Merging photoredox with copper catalysis: enantioselective remote cyanation *via* 1,4-heteroaryl migration

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Supporting Information

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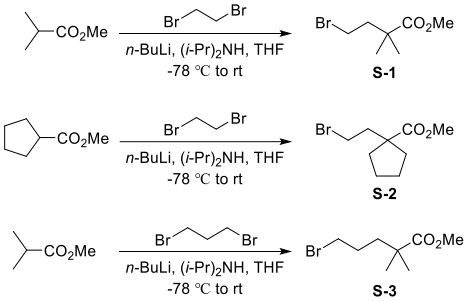
1. General information

All commercially available reagents were used without further purification unless otherwise stated. Solvents (DMF, DMA, THF, CH_3CN, CH_2Cl_2, $ClCH_2CH_2Cl$) were purified and dried according to standard methods before use. Column chromatography was performed on silica gel (200-300 mesh). ^1H NMR and ^{13}C NMR spectra were recorded on a 400 MHz NMR spectrometer or 500 MHz NMR spectrometer. Chemical shifts (δ) were reported in ppm, and coupling constants (J) were given in Hertz (Hz). Data were reported as s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, m = multiplet. High-performance liquid chromatography (HPLC) analyses were performed on a Shimadzu LC-16 HPLC system connected to SPD-16 UV detector using Daicel Chiralpak OJ-H, OD-H, or IC Column. Optical rotations were measured in $CHCl_3$ using a Rudolph Autopol IV automatic polarimeter. High-resolution mass spectra (HRMS) were recorded on an AB SCIEX Triple ESI -TOF 5600+ mass spectrometer or a Micromass CI-TOF mass spectrometer. Melting points were uncorrected.

2. The synthesis of substrates and ligands

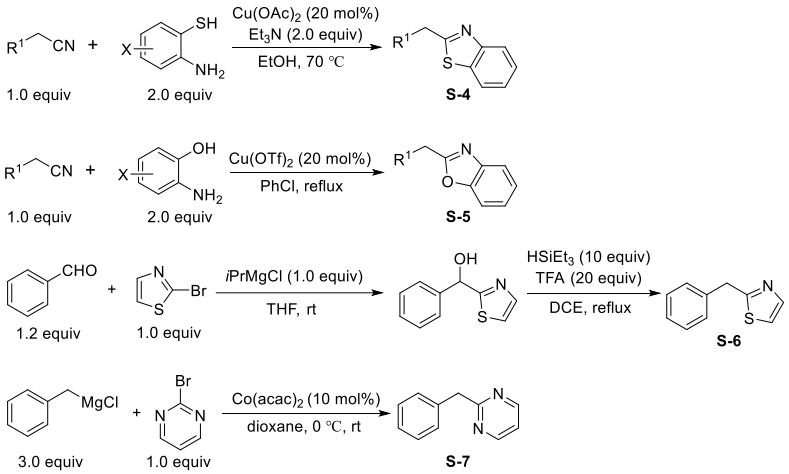
2.1 The procedures for the preparation of compounds S-1, S-2, and S-3



To a solution of diisopropylamine (3.04 g, 30.0 mmol) in dry THF (10 mL) was added dropwise *n*-BuLi (2.5 M in hexanes, 12 mL, 30.0 mmol) at -78 ℃. After stirring for 0.5 h at the same temperature, a solution of methyl isobutyrate (30.0 mmol) in dry THF (10 mL) was added dropwise. The resulting mixture was stirred for 0.5 h at -78 ℃. After the dropwise addition of 1,2-dibromoethane (5.64 g, 30.0 mmol) at -78 ℃, the reaction mixture was warmed to room temperature, stirred for 12 h, quenched with saturated aq. NH_4Cl (20 mL), and extracted with EtOAc (20 mL×3).

The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was roughly purified by vacuum distillation to give **S-1**. Compound **S-2** was prepared using the same method with methyl cyclopentanoate and 1,2-dibromoethane. **S-3** was synthesized using the same method with methyl isobutyrate and 1,3-dibromopropane.

2.2 Procedures for the preparation of compounds S-4~S-8



General procedure for the synthesis of **S-4**[1]: To a round-bottomed flask equipped with a reflux condenser and a magnetic stir bar were added arylacetonitrile (15.0 mmol), 2-aminobenzenethiol (30.0 mmol), $Cu(OAc)_2$ (3.0 mmol, 20 mol%), Et_3N (30.0 mmol), and ethanol (30 mL). The reaction mixture was stirred at 70 ℃ for 12 h. After completion of the reaction, the mixture was cooled to room temperature, quenched with saturated aq. Na_2CO_3 (30 mL), and extracted with ethyl acetate (30 mL×3). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate as eluent to give **S-4**.

General procedure for the synthesis of **S-5**[2]: To a round-bottomed flask equipped with a reflux condenser and a magnetic stir bar were added arylacetonitrile (15.0 mmol), 2-aminophenol (30.0 mmol), $Cu(OTf)_2$ (3.0 mmol, 20 mol%), and chlorobenzene (30 mL). The reaction mixture was stirred under reflux for 72 h. The

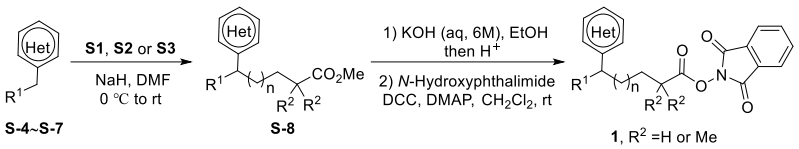
mixture was cooled to room temperature and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate as eluent to give **S-5**.

The procedure for the synthesis of **S-6**[3,4]: To a round-bottomed flask equipped with a magnetic stir bar were added *i*PrMgCl (15.0 mmol, 1.0 mol/L in THF) and 2-bromothiazole (15.0 mmol) at rt. After stirring for 2 h, benzaldehyde (18.0 mmol) was added. The resulting mixture was stirred for 3 h, quenched with H_2O (75 mL), and extracted with dichloromethane (30 mL×3). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1) as eluent to give phenyl(thiazol-2-yl)methanol (white solid, 1.91 g, 67% yield).

To a round-bottomed flask equipped with a reflux condenser and a magnetic stir bar were added phenyl(thiazol-2-yl)methanol (8.0 mmol), triethylsilane (80.0 mmol), trifluoroacetic acid (160.0 mmol), and dichloroethane (30 mL). The reaction mixture was stirred under reflux for 12 h. Then the mixture was concentrated under reduced pressure. The residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1) as eluent to give **S-6** (yellow oil, 0.98 g, 70% yield).

The procedure for the synthesis of **S-7**[5]: Anhydrous cobalt(II) acetylacetonate (1.0 mmol) was placed in a 100 mL flask. Anhydrous dioxane (30 mL) was then added under argon. Afterwards, benzylmagnesium chloride (2.0 M in THF, 15 mL, 30.0 mmol) was added at 0 ℃. The mixture was stirred for about 5 min at rt. Then, 2-bromo-pyrimidine (10.0 mmol) was added dropwise to the reaction mixture. After stirring for 2 h at rt, the mixture was quenched with H_2O (70 mL) and extracted with ethyl acetate (50 mL×3). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate (5:1) as eluent to give **S-7** (yellow oil, 0.90 g, 53% yield).

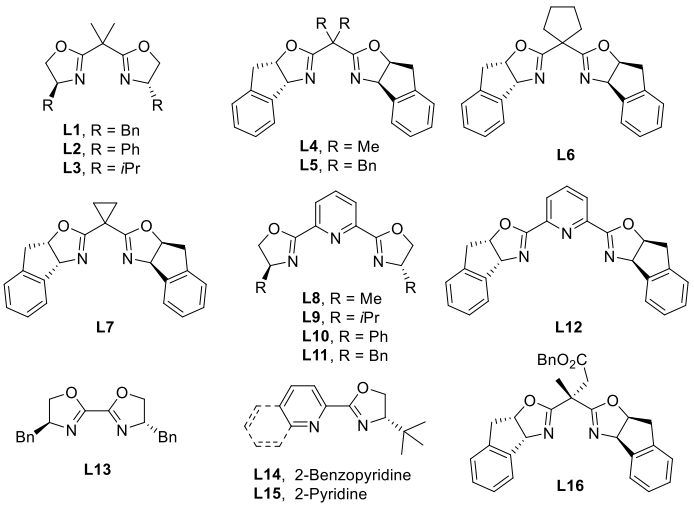
2.3 General procedure for the preparation of substrates 1

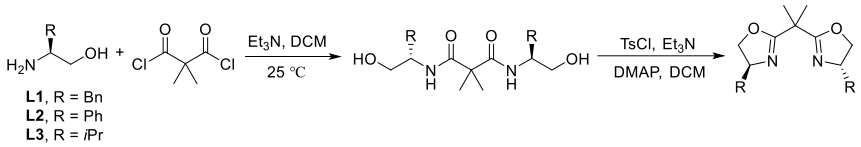


General procedure for the preparation of **S-8**: Under nitrogen atmosphere, to the suspension of NaH (15 mmol) in dry DMF (10.0 mL) was added dropwise **S-4**, **S-5**, **S-6**, or **S-7** (10 mmol, in 5 mL DMF) at rt. After stirring for 1 h at the same temperature, bromide **S-1** or **S-2** or **S-3** (20.0 mmol) was added dropwise *via* a syringe at 0 ℃. Then the reaction mixture was warmed to room temperature, stirred for 12 h, quenched with saturated aq. NH_4Cl (10 mL), and extracted with ethyl acetate (15 mL×3). The combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure. The resulting residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate as eluent to afford **S-8**.

General procedure for the preparation of substrates **1**: To a round-bottomed flask equipped with a magnetic stir bar were added **S-8** (5 mmol) and EtOH (10 mL). Then the KOH solution (2.5 mL, aq, 6 M) was added dropwise, and the reaction mixture was stirred at rt for 12 h. After that, the reaction mixture was brought to pH = 2~4 with HCl (1 M), and extracted with EtOAc (10 mL×3). The combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure. To the residue were added *N*-hydroxyphthalimide (7.5 mmol), *N*,*N*-dimethylpyridine (0.5 mmol), *N*,*N*-dicyclohexylcarbodiimide (7.5 mmol), and CH_2Cl_2 (10 mL). The reaction mixture was stirred at rt for 12 h. After that, the mixture was filtered through a pad of silica gel and rinsed with CH_2Cl_2. The filtrate was concentrated under reduced pressure. The residue was purified by column chromatography on silica gel to afford substrates **1**.

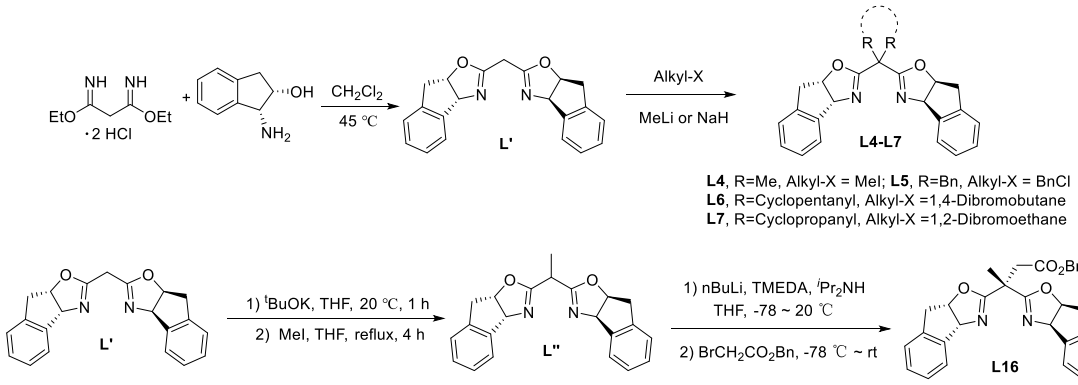
2.4 General procedure for the preparation of ligands





L1-L3 were prepared according to the reported literature.[6] in a three-necked round-bottom flask a solution *S*-amino alcohol (20.0 mmol, 2.0 equiv.) was taken in DCM. The solution was cooled to 0 ℃ and triethyl amine (50.0 mmol, 5.0 equiv.) was added to the mixture. Next a solution of dimethylmalonyl dichloride (10.0 mmol, 1.0 equiv) in DCM was added dropwise to the flask over 10 minutes. Ice bath was removed after 20 minutes and stirred at room temperature until complete loss of dimethylmalonyl dichloride was observed by TLC. After the reaction was completed, water (20 mL) and CH_2Cl_2 (30 mL) were added, and the combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The resultant residue was purified by coloum chromatography on silica gel. Pure diamide was used for further reaction.

Diamide (5.0 mmol, 1.0 equiv.) and 4-(dimethylamino)pyridine (0.5 mmol, 0.1 equiv.) was suspended in DCM (30 mL) and Triethylamine (50.0 mmol, 5.0 equiv.) was added to the mixture. Next p-toluenesulfonyl chloride (10.0 mmol, 2.0 equiv.) in DCM was added at 25 ℃ through cannula. The whole solution was stirred for 36 h. The solution was washed with NH_4Cl and then $NaHCO_3$. The resultant solution was concentrated by vacuo and purified by silica gel column chromatography.



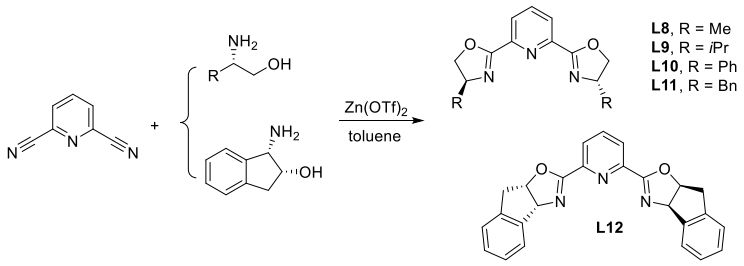
L' was prepared following known literature procedures.[7] The diethyl malonimidate dihydrochloride (50.0 mmol, 1.0 equiv) and (1*S*, 2*R*)-(–)-*cis*-1-amino-2-indanol (105.0 mmol, 2.1 equiv) were added to a flame-dried round bottom flask fitted with a magnetic sttir bar and a reflux condenser, and placed under N_2 atmosphere. Anhydrous CH_2Cl_2 (400 mL) was added and then the reaction mixture was stirred at 45 ℃ for 24 h. The reaction mixture was quenched with $NaHCO_3$ (aq.) at 0 ℃ and extracted with CH_2Cl_2 three times. The combined organic layers were dried over Na_2SO_4 and evaporated under reduced pressure. The residue was purifired by recrystallization from hexane/acetone system to afford **L'** as a white solid.

L' (5.0 mmol, 1.0 equiv) was added to a flamedried round bottom flask with a magnetic stir bar, and placed under N_2 atmosphere. Anhydrous THF (100 mL) was added and the solution was cooled to 0 ℃ (**L4**, **L6** and **L7**) or -55℃ (**L5**). After NaH (60% in oil, 15.0 mmol, 3.0 equiv, for **L4**, **L6** and **L7**) or MeLi (10.0 mmol, 2.0 equiv, for **L5**) was added in portions to the solution, the reaction mixture was stirred at the same temperature for 30 min and then corresponding alkyl halides (12.0 mmol, 2.4 equiv; for dihalides 6.0 mmol, 1.2 equiv) was added dropwise to the reaction mixture. The reaction was warmed to 50 ℃ and stirred for 3 h. The reaction mixture was quenched with sat. NH_4Cl aq. at 0 ℃ and extracted with CH_2Cl_2 three times. The combined organic layers were dried over Na_2SO_4 and evaporated under reduced pressure. The residue was purifired by flash column chromatography on silica-gel to afford following product **L4-L7**.

The preparation of **L16** were also following the above procedure with some minor modifications. To a dried three-necked round-bottom flask, chiral bis(oxazoline)

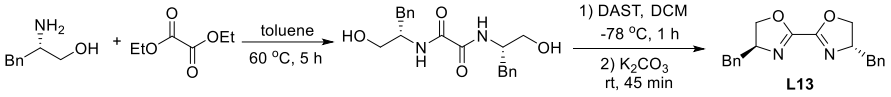
ligand **L'** (6.0 mmol) and THF (30 ml) were added, then ^{t}BuOK (6.0 mmol) was added to a solution at room temperature and the mixture was stirred for 1 h. Methyl iodide (6.0 mmol) was added and the reaction was heated to reflux for 4 h. After evaporating solvent under reduced pressure, brine (20 mL) was added to the crude product and the aqueous phase was extracted with ethyl acetate (3×30 mL). The combined organic phases were dried over Na_2SO_4 and filtered. The monomethylation product **L''** was afforded after concentrating under vacuum and was used for next step directly.

To a dried three-necked round-bottom flask, **L''** (5.0 mmol, 1.0 equiv.), Diisopropylamine (7.0 mmol, 1.4 equiv.), and TMEDA (6.0 mmol, 1.2 equiv) were sequentially dissolved in anhydrous THF (100 mL) in the presence of N_2 atmosphere, and the mixture was cooled to -78 ℃. Then nBuLi (7.0 mmol, 1.4 equiv., 2.5 M in hexane) was added dropwisely to the mixture. The resulting mixture was warmed to -20 ℃ for 1 hour then cooled to -78 ℃ again. Benzyl 2-bromoacetate (7.0 mmol, 1.4 equiv.) was added to the mixture and the reaction mixture was warmed to room temperature for overnight. After that, the reaction was quenched with saturated NH_4Cl (40 mL) and water (40 mL). The aqueous layer was extracted with EA. The combined organic layer were washed with brine (100 mL), dried over Na_2SO_4, and concentrated in vacuum. The residue was purified by flash chromatography on silica gel (PE/Acetone = 3:1) to give the product **L16**.[8]

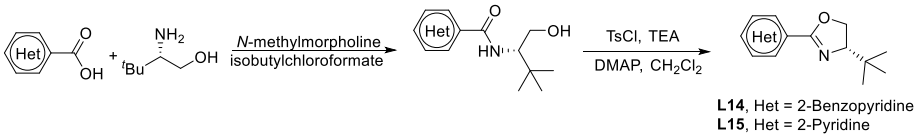


L8-L12 were prepared following known literature procedures.[9] A solution of the appropriate 2,6-pyridinedicarbonitrile (10.0 mmol, 1.0 equiv.), the appropriate amino alcohol (20.0 mmol, 2.0 equiv.) and zinc(II) triflate (1.0 mmol, 0.1 equiv.) in toluene (150 mL) was heated under reflux for 48 h. The reaction mixture was then cooled to rt

and diluted with EtOAc (100 mL). The organic layer was washed with brine (3 × 100 mL), saturated aqueous $NaHCO_3$ solution (3 × 100 mL), dried over Na_2SO_4 and evaporated under reduced pressure. The residue was further purified by silica gel column chromatography.



L13 was prepared following known literature procedures.[10] To an oven-dried round-bottom flask under N_2 equipped with a reflux condenser and a magnetic stir bar was added diethyl oxalate (10.0 mmol, 1.0 equiv) and dry toluene (83 mL). The (S)-2-amino-3-phenylpropan-1-ol (20.0 mmol, 2.0 equiv) was added and the reaction was heated to 60 ºC for 5 hours. A white precipitate formed and the reaction was cooled to room temperature before filtering. The white precipitate (diamide) was then washed with toluene and dried under high vacuum in a 100 mL round-bottom flask, which was directly used in the next step without further purification. To another oven-dried flask diamide (5.0 mmol, 1.0 equiv) and DCM (80 mL) were added under an N_2 atmosphere. The flask was cooled to -78 ℃, and diethylaminosulfur trifluoride (DAST, 14.0 mmol, 2.8 equiv) was added dropwise. The reaction mixture was stirred for 1 h, then K_2CO_3 (20.0 mmol, 4.0 equiv) was added slowly. The flask was removed from the cold bath and allowed to warm to rt. The stirring was continued for an additional 45 min. After that the reaction mixture was diluted with DCM (40 mL) and water (60 mL). The organic layer was washed with aqueous $NaHCO_3$ (40 mL) and brine (60 mL), dried over Na_2SO_4, and concentrated under reduced pressure. The crude product was purified by flash column chromatography on silica gel using a mixture of petroleum ether/ethyl acetate (2:1) as eluent to afford the ligand **L13**.



L14-L15 were prepared following known literature procedures.[11] To a flame dried

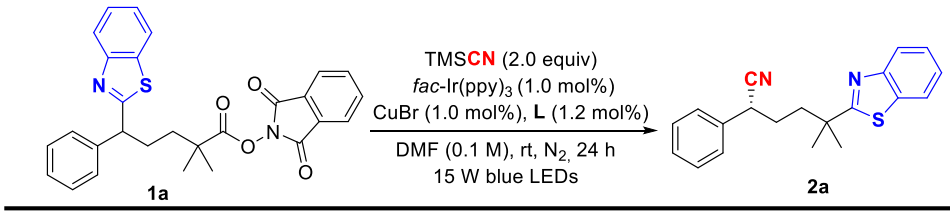
round bottom flask equipped with a stir bar was added heterocyclic acid (4.0 mmol, 1.0 equiv.) and dichloromethane (18 mL) under nitrogen atmosphere. The mixture was cooled to -5 ℃ in an ice bath, then *N*-methylmorpholine (6.0 mmol, 1.5 equiv.) was added dropwise *via* a syringe. The isobutylchloroformate (4.6 mmol, 1.15 equiv.) was added dropwise over a period of 2 minutes after the mixture was stirred for 15 minutes. The resulting mixture was stirred for 0.5 h at the same temperature. Then 4.8 mmol of (*S*)-tert-leucinol and *N*-methylmorpholine (4.6 mmol, 1.15 equiv.) in dichloromethane were added dropwise *via* a syringe. The reaction mixture was stirred for 0.5 h at the same temperature and then warmed to room temperature for another 12 h. The reaction solution was diluted with 50 mL dichloromethane and washed with 1.0 M aqueous HCl solution (1x 4 mL), brine (1x 20 mL) and H_2O (1x 20 mL), dried over Na_2SO_4 and evaporated under reduced pressure. The residue was further purified by silica gel column chromatography to afford the *N*-acyl amino alcohol product.

To a flame dried round bottom flask equipped with a stir bar was placed tosyl chloride (2.0 mmol, 1.5 equiv), DMAP (0.3 mmol, 0.1 equiv), *N*-acyl amino alcohol (2.0 mmol), and dichloroethane (20 mL) under nitrogen atmosphere. The triethylamine (8.0 mmol, 4.0 equiv) was added dropwise via a syringe to the mixture solution. The mixture was heated to reflux for 12 h after 3 hour's stirring at room temperature. The reaction solution was diluted with 50 mL dichloromethane and washed with aq. $NaHCO_3$ (1x 10 mL), brine (1x 10 mL) and H_2O (1x 10 mL), dried over Na_2SO_4, and evaporated under reduced pressure. The heterocyclic oxazoline **L14-L15** were purified with flash silica-gel column chromatography with petroleum ether/ethyl acetate as eluent.

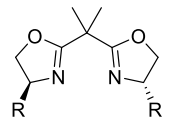
3. Experiments for the enantioselective remote cyanation *via* 1,4-heteroaryl migration

3.1 Optimization of reaction conditions

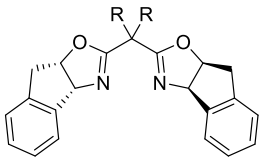
Table S1 Screening of ligands[a,b,c]



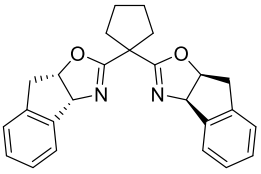
1a **2a**



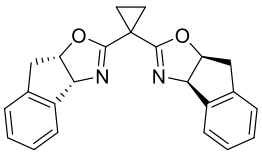
L1, R = Bn, 70% yield, 80:20 er
L2, R = Ph, 66% yield, 75.5:24.5 er
L3, R = *i*Pr, 52% yield, 69:31 er



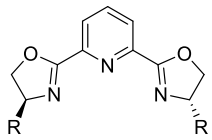
L4, R = Me, 59% yield, 85:15 er
L5, R = Bn, 31% yield, 78:22 er



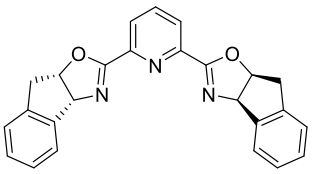
L6
64% yield, 86:14 er



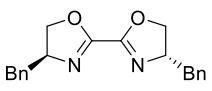
L7
83% yield, 92.5:7.5 er



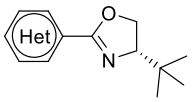
L8, R = Me, 68% yield, 57:43 er
L9, R = *i*Pr, 74% yield, 60.5:39.5 er
L10, R = Ph, 51% yield, 68.5:31.5 er
L11, R = Bn, 39% yield, 65:35 er



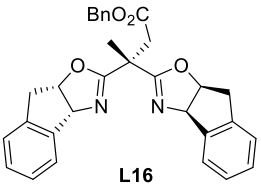
L12
62% yield, 72.5:27.5 er



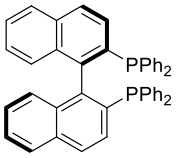
L13
59% yield, 51:49 er



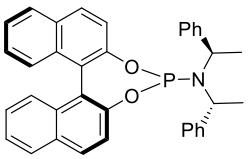
L14, Het = 2-Benzopyridine
46% yield, 52.5:47.5 er
L15, Het = 2-Pyridine
51% yield, 57.5:42.5 er



L16
52% yield, 66:34 er



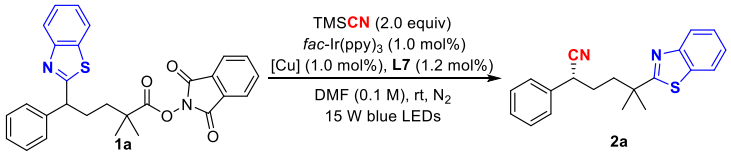
L17
32% yield, 48.5:51.5 er



L18
55% yield, 52.5:47.5 er

[a]All reactions were carried out with **1a** (0.20 mmol), TMSCN (0.40 mmol), *fac*-Ir(ppy)$_3$ (1.0 mol%), CuBr (1.0 mol%), and **L** (1.2 mol%) in DMF (2.0 mL) at room temperature for 24 h under the irradiation with a 15 W blue LED lamp. [b]Isolated yield based on **1a**. [c]The enantiomeric ratios were determined by HPLC on a chiral stationary phase.

