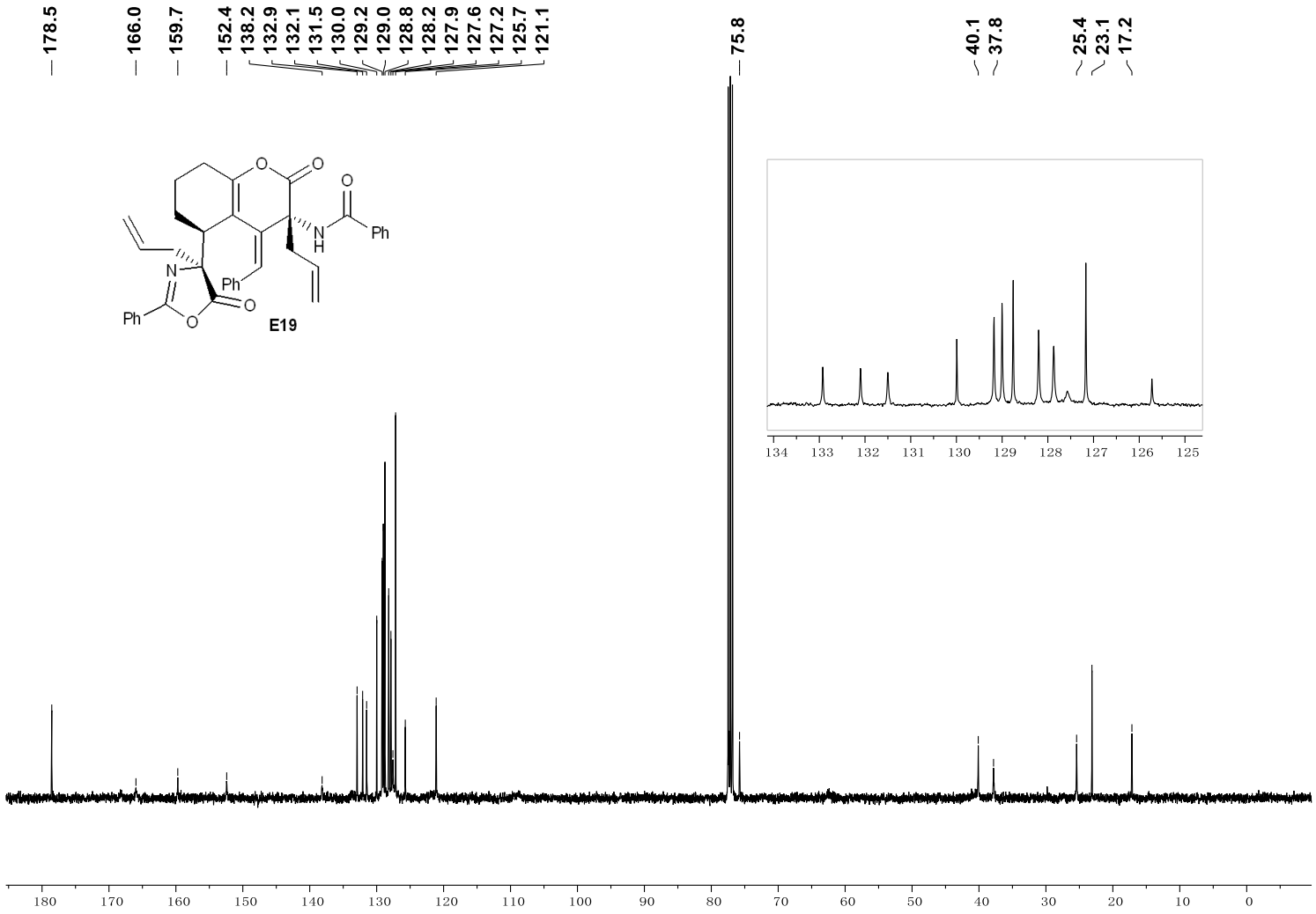
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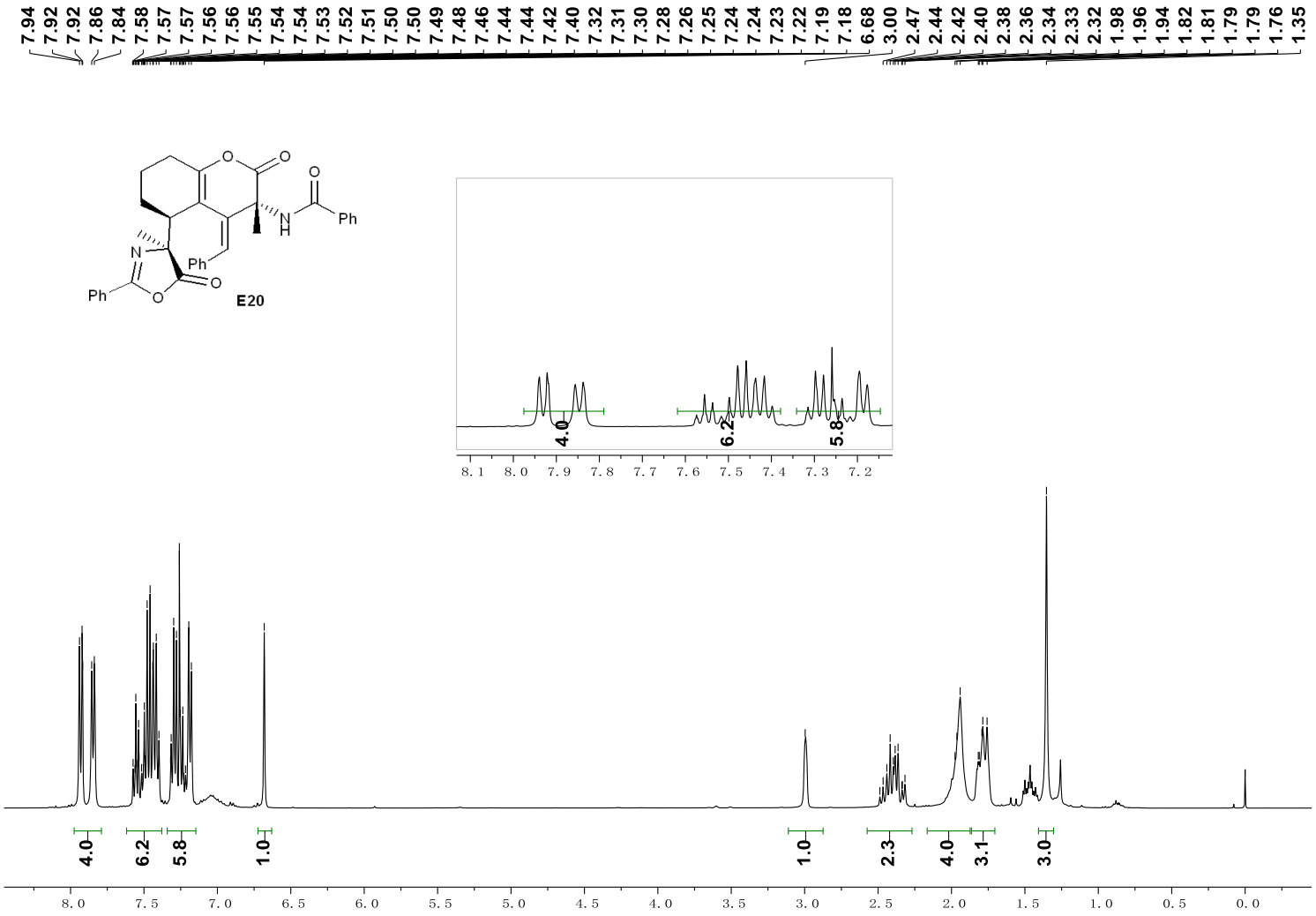
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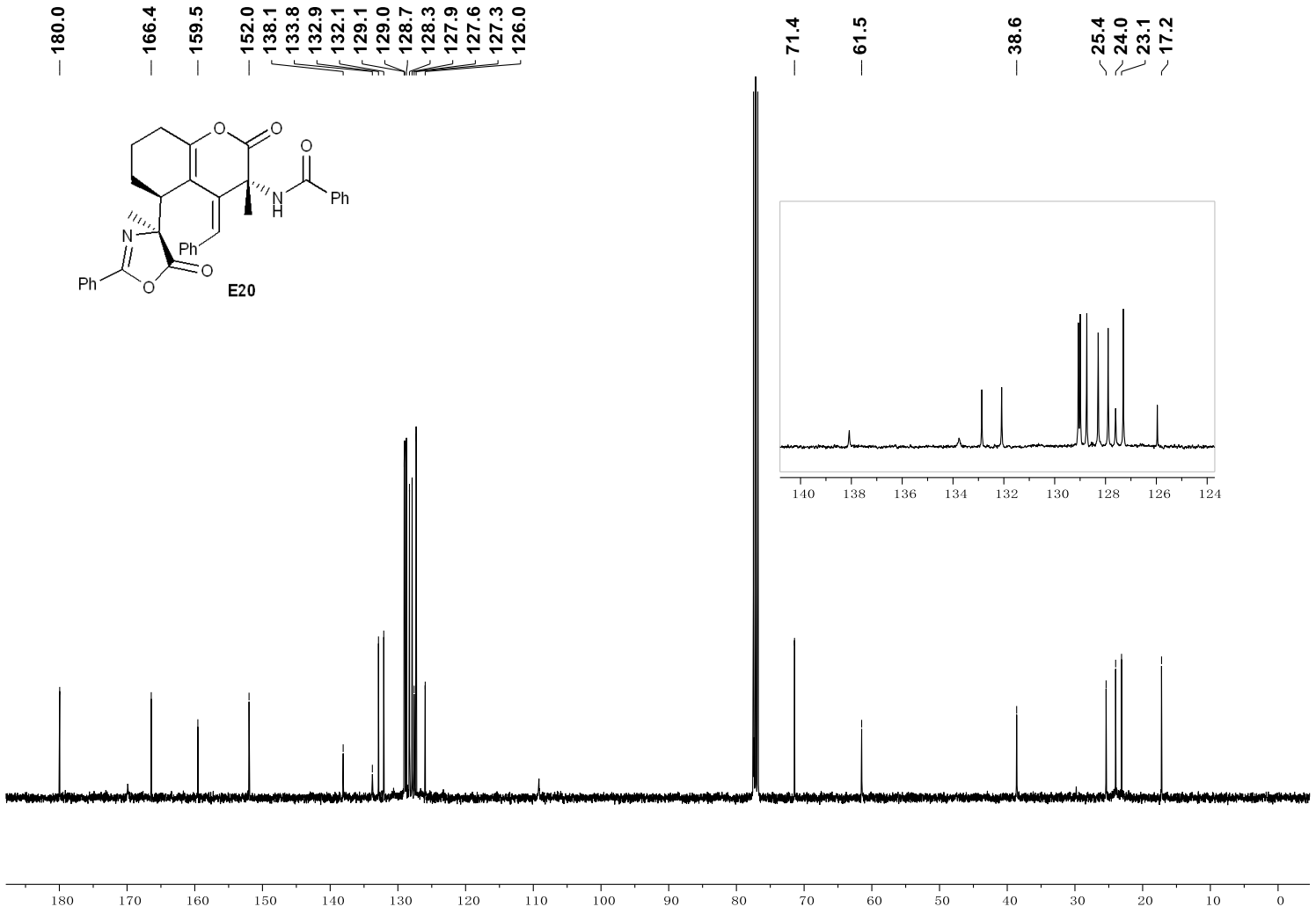
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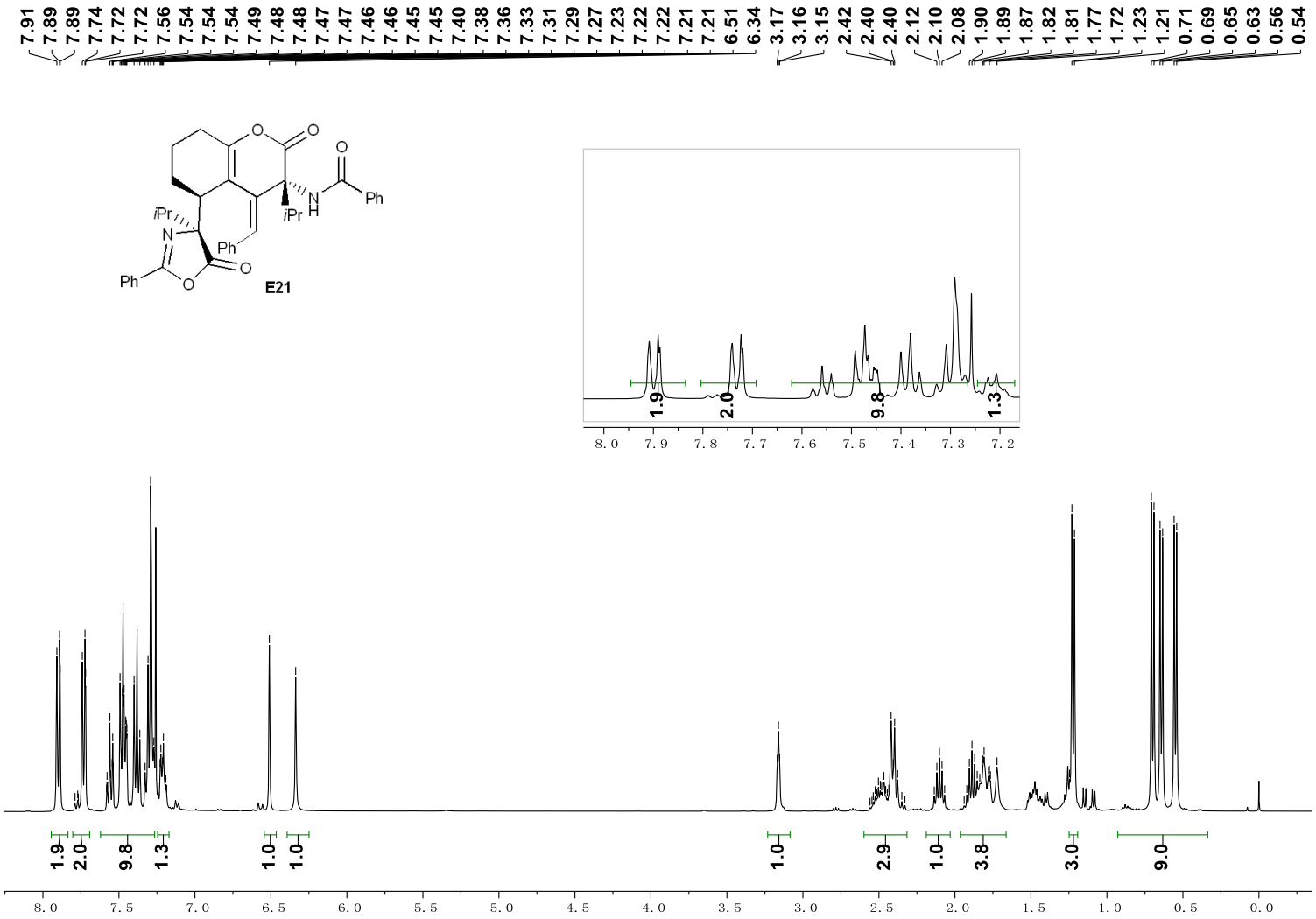