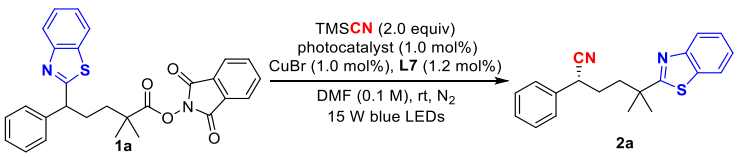
Table S2 Screening of the copper catalysts and ratios to ligands[a]



entry	[Cu]	yield (%)[b]	er[c]
1	CuCl	54	92.5:7.5
2	CuBr	83	92.5:7.5
3	CuI	62	92:8
4	CuCN	59	91.5:8.5
5	$Cu(MeCN)_4PF_6$	60	91.5:8.5
6	$CuCl_2$	48	92.5:7.5
7	$Cu(OAc)_2$	71	92:8
8	$Cu(OTf)_2$	41	91.5:8.5
9[d]	CuBr	79	89.5:10.5
10[e]	CuBr	76	92:8
11[f]	CuBr	84	90:10
12	–	0	–
13[g]	CuBr	43	50:50

[a]All reactions were carried out with **1a** (0.20 mmol), TMSCN (0.40 mmol), *fac*-Ir(ppy)$_3$ (1.0 mol%), copper catalyst (1.0 mol%), and **L7** (1.2 mol%) in DMF (2.0 mL) at room temperature for 24 h under irradiation with a 15 W blue LED lamp unless otherwise stated. [b]Isolated yield based on **1a**. [c]The enantiomeric ratios were determined by chiral HPLC analysis. [d]CuBr:**L7**=1:1. [e]CuBr:**L7**=1:2. [f]CuBr:**L7**=2:1. [g]Without **L7**

Table S3 Screening of the photocatalysts[a]



entry	photocatalyst	yield (%)[b]	er[c]
1	*fac*-Ir(ppy)$_3$	83	92.5:7.5
2	$Ir(ppy)_2(dtbpy)PF_6$.	66	92:8
3	$Ir[dF(CF_3)ppy]_2(dtbpy)PF_6$	84	90:10
4	$Ru(bpy)_2Cl_2$	55	90:10
5	–	0	–
6[d]	*fac*-Ir(ppy)$_3$	0	–

[a]All reactions were carried out with **1a** (0.20 mmol), TMSCN (0.40 mmol), photocatalyst (1.0 mol%), CuBr (1.0 mol%), and **L7** (1.2 mol%) in DMF (2.0 mL) at room temperature for 24 h under irradiation with a 15 W blue

LED lamp unless otherwise stated. [b]Isolated yield based on **1a**. [c]The enantiomeric ratios were determined by chiral HPLC analysis. [d]In the dark.

Table S4 Screening of the solvents and reaction temperature[a]

entry	solvent	yield (%)[b]	er[c]
1	DMF	83	92.5:7.5
2	DMA	67	92.5:7.5
3	DMSO	0	–
4	MeOH	57	81:19
5	EtOH	<10	–
6	CH_2Cl_2	0	–
7	PhCl	0	–
8	*p*-xylene	0	–
9	THF	0	–
10	MeCN	0	–
11[d]	DMF	50	90:10
12[e]	DMF	41	92.5:7.5

[a]All reactions were carried out with **1a** (0.20 mmol), TMSCN (0.40 mmol), *fac*-Ir(ppy)$_3$ (1.0 mol%), CuBr (1.0 mol%), and **L7** (1.2 mol%) in solvent (2.0 mL) at room temperature for 24 h under irradiation with a 15 W blue LED lamp unless otherwise stated. [b]Isolated yield based on **1a**. [c]The enantiomeric ratios were determined by chiral HPLC analysis. [d]At 50 ℃. [e]At -10 ℃.

3.2 General procedure for the enantioselective remote cyanation *via* 1,4-heteroaryl migration

3.2.1 Preparation of catalyst stock solution A

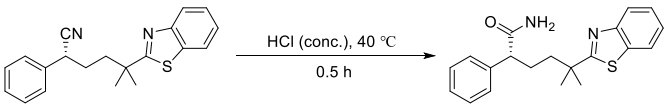
To a 10 mL reaction tube were added CuBr (7.2 mg, 0.05 mmol), chiral bisoxazoline ligand **L7** (21.4 mg, 0.06 mmol), and DMF (5 mL). The tube was sealed with a cap, then the mixture was degassed with nitrogen and stirred at room temperature until all the solids were dissolved. The **stock solution A** was stored under nitrogen atmosphere.

3.2.2 General procedure for the enantioselective remote cyanation *via* 1,4-heteroaryl migration

To a reaction tube equipped with a magnetic stir bar were added substrates **1** (0.20 mmol), *fac*-Ir(ppy)$_3$ (1.3 mg, 0.0020 mmol), catalyst stock solution A (0.20 mL), and DMF (1.8 mL). The mixture was degassed by three freeze-pump-thaw cycles and finally backfilled with nitrogen. Then, TMSCN (0.40 mmol) was added in one portion via a syringe. The reaction mixture was irradiated with a 15 W blue LED lamp and stirred at rt under nitrogen atmosphere for 24 h. After that, the mixture was diluted with water (15 mL) and extracted with EtOAc (15 mL×3). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate) to give product **2**.

4. Transformations of product 2a

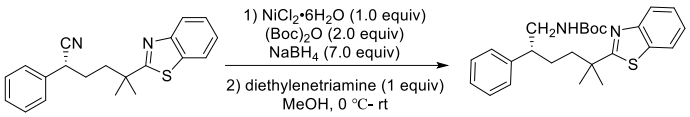
4.1 The procedure for the synthesis of amide 3[12]



2a, 92.5:7.5 er — **3**, 85% yield, 90.5:9.5 er

To a reaction tube equipped with a magnetic stir bar were added **2a** (64.9 mg, 0.20 mmol) and conc. HCl (0.40 mL). The mixture was heated to 40 ℃ and stirred for 0.5 h. After that, ice water (5 mL) was added, and the mixture was extracted with EtOAc (10 mL×3). The combined organic layers were dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate/EtOH = 6:2:1) to give **3** as colorless oil (57.6 mg, 85%).

4.2 The procedure for the reduction of 2a to a Boc-protected amine 4[13]



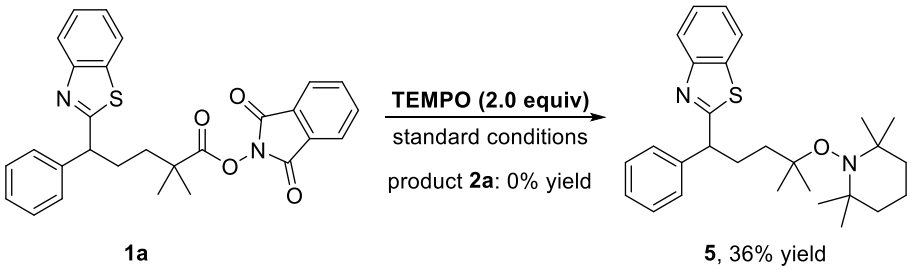
2a, 92.5:7.5 er — **4**, 69% yield, 92:8 er

To a reaction tube equipped with a magnetic stir bar were added **2a** (64.9 mg, 0.20 mmol) and dry methanol (2.0 mL). The reaction was cooled to 0 ℃, and Boc_2O (92

μL, 0.40 mmol) and $NiCl_2 \cdot 6H_2O$ (47.6 mg, 0.20 mmol) were added. $NaBH_4$ (53.0 mg, 1.4 mmol) was then added in small portions. The resulting reaction mixture was allowed to warm to room temperature and stirred for 1 h. Then diethylenetriamine (22 μL, 0.2 mmol) was added and the reaction was stirred for another 12 h. The reaction mixture was concentrated under reduced pressure. The residue was dissolved in EtOAc (5 mL) and washed with saturated aq. $NaHCO_3$ (2×5 mL). The organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 10:1) to give **4** as colorless oil (58.7 mg, 69%).

5. Mechanistic studies

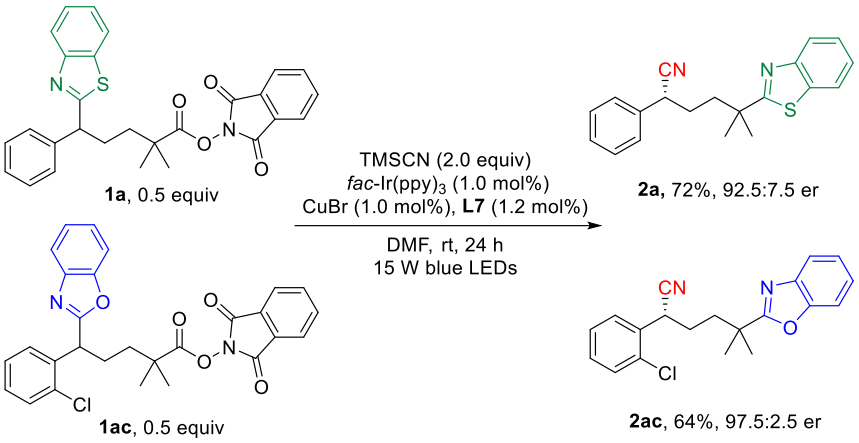
5.1 Radical-trapping experiment



Scheme S1 Radical-trapping experiment.

To a reaction tube equipped with a magnetic stir bar were added substrate **1a** (0.20 mmol), *fac*-$Ir(ppy)_3$ (1.3 mg, 0.0020 mmol), TMEPO (62.5mg, 0.40 mmol), catalyst stock solution A (0.20 mL), and DMF (1.8 mL). The mixture was degassed by three freeze-pump-thaw cycles and finally backfilled with nitrogen. Then, TMSCN (39.7 mg, 0.40 mmol) was added in one portion via a syringe. The reaction mixture was irradiated with a 15 W blue LED lamp and stirred at rt under nitrogen atmosphere for 24 h. Thin-layer chromatography (TLC) analysis indicated that the formation of product **2a** was not observed. The mixture was diluted with water (15 mL) and extracted with EtOAc (15 mL×3). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 30:1) to give **5** as colorless oil (32.7 mg, 36%).

5.2 Crossover experiment



Scheme S2 Crossover experiment.

To a reaction tube equipped with a magnetic stir bar were added substrate **1a** (0.10 mmol), substrate **1ac** (0.10 mmol), *fac*-Ir(ppy)$_3$ (1.3 mg, 0.0020 mmol), catalyst stock solution A (0.20 mL), and DMF (1.8 mL). The mixture was degassed by three freeze-pump-thaw cycles and finally backfilled with nitrogen. Then, TMSCN (39.7 mg, 0.40 mmol) was added in one portion *via* a syringe. The reaction mixture was irradiated with a 15 W blue LED lamp and stirred at rt under nitrogen atmosphere for 24 h. After that, the mixture was diluted with water (15 mL) and extracted with EtOAc (15 mL×3). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 30:1) to give **2a** (72%, 92.5:7.5 er) and **2ac** (64%, 97.5:2.5 er) (The yields of **2a** and **2ac** were determined by ^{1}H NMR spectroscopy).

5.3 Non-linear effect studies

To a reaction tube equipped with a magnetic stir bar were added substrate **1a** (0.20 mmol), *fac*-Ir(ppy)$_3$ (1.3 mg, 1.0 mol%), CuBr (1.0 mol%), **L7** (1.2 mol%, x% ee), and DMF (2.0 mL). The mixture was degassed by three freeze-pump-thaw cycles and finally backfilled with nitrogen. Then, TMSCN (0.40 mmol) was added in one portion via a syringe. The reaction mixture was irradiated with a 15 W blue LED lamp and stirred at rt under nitrogen atmosphere for 24 h. After that, the mixture was diluted with water (15 mL) and extracted with EtOAc (15 mL×3). The combined organic

layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (eluent: petroleum ether/ethyl acetate) to give product **2a**. Chiral HPLC analysis gave the corresponding ee values of product **2a**. An excellent linear relationship was found between the optical purity of **2a** and the enantiopurity of ligand.

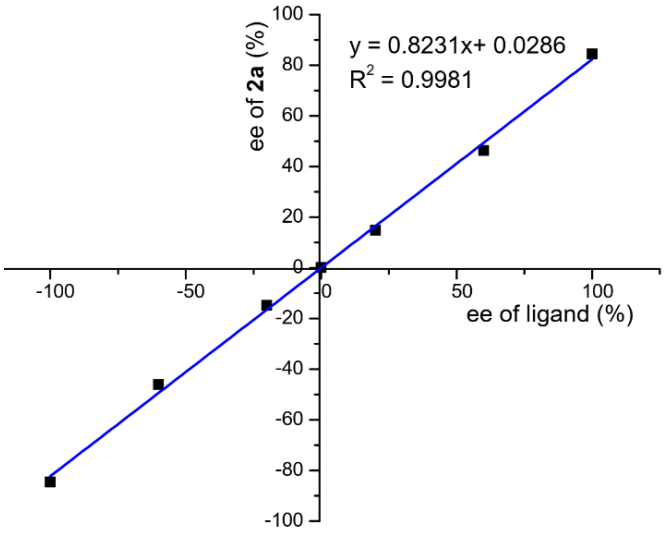


Fig. S1 Relationship between ee values of **2a** and the enantiopurity of ligand.

5.4 Light on/off experiment

To a reaction tube equipped with a magnetic stir bar were added substrate **1a** (0.20 mmol), *fac*-Ir(ppy)$_3$ (1.3 mg, 0.0020 mmol), catalyst stock solution A (0.20 mL), and DMF (1.8 mL). The mixture was degassed by three freeze-pump-thaw cycles and finally backfilled with nitrogen. Then, TMSCN (39.7 mg, 0.40 mmol) was added in one portion via a syringe. The reaction mixture was stirred at rt under nitrogen atmosphere with the light turned on and off at intervals, and the yields were determined by ^{1}H NMR with 1,3,5-trimethoxybenzene as an internal standard.

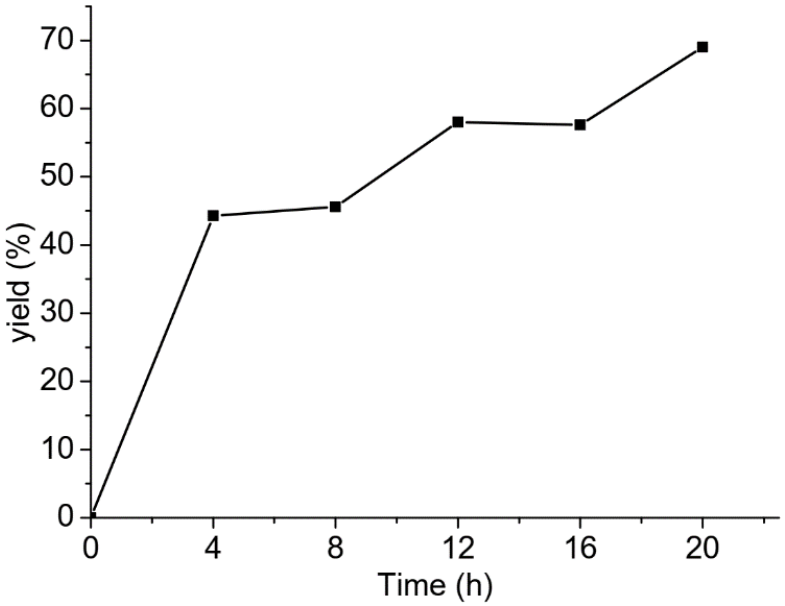
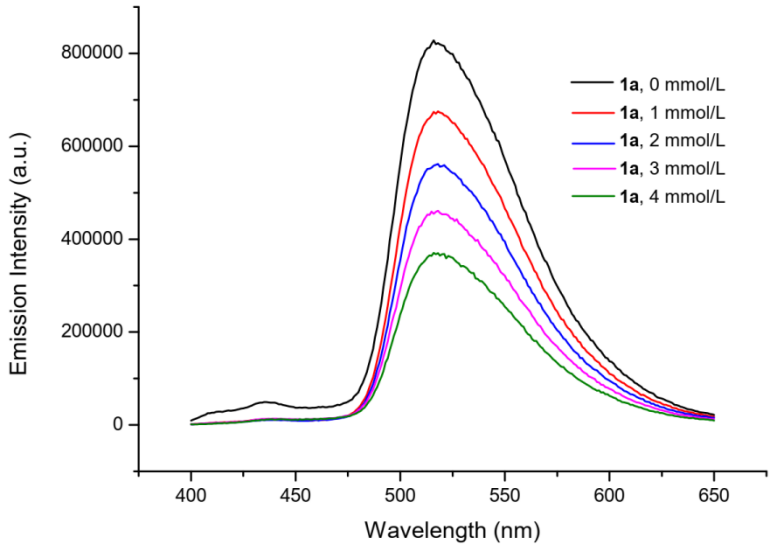


Fig. S2 Reaction profile with the light on/off over time.

5.5 Stern-Volmer fluorescence quenching experiments

The luminescence quenching experiment was taken using a FluoroMax-4 Spectrophotometer. The experiments were carried out in 3 x 10^{-5} mol/L of $Ir(ppy)_3$ in DMF at rt. The excitation wavelength was 384 nm and the emission intensity was collected at 517 nm. The concentrations of quencher (**1a**, CuBr/**L7**) in DMF were 1 mmol/L, 2 mmol/L, 3 mmol/L, and 4 mmol/L.



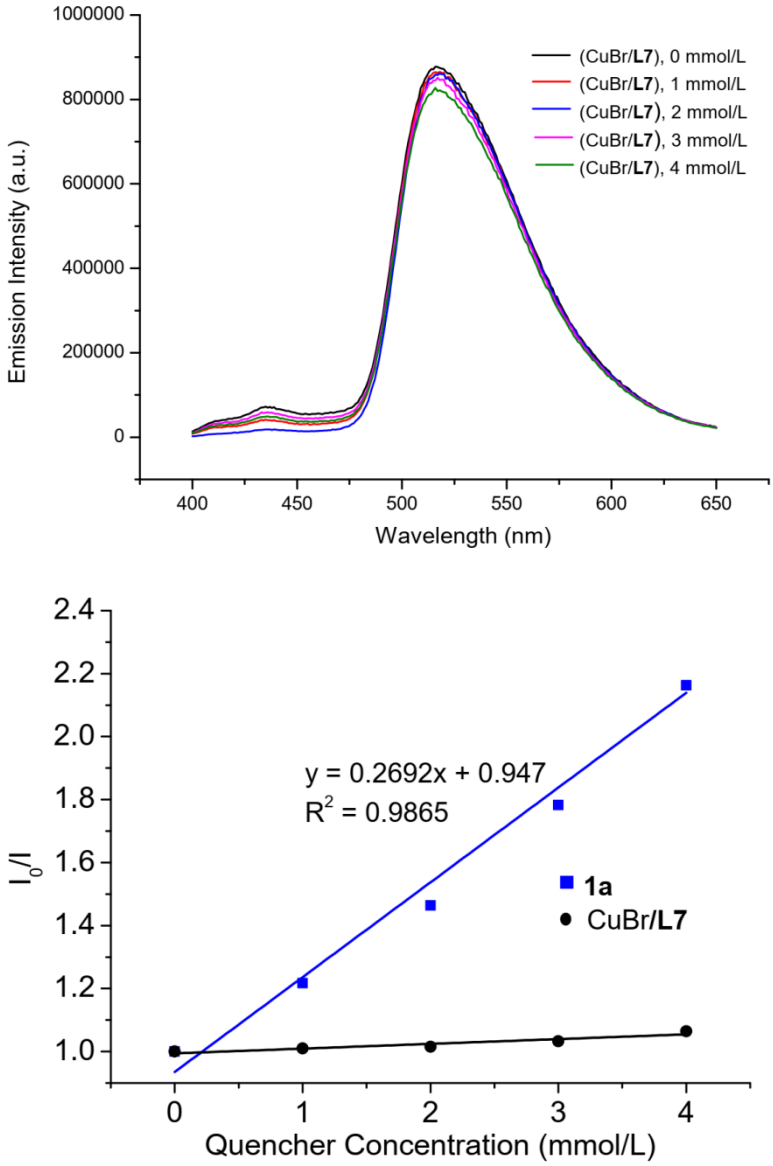


Fig. S3 Emission quenching experiments with **1a** or CuBr/**L7** as quenchers.

5.6 Cyclic voltammetry experiment

Cyclic Voltammetry was performed on a CHI 660E electrochemical analyzer. CV measurement of substrate **1a** (0.0010 M) was carried out in 0.10 M of Bu_4NPF_6/MeCN at a scan rate of 50 mV/s with the protection of N_2. The working electrode is a glassy carbon, the counter electrode is a Pt wire, and the reference electrode is Ag/AgCl (3.5 M KCl). As showed in Figure S4, the reduction peak at -1.272 V (-1.131 V vs SCE) is corresponding to the **1a**.

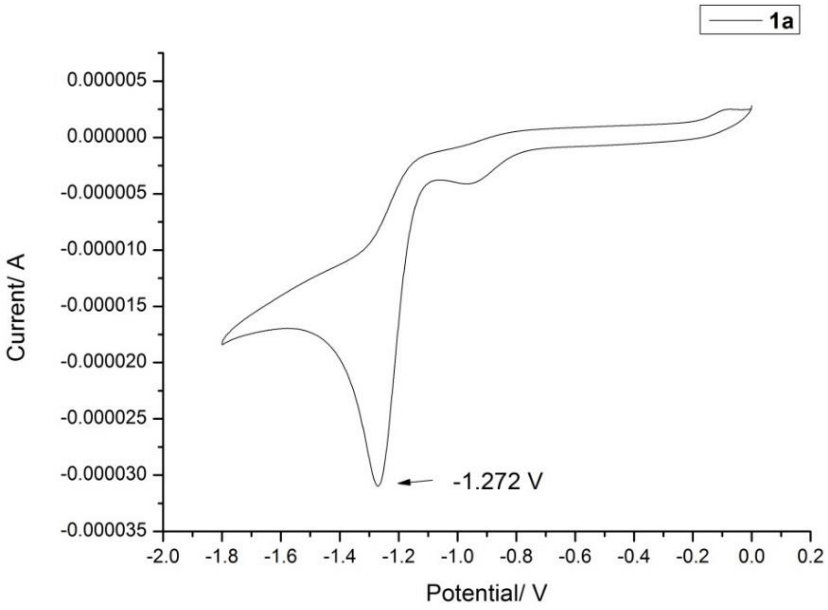
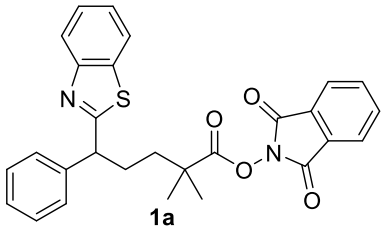


Fig. S4 Cyclic Voltammogram of **1a**.

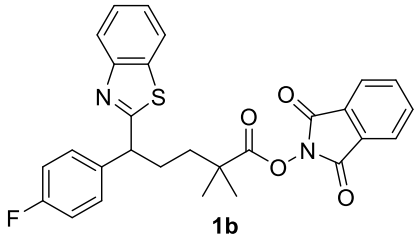
6. Characterization data

1,3-dioxoisoindolin-2-yl 5-(benzo[d]thiazol-2-yl)-2,2-dimethyl-5-phenylpentanoate (1a)



White solid, mp 83-84 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, J = 8.0 Hz, 1H), 7.91 – 7.83 (m, 2H), 7.82 – 7.70 (m, 3H), 7.50 (d, J = 7.6 Hz, 2H), 7.41 – 7.30 (m, 1H), 7.39 – 7.31 (m, 3H), 7.30 – 7.27 (m, 1H), 4.44 (t, J = 8.0 Hz, 1H), 2.65 – 2.52 (m, 1H), 2.46 – 2.33 (m, 1H), 1.87 – 1.74 (m, 2H), 1.41 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.9, 173.5, 162.0, 153.0, 141.1, 135.3, 134.6, 129.0, 128.8, 128.1, 127.4, 125.8, 124.7, 123.8, 122.9, 121.5, 51.3, 41.9, 38.6, 30.7, 25.6, 24.7; HRMS (CI-TOF) m/z: $[M+H]^+$ calcd for $C_{28}H_{25}N_2O_4S$ 485.1530, found 485.1543.

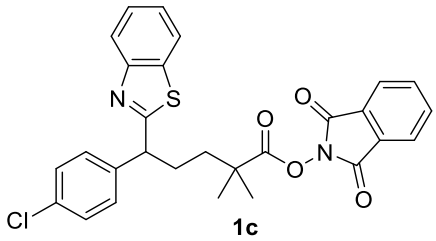
1,3-dioxoisoindolin-2-yl 5-(benzo[d]thiazol-2-yl)-5-(4-fluorophenyl)-2,2-dimethylpentanoate (1b)



1b

White solid, mp 97-99 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, J = 8.2 Hz, 1H), 7.85 – 7.82 (m, 2H), 7.80 (d, J = 8.0 Hz, 1H), 7.73 – 7.70 (m, 2H), 7.54 – 7.39 (m, 3H), 7.37 – 7.27 (m, 1H), 7.05 (t, J = 8.7 Hz, 2H), 4.43 (t, J = 7.7 Hz, 1H), 2.66 – 2.51 (m, 1H), 2.44 – 2.29 (m, 1H), 1.88 – 1.70 (m, 2H), 1.41 (s, 3H), 1.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.4, 173.4, 161.883 (d, J = 245.9 Hz), 161.878, 152.9, 136.8 (d, J = 3.2 Hz), 135.1, 134.5, 129.6 (d, J = 8.0 Hz), 128.8, 125.8, 124.7, 123.7, 122.8, 121.4, 115.6 (d, J = 21.4 Hz), 50.3, 41.8, 38.5, 30.8, 25.6, 24.5; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{28}H_{24}FN_2O_4S$ 503.1435, found 503.1439.

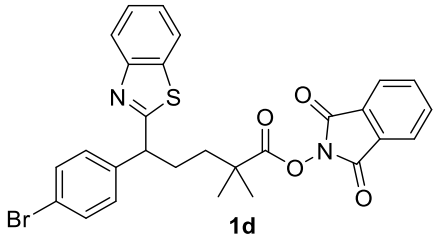
1,3-dioxoisoindolin-2-yl 5-(benzo[d]thiazol-2-yl)-5-(4-chlorophenyl)-2,2-dimethylpentanoate (1c)



1c

White solid, mp 105-107 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, J = 8.1 Hz, 1H), 7.91 – 7.86 (m, 2H), 7.81 (d, J = 8.0 Hz, 1H), 7.78 – 7.75 (m, 2H), 7.48 – 7.44 (m, 3H), 7.41 – 7.30 (m, 3H), 4.44 (t, J = 7.7 Hz, 1H), 2.68 – 2.51 (m, 1H), 2.45 – 2.31 (m, 1H), 1.91 – 1.71 (m, 2H), 1.41 (s, 3H), 1.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.0, 173.4, 161.9, 152.9, 139.5, 135.1, 134.6, 133.1, 129.5, 128.9, 128.8, 125.9, 124.8, 123.8, 122.9, 121.5, 50.5, 41.8, 38.6, 30.7, 25.7, 24.5; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{28}H_{24}ClN_2O_4S$ 519.1140, found 519.1137.

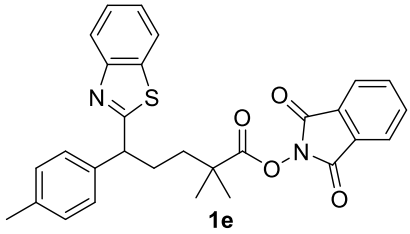
1,3-dioxoisoindolin-2-yl 5-(benzo[d]thiazol-2-yl)-5-(4-bromophenyl)-2,2-dimethylpentanoate (1d)



1d

White solid, mp 50-52 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, J = 8.1 Hz, 1H), 7.90 – 7.85 (m, 2H), 7.83 – 7.74 (m, 3H), 7.51 – 7.40 (m, 3H), 7.42 – 7.35 (m, 2H), 7.38 – 7.29 (m, 1H), 4.39 (t, J = 7.7 Hz, 1H), 2.64 – 2.47 (m, 1H), 2.41 – 2.27 (m, 1H), 1.88 – 1.67 (m, 2H), 1.41 (s, 3H), 1.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.0, 173.4, 162.0, 153.0, 140.1, 135.2, 134.7, 131.9, 129.9, 129.0, 125.9, 124.9, 123.9, 122.9, 121.5, 121.4, 50.6, 41.9, 38.6, 30.7, 25.8, 24.6; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{28}H_{24}BrN_2O_4S$ 563.0635, found 563.0638.

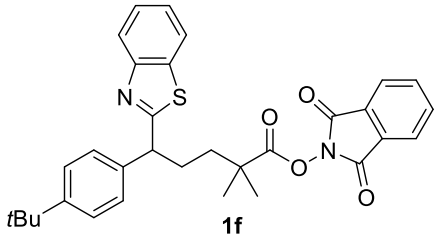
1,3-dioxoisoindolin-2-yl 5-(benzo[d]thiazol-2-yl)-2,2-dimethyl-5-(p-tolyl)pentanoate (1e)



1e

White solid, mp 104-106 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, J = 8.1 Hz, 1H), 7.93 – 7.84 (m, 2H), 7.82 – 7.72 (m, 3H), 7.50 – 7.41 (m, 1H), 7.42 – 7.35 (m, 2H), 7.34 – 7.28 (m, 1H), 7.22 – 7.13 (m, 2H), 4.40 (t, J = 7.8 Hz, 1H), 2.62 – 2.50 (m, 1H), 2.45 – 2.33 (m, 1H), 2.33 (s, 3H), 1.88 – 1.73 (m, 2H), 1.41 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.4, 173.5, 162.0, 153.0, 138.1, 137.0, 135.3, 134.6, 129.5, 129.0, 128.0, 125.7, 124.6, 123.8, 122.8, 121.5, 50.9, 41.9, 38.6, 30.6, 26.0, 24.7, 21.1; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{29}H_{27}N_2O_4S$ 499.1686, found 499.1681.

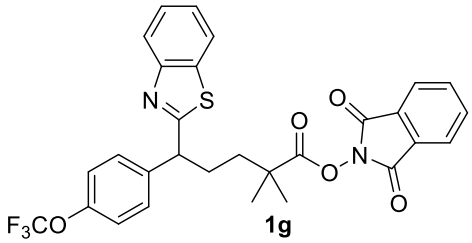
1,3-dioxoisoindolin-2-yl 5-(benzo[d]thiazol-2-yl)-5-(4-(tert-butyl)phenyl)-2,2-dimethylpentan-oate (1f)



1f

White solid, mp 140-142 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, J = 8.1 Hz, 1H), 7.95 – 7.85 (m, 2H), 7.84 – 7.74 (m, 3H), 7.50 – 7.41 (m, 3H), 7.39 (d, J = 8.2 Hz, 2H), 7.38 – 7.28 (m, 1H), 4.46 (t, J = 7.7 Hz, 1H), 2.67 – 2.51 (m, 1H), 2.48 – 2.32 (m, 1H), 1.94 – 1.75 (m, 2H), 1.42 (s, 3H), 1.41 (s, 3H), 1.30 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.3, 173.5, 162.0, 153.0, 150.1, 138.0, 135.3, 134.6, 128.9, 127.6, 125.7, 125.7, 124.6, 123.8, 122.8, 121.5, 50.8, 41.9, 38.6, 34.4, 31.3, 30.7, 25.5, 24.8; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{32}H_{33}N_2O_4S$ 541.2156, found 541.2152.

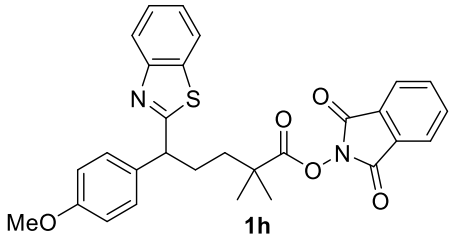
1,3-dioxoisoindolin-2-yl 5-(benzo[d]thiazol-2-yl)-2,2-dimethyl-5-(4-(trifluoromethoxy)phenyl)-pentanoate (1g)



1g

White solid, mp 72-74 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, J = 8.1 Hz, 1H), 7.92 – 7.84 (m, 2H), 7.84 – 7.73 (m, 3H), 7.57 – 7.52 (m, 2H), 7.50 – 7.41 (m, 1H), 7.37 – 7.31 (m, 1H), 7.25 – 7.17 (m, 2H), 4.46 (t, J = 7.7 Hz, 1H), 2.72 – 2.50 (m, 1H), 2.45 – 2.28 (m, 1H), 1.90 – 1.69 (m, 2H), 1.41 (s, 3H), 1.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.9, 173.4, 162.0, 153.0, 148.4, 139.8, 135.2, 134.7, 129.5, 128.9, 125.9, 124.9, 123.9, 122.9, 121.6, 121.2, 120.4 (q, J = 255.8 Hz), 50.5, 41.9, 38.6, 30.9, 25.7, 24.6; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{29}H_{24}F_3N_2O_5S$ 569.1353, found 569.1347.

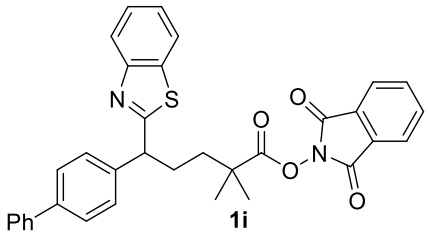
1,3-dioxoisoindolin-2-yl 5-(benzo[d]thiazol-2-yl)-5-(4-methoxyphenyl)-2,2-dimethylpentanoat-e (1h)



1h

White solid, mp 117-119 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, J = 8.1 Hz, 1H), 7.91 – 7.86 (m, 2H), 7.82 – 7.74 (m, 3H), 7.48 – 7.35 (m, 3H), 7.36 – 7.27 (m, 1H), 6.93 – 6.85 (m, 2H), 4.38 (t, J = 7.8 Hz, 1H), 3.79 (s, 3H), 2.61 – 2.48 (m, 1H), 2.43 – 2.27 (m, 1H), 1.87 – 1.70 (m, 2H), 1.41 (s, 3H), 1.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.6, 173.6, 162.0, 158.8, 153.1, 135.3, 134.6, 133.2, 129.2, 129.0, 125.8, 124.6, 123.9, 122.8, 121.5, 114.2, 55.2, 50.4, 41.9, 38.7, 30.7, 25.7, 24.7; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{29}H_{27}N_2O_5S$ 515.1635, found 515.1635.

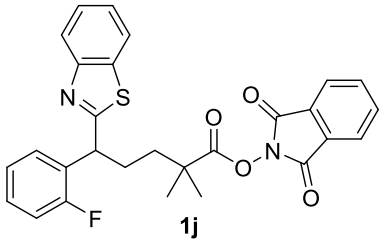
1,3-dioxoisoindolin-2-yl 5-([1,1'-biphenyl]-4-yl)-5-(benzo[*d*]thiazol-2-yl)-2,2-dimethylpentano-ate (1i)



1i

White solid, mp 57-59 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, J = 8.3 Hz, 1H), 7.90 – 7.77 (m, 3H), 7.72 – 7.58 (m, 8H), 7.52 – 7.38 (m, 3H), 7.33 (t, J = 7.5 Hz, 2H), 4.55 (t, J = 7.7 Hz, 1H), 2.82 – 2.59 (m, 1H), 2.58 – 2.43 (m, 1H), 2.01 – 1.75 (m, 2H), 1.46 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.6, 173.4, 161.8, 152.9, 140.3, 140.03, 140.00, 135.1, 134.4, 128.7, 128.5, 128.4, 127.3, 127.1, 126.8, 125.7, 124.6, 123.6, 122.7, 121.4, 50.7, 41.8, 38.5, 30.6, 25.5, 24.6; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{34}H_{29}N_2O_4S$ 561.1843, found 561.1837.

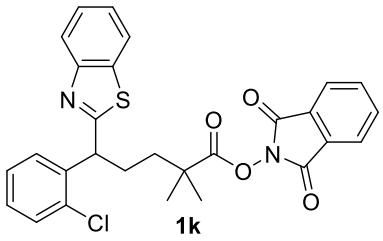
1,3-dioxoisoindolin-2-yl 5-(benzo[d]thiazol-2-yl)-5-(2-fluorophenyl)-2,2-dimethylpentanoate (1j)



1j

White solid, mp 63-64 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 – 7.98 (m, 1H), 7.92 – 7.82 (m, 2H), 7.83 – 7.72 (m, 3H), 7.64 – 7.55 (m, 1H), 7.52 – 7.40 (m, 1H), 7.37 – 7.28 (m, 1H), 7.30 – 7.21 (m, 1H), 7.20 – 7.11 (m, 1H), 7.13 – 7.03 (m, 1H), 4.82 (dd, *J* = 8.5, 7.0 Hz, 1H), 2.75 – 2.51 (m, 1H), 2.47 – 2.30 (m, 1H), 1.86 – 1.74 (m, 2H), 1.42 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.5, 162.0, 160.6 (d, *J* = 246.4 Hz), 153.1, 135.2, 134.6, 129.1 (d, *J* = 3.5 Hz), 129.0 (d, *J* = 8.2 Hz), 128.9, 128.1, 128.0, 125.8, 124.8, 124.6 (d, *J* = 3.6 Hz), 123.8, 123.0, 121.5, 115.6 (d, *J* = 22.4 Hz), 43.0 (d, *J* = 3.0 Hz), 41.9, 38.4, 29.9, 25.6, 24.8; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{28}H_{24}FN_2O_4S$ 503.1435, found 503.1432.

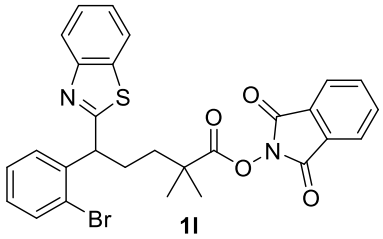
1,3-dioxoisoindolin-2-yl 5-(benzo[d]thiazol-2-yl)-5-(2-chlorophenyl)-2,2-dimethylpentanoate (1k)



1k

White solid, mp 100-102 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.03 (d, *J* = 8.2 Hz, 1H), 7.90 – 7.82 (m, 2H), 7.82 – 7.75 (m, 1H), 7.77 – 7.70 (m, 2H), 7.69 – 7.62 (m, 1H), 7.53 – 7.38 (m, 2H), 7.35 – 7.25 (m, 2H), 7.26 – 7.16 (m, 1H), 5.04 (t, *J* = 7.6 Hz, 1H), 2.70 – 2.55 (m, 1H), 2.49 – 2.33 (m, 1H), 1.89 – 1.78 (m, 2H), 1.43 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 173.4, 173.2, 161.9, 153.1, 138.6, 135.1, 134.6, 134.2, 129.7, 129.0, 128.9, 128.5, 127.4, 125.8, 124.7, 123.8, 122.9, 121.4, 46.4, 41.8, 38.2, 30.3, 25.6, 24.6; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{28}H_{24}ClN_2O_4S$ 519.1140, found 519.1141.

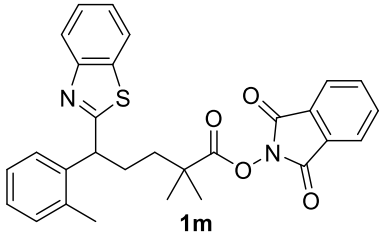
1,3-dioxoisoindolin-2-yl 5-(benzo[d]thiazol-2-yl)-5-(2-bromophenyl)-2,2-dimethylpentanoate (1l)



1l

White solid, mp 70-72 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 – 7.99 (m, 1H), 7.91 – 7.82 (m, 2H), 7.82 – 7.71 (m, 3H), 7.68 – 7.57 (m, 2H), 7.50 – 7.40 (m, 1H), 7.38 – 7.28 (m, 2H), 7.20 – 7.09 (m, 1H), 5.02 (dd, *J* = 8.3, 6.8 Hz, 1H), 2.70 – 2.54 (m, 1H), 2.50 – 2.31 (m, 1H), 1.89 – 1.77 (m, 2H), 1.42 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.5, 173.2, 162.0, 153.1, 140.3, 135.2, 134.6, 133.0, 129.2, 128.9, 128.9, 128.1, 125.8, 125.2, 124.8, 123.8, 123.0, 121.5, 49.2, 41.9, 38.2, 30.5, 25.7, 24.6; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{28}H_{24}BrN_2O_4S$ 563.0635, found 563.0627.

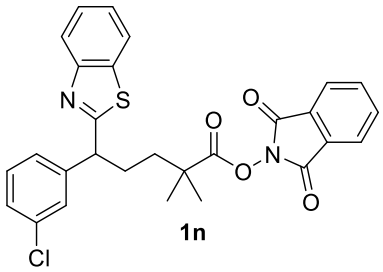
1,3-dioxoisoindolin-2-yl 5-(benzo[d]thiazol-2-yl)-2,2-dimethyl-5-(o-tolyl)pentanoate (1m)



1m

White solid, mp 48-50 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.02 (d, *J* = 8.2 Hz, 1H), 7.85 – 7.83 (m, 2H), 7.80 – 7.66 (m, 3H), 7.61 (d, *J* = 7.7 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 1H), 7.32 – 7.26 (m, 2H), 7.20 (d, *J* = 4.4 Hz, 2H), 4.72 (t, *J* = 7.6 Hz, 1H), 2.69 – 2.55 (m, 1H), 2.45 (s, 3H), 2.46 – 2.34 (m, 1H), 1.98 – 1.75 (m, 2H), 1.43 (s, 3H), 1.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 175.0, 173.4, 161.9, 152.9, 139.2, 136.5, 135.2, 134.5, 130.6, 128.8, 127.2, 126.8, 126.5, 125.6, 124.6, 123.7, 122.7, 121.4, 46.5, 41.8, 38.5, 30.4, 25.6, 24.6, 19.8; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{29}H_{27}N_2O_4S$ 499.1686, found 499.1684.

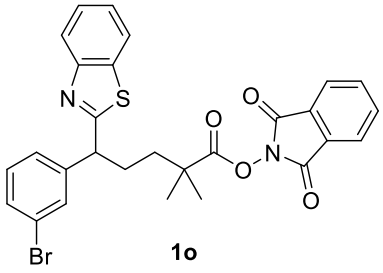
1,3-dioxoisoindolin-2-yl 5-(benzo[d]thiazol-2-yl)-5-(3-chlorophenyl)-2,2-dimethylpentanoate (1n)



1n

White solid, mp 91-93 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, J = 8.1 Hz, 1H), 7.88 – 7.86 (m, 2H), 7.84 – 7.72 (m, 3H), 7.52 – 7.37 (m, 3H), 7.36 – 7.20 (m, 3H), 4.41 (t, J = 7.8 Hz, 1H), 2.69 – 2.50 (m, 1H), 2.45 – 2.29 (m, 1H), 1.97 – 1.64 (m, 2H), 1.41 (s, 3H), 1.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.7, 173.4, 162.0, 153.0, 143.1, 135.2, 134.6, 134.5, 130.1, 128.9, 128.3, 127.6, 126.3, 125.9, 124.9, 123.8, 123.0, 121.5, 50.8, 41.9, 38.5, 30.7, 25.7, 24.6; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{28}H_{24}ClN_2O_4S$ 519.1140, found 519.1145.

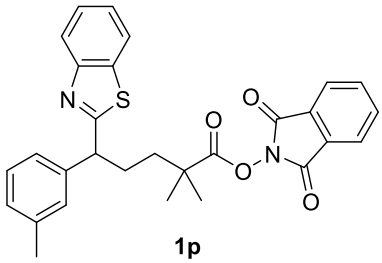
1,3-dioxoisoindolin-2-yl 5-(benzo[d]thiazol-2-yl)-5-(3-bromophenyl)-2,2-dimethylpentanoate (1o)



1o

White solid, mp 51-53 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, J = 8.1 Hz, 1H), 7.96 – 7.87 (m, 2H), 7.87 – 7.76 (m, 3H), 7.68 (t, J = 1.9 Hz, 1H), 7.51 – 7.45 (m, 2H), 7.44 – 7.33 (m, 2H), 7.29 – 7.20 (m, 1H), 4.42 (t, J = 7.8 Hz, 1H), 2.65 – 2.51 (m, 1H), 2.46 – 2.30 (m, 1H), 1.92 – 1.71 (m, 2H), 1.43 (s, 3H), 1.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.7, 173.4, 162.0, 153.0, 143.4, 135.2, 134.7, 131.2, 130.5, 130.4, 129.0, 126.8, 125.9, 124.9, 123.9, 123.0, 122.8, 121.6, 50.8, 41.9, 38.6, 30.8, 25.8, 24.6; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{28}H_{24}BrN_2O_4S$ 563.0635, found 563.0630.

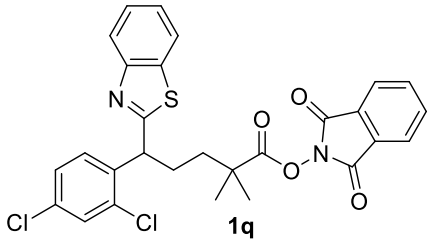
1,3-dioxoisoindolin-2-yl 5-(benzo[d]thiazol-2-yl)-2,2-dimethyl-5-(m-tolyl)pentanoate (1p)



1p

White solid, mp 51-53 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, J = 8.1 Hz, 1H), 7.86 – 7.74 (m, 3H), 7.69 – 7.67 (m, 2H), 7.48 – 7.39 (m, 1H), 7.37 – 7.32 (m, 2H), 7.30 – 7.26 (m, 2H) 7.10 (d, J = 7.4 Hz, 1H), 4.43 (t, J = 7.7 Hz, 1H), 2.70 – 2.54 (m, 1H), 2.49 – 2.37 (m, 1H), 2.36 (s, 3H), 1.92 – 1.74 (m, 2H), 1.43 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.9, 173.4, 161.8, 152.9, 140.9, 138.3, 135.1, 134.4, 128.8, 128.7, 128.6, 128.0, 125.6, 124.9, 124.5, 123.6, 122.7, 121.4, 51.1, 41.8, 38.5, 30.5, 25.4, 24.8, 21.3; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{29}H_{27}N_2O_4S$ 499.1686, found 499.1689.

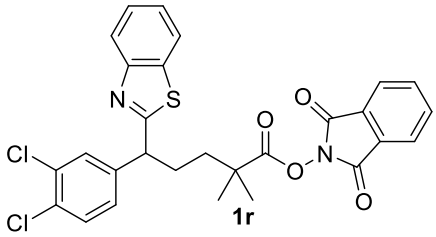
1,3-dioxoisoindolin-2-yl 5-(benzo[*d*]thiazol-2-yl)-5-(2,4-dichlorophenyl)-2,2-dimethylpentano -ate (1q)



1q

White solid, mp 118-120 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, J = 8.2 Hz, 1H), 7.91 – 7.84 (m, 2H), 7.83 – 7.73 (m, 3H), 7.62 (d, J = 8.4 Hz, 1H), 7.49 – 7.40 (m, 2H), 7.38 – 7.29 (m, 1H), 7.31 – 7.24 (m, 1H), 4.96 (t, J = 7.6 Hz, 1H), 2.68 – 2.52 (m, 1H), 2.42 – 2.29 (m, 1H), 1.89 – 1.73 (m, 2H), 1.42 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.4, 172.6, 162.0, 153.1, 137.2, 135.1, 134.9, 134.6, 133.6, 130.1, 129.4, 128.9, 127.8, 125.9, 124.9, 123.9, 123.0, 121.5, 45.9, 41.9, 38.2, 30.4, 25.9, 24.5; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{28}H_{23}Cl_2N_2O_4S$ 553.0750, found 553.0754.

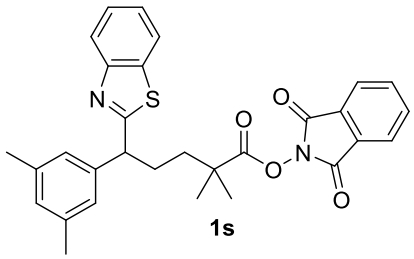
1,3-dioxoisoindolin-2-yl 5-(benzo[*d*]thiazol-2-yl)-5-(3,4-dichlorophenyl)-2,2-dimethylpentano -ate (1r)



1r

White solid, mp 49-51 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, J = 8.1 Hz, 1H), 7.93 – 7.85 (m, 2H), 7.85 – 7.74 (m, 3H), 7.60 (d, J = 1.9 Hz, 1H), 7.51 – 7.39 (m, 2H), 7.40 – 7.30 (m, 2H), 4.39 (t, J = 7.8 Hz, 1H), 2.62 – 2.47 (m, 1H), 2.43 – 2.26 (m, 1H), 1.86 – 1.68 (m, 2H), 1.41 (s, 3H), 1.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.4, 173.1, 162.0, 153.0, 141.3, 135.1, 134.7, 132.7, 131.4, 130.7, 130.1, 128.9, 127.5, 126.0, 125.0, 123.9, 123.0, 121.6, 50.2, 41.9, 38.6, 30.8, 25.8, 24.5; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{28}H_{23}Cl_2N_2O_4S$ 553.0750, found 553.0747.