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9.8
1.3
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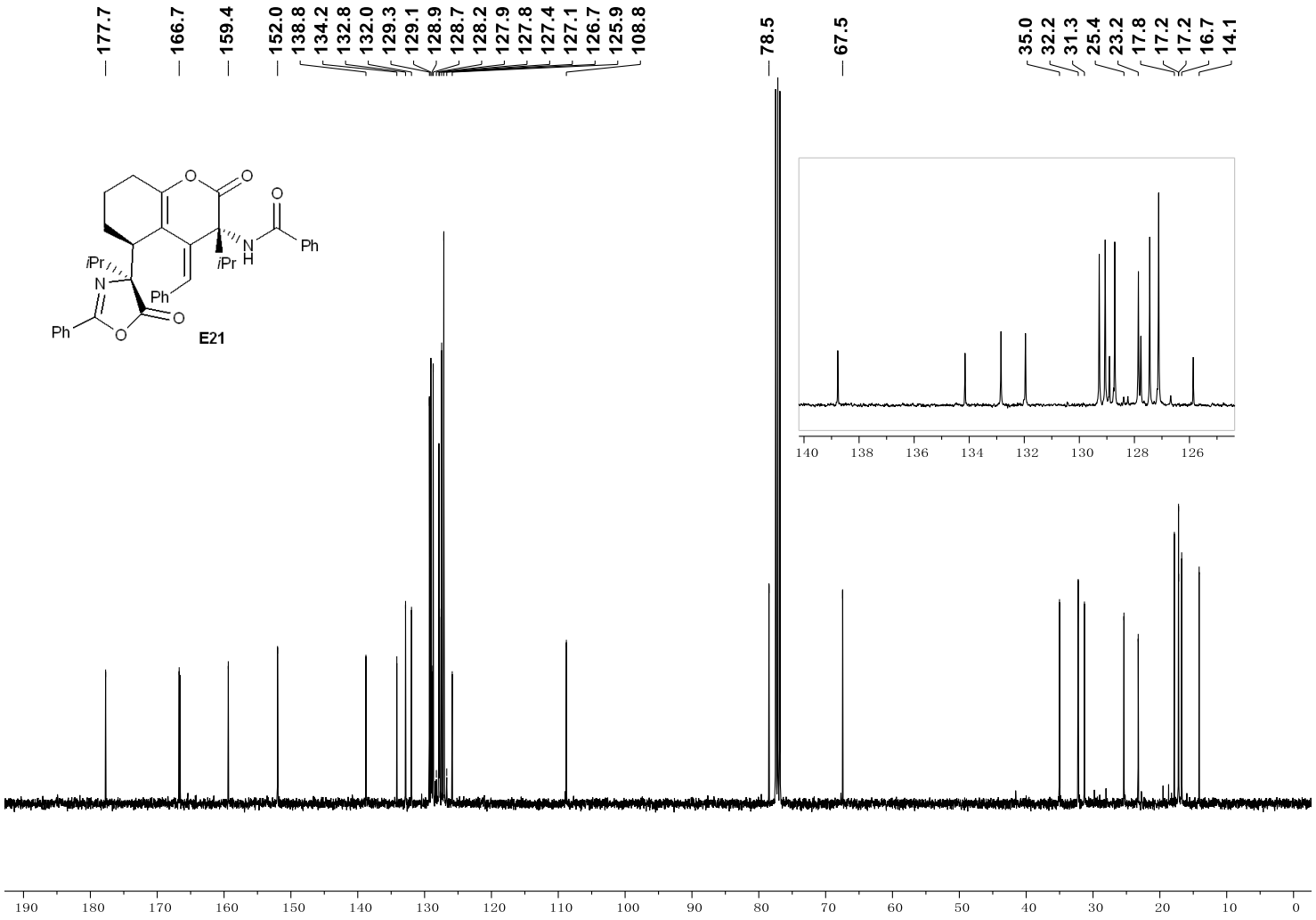
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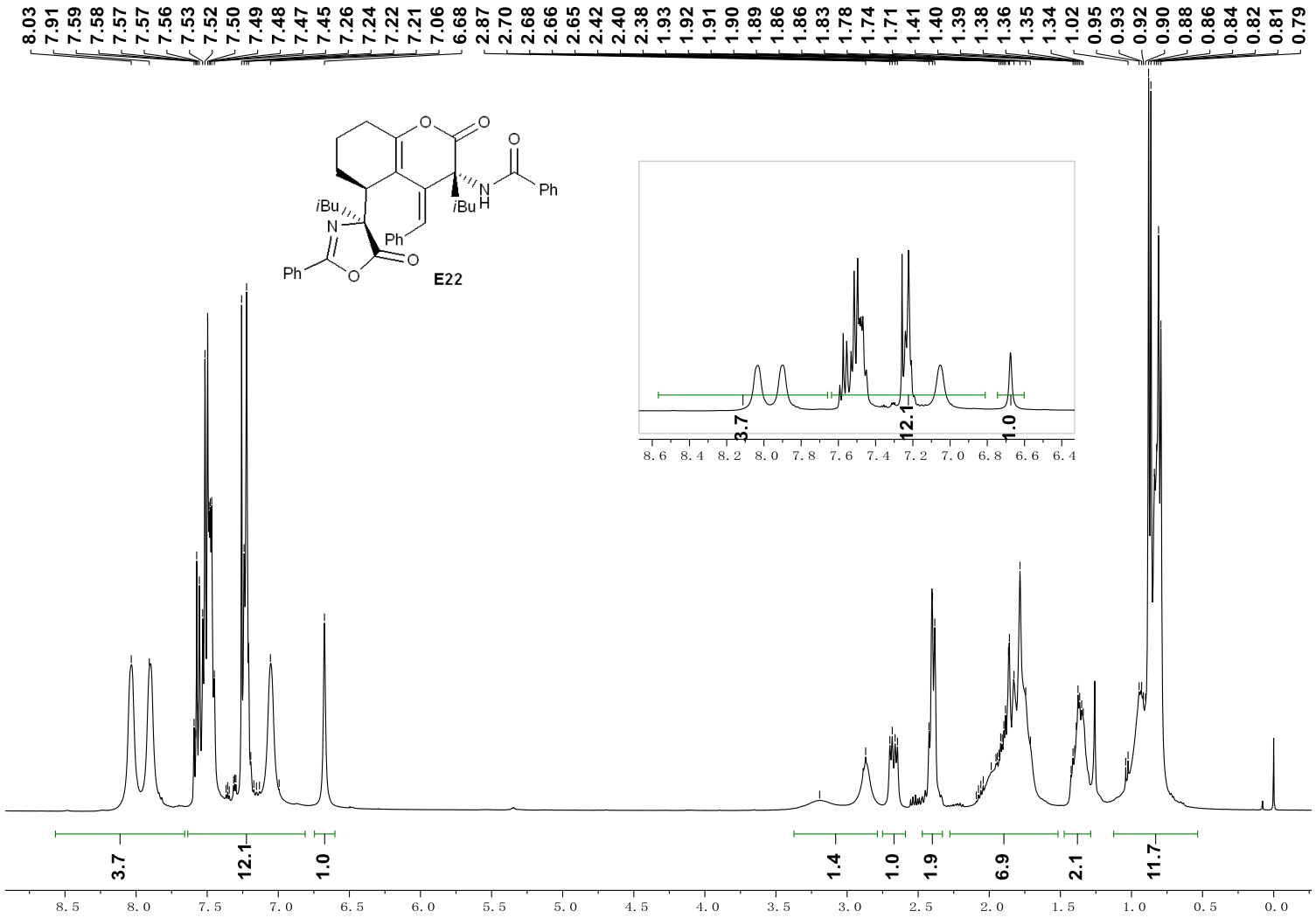
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1.4