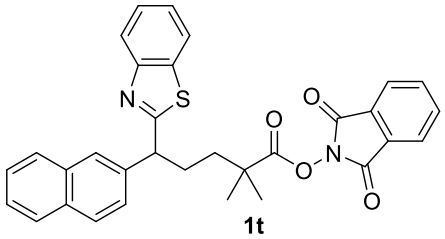
1,3-dioxoisoindolin-2-yl 5-(benzo[d]thiazol-2-yl)-5-(3,5-dimethylphenyl)-2,2-dimethylpentan -oate (1s)



1s

White solid, mp 118-120 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, J = 8.2 Hz, 1H), 7.84 – 7.73 (m, 3H), 7.70 – 7.61 (m, 2H), 7.42 (t, J = 7.8 Hz, 1H), 7.34 – 7.24 (m, 1H), 7.15 (s, 2H), 6.91 (s, 1H), 4.40 (t, J = 7.7 Hz, 1H), 2.66 – 2.53 (m, 1H), 2.49 – 2.35 (m, 1H), 2.32 (s, 6H), 1.93 – 1.75 (m, 2H), 1.43 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.0, 173.4, 161.8, 152.8, 140.8, 138.1, 135.1, 134.4, 128.9, 128.6, 125.7, 125.6, 124.5, 123.5, 122.6, 121.3, 51.0, 41.7, 38.5, 30.4, 25.4, 24.5, 21.1; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{30}H_{29}N_2O_4S$ 513.1843, found 513.1843.

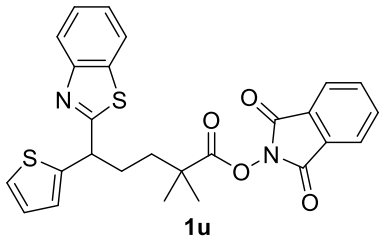
1,3-dioxoisoindolin-2-yl 5-(benzo[d]thiazol-2-yl)-2,2-dimethyl-5-(naphthalen-2-yl)pentanoate (1t)



1t

White solid, mp 57-59 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 – 8.01 (m, 1H), 8.01 – 7.96 (m, 1H), 7.91 – 7.82 (m, 4H), 7.85 – 7.74 (m, 2H), 7.77 – 7.70 (m, 2H), 7.70 – 7.60 (m, 1H), 7.55 – 7.41 (m, 3H), 7.36 – 7.27 (m, 1H), 4.63 (dd, J = 8.4, 7.0 Hz, 1H), 2.78 – 2.62 (m, 1H), 2.61 – 2.45 (m, 1H), 1.90 – 1.78 (m, 2H), 1.43 (s, 3H), 1.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.8, 173.5, 162.0, 153.0, 138.5, 135.3, 134.6, 133.5, 132.7, 128.9, 128.6, 127.9, 127.6, 126.9, 126.1, 126.0, 125.9, 125.8, 124.7, 123.8, 122.9, 121.5, 51.3, 41.9, 38.7, 30.5, 25.6, 24.7; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{32}H_{27}N_2O_4S$ 535.1686, found 535.1686.

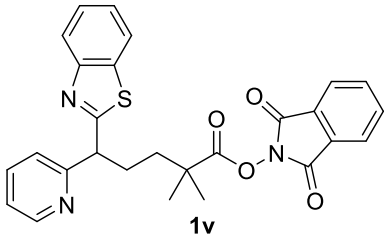
1,3-dioxoisoindolin-2-yl 5-(benzo[*d*]thiazol-2-yl)-2,2-dimethyl-5-(thiophen-2-yl)pentanoate (1u)



1u

Brown solid, mp 47-49 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 – 7.98 (m, 1H), 7.91 – 7.83 (m, 2H), 7.84 – 7.77 (m, 1H), 7.80 – 7.71 (m, 2H), 7.49 – 7.40 (m, 1H), 7.40 – 7.29 (m, 1H), 7.28 – 7.21 (m, 1H), 7.20 – 7.13 (m, 1H), 7.07 – 6.96 (m, 1H), 4.74 (t, J = 7.7 Hz, 1H), 2.63 – 2.50 (m, 1H), 2.50 – 2.35 (m, 1H), 1.98 – 1.85 (m, 1H), 1.86 – 1.71 (m, 1H), 1.42 (s, 3H), 1.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.3, 173.4, 162.0, 152.9, 144.2, 135.3, 134.6, 129.0, 127.0, 125.9, 125.5, 124.9, 124.8, 123.8, 123.0, 121.6, 46.2, 41.8, 38.5, 32.1, 25.5, 24.8; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{26}H_{23}N_2O_4S_2$ 491.1094, found 491.1101.

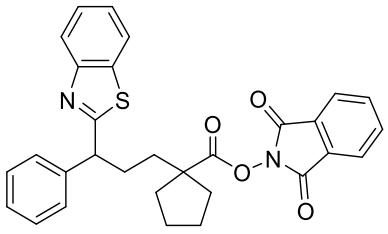
1,3-dioxoisoindolin-2-yl 5-(benzo[*d*]thiazol-2-yl)-2,2-dimethyl-5-(pyridin-2-yl)pentanoate (1v)



1v

White solid, mp 103-105 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.63 (d, J = 4.3 Hz, 1H), 8.00 (d, J = 8.2 Hz, 1H), 7.90 – 7.75 (m, 5H), 7.71 – 7.62 (m, 1H), 7.52 – 7.44 (m, 1H), 7.48 – 7.38 (m, 1H), 7.37 – 7.28 (m, 1H), 7.24 – 7.16 (m, 1H), 4.66 (t, J = 7.7 Hz, 1H), 2.64 – 2.43 (m, 2H), 1.90 – 1.70 (m, 2H), 1.40 (s, 3H), 1.38 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 173.6, 173.1, 162.0, 160.0, 152.7, 149.5, 137.0, 135.5, 134.6, 129.0, 125.8, 124.7, 123.9, 123.2, 122.9, 122.3, 121.5, 53.4, 41.9, 38.3, 30.6, 25.3, 24.7; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{27}H_{24}N_3O_4S$ 486.1482, found 486.1489.

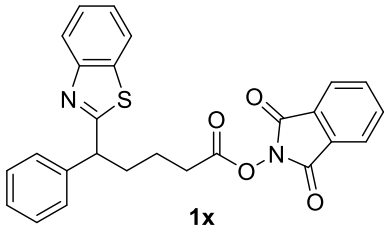
1,3-dioxoisoindolin-2-yl 1-(3-(benzo[*d*]thiazol-2-yl)-3-phenylpropyl)cyclopentane-1-carboxyl -ate (1w)



1w

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, J = 8.1 Hz, 1H), 7.93 – 7.85 (m, 2H), 7.83 – 7.74 (m, 3H), 7.55 – 7.48 (m, 2H), 7.48 – 7.39 (m, 1H), 7.40 – 7.29 (m, 3H), 7.29 – 7.24 (m, 1H), 4.46 (t, J = 7.8 Hz, 1H), 2.63 – 2.50 (m, 1H), 2.50 – 2.30 (m, 3H), 1.98 – 1.81 (m, 2H), 1.79 – 1.57 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.9, 173.5, 162.0, 152.9, 141.1, 135.2, 134.5, 128.9, 128.7, 128.1, 127.3, 125.7, 124.6, 123.7, 122.8, 121.4, 53.0, 51.2, 37.01, 36.95, 35.9, 31.6, 24.8, 24.7; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{30}H_{27}N_2O_4S$ 511.1686, found 511.1681.

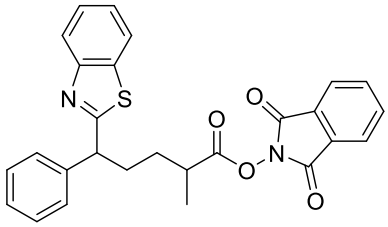
1,3-dioxoisoindolin-2-yl 5-(benzo[d]thiazol-2-yl)-5-phenylpentanoate (1x)



1x

White solid, mp 119-120 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, J = 8.0 Hz, 1H), 7.90 – 7.84 (m, 2H), 7.82 – 7.74 (m, 3H), 7.48 – 7.40 (m, 3H), 7.39 – 7.31 (m, 3H), 7.31 – 7.27 (m, 1H), 4.43 (t, J = 7.7 Hz, 1H), 2.82 – 2.67 (m, 2H), 2.64 – 2.52 (m, 1H), 2.43 – 2.30 (m, 1H), 1.93 – 1.79 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.6, 169.1, 161.8, 152.9, 141.0, 135.1, 134.7, 128.9, 128.8, 128.0, 127.5, 125.9, 124.8, 123.9, 122.9, 121.5, 50.5, 34.5, 30.7, 22.8; HRMS (CI-TOF) m/z: $[M+H]^+$ calcd for $C_{26}H_{21}N_2O_4S$ 457.1217, found 457.1210;

1,3-dioxoisoindolin-2-yl 5-(benzo[d]thiazol-2-yl)-2-methyl-5-phenylpentanoate

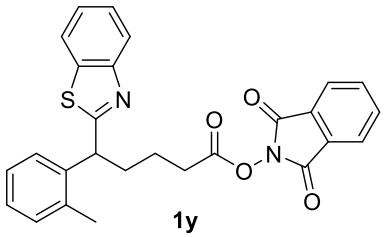


1x'

dr =1:1, Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 – 8.00 (d, J = 8.0 Hz, 1H, two isomers), 7.90 – 7.87 (m, 2H, two isomers), 7.79 – 7.78 (m, 3H, two isomers), 7.46 – 7.43 (m, 3H, two isomers), 7.37 – 7.31 (m, 3H, two isomers), 7.29 – 7.27 (m, 1H, two isomers), 4.44 (dd, J_1 = 7.5 Hz, J_2 = 14.0 Hz, 1H, two isomers), 2.94 – 2.87 (m, 1H, two isomers), 2.64 – 2.54 (m, 1H, two isomers), 2.46 – 2.33 (m, 1H, two isomers), 1.95 – 1.82 (m, 1H, two isomers), 1.75 – 1.65 (m, 1H, two isomers), 1.36 (t, J= 7.0 Hz, 3H, two isomers); ^{13}C NMR (125 MHz, $CDCl_3$) δ 175.0 & 174.8 (two isomers), 172.5 & 172.5 (overlap, two isomers), 162.1, 153.2 & 153.2 (overlap, two isomers), 141.3 & 141.2 (two isomers), 134.8, 129.1 & 129.0 (two isomers), 128.2, 127.6 & 127.6 (overlap, two isomers), 126.0, 124.9, 124.1, 123.1 & 123.1 (overlap, two isomers), 121.7 & 121.7 (overlap, two isomers), 50.1 & 50.1 (overlap, two isomers),

37.3 & 37.0 (two isomers), 33.0 & 32.6 (two isomers), 32.0 & 31.7 (two isomers), 17.4 & 17.0 (two isomers).

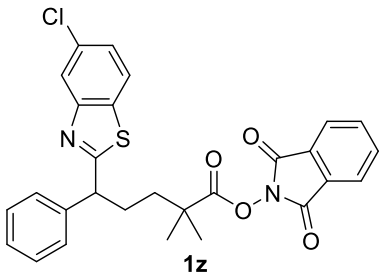
1,3-dioxoisoindolin-2-yl 5-(benzo[*d*]thiazol-2-yl)-5-(o-tolyl)pentanoate (1y)



1y

White solid, mp 91-92 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, J = 8.0 Hz, 1H), 7.90 – 7.84 (m, 2H), 7.82 – 7.73 (m, 3H), 7.49 – 7.40 (m, 2H), 7.35 – 7.29 (m, 1H), 7.25 – 7.21 (m, 1H), 7.21 – 7.17 (m, 2H), 4.70 (t, J = 7.6 Hz, 1H), 2.84 – 2.66 (m, 2H), 2.66 – 2.51 (m, 1H), 2.42 (s, 3H), 2.41 – 2.27 (m, 1H), 1.99 – 1.81 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.8, 169.2, 161.9, 153.0, 139.3, 136.4, 135.3, 134.7, 130.8, 128.9, 127.4, 127.0, 126.7, 125.8, 124.8, 123.9, 122.9, 121.5, 46.0, 34.3, 30.8, 22.9, 19.9; HRMS (CI-TOF) m/z: $[M+H]^+$ calcd for $C_{27}H_{23}N_2O_4S$ 471.1373, found 471.1383.

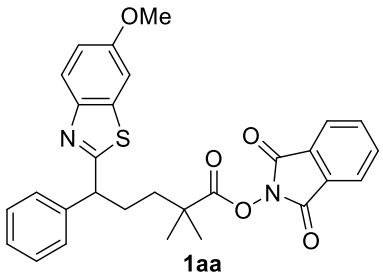
1,3-dioxoisoindolin-2-yl 5-(5-chlorobenzo[*d*]thiazol-2-yl)-2,2-dimethyl-5-phenylpentanoate (1z)



1z

White solid, mp 36-38 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, J = 2.0 Hz, 1H), 7.90 – 7.81 (m, 2H), 7.78 – 7.71 (m, 2H), 7.70 – 7.60 (m, 1H), 7.50 – 7.44 (m, 2H), 7.43 – 7.32 (m, 2H), 7.32 – 7.25 (m, 2H), 4.41 (t, J = 7.8 Hz, 1H), 2.65 – 2.51 (m, 1H), 2.46 – 2.29 (m, 1H), 1.83 – 1.73 (m, 2H), 1.40 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.0, 173.5, 162.0, 154.0, 140.8, 134.6, 133.6, 131.8, 129.0, 128.9, 128.1, 127.5, 125.2, 123.9, 122.8, 122.2, 51.3, 41.9, 38.6, 30.6, 25.5, 24.8; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{28}H_{24}ClN_2O_4S$ 519.1140, found 519.1139.

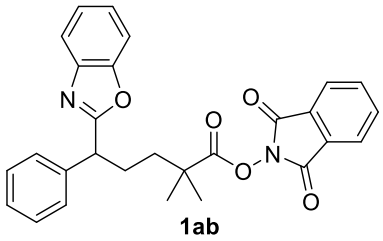
1,3-dioxoisoindolin-2-yl 5-(6-methoxybenzo[*d*]thiazol-2-yl)-2,2-dimethyl-5-phenylpentanoate (1aa)



1aa

White solid, mp 69-71 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (d, J = 8.1 Hz, 1H), 7.94 – 7.86 (m, 2H), 7.82 – 7.76 (m, 4H), 7.54 – 7.40 (m, 1H), 7.37 – 7.23 (m, 3H), 7.08 (d, J = 7.7 Hz, 1H), 4.41 (t, J = 7.8 Hz), 3.80 (s, 3H), 2.61 – 2.50 (m, 1H), 2.44 – 2.32 (m, 1H), 1.89 – 1.73 (m, 2H), 1.41 (s, 3H), 1.40 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 174.8, 173.5, 162.0, 159.8, 153.0, 142.6, 134.6, 129.8, 129.0, 125.8, 123.8, 122.9, 121.5, 120.4, 113.7, 103.8, 55.2, 51.3, 41.9, 38.6, 30.6, 25.6, 24.7; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{29}H_{27}N_2O_5S$ 515.1635, found 515.1654.

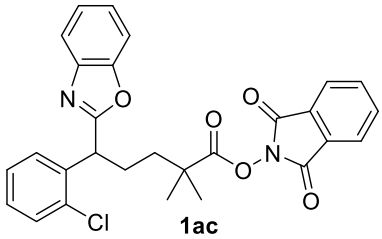
1,3-dioxoisoindolin-2-yl 5-(benzo[d]oxazol-2-yl)-2,2-dimethyl-5-phenylpentanoate (1ab)



1ab

White solid, mp 117-119 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 – 7.82 (m, 2H), 7.82 – 7.68 (m, 3H), 7.51 – 7.39 (m, 3H), 7.40 – 7.30 (m, 2H), 7.31 – 7.19 (m, 3H), 4.29 (t, J = 7.8 Hz, 1H), 2.63 – 2.46 (m, 1H), 2.42 – 2.24 (m, 1H), 1.82 – 1.74 (m, 2H), 1.41 (s, 3H), 1.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.5, 167.6, 161.9, 150.8, 141.2, 139.2, 134.6, 129.0, 128.8, 128.0, 127.4, 124.6, 124.1, 123.8, 119.9, 110.5, 46.4, 41.9, 38.3, 29.3, 25.3, 24.7; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{28}H_{25}N_2O_5$ 469.1758, found 469.1751.

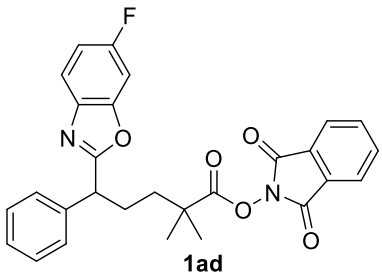
1,3-dioxoisoindolin-2-yl 5-(benzo[*d*]oxazol-2-yl)-5-(2-chlorophenyl)-2,2-dimethylpentanoate (1ac)



1ac

White solid, mp 92-94 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 – 7.83 (m, 2H), 7.81 – 7.70 (m, 3H), 7.56 – 7.39 (m, 3H), 7.34 – 7.27 (m, 2H), 7.25 – 7.16 (m, 2H), 4.91 (t, *J* = 7.6 Hz, 1H), 2.62 – 2.48 (m, 1H), 2.42 – 2.22 (m, 1H), 1.91 – 1.71 (m, 2H), 1.42 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.4, 166.8, 161.9, 150.7, 141.1, 136.9, 134.6, 134.0, 129.7, 129.02, 128.95, 128.6, 127.4, 124.7, 124.1, 123.8, 120.0, 110.6, 41.9, 41.8, 37.9, 28.9, 25.4, 24.8; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{28}H_{24}ClN_2O_5$ 503.1368, found 503.1372.

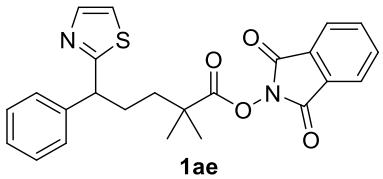
1,3-dioxoisoindolin-2-yl 5-(6-fluorobenzo[*d*]oxazol-2-yl)-2,2-dimethyl-5-phenylpentanoate (1ad)



1ad

White solid, mp 35-37 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 – 7.80 (m, 2H), 7.78 – 7.68 (m, 2H), 7.62 (dd, *J* = 8.7, 4.9 Hz, 1H), 7.49 – 7.41 (m, 2H), 7.40 – 7.30 (m, 2H), 7.31 – 7.21 (m, 1H), 7.21 – 7.12 (m, 1H), 7.11 – 6.97 (m, 1H), 4.29 – 4.22 (m, 1H), 2.58 – 2.47 (m, 1H), 2.42 – 2.25 (m, 1H), 1.80 – 1.74 (m, 2H), 1.40 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 173.4, 168.2 (d, *J* = 3.3 Hz), 161.9, 160.2 (d, *J* = 243.3 Hz), 150.6 (d, *J* = 14.7 Hz), 138.9, 137.3 (d, *J* = 1.6 Hz), 134.6, 128.8, 128.8, 127.9, 127.4, 123.7, 120.0 (d, *J* = 10.2 Hz), 111.9 (d, *J* = 24.5 Hz), 98.5 (d, *J* = 28.2 Hz), 46.3, 41.8, 38.2, 29.1, 25.1, 24.7; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{28}H_{24}FN_2O_5$ 487.1664, found 487.1652.

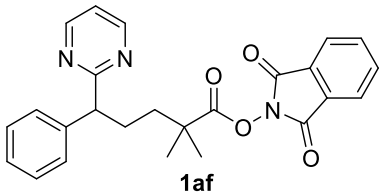
1,3-dioxoisoindolin-2-yl 2,2-dimethyl-5-phenyl-5-(thiazol-2-yl)pentanoate (1ae)



1ae

White solid, mp 109-112 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 – 7.84 (m, 2H), 7.83 – 7.74 (m, 2H), 7.71 (d, J = 3.3 Hz, 1H), 7.46 – 7.39 (m, 2H), 7.38 – 7.30 (m, 2H), 7.29 – 7.23 (m, 1H), 7.19 (d, J = 3.3 Hz, 1H), 4.37 – 4.30 (m, 1H), 2.58 – 2.41 (m, 1H), 2.40 – 2.23 (m, 1H), 1.81 – 1.65 (m, 2H), 1.38 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.3, 173.5, 162.0, 142.2, 141.8, 134.6, 129.0, 128.8, 128.0, 127.2, 123.9, 118.6, 50.3, 41.9, 38.6, 31.1, 25.5, 24.8; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{24}H_{23}N_2O_4S$ 435.1373, found 435.1388.

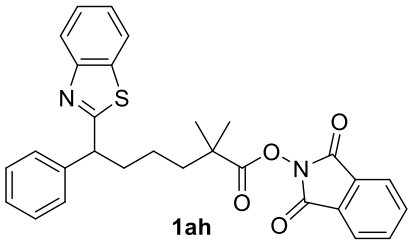
1,3-dioxoisoindolin-2-yl 2,2-dimethyl-5-phenyl-5-(pyrimidin-2-yl)pentanoate (1af)



1af

White solid, mp 97-99 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.67 (d, J = 4.9 Hz, 2H), 7.84 (dd, J = 5.4, 3.1 Hz, 2H), 7.74 (dd, J = 5.4, 3.1 Hz, 2H), 7.51 – 7.43 (m, 2H), 7.34 – 7.24 (m, 2H), 7.24 – 7.14 (m, 1H), 7.12 – 7.03 (m, 1H), 4.24 (t, J = 7.7 Hz, 1H), 2.53 – 2.39 (m, 1H), 2.39 – 2.24 (m, 1H), 1.79 – 1.58 (m, 2H), 1.38 (s, 3H), 1.37 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 173.7, 172.0, 161.9, 157.1, 142.1, 134.5, 128.9, 128.4, 128.1, 126.6, 123.7, 118.6, 55.3, 41.9, 38.5, 29.6, 25.1, 24.8; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{25}H_{24}N_3O_4$ 430.1761, found 430.1778.

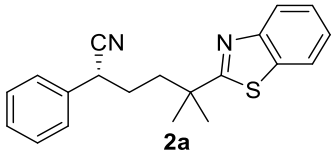
1,3-dioxoisoindolin-2-yl 6-(benzo[*d*]thiazol-2-yl)-2,2-dimethyl-6-phenylhexanoate



1ah

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, J = 8.1 Hz, 1H), 7.85 – 7.81 (m, 2H), 7.78 – 7.75 (m, 1H), 7.75 – 7.72 (m, 2H), 7.46 – 7.40 (m, 3H), 7.38 – 7.29 (m, 3H), 7.30 – 7.23 (m, 1H), 4.47 (t, J = 7.7 Hz, 1H), 2.57 – 2.43 (m, 1H), 2.36 – 2.19 (m, 1H), 1.88 – 1.77 (m, 2H), 1.64 – 1.46 (m, 2H), 1.33 (s, 3H), 1.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.1, 173.7, 161.9, 153.1, 141.5, 135.2, 134.5, 128.9, 128.7, 128.0, 127.2, 125.7, 124.6, 123.7, 122.8, 121.4, 50.5, 42.0, 40.1, 35.8, 25.0, 24.9, 22.8; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{29}H_{27}N_2O_4S$ 499.1686, found 499.1691.

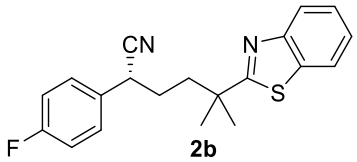
(*R*)-5-(benzo[*d*]thiazol-2-yl)-5-methyl-2-phenylhexanenitrile (2a)



2a

White solid (52.9 mg, 83%), mp 39-40 ℃; 92.5:7.5 er, HPLC condition: Daicel Chiralpak OJ-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, retention time = 9.2 min (major) and 10.4 min (minor); $[\alpha]_D^{23}$ = -7.2 (*c* 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, J = 8.0 Hz, 1H), 7.85 (d, J = 8.0 Hz, 1H), 7.50 – 7.42 (m, 1H), 7.39 – 7.30 (m, 4H), 7.30 – 7.23 (m, 2H), 3.75 (dd, J = 7.9, 6.1 Hz, 1H), 2.10 – 1.94 (m, 2H), 1.95 – 1.81 (m, 2H), 1.51 (s, 3H), 1.50 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.5, 153.0, 135.4, 134.9, 129.0, 128.0, 127.2, 125.8, 124.7, 122.8, 121.5, 120.6, 41.0, 40.8, 37.5, 31.1, 28.9, 28.3; HRMS (CI-TOF) m/z: $[M+H]^+$ calcd for $C_{20}H_{21}N_2S$ 321.1420, found 321.1427.

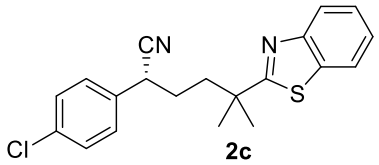
(*R*)-5-(benzo[*d*]thiazol-2-yl)-2-(4-fluorophenyl)-5-methylhexanenitrile (2b)



2b

Colorless oil (51.5 mg, 76%); 90:10 er, HPLC condition: Daicel Chiralpak OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 95:5, 0.7 mL/min, 254 nm UV detector, retention time = 11.9 min (minor) and 12.5 min (major); $[\alpha]_D^{23}$ = -12.6 (*c* 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.2 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.52 – 7.41 (m, 1H), 7.40 – 7.31 (m, 1H), 7.27 – 7.19 (m, 2H), 7.06 – 6.96 (m, 2H), 3.73 (t, *J* = 7.0 Hz, 1H), 2.05 – 1.93 (m, 2H), 1.92 – 1.81 (m, 2H), 1.51 (s, 3H), 1.50 (s, 3H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -133.6; ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.4, 162.3 (d, *J* = 247.3 Hz), 153.0, 134.9, 131.2 (d, *J* = 3.3 Hz), 128.9 (d, *J* = 8.3 Hz), 125.9, 124.8, 122.7, 121.5, 120.4, 116.0 (d, *J* = 21.8 Hz), 41.0, 40.6, 36.7, 31.1, 28.9, 28.3; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{20}H_{20}FN_2S$ 339.1326, found 339.1333.

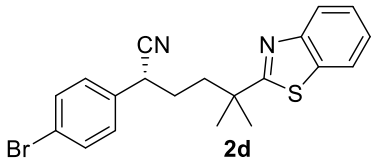
(*R*)-5-(benzo[*d*]thiazol-2-yl)-2-(4-chlorophenyl)-5-methylhexanenitrile (2c)



2c

White solid (60.2 mg, 85%), mp 76-78 ℃; 92.5:7.5 er, HPLC condition: Daicel Chiralpak OJ-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 85:15, 1.0 mL/min, 254 nm UV detector, retention time = 12.8 min (major) and 15.0 min (minor); $[\alpha]_D^{23}$ = -10.2 (*c* 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.1 Hz, 1H), 7.85 (d, *J* = 7.9 Hz, 1H), 7.51 – 7.41 (m, 1H), 7.40 – 7.31 (m, 1H), 7.33 – 7.26 (m, 2H), 7.22 – 7.15 (m, 2H), 3.72 (t, *J* = 6.9 Hz, 1H), 2.04 – 1.93 (m, 2H), 1.94 – 1.79 (m, 2H), 1.50 (s, 3H), 1.49 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.4, 153.0, 134.9, 134.1, 133.8, 129.2, 128.6, 125.9, 124.8, 122.8, 121.5, 120.1, 41.0, 40.6, 36.9, 31.0, 28.9, 28.3; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{20}H_{20}ClN_2S$ 355.1030, found 355.1033.

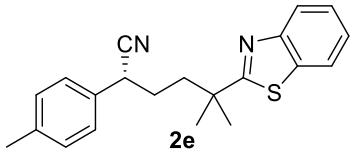
(*R*)-5-(benzo[*d*]thiazol-2-yl)-2-(4-bromophenyl)-5-methylhexanenitrile (2d)



2d

White solid (70.8 mg, 89%), mp 64-65 ℃; 92.5:7.5 er, HPLC condition: Daicel Chiralpak OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 95:5, 0.4 mL/min, 254 nm UV detector, retention time = 27.3 min (minor) and 28.3 min (major); $[\alpha]_D^{23}$ = -15.3 (*c* 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.3 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.51 – 7.41 (m, 3H), 7.41 – 7.31 (m, 1H), 7.17 – 7.08 (m, 2H), 3.70 (t, *J* = 6.8 Hz, 1H), 2.05 – 1.90 (m, 2H), 1.93 – 1.78 (m, 2H), 1.49 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.2, 153.0, 134.9, 134.4, 132.2, 128.9, 125.9, 124.8, 122.8, 122.1, 121.5, 120.1, 41.0, 40.6, 36.9, 30.9, 28.9, 28.3; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{20}H_{20}BrN_2S$ 399.0525, found 399.0536.

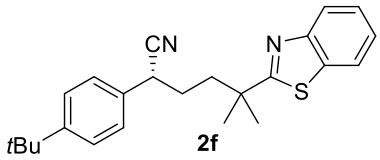
(*R*)-5-(benzo[*d*]thiazol-2-yl)-5-methyl-2-(p-tolyl)hexanenitrile (2e)



2e

Colorless oil (51.4 mg, 77%); 90.5:9.5 er, HPLC condition: Daicel Chiralpak OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 98:2, 0.6 mL/min, 254 nm UV detector, retention time = 18.8 min (major) and 20.0 min (minor); $[\alpha]_D^{23}$ = -6.4 (*c* 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.1 Hz, 1H), 7.85 (d, *J* = 7.9 Hz, 1H), 7.53 – 7.41 (m, 1H), 7.40 – 7.31 (m, 1H), 7.17 – 7.11 (m, 4H), 3.70 (dd, *J* = 7.8, 6.1 Hz, 1H), 2.33 (s, 3H), 2.07 – 1.94 (m, 2H), 1.93 – 1.80 (m, 2H), 1.50 (s, 3H), 1.49 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.6, 153.1, 137.9, 134.9, 132.4, 129.7, 127.1, 125.8, 124.7, 122.8, 121.5, 120.8, 41.1, 40.9, 37.1, 31.1, 28.9, 28.3, 21.0; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{21}H_{23}N_2S$ 335.1576, found 335.1580.

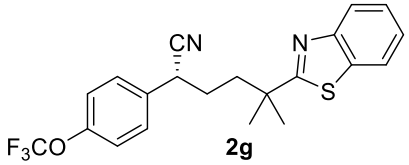
(*R*)-5-(benzo[*d*]thiazol-2-yl)-2-(4-(tert-butyl)phenyl)-5-methylhexanenitrile (2f)



2f

White solid (48.4 mg, 64%), mp 94-96 ℃; 89:11 er, HPLC condition: Daicel Chiralpak OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 95:5, 0.7 mL/min, 254 nm UV detector, retention time = 9.5 min (minor) and 10.7 min (major); $[\alpha]_D^{23}$ = -8.8 (*c* 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.1 Hz, 1H), 7.85 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.52 – 7.41 (m, 1H), 7.40 – 7.29 (m, 3H), 7.29 – 7.11 (m, 2H), 3.71 (dd, *J* = 8.3, 6.2 Hz, 1H), 2.12 – 1.96 (m, 2H), 1.94 – 1.81 (m, 2H), 1.51 (s, 3H), 1.51 (s, 3H), 1.30 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.6, 153.0, 151.1, 134.9, 132.4, 126.8, 125.9, 125.8, 124.7, 122.7, 121.5, 120.8, 41.1, 41.0, 37.1, 34.5, 31.2, 31.1, 29.0, 28.2; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{24}H_{29}N_2S$ 377.2046, found 377.2046.

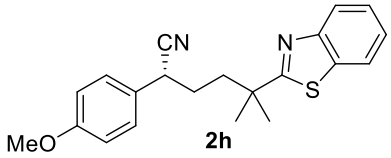
(*R*)-5-(benzo[*d*]thiazol-2-yl)-5-methyl-2-(4-(trifluoromethoxy)phenyl)hexanenitrile (2g)



2g

Colorless oil (62.8 mg, 78%); 91.5:8.5 er, HPLC condition: Daicel Chiralpak OJ-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, retention time = 14.9 min (major) and 17.2 min (minor); $[\alpha]_D^{23}$ = -8.5 (*c* 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.1 Hz, 1H), 7.85 (d, *J* = 7.8 Hz, 1H), 7.51 – 7.41 (m, 1H), 7.41 – 7.31 (m, 1H), 7.33 – 7.25 (m, 2H), 7.22 – 7.15 (m, 2H), 3.76 (dd, *J* = 7.7, 6.2 Hz, 1H), 2.05 – 1.97 (m, 2H), 1.95 – 1.85 (m, 2H), 1.51 (s, 3H), 1.50 (s, 3H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.8; ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.3, 153.0, 148.9, 134.9, 134.1, 128.7, 125.9, 124.8, 122.8, 121.51, 121.49, 120.4 (q, *J* = 256.2 Hz), 120.1, 41.0, 40.6, 36.9, 31.1, 28.9, 28.3; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{21}H_{20}F_3N_2OS$ 405.1243, found 405.1240.

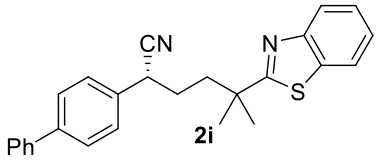
(*R*)-5-(benzo[*d*]thiazol-2-yl)-2-(4-methoxyphenyl)-5-methylhexanenitrile (2h)



2h

White solid (50.6 mg, 72%), mp 83-85 ℃; 85:15 er, HPLC condition: Daicel Chiralpak OJ-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 85:15, 1.0 mL/min, 254 nm UV detector, retention time = 18.8 min (major) and 21.4 min (minor); $[\alpha]_D^{23}$ = -4.2 (*c* 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.1 Hz, 1H), 7.85 (d, *J* = 7.9 Hz, 1H), 7.50 – 7.41 (m, 1H), 7.41 – 7.31 (m, 1H), 7.21 – 7.10 (m, 2H), 6.94 – 6.77 (m, 2H), 3.79 (s, 3H), 3.68 (dd, *J* = 7.8, 6.3 Hz, 1H), 2.03 – 1.92 (m, 2H), 1.91 – 1.80 (m, 2H), 1.50 (s, 3H), 1.49 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.6, 159.3, 153.0, 134.9, 128.3, 127.4, 125.8, 124.7, 122.8, 121.5, 120.9, 114.3, 55.3, 41.1, 40.8, 36.7, 31.1, 28.9, 28.3; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{21}H_{23}N_2OS$ 351.1526, found 351.1522.

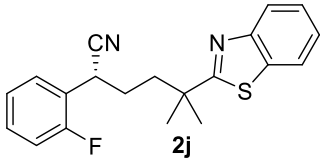
(*R*)-2-([1,1'-biphenyl]-4-yl)-5-(benzo[*d*]thiazol-2-yl)-5-methylhexanenitrile (2i)



2i

White solid (56.1 mg, 71%), mp 122-124 ℃; 92.5:7.5 er, HPLC condition: Daicel Chiralpak OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 90:10, 0.7 mL/min, 254 nm UV detector, retention time = 12.1 min (major) and 16.3 min (minor); $[\alpha]_D^{23}$ = -5.7 (*c* 0.80, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.2 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.60 – 7.53 (m, 4H), 7.51 – 7.40 (m, 3H), 7.41 – 7.30 (m, 4H), 3.79 (t, *J* = 7.0 Hz, 1H), 2.14 – 1.99 (m, 2H), 1.98 – 1.88 (m, 2H), 1.52 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.5, 153.0, 141.0, 140.2, 134.9, 134.3, 128.8, 127.7, 127.63, 127.55, 127.0, 125.9, 124.7, 122.8, 121.5, 120.5, 41.1, 40.8, 37.2, 31.1, 28.9, 28.3; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{26}H_{25}N_2S$ 397.1733, found 397.1729.

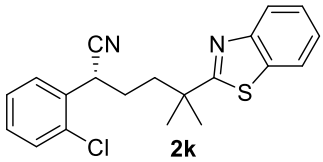
(*R*)-5-(benzo[*d*]thiazol-2-yl)-2-(2-fluorophenyl)-5-methylhexanenitrile (2j)



2j

Colorless oil (59.2 mg, 88%); 95.5:4.5 er, HPLC condition: Daicel Chiralpak OJ-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, retention time = 8.1 min (major) and 10.7 min (minor); $[\alpha]_D^{23}$ = -8.4 (*c* 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (dd, *J* = 8.1, 1.0 Hz, 1H), 7.85 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.50 – 7.25 (m, 4H), 7.20 – 7.10 (m, 1H), 7.09 – 6.99 (m, 1H), 4.06 (dd, *J* = 7.9, 6.2 Hz, 1H), 2.12 – 1.96 (m, 2H), 1.97 – 1.82 (m, 2H), 1.50 (s, 6H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -118.2; ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.4, 159.65 (d, *J* = 247.8 Hz), 153.0, 134.9, 130.0 (d, *J* = 8.3 Hz), 128.9 (d, *J* = 3.1 Hz), 125.8, 124.74, 124.71, 122.8, 122.6, 121.5, 119.8, 115.8 (d, *J* = 21.4 Hz), 41.0, 40.8, 31.2 (d, *J* = 3.3 Hz), 29.6, 28.8, 28.4; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{20}H_{20}FN_2S$ 339.1326, found 339.1338.

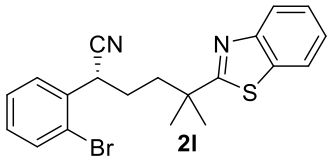
(*R*)-5-(benzo[*d*]thiazol-2-yl)-2-(2-chlorophenyl)-5-methylhexanenitrile (2k)



2k

Colorless oil (59.8 mg, 84%); 97.5:2.5 er, HPLC condition: Daicel Chiralpak OJ-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, retention time = 6.9 min (major) and 8.0 min (minor); $[\alpha]_D^{23}$ = -10.4 (*c* 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.1 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.53 – 7.46 (m, 1H), 7.49 – 7.40 (m, 1H), 7.39 – 7.31 (m, 2H), 7.35 – 7.20 (m, 2H), 4.23 (dd, *J* = 8.7, 5.7 Hz, 1H), 2.18 – 1.98 (m, 2H), 1.97 – 1.80 (m, 2H), 1.51 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.4, 153.0, 134.9, 133.3, 132.6, 129.9, 129.5, 128.8, 127.5, 125.8, 124.7, 122.7, 121.5, 120.0, 41.1, 40.9, 34.9, 29.5, 28.9, 28.2; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{20}H_{20}ClN_2S$ 355.1030, found 355.1023.

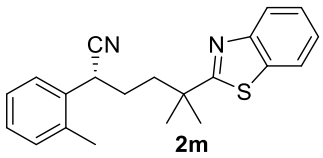
(*R*)-5-(benzo[*d*]thiazol-2-yl)-2-(2-bromophenyl)-5-methylhexanenitrile (2l)



2l

Colorless oil (53.7 mg, 67%); 97.5:2.5 er, HPLC condition: Daicel Chiralpak OJ-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, retention time = 7.7 min (major) and 9.0 min (minor); $[\alpha]_D^{23}$ = -25.2 (*c* 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 – 7.92 (m, 1H), 7.90 – 7.79 (m, 1H), 7.56 – 7.48 (m, 2H), 7.49 – 7.40 (m, 1H), 7.39 – 7.28 (m, 2H), 7.23 – 7.10 (m, 1H), 4.22 (dd, *J* = 9.2, 5.3 Hz, 1H), 2.18 – 1.99 (m, 2H), 1.98 – 1.77 (m, 2H), 1.51 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.4, 153.0, 135.0, 134.9, 133.3, 129.7, 128.8, 128.2, 125.8, 124.7, 122.9, 122.8, 121.5, 120.1, 41.1, 40.9, 37.5, 29.8, 28.9, 28.2; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{20}H_{20}BrN_2S$ 399.0525, found 399.0533.

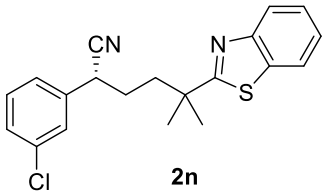
(*R*)-5-(benzo[*d*]thiazol-2-yl)-5-methyl-2-(o-tolyl)hexanenitrile (2m)



2m

Colorless oil (46.9 mg, 70%); 95:5 er, HPLC condition: Daicel Chiralpak OJ-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 95:5, 1.0 mL/min, 254 nm UV detector, retention time = 12.6 min (major) and 14.4 min (minor); $[\alpha]_D^{23}$ = -3.4 (*c* 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.1 Hz, 1H), 7.90 – 7.77 (m, 1H), 7.50 – 7.41 (m, 1H), 7.42 – 7.31 (m, 2H), 7.25 – 7.15 (m, 2H), 7.16 – 7.09 (m, 1H), 3.90 (dd, *J* = 9.2, 5.6 Hz, 1H), 2.24 (s, 3H), 2.15 – 2.00 (m, 2H), 1.91 – 1.73 (m, 2H), 1.52 (s, 3H), 1.51 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.6, 153.0, 134.9, 134.8, 133.9, 130.9, 128.0, 127.2, 126.8, 125.8, 124.7, 122.7, 121.5, 120.9, 41.2, 41.1, 34.6, 29.9, 29.5, 27.9, 19.0; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{21}H_{23}N_2S$ 335.1576, found 335.1579.

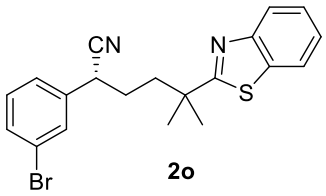
(*R*)-5-(benzo[*d*]thiazol-2-yl)-2-(3-chlorophenyl)-5-methylhexanenitrile (2n)



2n

Colorless oil (57.9 mg, 82%); 93:7 er, HPLC condition: Daicel Chiralpak IC column (25 cm × 0.46 cm ID), hexane/2-propanol = 98:2, 1.0 mL/min, 254 nm UV detector, retention time = 13.3 min (minor) and 14.7 min (major); $[\alpha]_D^{23}$ = -6.5 (*c* 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.1 Hz, 1H), 7.86 (d, *J* = 7.9 Hz, 1H), 7.49 – 7.43 (m, 1H), 7.41 – 7.34 (m, 1H), 7.31 – 7.23 (m, 3H), 7.20 – 7.11 (m, 1H), 3.72 (dd, *J* = 7.7, 6.1 Hz, 1H), 2.11 – 1.93 (m, 2H), 1.90 – 1.78 (m, 2H), 1.51 (s, 3H), 1.50 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.3, 153.0, 137.3, 134.9, 134.9, 130.3, 128.4, 127.4, 125.9, 125.5, 124.8, 122.8, 121.5, 120.0, 41.1, 40.7, 37.2, 30.9, 29.0, 28.4; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{20}H_{20}ClN_2S$ 355.1030, found 355.1027.

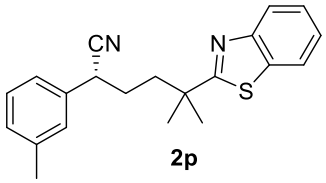
(*R*)-5-(benzo[*d*]thiazol-2-yl)-2-(3-bromophenyl)-5-methylhexanenitrile (2o)



2o

Colorless oil (56.1 mg, 70%); 92.5:7.5 er, HPLC condition: Daicel Chiralpak OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 95:5, 1.0 mL/min, 254 nm UV detector, retention time = 25.6 min (major) and 34.7 min (minor); $[\alpha]_D^{23}$ = -1.8 (*c* 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 – 7.94 (m, 1H), 7.87 – 7.80 (m, 1H), 7.48 – 7.41 (m, 3H), 7.40 – 7.31 (m, 1H), 7.24 – 7.17 (m, 2H), 3.71 (dd, *J* = 7.9, 6.2 Hz, 1H), 2.09 – 1.95 (m, 2H), 1.94 – 1.82 (m, 2H), 1.51 (s, 3H), 1.50 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.3, 153.0, 137.5, 134.8, 131.3, 130.5, 130.3, 125.89, 125.87, 124.8, 123.0, 122.8, 121.5, 119.9, 41.0, 40.6, 371, 30.9, 28.9, 28.4; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{20}H_{20}BrN_2S$ 399.0525, found 399.0519.

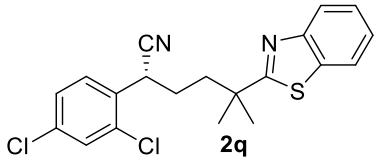
(*R*)-5-(benzo[*d*]thiazol-2-yl)-5-methyl-2-(m-tolyl)hexanenitrile (2p)



2p

Colorless oil (47.0 mg, 70%); 91.5:8.5 er, HPLC condition: Daicel Chiralpak OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 95:5, 0.7 mL/min, 254 nm UV detector, retention time = 11.5 min (major) and 12.6 min (minor); $[\alpha]_D^{23}$ = -8.1 (*c* 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.2 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.55 – 7.41 (m, 1H), 7.40 – 7.30 (m, 1H), 7.29 – 7.16 (m, 1H), 7.15 – 7.00 (m, 3H), 3.69 (t, *J* = 7.1 Hz, 1H), 2.32 (s, 3H), 2.07 – 1.95 (m, 2H), 1.94 – 1.80 (m, 2H), 1.50 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.6, 153.0, 138.9, 135.3, 134.9, 128.9, 128.8, 127.8, 125.8, 124.7, 124.3, 122.8, 121.5, 120.7, 41.1, 40.9, 37.5, 31.1, 28.9, 28.3, 21.3; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{21}H_{23}N_2S$ 335.1576, found 335.1572.

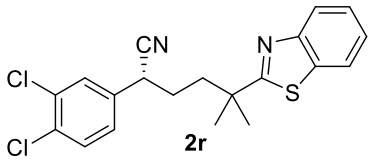
(*R*)-5-(benzo[*d*]thiazol-2-yl)-2-(2,4-dichlorophenyl)-5-methylhexanenitrile (2q)



2q

Colorless oil (47.4 mg, 61%); 95.5:4.5 er, HPLC condition: Daicel Chiralpak OJ-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, retention time = 6.9 min (major) and 10.4 min (minor); $[\alpha]_D^{23}$ = +16.8 (*c* 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.1 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.50 – 7.39 (m, 2H), 7.40 – 7.31 (m, 2H), 7.30 – 7.22 (m, 1H), 4.17 (dd, *J* = 8.3, 5.9 Hz, 1H), 2.13 – 1.95 (m, 2H), 1.93 – 1.78 (m, 2H), 1.50 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.2, 153.0, 134.9, 134.8, 133.4, 131.9, 129.8, 129.6, 127.9, 125.9, 124.8, 122.8, 121.5, 119.6, 41.1, 40.6, 34.5, 29.4, 28.9, 28.2; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{20}H_{19}Cl_2N_2S$ 389.0641, found 389.0645.

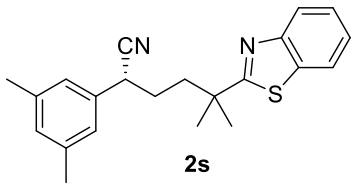
(*R*)-5-(benzo[*d*]thiazol-2-yl)-2-(3,4-dichlorophenyl)-5-methylhexanenitrile (2r)



2r

Colorless oil (61.4 mg, 79%); 92:8 er, HPLC condition: Daicel Chiralpak OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 90:10, 0.7 mL/min, 254 nm UV detector, retention time = 17.0 min (major) and 19.4 min (minor); $[\alpha]_D^{23}$ = -4.2 (*c* 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.1 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.51 – 7.41 (m, 1H), 7.43 – 7.32 (m, 3H), 7.14 – 7.06 (m, 1H), 3.71 (t, *J* = 6.9 Hz, 1H), 2.02 – 1.94 (m, 2H), 1.93 – 1.82 (m, 2H), 1.51 (s, 3H), 1.50 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.2, 153.0, 135.4, 134.8, 133.2, 132.5, 131.0, 129.2, 126.6, 125.9, 124.8, 122.8, 121.5, 119.6, 41.0, 40.4, 36.6, 30.8, 28.9, 28.4; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{20}H_{19}Cl_2N_2S$ 389.0641, found 389.0639.

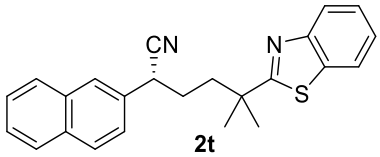
(*R*)-5-(benzo[*d*]thiazol-2-yl)-2-(3,5-dimethylphenyl)-5-methylhexanenitrile (2s)



2s

Colorless oil (46.8 mg, 67%); 90:10 er, HPLC condition: Daicel Chiralpak OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 95:5, 0.7 mL/min, 254 nm UV detector, retention time = 10.8 min (minor) and 12.4 min (major); $[\alpha]_D^{23}$ = -5.4 (*c* 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.1 Hz, 1H), 7.86 (d, *J* = 7.9 Hz, 1H), 7.52 – 7.42 (m, 1H), 7.42 – 7.31 (m, 1H), 6.92 (s, 1H), 6.87 (s, 2H), 3.65 (dd, *J* = 8.1, 6.1 Hz, 1H), 2.28 (s, 6H), 2.10 – 1.97 (m, 2H), 1.94 – 1.83 (m, 2H), 1.52 (s, 3H), 1.51 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.6, 153.0, 138.7, 135.2, 134.9, 129.6, 125.8, 124.9, 124.7, 122.7, 121.5, 120.8, 41.1, 40.9, 37.4, 31.1, 28.9, 28.3, 21.2; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{22}H_{25}N_2S$ 349.1733, found 349.1728.