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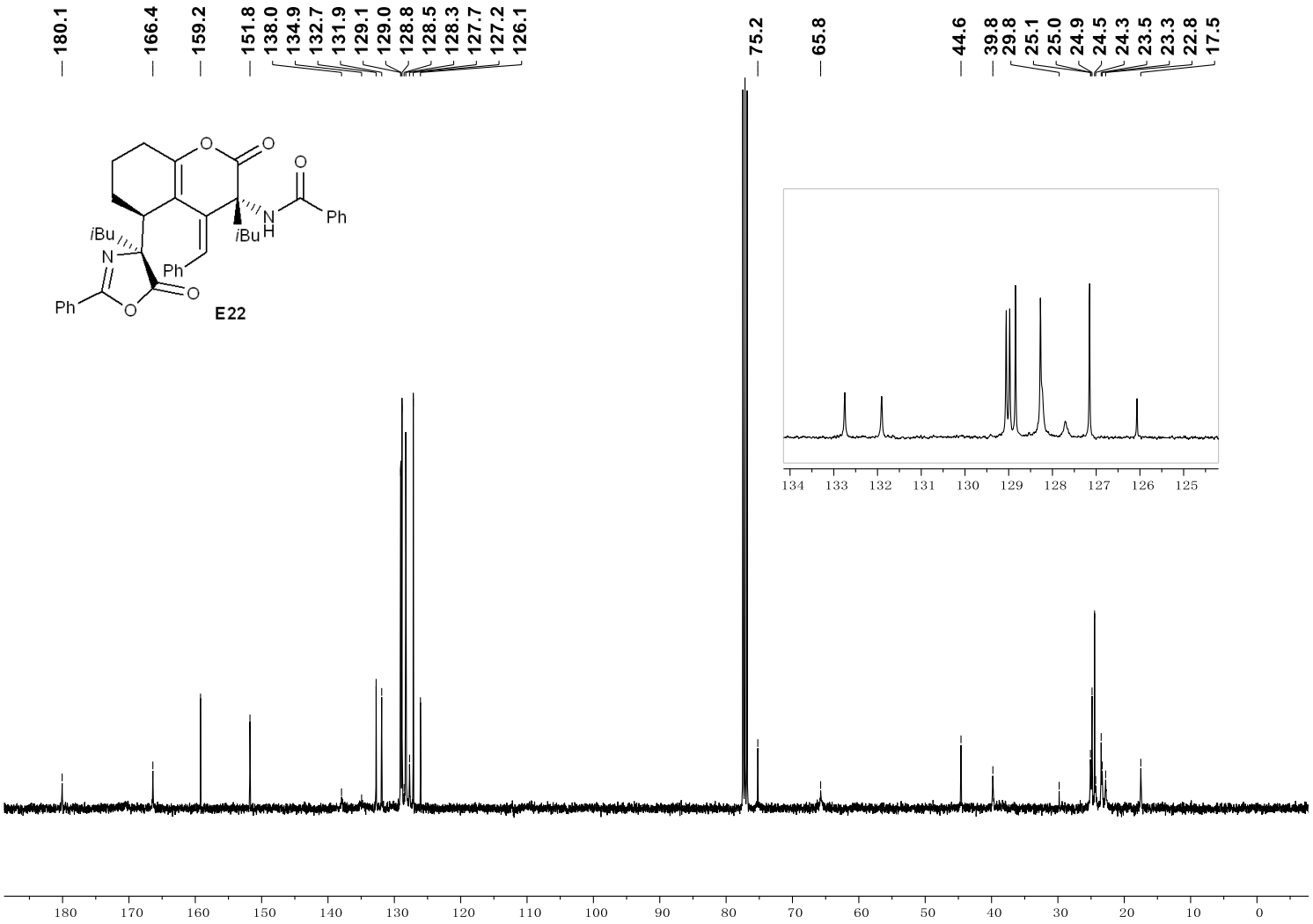
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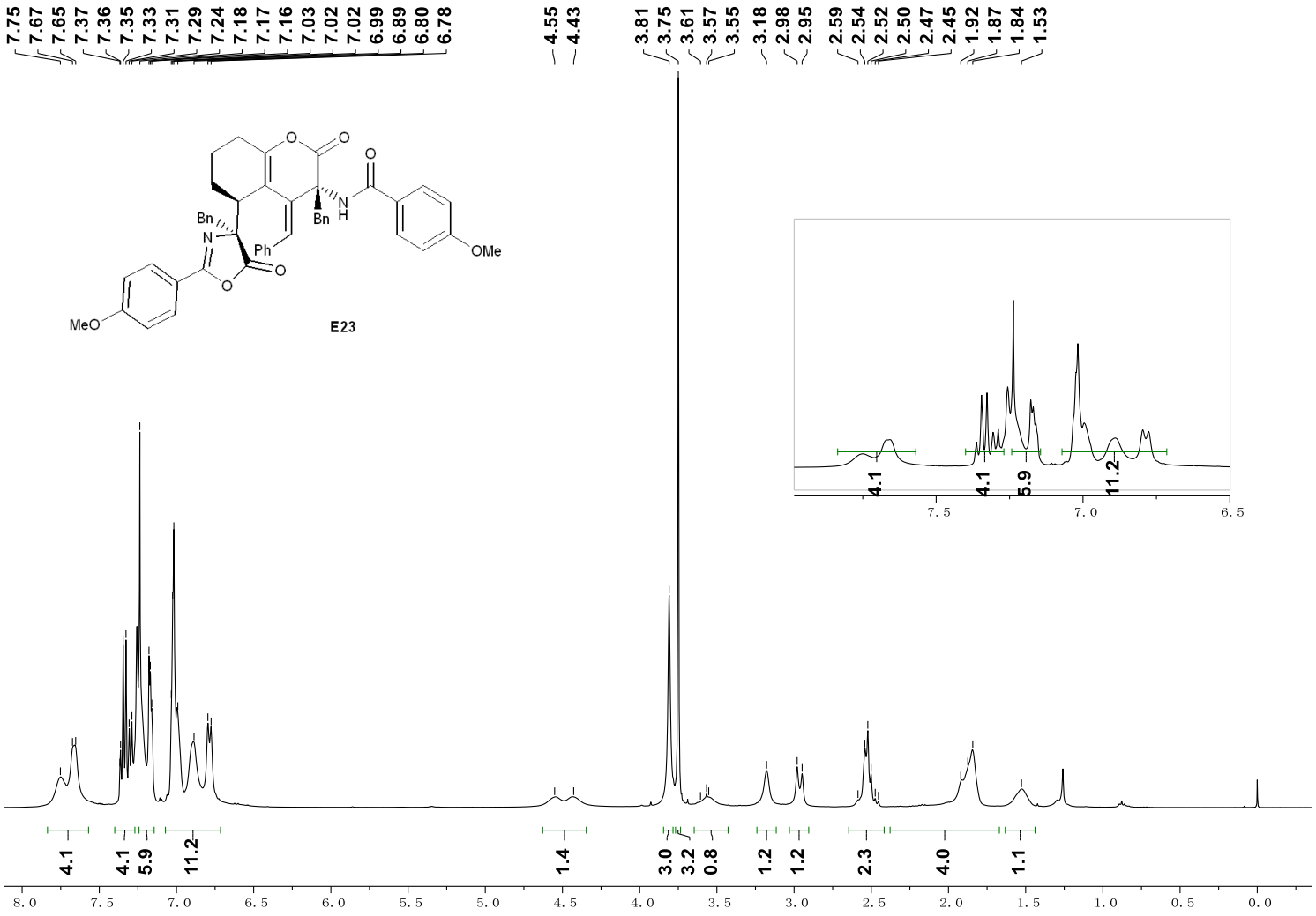
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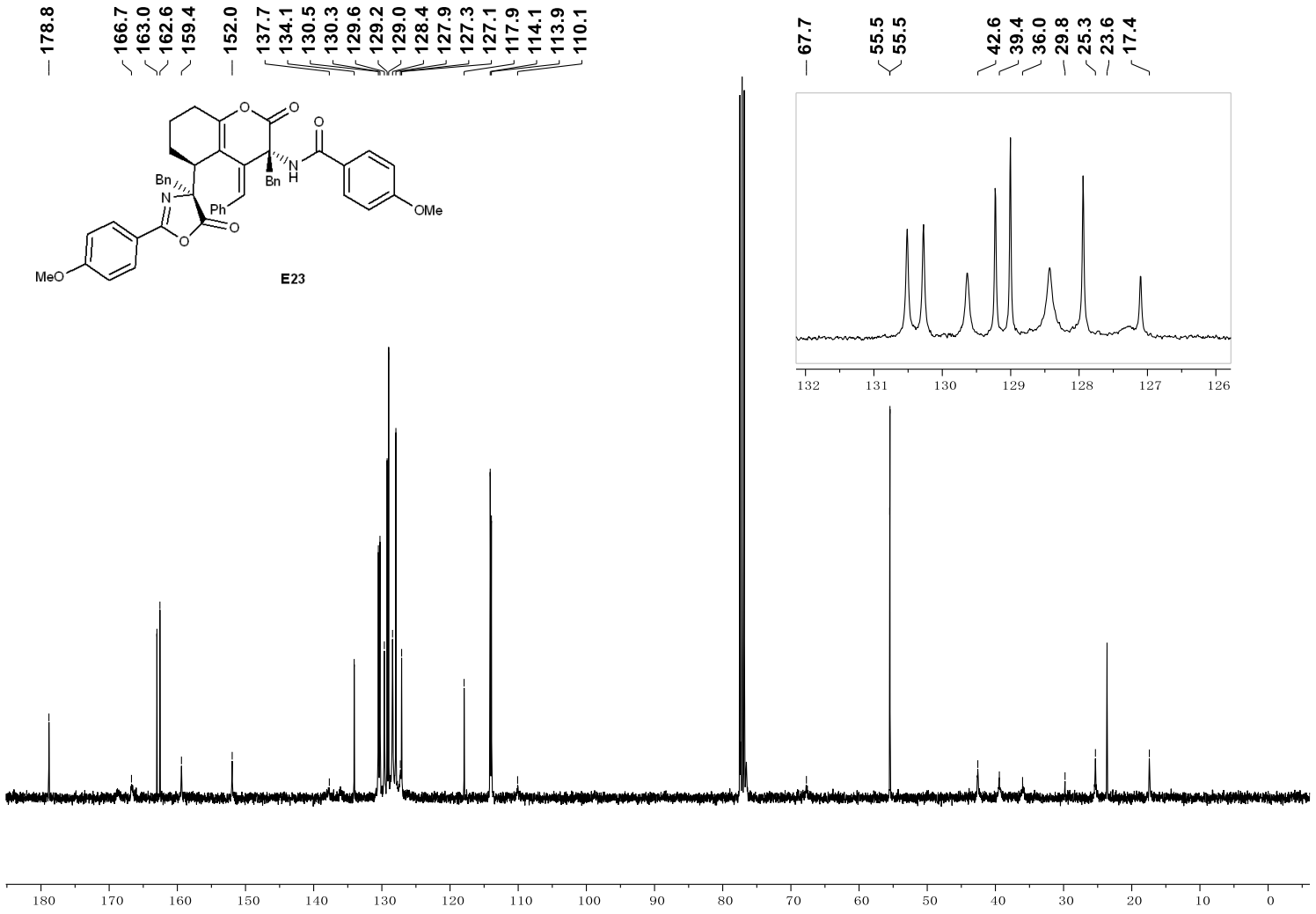