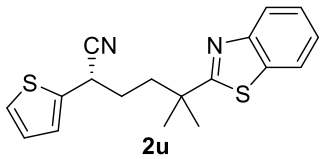
(*R*)-5-(benzo[*d*]thiazol-2-yl)-5-methyl-2-(naphthalen-2-yl)hexanenitrile (2t)



2t

Colorless oil (38.6 mg, 52%); 92:8 er, HPLC condition: Daicel Chiralpak OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, retention time = 10.9 min (major) and 12.5 min (minor); $[\alpha]_D^{23}$ = -14.6 (*c* 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.94 (m, 1H), 7.85 – 7.78 (m, 4H), 7.79 – 7.73 (m, 1H), 7.53 – 7.49 (m, 2H), 7.50 – 7.41 (m, 1H), 7.38 – 7.30 (m, 2H), 3.96 – 3.87 (m, 1H), 2.10 – 1.92 (m, 4H), 1.50 (s, 3H), 1.49 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.5, 153.1, 134.9, 133.2, 132.8, 132.6, 129.0, 127.8, 127.7, 126.7, 126.5, 126.3, 125.8, 124.7, 124.7, 122.8, 121.5, 120.6, 41.1, 40.8, 37.6, 30.9, 28.9, 28.4; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{24}H_{23}N_2S$ 371.1576, found 371.1588.

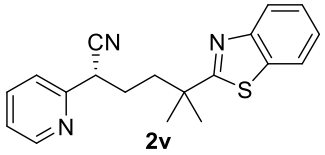
(*S*)-5-(benzo[*d*]thiazol-2-yl)-5-methyl-2-(thiophen-2-yl)hexanenitrile (2u)



2u

Colorless oil (46.4 mg, 71%); 96.5:3.5 er, HPLC condition: Daicel Chiralpak OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, retention time = 7.1 min (major) and 7.9 min (minor); $[\alpha]_D^{23}$ = -6.7 (*c* 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 7.9 Hz, 1H), 7.89 (d, *J* = 7.8 Hz, 1H), 7.54 – 7.44 (m, 1H), 7.44 – 7.34 (m, 1H), 7.27 (dd, *J* = 7.4, 4.9 Hz, 1H), 7.08 – 7.02 (m, 1H), 7.04 – 6.94 (m, 1H), 4.06 (t, *J* = 6.1 Hz, 1H), 2.12 – 1.94 (m, 4H), 1.55 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.4, 153.0, 137.4, 134.9, 127.0, 126.2, 125.8, 125.5, 124.7, 122.8, 121.5, 119.6, 41.0, 40.5, 32.6, 31.2, 28.8, 28.4; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{18}H_{19}N_2S_2$ 327.0984, found 327.0986.

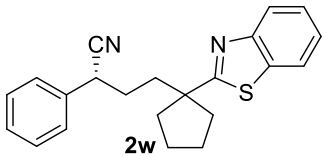
(*R*)-5-(benzo[*d*]thiazol-2-yl)-5-methyl-2-(pyridin-2-yl)hexanenitrile (2v)



2v

Colorless oil (41.5 mg, 65%); 81.5:18.5 er, HPLC condition: Daicel Chiralpak OJ-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, retention time = 11.4 min (major) and 12.7 min (minor); $[\alpha]_D^{23}$ = -11.3 (*c* 1.0, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.57 – 8.49 (m, 1H), 8.00 – 7.91 (m, 1H), 7.88 – 7.79 (m, 1H), 7.68 (td, *J* = 7.7, 1.8 Hz, 1H), 7.49 – 7.39 (m, 1H), 7.40 – 7.29 (m, 2H), 7.27 – 7.17 (m, 1H), 3.95 – 3.91 (m, 1H), 2.11 – 1.93 (m, 4H), 1.50 (s, 3H), 1.50 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 179.6, 154.8, 153.0, 149.8, 137.3, 134.9, 125.8, 124.7, 123.0, 122.7, 121.7, 121.5, 119.8, 41.1, 40.8, 39.9, 29.5, 28.7, 28.4; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{19}H_{20}N_3S$ 322.1372, found 322.1359.

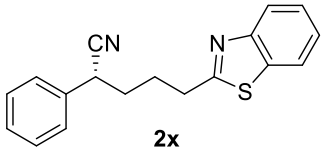
(*R*)-4-(1-(benzo[*d*]thiazol-2-yl)cyclopentyl)-2-phenylbutanenitrile (2w)



2w

White solid (32.4 mg, 47%), mp 61-63 ℃; 90.5:9.5 er, HPLC condition: Daicel Chiralpak OJ-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, retention time = 11.0 min (minor) and 12.5 min (major); $[\alpha]_D^{23}$ = -4.6 (c = 0.6, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.1 Hz, 1H), 7.84 (d, *J* = 7.9 Hz, 1H), 7.52 – 7.41 (m, 1H), 7.39 – 7.27 (m, 4H), 7.27 – 7.20 (m, 2H), 3.72 (dd, *J* = 8.1, 6.3 Hz, 1H), 2.47 – 2.22 (m, 2H), 2.13 – 1.95 (m, 2H), 1.90 – 1.77 (m, 4H), 1.78 – 1.69 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.1, 153.0, 135.4, 135.1, 129.0, 128.0, 127.2, 125.8, 124.7, 122.7, 121.5, 120.6, 53.1, 39.5, 39.2, 39.0, 37.4, 31.9, 24.2; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{22}H_{23}N_2S$ 347.1576, found 347.1573.

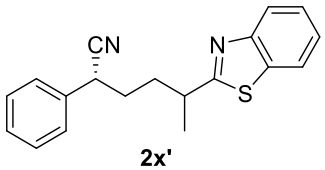
(*R*)-5-(benzo[*d*]thiazol-2-yl)-2-phenylpentanenitrile (2x)



2x

Colorless oil (33.8 mg, 58%); 93:7 er, HPLC condition: Daicel Chiralpak OJ-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, retention time = 12.4 min (major) and 14.5 min (minor); $[\alpha]_D^{23}$ = -7.1 (*c* 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.0 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.51 – 7.45 (m, 1H), 7.39 – 7.30 (m, 6H), 3.87 (t, *J* = 6.6 Hz, 1H), 3.16 (t, *J* = 6.5 Hz, 2H), 2.15 – 1.97 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.4, 153.1, 135.3, 135.0, 129.1, 128.1, 127.2, 126.0, 124.9, 122.6, 121.5, 120.5, 37.0, 34.9, 33.3, 26.7; HRMS (CI-TOF) m/z: $[M+H]^+$ calcd for $C_{18}H_{17}N_2S$ 293.1107, found 293.1111.

(2R)-5-(benzo[*d*]thiazol-2-yl)-2-phenylhexanenitrile

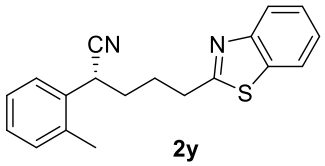


2x'

dr = 1.2:1, Colorless oil (54.0 mg, 88%); 91.5:8.5 er, HPLC condition: Daicel Chiralpak OJ-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, retention time = 12.4 min (major) and 14.5 min (minor); ^1H NMR (500 MHz, $CDCl_3$) δ 7.98 – 7.96 (d, *J* = 8.0 Hz, 1H, two isomers), 7.86 – 7.85 (d, *J* = 8.0 Hz, 1H, two isomers), 7.48 – 7.45 (m, 1H, two isomers), 7.48 – 7.45 (m, 3H, two isomers), 7.39 – 7.33 (m, 3H, two isomers), 3.90 – 3.76 (m, 1H, two isomers), 3.39 – 3.28 (m, 1H, two isomers), 2.06 – 1.98 (m, 2H, two isomers), 1.98 – 1.89 (m, 2H, two isomers), 1.47 (dd, J_1 = 1.5 Hz, J_2 = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 176.4 & 176.3 (two isomers), 153.1 & 153.0 (two isomers), 135.5 & 135.5 (overlap, two isomers), 134.7 & 134.7 (overlap, two isomers), 129.2 & 129.2 (overlap, two isomers), 128.3 & 128.2 (two isomers), 127.3, 126.1, 125.0, 122.8, 121.8 & 121.8 (overlap, two isomers), 120.7 & 120.6 (two isomers), 39.2 & 38.8 (two

isomers), 37.5 & 37.1 (two isomers), 34.8 & 34.7 (two isomers), 33.7 & 33.4 (two isomers), 21.5; HRMS (ESI) m/z: $[M+Na]^+$ calcd for $C_{19}H_{18}N_2SNa$ 329.1083, found 329.1080.

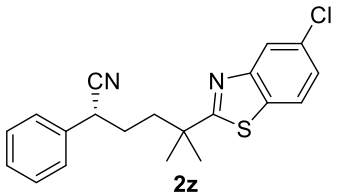
(*R*)-5-(benzo[*d*]thiazol-2-yl)-2-(o-tolyl)pentanenitrile (2y)



2y

Colorless oil (36.6 mg, 60%); 94:6 er, HPLC condition: Daicel Chiralpak OJ-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, retention time = 8.2 min (major) and 9.1 min (minor); $[\alpha]_D^{23}$ = -4.3 (*c* 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.4 Hz, 1H), 7.88 – 7.81 (m, 1H), 7.51 – 7.39 (m, 2H), 7.41 – 7.32 (m, 1H), 7.25 – 7.19 (m, 2H), 7.19 – 7.15 (m, 1H), 4.03 (dd, *J* = 8.7, 5.7 Hz, 1H), 3.23 – 3.14 (m, 2H), 2.32 (s, 3H), 2.26 – 2.07 (m, 2H), 2.08 – 1.91 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.4, 153.1, 135.0, 134.8, 133.7, 131.0, 128.2, 127.3, 126.9, 126.0, 124.9, 122.6, 121.5, 120.7, 33.89, 33.5, 33.3, 27.0, 19.1; HRMS (CI-TOF) m/z: $[M+H]^+$ calcd for $C_{19}H_{19}N_2S$ 307.1263, found 307.1271.

(*R*)-5-(5-chlorobenzo[*d*]thiazol-2-yl)-5-methyl-2-phenylhexanenitrile (2z)

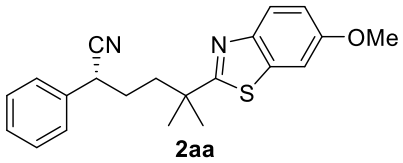


2z

Colorless oil (43.4 mg, 61%); 90:10 er, HPLC condition: Daicel Chiralpak OJ-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, retention time = 10.3 min (major) and 12.5 min (minor); $[\alpha]_D^{23}$ = -9.2 (*c* 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 2.0 Hz, 1H), 7.75 (d, *J* = 8.5 Hz, 1H), 7.40 – 7.29 (m, 4H), 7.28 – 7.23 (m, 2H), 3.74 (dd, *J* = 7.8, 6.1 Hz, 1H), 2.07 – 1.94 (m, 2H), 1.93 – 1.81 (m, 2H), 1.49 (s, 3H), 1.48 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 181.6, 153.9, 135.3, 133.1, 131.8, 129.0, 128.1, 127.1, 125.2, 122.7, 122.2,

120.5, 41.2, 40.7, 37.5, 31.1, 28.8, 28.2; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{20}H_{20}ClN_2S$ 355.1030, found 355.1026.

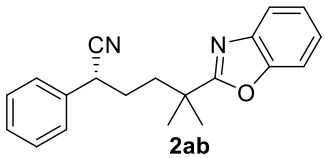
(*R*)-5-(6-methoxybenzo[*d*]thiazol-2-yl)-5-methyl-2-phenylhexanenitrile (2aa)



2aa

Colorless oil (39.4 mg, 56%); 93:7 er, HPLC condition: Daicel Chiralpak OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, retention time = 6.5 min (major) and 7.1 min (minor); $[\alpha]_D^{23}$ = -7.6 (*c* 1.0, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 – 7.79 (m, 1H), 7.39 – 7.29 (m, 1H), 7.27 – 7.21 (m, 5H), 7.03 – 7.08 (m, 1H), 3.75 (s, 3H), 3.69 (t, *J* = 7.0 Hz, 1H), 2.06 – 1.79 (m, 4H), 1.49 (s, 3H), 1.48 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 179.6, 160.0, 153.0, 136.8, 130.1, 125.8, 124.7, 122.8, 121.5, 119.5, 113.4, 103.8, 55.3, 41.1, 40.8, 37.5, 31.0, 28.9, 28.3; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{21}H_{23}N_2OS$ 351.1526, found 351.1515.

(*R*)-5-(benzo[*d*]oxazol-2-yl)-5-methyl-2-phenylhexanenitrile (2ab)

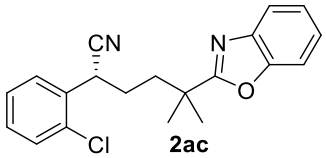


2ab

Colorless oil (35.5 mg, 58%); 92:8 er, HPLC condition: Daicel Chiralpak OJ-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, retention time = 8.1 min (major) and 10.0 min (minor); $[\alpha]_D^{23}$ = -6.3 (*c* 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 – 7.68 (m, 1H), 7.54 – 7.48 (m, 1H), 7.39 – 7.27 (m, 7H), 3.78 (dd, *J* = 7.8, 6.2 Hz, 1H), 2.10 – 1.96 (m, 2H), 1.95 – 1.84 (m, 2H), 1.51 (s, 3H), 1.50 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.5, 150.7, 140.9, 135.3, 129.0, 128.1, 127.2, 124.6, 124.1, 120.5, 119.7, 110.4, 38.6, 37.4, 37.2, 31.1,

26.6, 26.0; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{20}H_{21}N_2O$ 305.1648, found 305.1641.

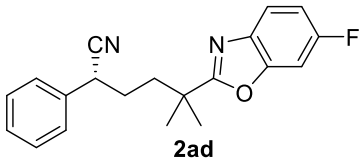
(*R*)-5-(benzo[*d*]oxazol-2-yl)-2-(2-chlorophenyl)-5-methylhexanenitrile (2ac)



2ac

Colorless oil (46.8 mg, 69%); 97.5:2.5 er, HPLC condition: Daicel Chiralpak OJ-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 95:5, 1.0 mL/min, 254 nm UV detector, retention time = 6.9 min (major) and 7.7 min (minor); $[\alpha]_D^{23}$ = +29.0 (*c* 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.71 – 7.64 (m, 1H), 7.54 – 7.44 (m, 2H), 7.37 – 7.25 (m, 4H), 7.27 – 7.20 (m, 1H), 4.23 (dd, *J* = 8.5, 5.9 Hz, 1H), 2.16 – 1.94 (m, 2H), 1.91 – 1.78 (m, 2H), 1.49 (s, 3H), 1.49 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.5, 150.7, 140.9, 133.2, 132.6, 130.0, 129.5, 128.7, 127.6, 124.6, 124.1, 119.9, 119.7, 110.4, 38.7, 37.2, 34.9, 29.6, 26.6, 26.0; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{20}H_{2o}ClN_2O$ 339.1529, found 339.1533.

(*R*)-5-(6-fluorobenzo[*d*]oxazol-2-yl)-5-methyl-2-phenylhexanenitrile (2ad)

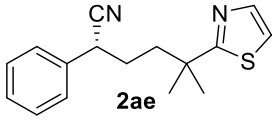


2ad

Colorless oil (46.2 mg, 72%); 92.5:7.5 er, HPLC condition: Daicel Chiralpak OJ-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, retention time = 9.1 min (major) and 10.1 min (minor); $[\alpha]_D^{23}$ = -1.2 (*c* 1.0, $CHCl_3$); ^1H NMR (500 MHz, $CDCl_3$) δ 7.59 (dd, *J* = 8.7, 4.9 Hz, 1H), 7.37 – 7.30 (m, 3H), 7.29 – 7.25 (m, 2H), 7.19 (dd, *J* = 8.0, 2.4 Hz, 1H), 7.10 – 6.99 (m, 1H), 3.76 (dd, *J* = 7.8, 6.2 Hz, 1H), 2.06 – 1.78 (m, 4H), 1.46 (s, 3H), 1.45 (s, 3H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -115.7; ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.2 (d, *J* = 3.2 Hz), 160.3 (d, *J* = 243.4 Hz), 150.6 (d, *J* = 14.6 Hz), 137.2 (d, *J* = 1.8 Hz), 135.3, 129.1, 128.1,

127.2, 120.4, 120.0 (d, J = 10.0 Hz), 112.0 (d, J = 24.7 Hz), 98.5 (d, J = 28.1 Hz), 38.5, 37.4, 37.2, 31.1, 26.5, 26.0; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{20}H_{20}FN_2O$ 323.1554, found 323.1563.

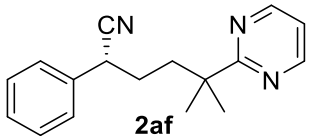
(*R*)-5-methyl-2-phenyl-5-(thiazol-2-yl)hexanenitrile (2ae)



2ae

Colorless oil (12.1 mg, 22%); 92.5:7.5 er, HPLC condition: Daicel Chiralpak OJ-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, retention time = 11.5 min (major) and 12.7 min (minor); $[\alpha]_D^{23}$ = -2.6 (*c* 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 – 7.43 (m, 1H), 7.42 – 7.26 (m, 5H), 7.22 – 7.18 (m, 1H), 3.77 (dd, J = 8.6, 6.2 Hz, 1H), 2.09 – 1.85 (m, 4H), 1.53 (s, 3H), 1.52 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.6, 141.6, 135.5, 129.1, 127.3, 125.9, 120.7, 117.7, 41.1, 40.9, 37.6, 31.2, 29.0, 28.4; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{16}H_{19}N_2S$ 271.1263, found 271.1250.

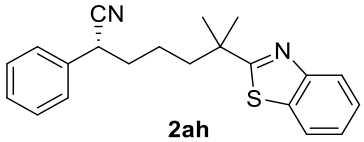
(*R*)-5-methyl-2-phenyl-5-(pyrimidin-2-yl)hexanenitrile (2af)



2af

Colorless oil (21.9 mg, 41%); 92:8 er, HPLC condition: Daicel Chiralpak OJ-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, retention time = 7.0 min (major) and 8.0 min (minor); $[\alpha]_D^{23}$ = -8.1 (*c* 1.0, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.67 (d, J = 4.8 Hz, 2H), 7.39 – 7.23 (m, 5H), 7.10 (t, J = 4.8 Hz, 1H), 3.69 (dd, J = 8.5, 6.4 Hz, 1H), 2.09 – 1.87 (m, 2H), 1.83 – 1.66 (m, 2H), 1.38 (s, 3H), 1.37 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 175.7, 156.6, 135.9, 129.0, 127.2, 123.6, 120.9, 118.3, 42.2, 39.7, 37.8, 31.5, 27.6, 27.1; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{17}H_{20}N_3$ 266.1652, found 266.1643.

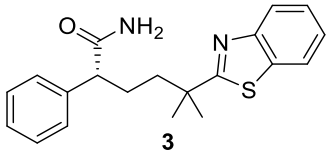
(*R*)-6-(benzo[*d*]thiazol-2-yl)-6-methyl-2-phenylheptanenitrile (2ah)



2ah

Colorless oil (36.9 mg, 55%); 92:8 er, HPLC condition: Daicel Chiralpak OJ-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 90:10, 0.8 mL/min, 254 nm UV detector, retention time = 19.0 min (major) and 20.7 min (minor); $[\alpha]_D^{23}$ = -6.6 (*c* 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.1 Hz, 1H), 7.92 – 7.79 (m, 1H), 7.53 – 7.41 (m, 2H), 7.40 – 7.30 (m, 2H), 7.33 – 7.21 (m, 3H), 3.72 (dd, *J* = 8.8, 6.3 Hz, 1H), 1.99 – 1.76 (m, 4H), 1.50 (s, 3H), 1.48 (s, 3H), 1.48 – 1.36 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 180.4, 153.2, 135.8, 134.8, 129.0, 128.0, 127.1, 125.8, 124.6, 122.7, 121.5, 120.7, 42.9, 41.3, 37.1, 36.2, 28.6, 28.4, 22.2; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{21}H_{23}N_2S$ 335.1576, found 335.1571.

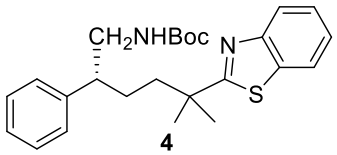
(*R*)-5-(benzo[*d*]thiazol-2-yl)-5-methyl-2-phenylhexanamide (3)



3

White solid (57.7 mg, 85%), mp 136-138 °C; 90.5:9.5 er, HPLC condition: Daicel Chiralpak OJ-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, retention time = 15.9 min (minor) and 24.6 min (major); $[\alpha]_D^{23}$ = -19.2 (*c* 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.1 Hz, 1H), 7.83 (d, *J* = 7.9 Hz, 1H), 7.47 – 7.40 (m, 1H), 7.35 – 7.19 (m, 6H), 5.90 (s, 1H), 5.76 (s, 1H), 3.31 (t, *J* = 7.4 Hz, 1H), 2.16 – 2.06 (m, 1H), 1.94 – 1.82 (m, 1H), 1.81 – 1.64 (m, 2H), 1.47 (s, 3H), 1.45 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 180.7, 175.8, 153.0, 139.6, 134.8, 128.8, 127.8, 127.3, 125.7, 124.5, 122.6, 121.4, 52.9, 41.5, 41.3, 28.8, 28.4, 28.0; HRMS (ESI) m/z: $[M+Na]^+$ calcd for $C_{20}H_{22}N_2NaOS$ 361.1345, found 361.1358.

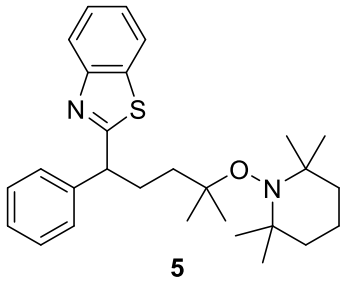
***tert*-butyl (*R*)-(5-(benzo[*d*]thiazol-2-yl)-5-methyl-2-phenylhexyl)carbamate (4)**



4

Colorless oil (58.7 mg, 69%); 92.5:7.5 er, HPLC condition: Daicel Chiralpak OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, retention time = 4.6 min (minor) and 5.4 min (major); $[\alpha]_D^{23}$ = +22.6 (*c* 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.1 Hz, 1H), 7.83 (d, *J* = 7.9 Hz, 1H), 7.47 – 7.41 (m, 1H), 7.36 – 7.31 (m, 1H), 7.33 – 7.24 (m, 2H), 7.24 – 7.19 (m, 1H), 7.13 – 7.07 (m, 2H), 4.41 (t, *J* = 6.0 Hz, 1H), 3.65 – 3.34 (m, 1H), 3.20 – 2.96 (m, 1H), 2.82 – 2.54 (m, 1H), 1.84 – 1.73 (m, 1H), 1.69 – 1.58 (m, 2H), 1.57 – 1.49 (m, 1H), 1.44 (s, 3H), 1.42 (s, 3H), 1.36 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 180.6, 155.8, 153.0, 142.5, 135.0, 128.7, 127.8, 126.6, 125.6, 124.5, 122.7, 121.4, 79.0, 46.3, 46.1, 41.5, 41.3, 28.6, 28.5, 28.3; HRMS (ESI) m/z: $[M+Na]^+$ calcd for $C_{25}H_{32}N_2NaO_2S$ 447.2077, found 447.2052.

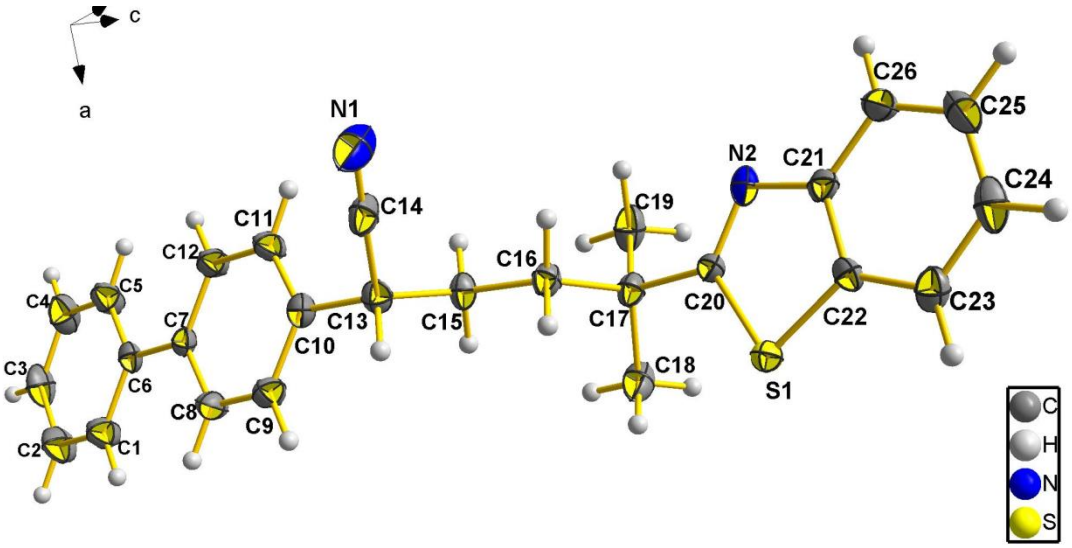
2-(4-methyl-1-phenyl-4-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)pentyl)benzo[*d*]thiazole (5)

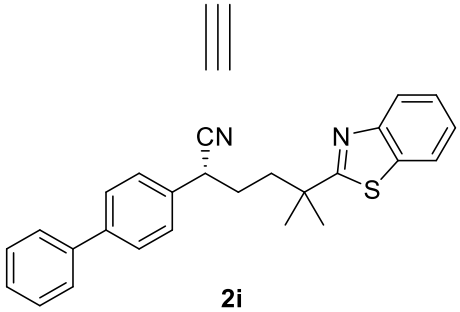


5

Colorless oil (32.5 mg, 36%); ^{1}H NMR (500 MHz, $CDCl_3$) *δ* 8.04 – 7.96 (m, 1H), 7.83 – 7.73 (m, 1H), 7.49 – 7.39 (m, 3H), 7.37 – 7.28 (m, 3H), 7.28 – 7.23 (m, 1H), 4.33 (t, *J* = 7.7 Hz, 1H), 2.61 – 2.50 (m, 1H), 2.45 – 2.32 (m, 1H), 1.70 – 1.35 (m, 8H), 1.26 (s, 3H), 1.25 (s, 3H), 1.06 (s, 6H), 1.03 (s, 3H), 0.98 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) *δ* 175.6, 153.1, 141.9, 135.2, 128.7, 128.1, 127.2, 125.8, 124.6, 122.8, 121.4, 78.2, 59.12, 59.09, 51.7, 41.8, 40.78, 40.77, 34.61, 34.59, 30.5, 27.1, 26.9, 20.8, 20.7, 17.1; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{28}H_{39}N_2OS$ 451.2778, found 451.2756.