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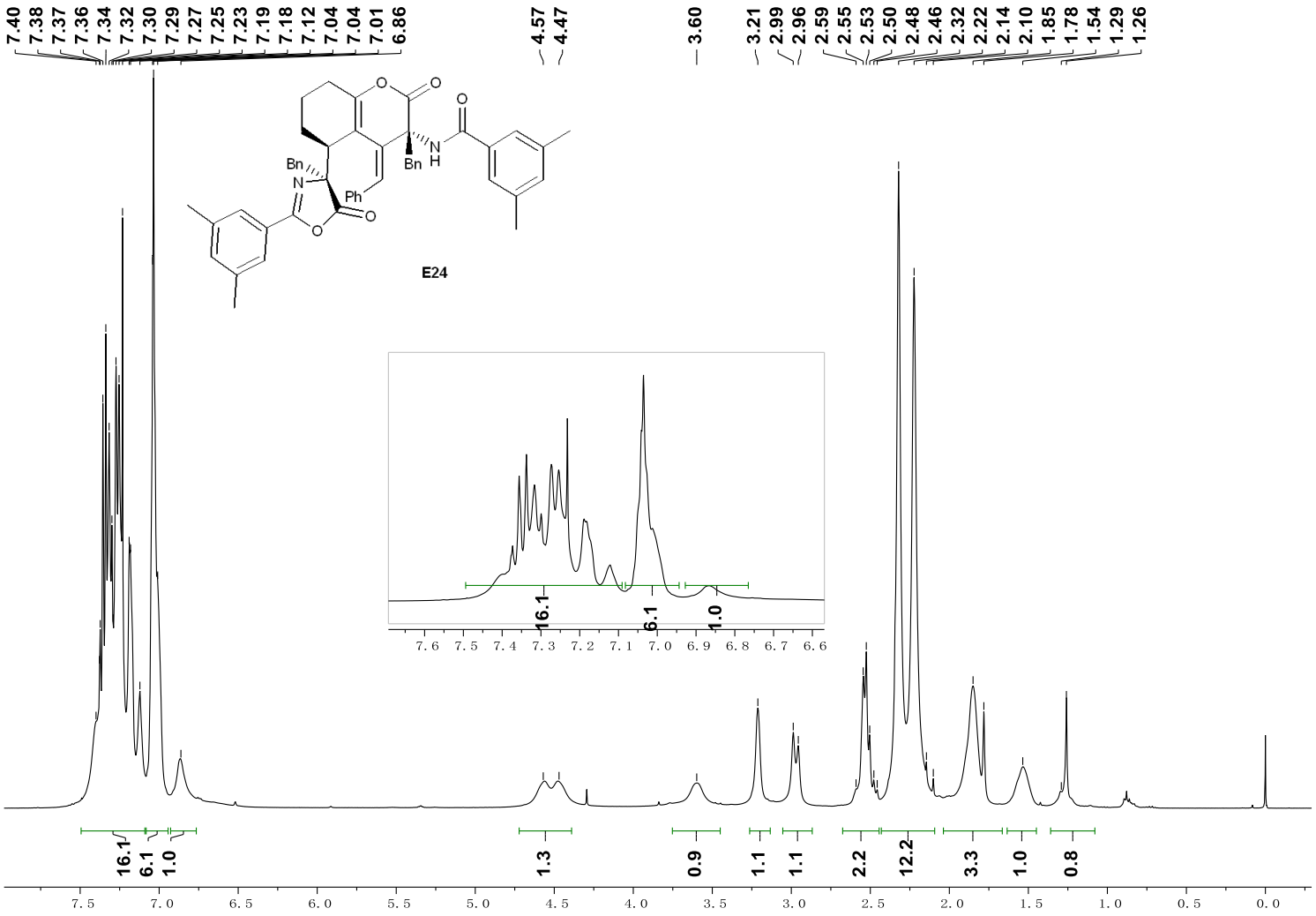
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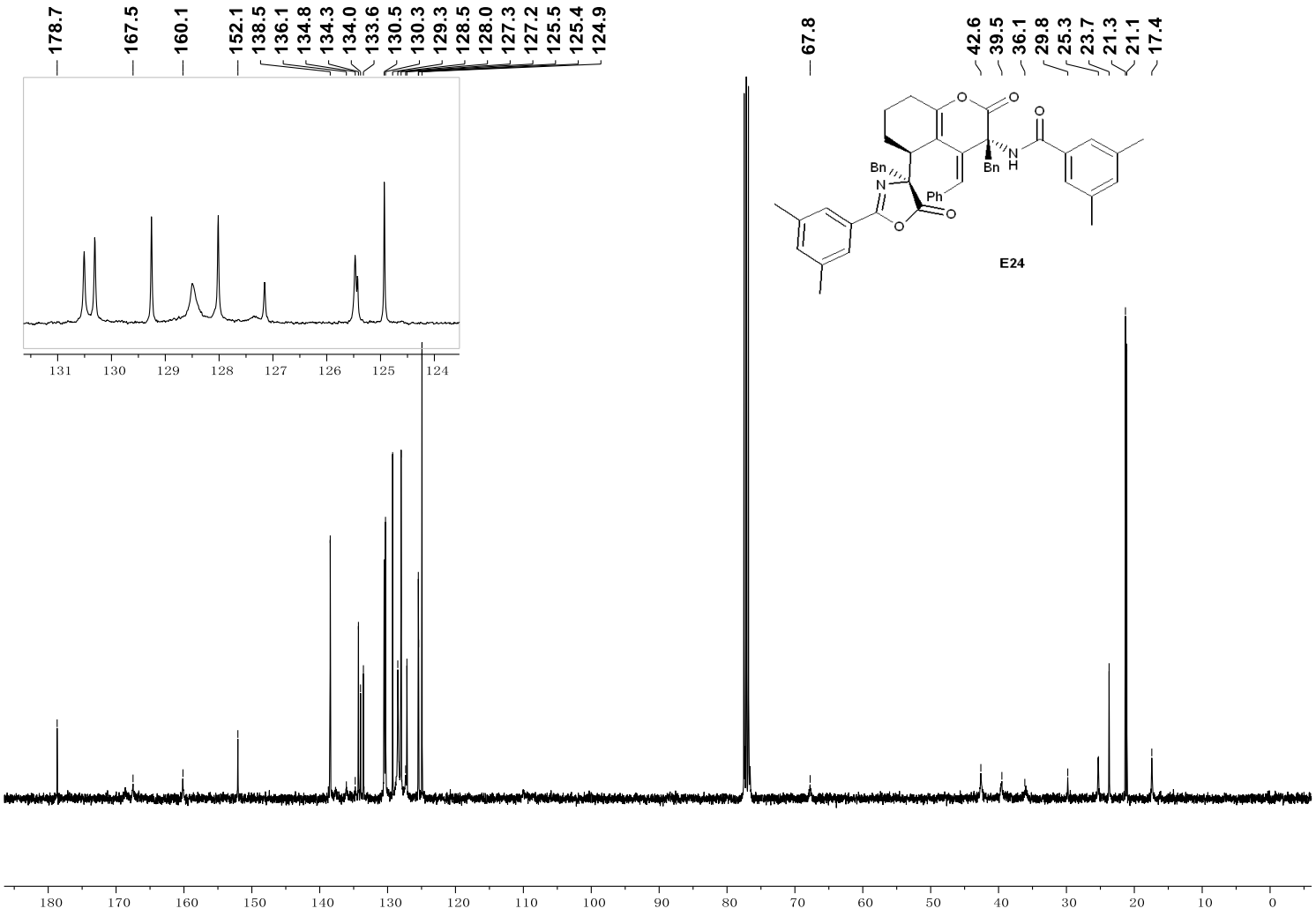
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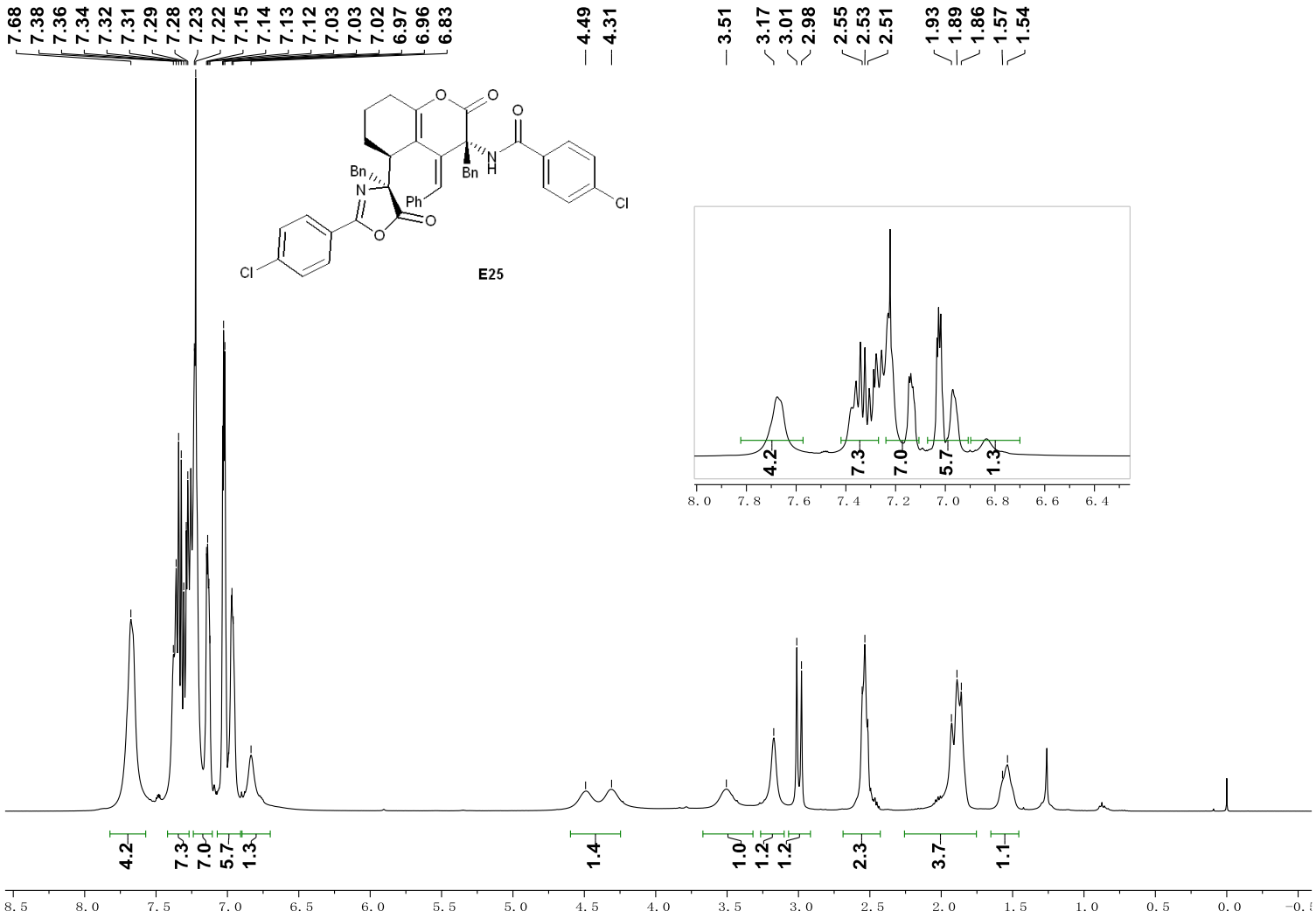
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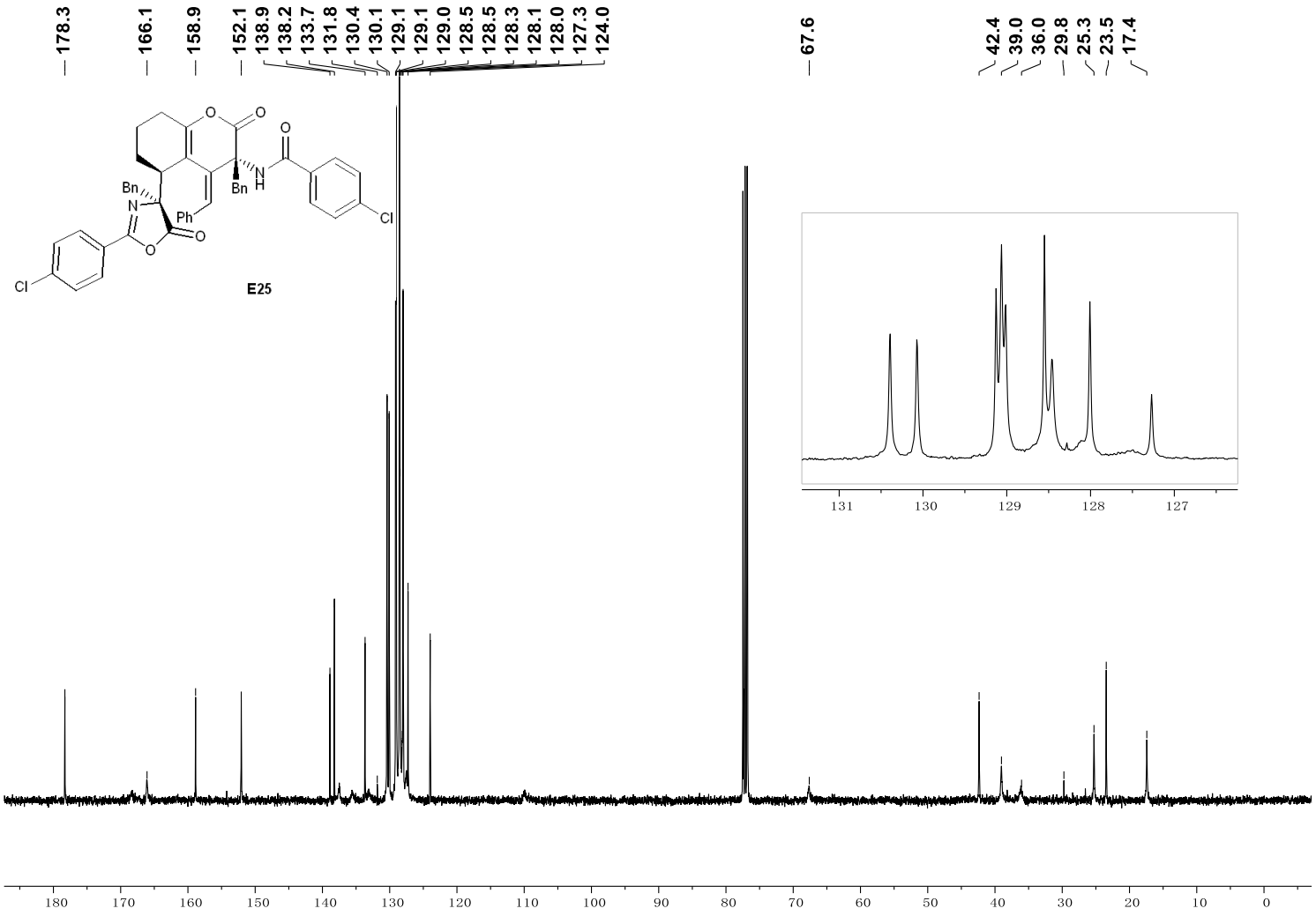