7. X-ray structure of (*R*)-2i (CCDC 1887624)





2i

Crystal data and structure refinement for 2i

Identification code	2i	
Empirical formula	$C_{26}\ H_{24}\ N_2\ S$	
Formula weight	396.53	
Temperature	173(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 5.9714(6) Å	α = 90°.
	b = 7.5838(7) Å	β = 96.615(3)°.
	c = 23.115(2) Å	γ = 90°.
Volume	1039.80(17) $Å^3$	
Z	2	
Density (calculated)	1.267 Mg/m^3	
Absorption coefficient	1.475 mm^{-1}	

F(000)	420
Crystal size	0.220 x 0.190 x 0.140 mm^3
Theta range for data collection	6.145 to 64.980°.
Index ranges	-6<=h<=7, -8<=k<=8, -27<=l<=27
Reflections collected	6701
Independent reflections	3237 [R(int) = 0.0268]
Completeness to theta = 64.980°	98.5 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3237 / 1 / 258
Goodness-of-fit on F^2	1.037
Final R indices [I>2sigma(I)]	R1 = 0.0341, wR2 = 0.0930
R indices (all data)	R1 = 0.0343, wR2 = 0.0932
Absolute structure parameter	0.066(7)
Extinction coefficient	n/a
Largest diff. peak and hole	0.320 and -0.209 e.$Å^{-3}$

8. DFT Calculations

Computational Methods All the DFT calculations were carried out with Gaussian 16. The functional of M06 with 6-31G(d) basis set (lanl2dz for Cu) was used for geometry optimizations. M062X functional with basis set 6-311+G(d, p) (SDD basis set for Cu) was employed to estimate solvation energies with single point calculations based on optimized structures, using the SMD continuum solvation model.

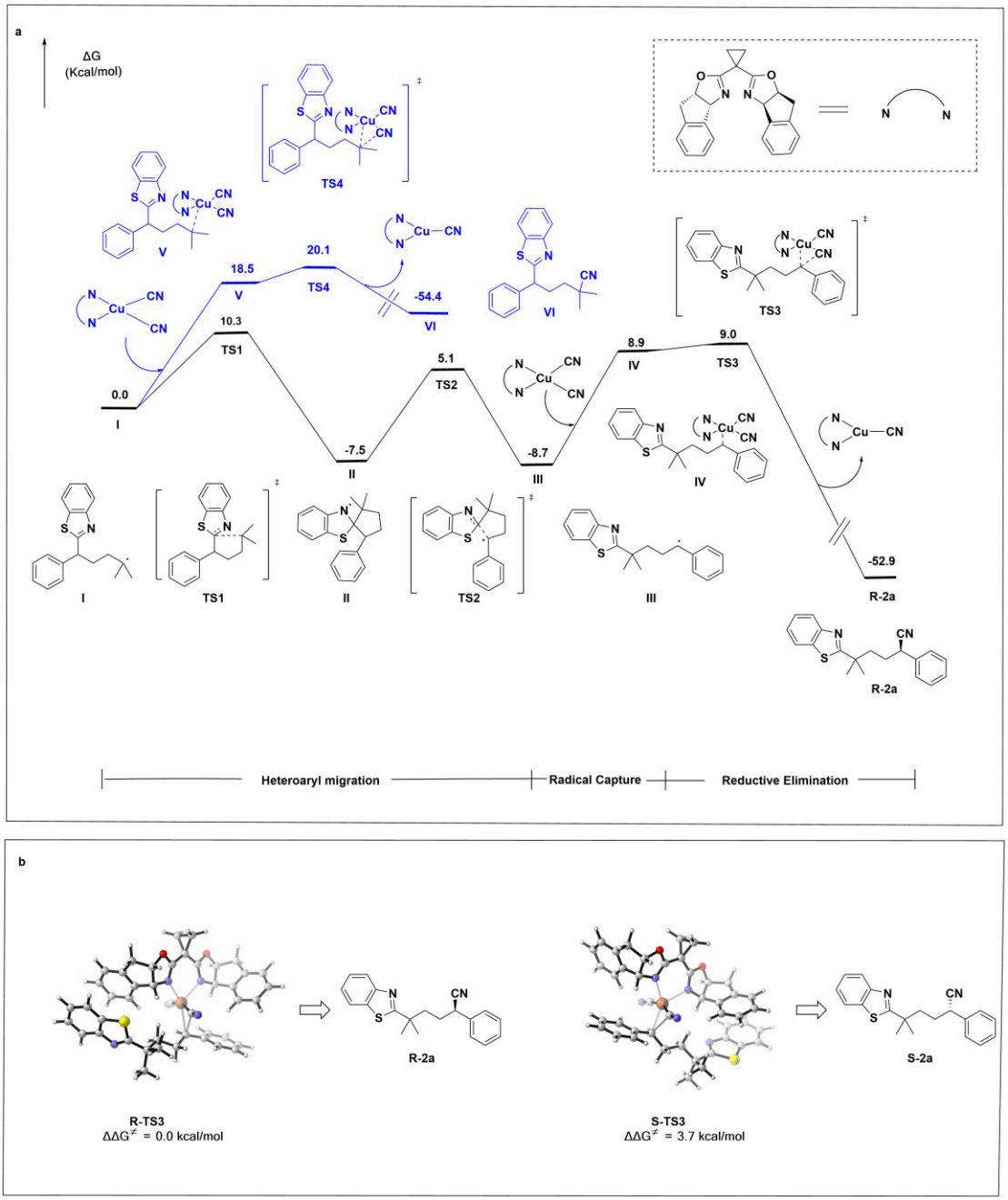


Fig. S5 DFT computational studies. (a) Free energy profile of photoredox/Cu dual catalyzed enantioselective remote cyanation via 1,4-heteroaryl migration. (b) The differences in activation free energy of transition states for enantiomers.

The Gibbs free energy barrier for the *ipso*-cyanation process (from **I** to **TS4**, 20.1

kcal/mol) is higher than that for the 1,4-heteroaryl migration pathway (from **III** to **TS3**, 17.7 kcal/mol) (Fig. S5a), which illustrates that the 1,4-heteroaryl migration/enantioselective remote cyanation process is more kinetically favored. These results clearly explain why remote cyanation products are exclusively obtained in this transformation. The stereoselectivity of remote cyanation is determined by the reductive elimination step. The difference in Gibbs free energies of the two key transition state structures (**R-TS3** and **S-TS3**, corresponding to products **R-2a** and **S-2a**, respectively) is 3.7 kcal/mol, suggesting the nitrile **2a** with R configuration is the more favored enantiomer (Fig. S5b). This result is consistent with our experimental observation.

CARTESIAN COORDINATES OF OPTIMIZED STRUCTURES

I

C	5.04456200	0.27575600	0.13124200
C	4.53377900	0.93054000	1.25954400
C	3.16821400	1.04086600	1.45864800
C	2.29855200	0.48668500	0.51591900
C	2.82477000	-0.17089900	-0.61504100
C	4.19837900	-0.28013200	-0.81710300
C	-2.94684100	3.32192800	1.41445600
C	-2.77332200	4.51789400	-0.84783500
C	-2.62612500	3.27688000	-0.03947600
C	-1.72242600	2.20958400	-0.56618600
C	-1.92607800	0.83135400	0.05303100
C	-1.09564300	-0.26440100	-0.62247200
C	-1.50340500	-1.64293500	-0.13726700
C	-1.16811100	-2.07459500	1.14753700
C	-2.25575600	-2.48207600	-0.95727300
C	-1.58326700	-3.32049500	1.60132300
C	-2.67218300	-3.72989600	-0.50429800
C	-2.33652000	-4.15190200	0.77707800
S	1.50873300	-0.74891400	-1.60617700
N	0.91877600	0.52705100	0.59093300
C	0.37909500	-0.05865900	-0.42296000
H	5.22083200	1.35749900	1.98764100
H	2.75307700	1.54624800	2.32811000
H	4.59807300	-0.78798600	-1.69250300
H	-3.67946300	4.10828200	1.63877800
H	-3.35497000	2.37100800	1.78752000
H	-2.05208500	3.53086300	2.03216100
H	-1.90875700	5.19996200	-0.73065900
H	-2.84674300	4.29889700	-1.92314400
H	-3.66301300	5.09349400	-0.55591200
H	-1.84804600	2.13785700	-1.66163200

H	-0.66342900	2.50485200	-0.41735000
H	-1.67585200	0.84980300	1.12354000
H	-2.98589100	0.54162500	-0.02121300
H	-1.29361200	-0.22357700	-1.70772600
H	-0.56890200	-1.42767600	1.78907700
H	-2.51982500	-2.15127200	-1.96278700
H	-1.31369300	-3.64669500	2.60460300
H	-3.25811400	-4.37492100	-1.15715600
H	-2.65859900	-5.12894700	1.13325000
H	6.12181000	0.20098400	-0.00549600

L*Cu^{II}(CN)$_2$

C	-3.04359600	1.36254400	1.71620300
O	-2.09647900	2.26402500	1.07391500
C	-2.53032400	-0.03390400	1.30212300
H	-2.38650100	-0.74252100	2.12596600
C	-1.10691300	1.51448100	0.57769100
N	-1.21717300	0.24434500	0.69052400
C	0.00000800	2.26449100	-0.03803300
C	-0.35480000	3.58925800	-0.71602700
C	0.34112000	3.62146900	0.57922900
H	-1.41457200	3.82754100	-0.74629200
H	0.20986800	3.81626600	-1.61647100
H	-0.22678400	3.88183600	1.46840600
H	1.39786500	3.87333700	0.59815500
C	3.07517400	1.32200400	-1.71642500
O	2.11540500	2.23599000	-1.11143600
C	2.55321300	-0.06466800	-1.28428100
H	2.43137900	-0.79153700	-2.09647500
C	1.11433300	1.49964900	-0.62017000
N	1.22537300	0.22644300	-0.70933600
C	-5.58213200	0.18931600	-0.78733100
C	-5.53152800	-0.95914800	-1.57261900
C	-4.49181300	-1.87774400	-1.42486000
C	-3.48049200	-1.65980600	-0.49402600
C	-3.52930000	-0.50316300	0.27724500
C	-4.57152700	0.41277600	0.14102500
H	-6.40138600	0.89963100	-0.89860700
H	-6.31466700	-1.14501900	-2.30595400
H	-4.47091900	-2.77531600	-2.04001300
H	-2.67519300	-2.38179800	-0.35963400
C	-4.43829300	1.54497900	1.12307700
H	-4.54219900	2.54193100	0.67368400
H	-5.19668400	1.47806200	1.91686200

C	3.45339700	-1.64383400	0.57798300
C	3.52525200	-0.50906800	-0.22324200
C	4.56549100	0.40867100	-0.08475300
C	5.55174900	0.20811300	0.87451600
C	5.47824400	-0.91881100	1.68863700
C	4.43982400	-1.83873800	1.53994500
H	2.64959600	-2.36903700	0.44868100
H	6.36942300	0.91984900	0.98795100
H	6.24194000	-1.08639700	2.44642400
H	4.39985300	-2.71859000	2.17914400
C	4.45733400	1.51588700	-1.09804500
H	4.55498200	2.52361600	-0.67199600
H	3.03900400	1.51199000	-2.79443300
H	5.23204300	1.42655600	-1.87365100
H	-2.98565000	1.57440300	2.78923800
C	-1.15309400	-3.19317600	2.10388000
N	-0.68932800	-2.50212000	1.26395700
Cu	-0.00553700	-1.24222400	-0.01683000
C	0.67584100	-2.52988400	-1.31761200
N	1.19466600	-3.19303500	-2.12907500

TS1

C	-3.85330200	-2.37044300	0.39004700
C	-3.63923600	-2.26246300	-0.99076500
C	-2.58733700	-1.51561800	-1.49027700
C	-1.72287900	-0.86283900	-0.59837300
C	-1.95156700	-0.98386900	0.79602900
C	-3.01485500	-1.72925100	1.29364100
C	1.47693300	1.98180500	-1.12394700
C	1.33563000	0.98815800	0.03919600
C	2.35730600	-0.12592800	-0.00201200
C	2.34015300	-1.10045600	-1.00323000
C	3.35800100	-0.17818700	0.96737900
C	3.30755900	-2.09719900	-1.03148400
C	4.32963100	-1.17345200	0.93941700
C	4.30685400	-2.13627400	-0.06234300
N	-0.65397900	-0.09812500	-0.96645100
C	-0.09068200	0.48942200	0.07559400
H	-4.31229700	-2.77184900	-1.67814100
H	-2.40823200	-1.41945000	-2.55944100
H	-3.18474300	-1.81277400	2.36543200
H	1.50114500	1.53105100	0.98223200
H	1.54745400	-1.07874100	-1.75100400
H	3.37591100	0.57471400	1.75692000

H	3.27954900	-2.85267700	-1.81534800
H	5.10360000	-1.19720600	1.70500000
H	5.06318600	-2.91907400	-0.08771000
H	-4.68705600	-2.96332200	0.76167000
C	0.16656200	2.77632800	-1.31652900
H	-0.33205600	2.43834100	-2.23361600
C	-0.77104100	2.58546900	-0.15773800
H	2.33800700	2.63535100	-0.92853400
H	1.71123700	1.43159800	-2.04416000
H	0.38334700	3.84997600	-1.44997000
C	-2.23029900	2.47052400	-0.44350000
H	-2.78496200	2.10801800	0.43429600
H	-2.65034000	3.45916800	-0.69925400
H	-2.43022100	1.79792100	-1.28653200
C	-0.44089700	3.31742100	1.10641800
H	-0.88493700	4.32789900	1.07490000
H	-0.86159100	2.81662500	1.99068500
H	0.63772600	3.45191900	1.25850100
S	-0.74288000	-0.07246900	1.66525500

II

C	-2.06877500	3.50884000	0.23712200
C	-2.02449400	3.17854000	-1.13077100
C	-1.18280600	2.19174000	-1.58903500
C	-0.34931400	1.49661500	-0.67067300
C	-0.41523600	1.84718800	0.72277800
C	-1.26766800	2.84729100	1.16547800
C	1.65666800	-2.25418700	-0.85907700
C	0.75796500	-1.57081600	0.19469700
C	-0.71916600	-1.84547900	0.10877000
C	-1.42137000	-1.76638900	-1.09830200
C	-1.42876700	-2.17403600	1.26480100
C	-2.78754700	-2.01385000	-1.14363100
C	-2.79679000	-2.42375600	1.22401300
C	-3.48071800	-2.34602700	0.01700500
N	0.48686000	0.53421900	-1.02088600
C	1.15614800	-0.06520000	0.07858000
H	-2.66714200	3.71103600	-1.82927700
H	-1.13237600	1.91430300	-2.63995600
H	-1.31351800	3.10992300	2.22050700
H	1.08514600	-1.88823900	1.19547300
H	-0.89240100	-1.48837100	-2.00920200
H	-0.89541300	-2.23183200	2.21477200
H	-3.31580000	-1.94631000	-2.09359900

H	-3.32733000	-2.68094200	2.13951500
H	-4.55097700	-2.54268900	-0.02110300
H	-2.74242100	4.29317600	0.57756000
C	2.75308200	-1.23900800	-1.23215300
H	2.54887700	-0.81134500	-2.22215000
C	2.69025500	-0.12059100	-0.17827000
H	2.07399000	-3.18188500	-0.44634600
H	1.07496100	-2.54422600	-1.74185100
H	3.75620300	-1.68664800	-1.27023800
C	3.23834300	1.20176500	-0.68926200
H	3.12594100	1.99421200	0.06475500
H	4.30954700	1.10463400	-0.91518500
H	2.72229800	1.52079800	-1.60248500
C	3.46972100	-0.53460400	1.06930200
H	4.53616300	-0.61174300	0.81605500
H	3.37698700	0.20959200	1.87202500
H	3.16226000	-1.51022100	1.46807500
S	0.68623700	0.87618900	1.65128800

TS2

C	-2.99133100	-2.45950500	0.00064500
C	-2.98474900	-1.74458700	1.20847800
C	-1.85863800	-1.05965600	1.62131500
C	-0.70575200	-1.08196300	0.81690300
C	-0.72944100	-1.81148600	-0.40322300
C	-1.86705600	-2.49680300	-0.81462000
C	2.16854900	2.13454800	-0.19496700
C	1.00202600	1.42594100	-0.83956300
C	-0.37694000	1.76920500	-0.56765800
C	-0.77207400	2.38617600	0.63256700
C	-1.38021200	1.39563100	-1.47845800
C	-2.11032300	2.62948300	0.89928100
C	-2.71998000	1.63061200	-1.20610400
C	-3.09122900	2.25049100	-0.01597000
N	0.45300100	-0.44129400	1.10547400
C	1.30417000	-0.46371700	0.08469400
H	-3.88317600	-1.72564800	1.82283100
H	-1.83806800	-0.48643700	2.54607700
H	-1.87847600	-3.04787200	-1.75313600
H	1.16964000	1.10001400	-1.86913600
H	-0.01716200	2.65480700	1.37108800
H	-1.08917700	0.90422700	-2.40796500
H	-2.39526000	3.11000600	1.83416400
H	-3.47946300	1.32652500	-1.92449500

H	-4.14182600	2.43738600	0.19965800
H	-3.89060100	-2.99192200	-0.30421700
C	2.85207500	1.23034200	0.83751800
H	2.31959000	1.29194900	1.79740100
C	2.78546300	-0.21741500	0.34552900
H	2.88993800	2.40822700	-0.97842800
H	1.85102500	3.07812500	0.26971800
H	3.89490100	1.53141200	1.01852700
C	3.27736500	-1.17925100	1.42573500
H	3.17194500	-2.22271000	1.09742200
H	4.33977300	-0.99667300	1.64208400
H	2.70249000	-1.05323300	2.35051400
C	3.63394200	-0.40835400	-0.90961300
H	4.67139200	-0.11254700	-0.70107700
H	3.65049500	-1.46240500	-1.21953900
H	3.28430300	0.18552300	-1.76384300
S	0.80509500	-1.65111500	-1.21380700

III

C	-3.78243900	-0.88210400	-1.46205300
C	-4.28274800	-2.14828300	-1.21039600
C	-3.85559200	-2.88049300	-0.09505900
C	-2.92049700	-2.35955300	0.78758000
C	-1.42657800	1.15080300	0.23190400
C	-2.83946000	-0.33981400	-0.58551100
C	-2.41667100	-1.08664700	0.53204300
S	-1.24692900	-0.15857000	1.43678900
N	-2.25954200	0.90746300	-0.71985400
C	-0.60376600	2.40742800	0.36522800
C	0.89253800	2.06559000	0.21566300
C	1.28551800	1.38608400	-1.10188700
C	2.74105300	1.07049200	-1.14637400
C	-1.04194800	3.41147700	-0.69856700
C	-0.82258200	3.02526300	1.75014200
C	3.34094700	-0.07974500	-0.59488500
C	4.75114900	-0.24160700	-0.65681700
C	2.59659700	-1.11245400	0.03611200
C	5.37166400	-1.35569400	-0.12743900
C	3.22885400	-2.22344100	0.56393200
C	4.61698700	-2.35807100	0.48890400
H	-4.10173100	-0.29791000	-2.32251500
H	-5.01729900	-2.58192200	-1.88627000
H	-4.26256000	-3.87403200	0.08392800
H	-2.59132000	-2.93056600	1.65341700

H	1.46423100	3.00160900	0.32841200
H	1.20555400	1.42070500	1.05336500
H	0.68071500	0.47405300	-1.23491000
H	1.02870800	2.04459600	-1.94375400
H	3.40834300	1.81799700	-1.58156900
H	-2.08226700	3.71896000	-0.53576900
H	-0.40309800	4.30402200	-0.64467800
H	-0.98524700	2.99435400	-1.70933000
H	-1.88521600	3.24245300	1.92167200
H	-0.47554600	2.36485900	2.55640800
H	-0.26416100	3.96814000	1.82839100
H	5.34225300	0.53905000	-1.13707800
H	1.51206000	-1.02836900	0.10699300
H	6.45460000	-1.45227000	-0.19097100
H	2.63472800	-3.00040000	1.04307500
H	5.10674300	-3.23582800	0.90641800

IV

Cu	-4.79999974	0.20000000	0.00000000
C	-4.69283974	0.87499900	-1.79082000
N	-4.62856874	1.25931800	-2.89399700
C	-3.77438774	-3.26165300	-0.85534100
C	-3.67717074	-4.75409700	-0.55424300
C	-3.15379874	-4.25014300	-1.83807000
H	-4.61996574	-5.29457300	-0.55640100
H	-2.97298774	-5.02941900	0.22574000
H	-2.07692074	-4.16899200	-1.96318900
H	-3.72407874	-4.43377300	-2.74445300
C	-2.82967574	-2.36288900	-0.16924000
O	-1.71719574	-2.96670200	0.30282500
C	-0.98607174	-1.96247500	1.04883400
C	-1.66088374	-0.66254800	0.57302100
H	-1.12764974	-2.19128500	2.11198000
H	-1.86347374	0.05627500	1.37959800
N	-2.92578674	-1.09928300	-0.02601400
C	-5.12798374	-2.75830600	-1.14978600
O	-5.87121174	-3.58190400	-1.91561300
C	-7.12431874	-2.90167300	-2.17388100
C	-7.09223874	-1.76075700	-1.13877600
H	-7.10050874	-2.57578300	-3.22030600
H	-7.42437974	-0.78979400	-1.53211900
N	-5.68416774	-1.69039900	-0.72303800
C	-8.29733974	-3.80959500	-1.82683800
C	-7.97389074	-2.26909900	-0.02708800

C	-8.16027074	-1.72111300	1.23630300
C	-8.61541474	-3.45033900	-0.40091500
C	-9.00838574	-2.37404600	2.12575200
H	-7.63586274	-0.81204000	1.53011100
C	-9.46216174	-4.10215400	0.48970300
C	-9.65481774	-3.55429200	1.75527100
H	-9.16225074	-1.96324900	3.12173000
H	-9.96458674	-5.02640800	0.20326800
H	-10.31242674	-4.05374400	2.46522100
H	-9.14744874	-3.58991400	-2.49164000
H	-8.04004374	-4.86636800	-1.97874400
C	0.47286026	-1.91483000	0.60835100
C	-0.70912374	-0.13913100	-0.47086900
C	0.48843926	-0.85317600	-0.45854200
C	-0.93887974	0.86280300	-1.40416300
C	1.49598026	-0.54363100	-1.36515300
C	0.07157426	1.17365100	-2.30903500
H	-1.90042174	1.37510400	-1.44093800
C	1.28215226	0.47990900	-2.28501700
H	2.43392926	-1.09920000	-1.36467700
H	-0.09153274	1.95521400	-3.04977000
H	2.06172926	0.73037400	-3.00319400
H	1.11231626	-1.64511500	1.46237300
H	0.81269926	-2.89883400	0.25810500
C	-11.38429874	-1.15030300	-0.54977100
C	-12.69932774	-1.49521600	-0.29187300
C	-13.68029474	-0.50998600	-0.11208200
C	-13.35909974	0.83786900	-0.18161900
H	-10.60784474	-1.90285800	-0.67729500
H	-12.97256174	-2.54708500	-0.22150300
H	-14.70896074	-0.80413600	0.08935000
H	-14.12081474	1.60174500	-0.03749600
C	-9.74016774	1.97645000	-0.84777500
C	-11.03924774	0.20186400	-0.62284400
C	-12.03296774	1.18359700	-0.43571800
S	-11.30836474	2.76525000	-0.55746300
N	-9.76768174	0.68639600	-0.85719600
C	-8.48452574	2.78286400	-1.09618500
C	-7.39690774	2.20732000	-0.16735100
C	-6.06572474	2.94195800	-0.21022800
H	-7.77582374	2.19455600	0.86936900
H	-7.23473174	1.15368700	-0.44227500
C	-5.00510974	2.29213900	0.62404400
H	-5.73078574	3.08196700	-1.24364300