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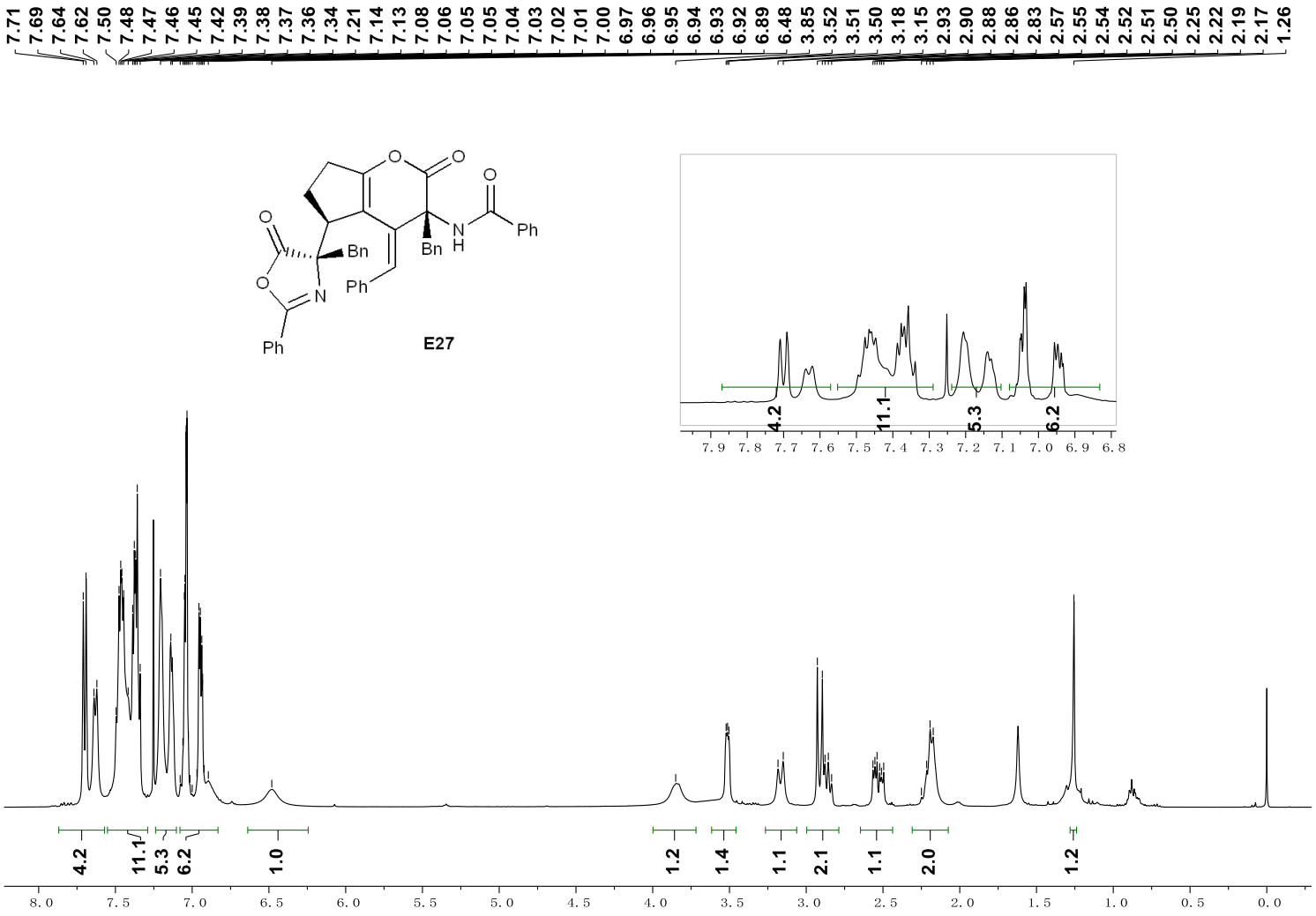
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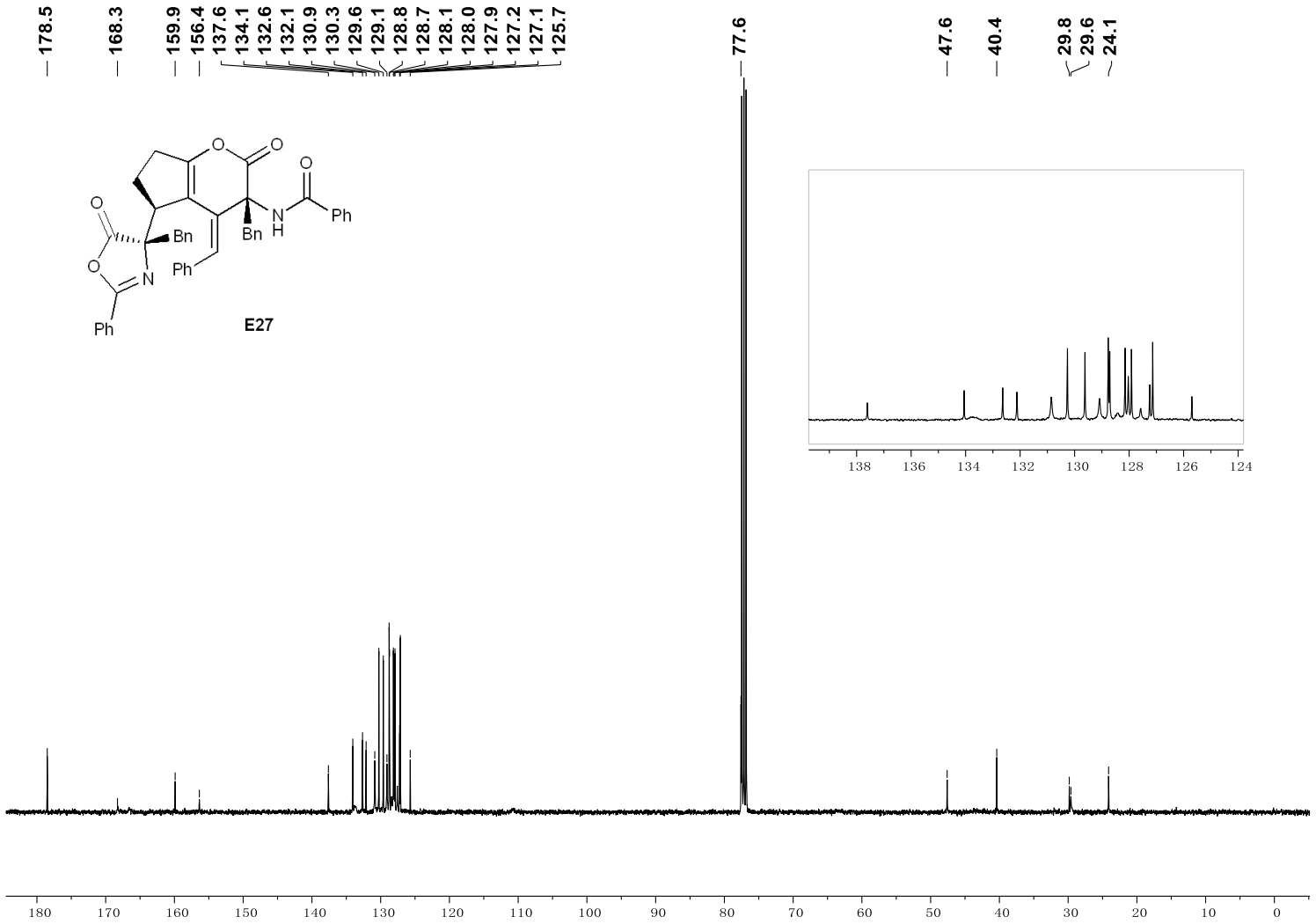
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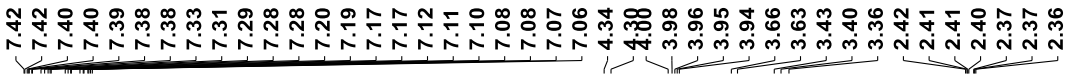
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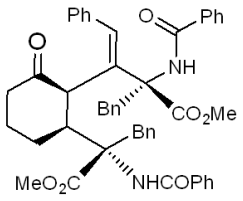
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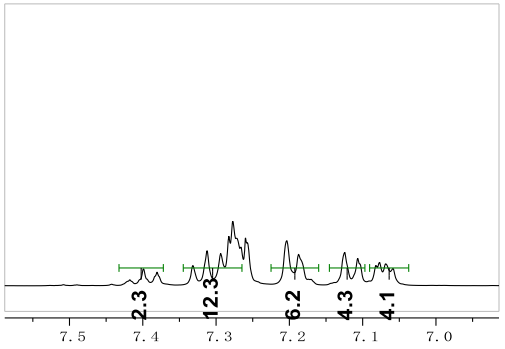
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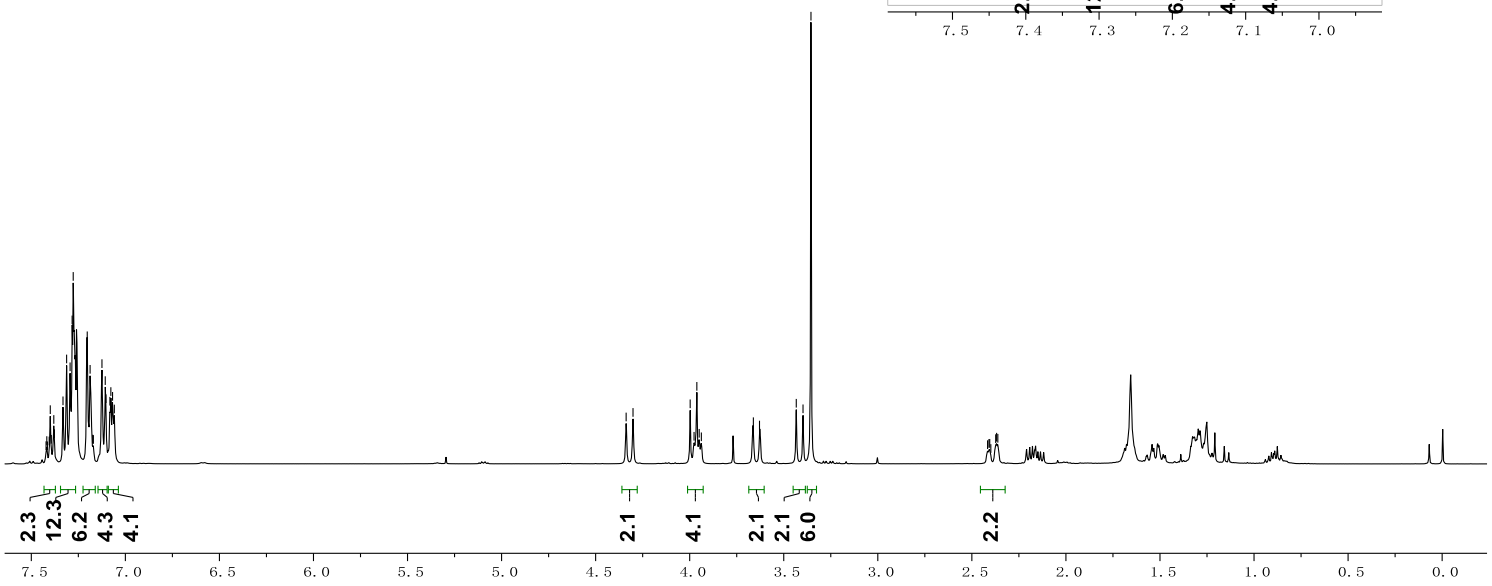
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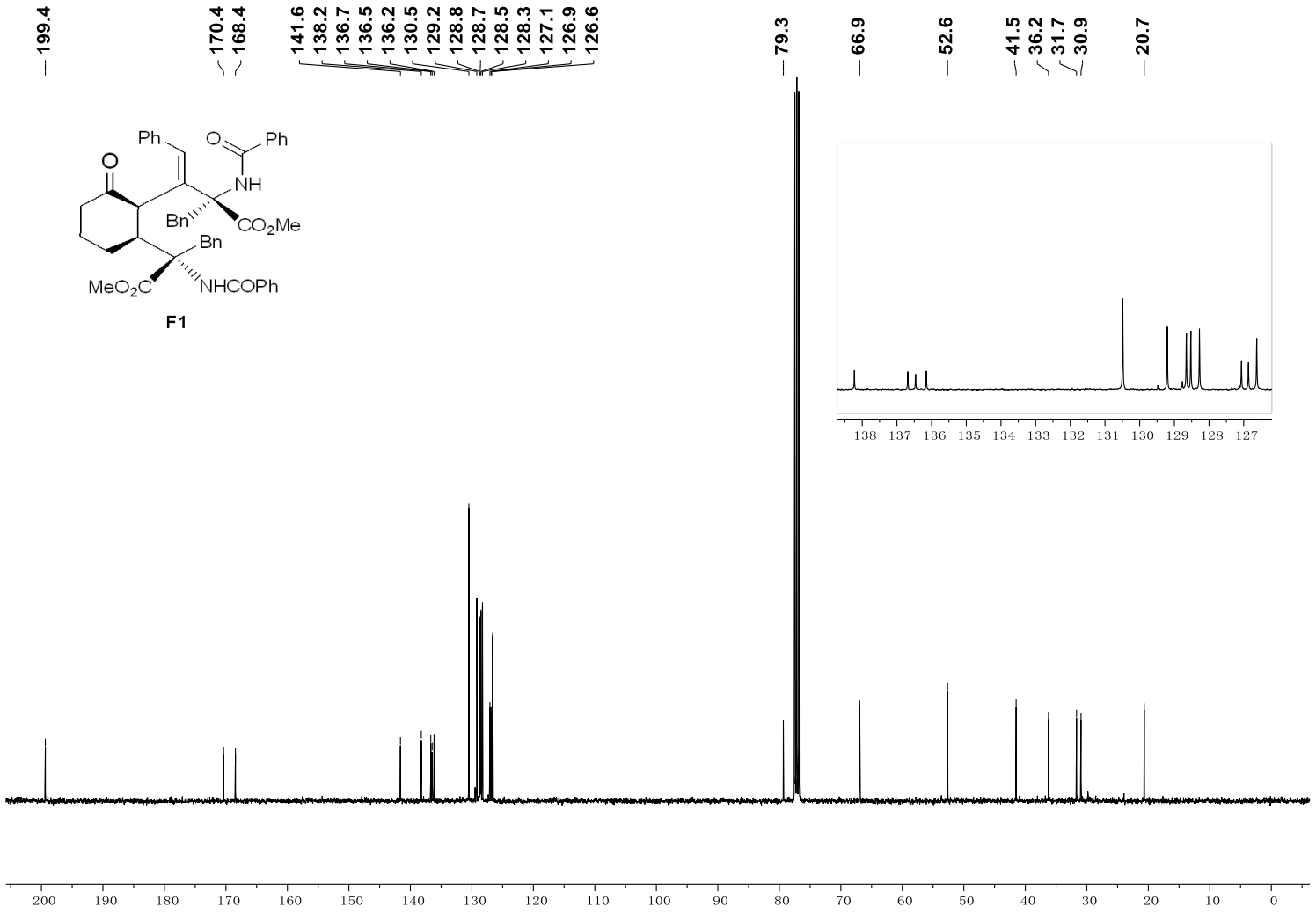
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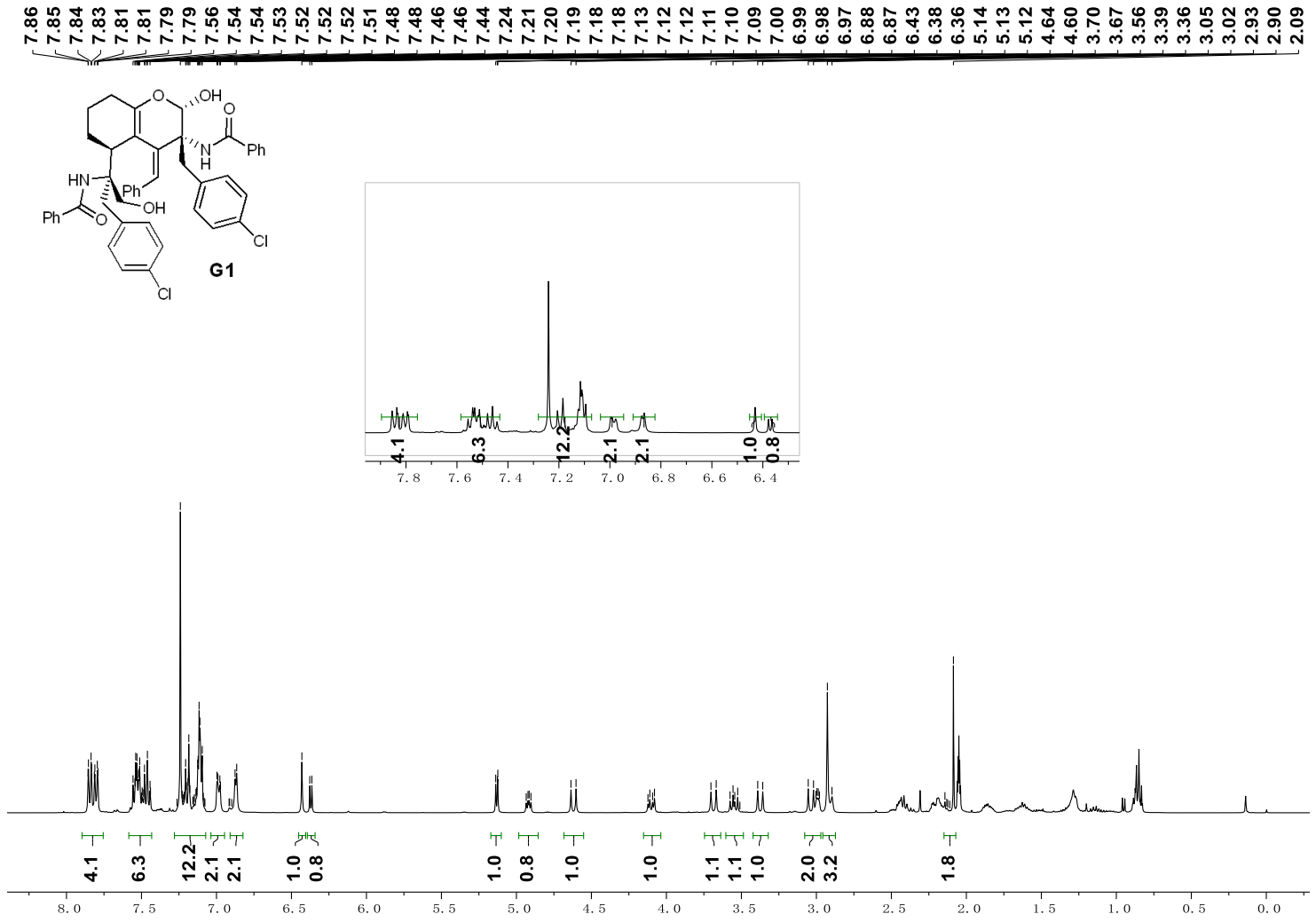
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G1
4.1 6.3 12.2 2.1 2.1 1.0 0.8 1.0 0.8 1.0 1.0 1.1 1.1 1.0 2.0 3.2 1.8
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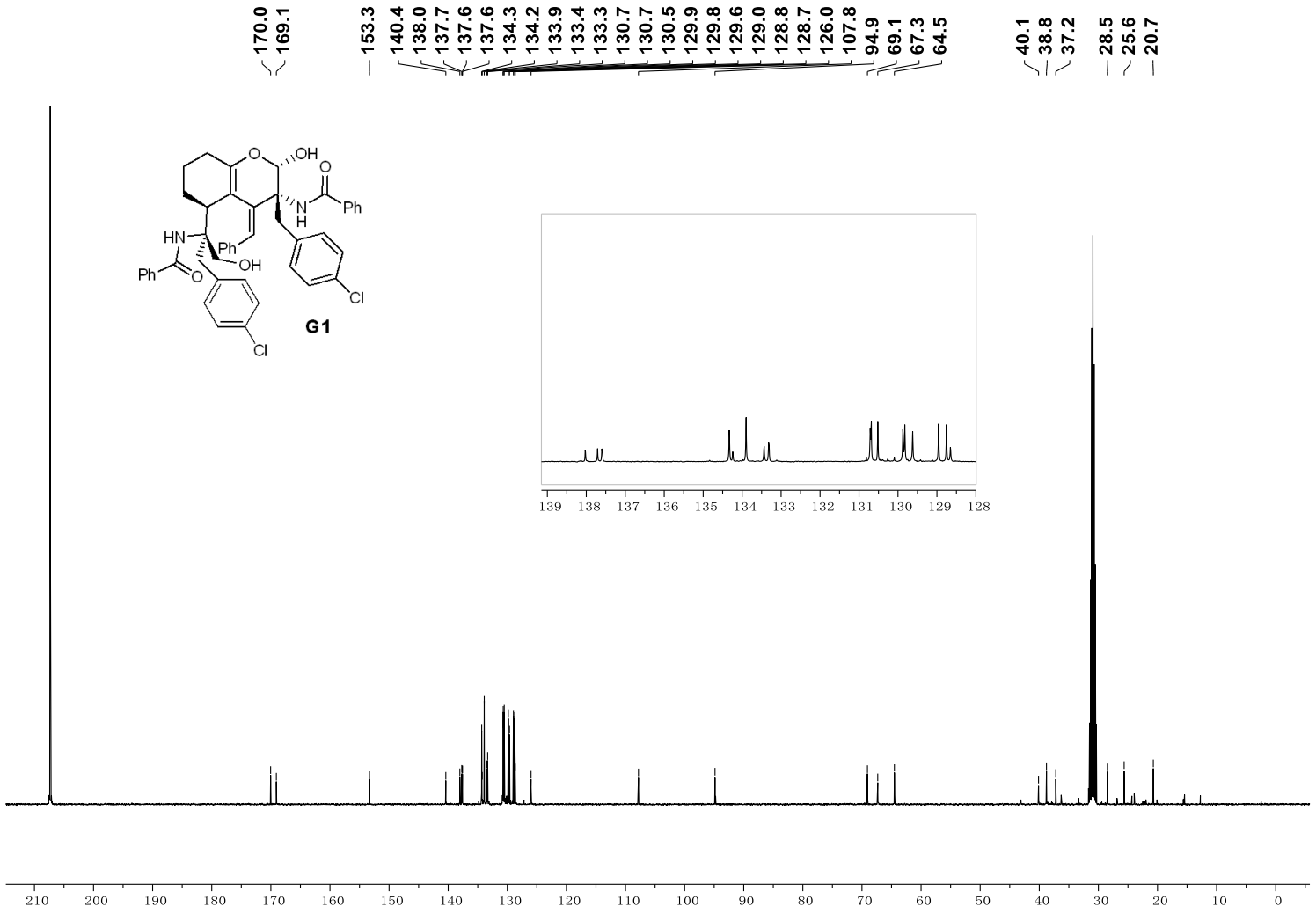
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94.9
69.1
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37.2
28.5
25.6
20.7
G1
139 138 137 136 135 134 133 132 131 130 129 128
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0