H	-6.18564974	3.95012500	0.23277900
H	-5.35805274	2.07007700	1.63183400
C	-8.11142574	2.59107800	-2.57244000
H	-7.94934474	1.53139700	-2.80257500
H	-8.91755474	2.96491600	-3.21936400
H	-7.19217274	3.13271200	-2.83002000
C	-8.70980174	4.26650500	-0.81557400
H	-8.94330874	4.45207000	0.24286500
H	-7.81425474	4.84557400	-1.07315200
H	-9.53020474	4.66912100	-1.42621700
C	-3.62644274	2.77341000	0.60976500
C	-2.81626274	2.53317400	1.73339500
C	-3.10168274	3.52751000	-0.45290100
C	-1.52398874	3.03348500	1.79343400
H	-3.22015774	1.93340100	2.55130700
C	-1.81452374	4.03969600	-0.38054000
H	-3.69963274	3.69308400	-1.34716900
C	-1.02024774	3.79022500	0.73692600
H	-0.90772274	2.83871100	2.66958400
H	-1.41952274	4.62359900	-1.21029000
H	-0.00528774	4.18115500	0.78162100
C	-4.98770174	-0.17049700	1.87033700
N	-4.99655774	-0.39780100	3.01804100

R-TS3

Cu	0.94902600	0.18264700	0.53900100
C	0.97394800	1.13030100	-1.11383400
N	0.98106300	1.37059400	-2.26080100
C	1.67225000	-3.26452700	-0.32882000
C	1.57702200	-4.70990100	0.15307200
C	2.18155400	-4.43459600	-1.16381000
H	0.57304200	-5.12558300	0.18569700
H	2.22592700	-4.97164900	0.98415800
H	3.26196200	-4.50290200	-1.26035300
H	1.60942900	-4.65980000	-2.05936900
C	2.70646300	-2.40771100	0.28305500
O	3.77035000	-3.07727800	0.77479600
C	4.61081100	-2.10210800	1.43899000
C	3.99906100	-0.76410700	0.97154700
H	4.52223500	-2.29167300	2.51473000
H	3.81394100	-0.05167100	1.78865400
N	2.71761400	-1.13475000	0.36371700
C	0.39736900	-2.64125800	-0.73160600
O	-0.39193700	-3.41498100	-1.50588000

C	-1.52325300	-2.60012300	-1.90102700
C	-1.40021100	-1.38679100	-0.95811200
H	-1.38613800	-2.36779100	-2.96360200
H	-1.50528100	-0.42123000	-1.47535400
N	-0.04985200	-1.49270000	-0.40127400
C	-2.84315800	-3.29654600	-1.58737600
C	-2.46063500	-1.62682700	0.08310600
C	-2.67354100	-0.92823900	1.26542000
C	-3.25025700	-2.72479800	-0.25638100
C	-3.71104400	-1.33274100	2.10060600
H	-2.02448800	-0.09807900	1.54597000
C	-4.27890800	-3.13359700	0.58429300
C	-4.50673200	-2.42730000	1.76209900
H	-3.89629800	-0.79496700	3.02865500
H	-4.90087500	-3.99091800	0.32512200
H	-5.31614700	-2.72946100	2.42508400
H	-3.58259600	-3.05694100	-2.36798000
H	-2.72499400	-4.38860900	-1.58864800
C	6.04343700	-2.16776300	0.91378900
C	4.97399900	-0.26049900	-0.05741700
C	6.11046900	-1.06560800	-0.10942500
C	4.81653400	0.81874600	-0.91719200
C	7.12276800	-0.78549000	-1.02091100
C	5.83148100	1.09957100	-1.82624400
H	3.90824900	1.42229900	-0.88981500
C	6.97692700	0.30388800	-1.87600300
H	8.01433300	-1.41084400	-1.07057000
H	5.72477100	1.94230900	-2.50801300
H	7.76150200	0.53226300	-2.59606200
H	6.75492900	-1.99968100	1.73590700
H	6.26501100	-3.16314000	0.50547400
C	-6.60165500	0.98438700	1.50057700
C	-7.48530800	-0.07436700	1.37051200
C	-7.42510000	-0.93074000	0.26250500
C	-6.47947000	-0.74191900	-0.73461500
H	-6.63438300	1.65920900	2.35360900
H	-8.23881800	-0.24383400	2.13774600
H	-8.12900400	-1.75759100	0.18276500
H	-6.42798200	-1.41243400	-1.59131900
C	-3.95496900	2.15882100	-0.54646900
C	-5.64071400	1.19138800	0.50605000
C	-5.59210100	0.32314100	-0.60310500
S	-4.31869900	0.82928800	-1.67966800
N	-4.70291700	2.20451700	0.50225200

C	-2.78796800	3.09033900	-0.79216800
C	-1.61645300	2.50494000	0.02219100
C	-0.30013000	3.26672400	-0.05927000
H	-1.92904800	2.42580500	1.07663800
H	-1.44005400	1.47388100	-0.32616800
C	0.81983600	2.53011100	0.61293800
H	-0.04469400	3.52975700	-1.09160300
H	-0.38408800	4.21371400	0.50677700
H	0.51433500	2.15235100	1.59110800
C	-2.43972100	3.14975600	-2.27986400
H	-2.02138200	2.20113800	-2.64709200
H	-3.32518600	3.40028600	-2.87938500
H	-1.68625800	3.92320600	-2.47269500
C	-3.16355300	4.48455600	-0.28942900
H	-3.40836000	4.46663700	0.77886300
H	-2.33644700	5.18798200	-0.45565800
H	-4.04077400	4.86643200	-0.82814500
C	2.19374300	3.03245900	0.61937600
C	2.99493300	2.76606200	1.74077600
C	2.71802300	3.79972900	-0.43050600
C	4.28772100	3.26671400	1.81338500
H	2.58756200	2.15361700	2.54821700
C	4.00872500	4.30292500	-0.34958700
H	2.11889700	3.97629700	-1.32245100
C	4.79629600	4.03566400	0.76925900
H	4.90091000	3.05626800	2.68776800
H	4.40934900	4.89778200	-1.16865500
H	5.81246300	4.42254000	0.82290600
C	0.88237900	-0.01771900	2.48627500
N	1.02399900	-0.03079800	3.64889500

S-TS3

Cu	-1.07968700	0.39446500	0.39592200
C	-0.75352000	1.21778900	-1.28952400
N	-0.55795700	1.37236800	-2.43467600
C	-1.50024500	-3.08025000	-0.47162500
C	-2.00310700	-4.43476500	0.01637100
C	-1.39487300	-4.33864300	-1.32483300
H	-3.08343200	-4.53335400	0.08977100
H	-1.43009700	-4.88685600	0.82130200
H	-0.38881700	-4.72582400	-1.46498500
H	-2.04208900	-4.37247500	-2.19680700
C	-0.22864900	-2.57245300	0.07932200
O	0.60591200	-3.51500400	0.56304500

C	1.71997700	-2.80325300	1.17078200
C	1.57305700	-1.40775700	0.54291100
H	1.56361200	-2.83856800	2.25608000
H	1.77591800	-0.57662000	1.23687600
N	0.18114700	-1.36251800	0.08568200
C	-2.54852100	-2.09818000	-0.81143200
O	-3.55375500	-2.56765400	-1.58013500
C	-4.40109600	-1.43026600	-1.89258200
C	-3.94680000	-0.40261800	-0.84011800
H	-4.18654200	-1.15205900	-2.93150500
H	-3.85107000	0.62459000	-1.22361900
N	-2.63727800	-0.89197600	-0.40460400
C	-5.86404300	-1.75378100	-1.61878600
C	-4.98346500	-0.54493400	0.24792500
C	-4.92183700	-0.08215600	1.55730100
C	-6.06215100	-1.31076300	-0.19435700
C	-5.98532200	-0.36088900	2.41124700
H	-4.03746800	0.44022000	1.92293300
C	-7.12426600	-1.58505100	0.65947900
C	-7.08284600	-1.09651300	1.96256200
H	-5.94869300	-0.01704400	3.44344800
H	-7.96859600	-2.18539000	0.32008700
H	-7.90489600	-1.30907800	2.64462400
H	-6.50500500	-1.19342900	-2.31616800
H	-6.07341600	-2.81932200	-1.78337700
C	3.05042400	-3.38025400	0.70706600
C	2.54632800	-1.44825900	-0.61043000
C	3.39189800	-2.55276300	-0.50198700
C	2.63735900	-0.58270200	-1.69461000
C	4.38436800	-2.77239300	-1.44932500
C	3.63059900	-0.80675100	-2.64508600
H	1.91934500	0.22960400	-1.82083700
C	4.50732100	-1.88416600	-2.51488700
H	5.05098900	-3.63084200	-1.36456400
H	3.71824800	-0.13602800	-3.49889800
H	5.28003000	-2.04469400	-3.26552500
H	3.80513100	-3.25997700	1.49951600
H	2.96931900	-4.45570400	0.49899700
C	4.97006500	-0.77213200	2.23760700
C	6.07484000	-1.60502800	2.15951400
C	7.04981600	-1.41671000	1.16969800
C	6.94095500	-0.38644700	0.24695400
H	4.20500900	-0.90052400	3.00320400
H	6.19101500	-2.41476300	2.87861900

H	7.90815400	-2.08492600	1.12675000
H	7.69895500	-0.24149800	-0.52039700
C	3.92116400	1.99822300	0.28851800
C	4.83862900	0.26736500	1.31122800
C	5.83301300	0.45350500	0.32954800
S	5.39973900	1.80607000	-0.67951100
N	3.78465000	1.15540000	1.25707600
C	2.92904100	3.10307800	-0.01054800
C	1.53713100	2.52854500	0.29980800
C	0.33685000	3.37434600	-0.10339300
H	1.44971800	1.56237500	-0.21918400
H	1.48000200	2.29568500	1.37436800
C	-0.94407800	2.71339000	0.31381500
H	0.34558700	4.33811600	0.44073200
H	0.34051800	3.60286600	-1.17554100
H	-0.89793200	2.42404000	1.36607900
C	3.25945400	4.28424400	0.91009100
H	3.20259600	3.98241900	1.96390100
H	4.27344000	4.66089300	0.71593700
H	2.55864700	5.11456500	0.74492300
C	3.02348000	3.54368700	-1.47038200
H	2.73903200	2.73442300	-2.15880900
H	2.35901800	4.39636700	-1.65760400
H	4.03894600	3.87707100	-1.72682500
C	-2.27266200	3.21386100	-0.04959600
C	-3.31121500	3.05088800	0.87892200
C	-2.54050200	3.84495000	-1.27171000
C	-4.59070300	3.50863000	0.59371400
H	-3.09765400	2.55012000	1.82525000
C	-3.81791900	4.30833400	-1.54983200
H	-1.75185100	3.93804200	-2.01640900
C	-4.84564400	4.13713300	-0.62224200
H	-5.39011100	3.36558500	1.31869300
H	-4.01975600	4.79637500	-2.50172500
H	-5.84896700	4.49249600	-0.85165700
C	-1.35626900	0.32820400	2.33196800
N	-1.62844800	0.42386900	3.46725000

L*Cu^{I}CN

C	3.06469500	1.35082800	-1.71123500
O	2.10756800	2.25603700	-1.09055400
C	2.54832400	-0.04214800	-1.29039800
H	2.41674300	-0.75876800	-2.11049900
C	1.11339200	1.51036400	-0.59644900

N	1.22794900	0.23901000	-0.69548600
C	0.00016000	2.26689000	0.00002500
C	0.34661500	3.60825000	0.64852100
C	-0.34637100	3.60812100	-0.64876600
H	1.40480400	3.85356500	0.67543500
H	-0.22165100	3.85236200	1.54212500
H	0.22187900	3.85208000	-1.54242300
H	-1.40457500	3.85337200	-0.67573500
C	-3.06449200	1.35101500	1.71119900
O	-2.10696900	2.25618300	1.09110400
C	-2.54829800	-0.04200800	1.29024700
H	-2.41651900	-0.75862800	2.11031400
C	-1.11311200	1.51041400	0.59651000
N	-1.22804800	0.23905300	0.69498600
C	5.57200700	0.20416000	0.83675800
C	5.51170200	-0.93659300	1.63251100
C	4.47458100	-1.85749900	1.48029300
C	3.47618100	-1.64919400	0.53358900
C	3.53459400	-0.50060400	-0.24874400
C	4.57381000	0.41777300	-0.10732700
H	6.38899800	0.91636000	0.95238900
H	6.28495000	-1.11456500	2.37816900
H	4.44544100	-2.74856200	2.10443100
H	2.67340700	-2.37457200	0.39957800
C	4.45130500	1.54100700	-1.10111600
H	4.54728000	2.54189100	-0.65878000
H	5.22040000	1.46885700	-1.88408000
C	-3.47673200	-1.64933300	-0.53314000
C	-3.53479300	-0.50049100	0.24884900
C	-4.57379700	0.41809400	0.10728900
C	-5.57216800	0.20441900	-0.83660000
C	-5.51222400	-0.93658700	-1.63201600
C	-4.47529300	-1.85769000	-1.47965900
H	-2.67410800	-2.37485300	-0.39897500
H	-6.38902100	0.91676200	-0.95233700
H	-6.28561300	-1.11461000	-2.37751600
H	-4.44644800	-2.74894800	-2.10353100
C	-4.45091500	1.54161900	1.10070600
H	-4.54625300	2.54237700	0.65793900
H	-3.02135200	1.55181700	2.78702800
H	-5.22024400	1.47021300	1.88350300
H	3.02121700	1.55190900	-2.78700300
C	-0.65554900	-2.52896700	1.32216500
N	-1.16672600	-3.18682400	2.14322900

Cu	-0.00005900	-1.24913800	-0.00018300
C	0.65555000	-2.52921400	-1.32220900
N	1.16719000	-3.18646400	-2.14346300

R-2a

C	-3.78243900	-0.88210400	-1.46205300
C	-4.28274800	-2.14828300	-1.21039600
C	-3.85559200	-2.88049300	-0.09505900
C	-2.92049700	-2.35955300	0.78758000
C	-1.42657800	1.15080300	0.23190400
C	-2.83946000	-0.33981400	-0.58551100
C	-2.41667100	-1.08664700	0.53204300
S	-1.24692900	-0.15857000	1.43678900
N	-2.25954200	0.90746300	-0.71985400
C	-0.60376600	2.40742800	0.36522800
C	0.89253800	2.06559000	0.21566300
C	1.28551800	1.38608400	-1.10188700
C	2.74105300	1.07049200	-1.14637400
C	-1.04194800	3.41147700	-0.69856700
C	-0.82258200	3.02526300	1.75014200
C	3.37514972	-0.14532531	-0.56344207
C	4.78535172	-0.30718731	-0.62537407
C	2.63079972	-1.17803431	0.06755493
C	5.40586672	-1.42127431	-0.09599607
C	3.26305672	-2.28902131	0.59537493
C	4.65118972	-2.42365131	0.52034693
H	-4.10173100	-0.29791000	-2.32251500
H	-5.01729900	-2.58192200	-1.88627000
H	-4.26256000	-3.87403200	0.08392800
H	-2.59132000	-2.93056600	1.65341700
H	1.46423100	3.00160900	0.32841200
H	1.20555400	1.42070500	1.05336500
H	0.68071500	0.47405300	-1.23491000
H	1.02870800	2.04459600	-1.94375400
H	2.70709256	0.67481095	-2.13994493
H	-2.08226700	3.71896000	-0.53576900
H	-0.40309800	4.30402200	-0.64467800
H	-0.98524700	2.99435400	-1.70933000
H	-1.88521600	3.24245300	1.92167200
H	-0.47554600	2.36485900	2.55640800
H	-0.26416100	3.96814000	1.82839100
H	5.37645572	0.47346969	-1.10563507
H	1.54626272	-1.09394931	0.13843593
H	6.48880272	-1.51785031	-0.15952807

H	2.66893072	-3.06598031	1.07451793
H	5.14094572	-3.30140831	0.93786093
C	3.65860633	2.30645908	-1.19199492
N	4.34176650	3.22669275	-1.22596175

V

C	0.92920800	3.38755400	1.61474500
O	2.35880500	3.17941100	1.69771800
C	0.51826300	2.33467000	0.56959200
H	-0.41826800	1.81625100	0.82376300
C	2.61320600	1.99250000	1.10007000
N	1.64178300	1.39287700	0.52722000
C	4.01246800	1.53675800	1.21037800
C	5.04087700	2.52387700	1.74854500
C	4.57602000	1.44137400	2.63150000
H	4.67498500	3.53174400	1.92063400
H	6.03383500	2.44734900	1.31483200
H	3.86662100	1.67128500	3.42303600
H	5.21685100	0.58378900	2.82102400
C	6.05117900	-0.89502700	-0.46577500
O	5.82983700	0.32223500	0.27790300
C	4.75407200	-1.06559700	-1.28084700
H	4.80487600	-0.71798900	-2.32295300
C	4.49882700	0.52314600	0.25816500
N	3.81291200	-0.19113400	-0.55441700
C	0.38619100	5.41566300	-1.48387400
C	0.24262000	4.94265300	-2.78618200
C	0.20115300	3.57110800	-3.04485000
C	0.28843600	2.65016400	-2.00423000
C	0.40812700	3.13074000	-0.70543000
C	0.47409600	4.49824800	-0.44257800
H	0.43768700	6.48672100	-1.28707500
H	0.17708500	5.64938200	-3.61228600
H	0.11179900	3.21539100	-4.06984800
H	0.28273500	1.57763200	-2.20668000
C	0.61508200	4.76059400	1.03208400
H	1.39776000	5.48915300	1.28269500
H	-0.32446200	5.13793400	1.46533600
C	3.50392300	-3.26746600	-1.88219900
C	4.43846200	-2.52900800	-1.16581500
C	5.23106700	-3.12272600	-0.18382200
C	5.08403900	-4.47147600	0.11086700
C	4.13866600	-5.21489000	-0.59256100
C	3.35823900	-4.62073500	-1.58420400

H	2.89255800	-2.79217800	-2.64929100
H	5.69367300	-4.94045600	0.88259900
H	4.01454200	-6.27411200	-0.37158100
H	2.63232900	-5.21875700	-2.13366400
C	6.14162700	-2.11759500	0.46180100
H	5.75418900	-1.84844700	1.45820800
H	6.94949300	-0.73986700	-1.07003600
H	7.17062200	-2.47615400	0.59321900
H	0.51776200	3.22575600	2.61939100
C	2.60149500	-1.47956000	1.56820900
N	3.24555600	-1.73603400	2.51146100
Cu	1.84544300	-0.88935000	-0.09900400
C	1.27832700	-0.80552000	-1.93341800
N	1.02567200	-0.76778100	-3.07548700
C	-9.41321800	-2.17428700	0.40988700
C	-8.70915500	-2.94680500	1.34322700
C	-7.33217400	-2.84788900	1.45169700
C	-6.64819300	-1.96246600	0.61438700
C	-7.36789000	-1.18985300	-0.32041100
C	-8.75307200	-1.28949500	-0.43088200
C	0.17357600	-3.23404800	-0.21118600
C	-0.15868900	-1.90237300	1.90191700
C	-0.04229400	-1.88231200	0.40124900
C	-1.08280200	-0.99901500	-0.25592300
C	-2.51618300	-1.35631900	0.15883200
C	-3.52772300	-0.41961600	-0.50922900
C	-3.37350800	1.01338900	-0.03368000
C	-3.65220100	1.34482300	1.29645000
C	-2.94371200	2.01313000	-0.90363500
C	-3.49958400	2.65167300	1.74303100
C	-2.79456400	3.32576600	-0.46029100
C	-3.07319100	3.64689900	0.86371800
S	-6.25573800	-0.18538200	-1.21631300
N	-5.27937300	-1.76699500	0.61634800
C	-4.93285100	-0.89514900	-0.26751800
H	-9.25308700	-3.63294600	1.98976100
H	-6.76798100	-3.44004700	2.16935200
H	-9.30317400	-0.69132200	-1.15460700
H	0.22878700	-3.19345000	-1.30430200
H	1.07795400	-3.71889600	0.17762100
H	-0.68543000	-3.87179900	0.07071100
H	0.62046600	-2.49620100	2.38253600
H	-0.14961000	-0.89074200	2.33004200
H	-1.13088600	-2.36201200	2.14985300

H	-0.89384200	0.05130100	0.01127700
H	-1.00098100	-1.06114200	-1.34794900
H	-2.74997700	-2.39510700	-0.11755300
H	-2.65479700	-1.28728500	1.24520000
H	-3.35101100	-0.43180800	-1.59882400
H	-4.00867200	0.57135100	1.97852000
H	-2.70818900	1.76095800	-1.93912700
H	-3.72735600	2.89888100	2.77895600
H	-2.45232800	4.09356600	-1.15323300
H	-2.97147600	4.67521700	1.20952200
H	-10.49555800	-2.26839700	0.34135300

TS4

C	-0.83116500	3.23079100	-1.69386300
O	-2.26992100	3.11398000	-1.78889100
C	-0.50167400	2.18088400	-0.61663500
H	0.40779900	1.60090400	-0.83925000
C	-2.60744400	1.95377700	-1.18182900
N	-1.67926900	1.30763000	-0.58427100
C	-4.02224300	1.56446000	-1.32616900
C	-4.97702800	2.55905300	-1.97386100
C	-4.51164800	1.41114700	-2.76994700
H	-4.56411100	3.54222200	-2.18040000
H	-5.99334300	2.54320100	-1.59005400
H	-3.75118200	1.57036700	-3.53108100
H	-5.16770200	0.56279300	-2.94704900
C	-6.23116500	-0.73162400	0.33134500
O	-5.92342400	0.41689700	-0.48636900
C	-4.99646000	-0.86198700	1.25033900
H	-5.14018200	-0.47847700	2.27090800
C	-4.59935600	0.62407800	-0.34633000
N	-3.98962700	-0.01947300	0.57779000
C	-0.22927200	5.30548200	1.35888000
C	-0.15059400	4.86270800	2.67754700
C	-0.19985500	3.49925600	2.97358000
C	-0.31429800	2.55575500	1.95584000
C	-0.37034900	3.00402100	0.64135700
C	-0.34633000	4.36556700	0.34104500
H	-0.21206000	6.37158800	1.13148300
H	-0.06713300	5.58793700	3.48588400
H	-0.16082000	3.16886500	4.01025500
H	-0.37811800	1.49161500	2.18842300
C	-0.43741800	4.59519900	-1.14272100
H	-1.16312100	5.36730700	-1.43107200

H	0.53537400	4.89445300	-1.56367900
C	-3.73774700	-3.01334000	1.99388400
C	-4.66335700	-2.32581500	1.21706800
C	-5.40142200	-2.97532400	0.22932300
C	-5.21006800	-4.33050000	-0.00728600
C	-4.27480000	-5.02310600	0.75743800
C	-3.54640900	-4.37228200	1.75393300
H	-3.16528700	-2.49544900	2.76274900
H	-5.77397700	-4.84110300	-0.78728600
H	-4.11576100	-6.08602200	0.58049900
H	-2.82824000	-4.93054300	2.35378900
C	-6.30003500	-2.02079100	-0.50280200
H	-5.89249200	-1.82987000	-1.50906000
H	-7.16350100	-0.50457100	0.85688800
H	-7.32637300	-2.39170800	-0.62281300
H	-0.42081400	3.01618600	-2.68907900
C	-2.92362500	-1.57687100	-1.70140100
N	-3.58095500	-1.84734500	-2.63327100
Cu	-2.06590700	-0.89236200	-0.05976400
C	-1.18293600	-0.96129300	1.60350900
N	-1.02304500	-0.85701200	2.75978800
C	9.49331500	-2.16362500	-0.86784900
C	8.69912500	-2.90563500	-1.75246000
C	7.31813000	-2.80899800	-1.71811200
C	6.72166000	-1.95688800	-0.78481700
C	7.53167300	-1.21507900	0.09960900
C	8.92094400	-1.31201800	0.06617300
C	-0.01599400	-3.26549400	0.65145300
C	0.13004100	-1.85663100	-1.41898000
C	0.16593700	-1.88937600	0.08751700
C	1.27700800	-1.03451400	0.66544000
C	2.65634100	-1.37610400	0.09432700
C	3.73116900	-0.47370500	0.71003700
C	3.52080500	0.98198300	0.33652900
C	3.70261100	1.40069700	-0.98535000
C	3.11591000	1.91260700	1.29178900
C	3.48531100	2.72743300	-1.33949500
C	2.89923200	3.24190800	0.94018900
C	3.08758500	3.65202100	-0.37491300
S	6.51572300	-0.24698200	1.13856800
N	5.35934000	-1.76726000	-0.64060700
C	5.10452400	-0.92880600	0.30459800
H	9.17551000	-3.56595400	-2.47470000
H	6.68511200	-3.37768700	-2.39621300

H	9.54077200	-0.73738000	0.75154500
H	0.03450600	-3.28114700	1.74449800
H	-0.96679800	-3.70560300	0.32635000
H	0.79632100	-3.89607800	0.24857400
H	-0.68333100	-2.44599100	-1.84437000
H	0.08628100	-0.83935800	-1.82837800
H	1.08224200	-2.30702800	-1.75254500
H	1.06025200	0.02408900	0.45814200
H	1.30188800	-1.13803800	1.75762800
H	2.91234000	-2.42809200	0.28931300
H	2.69021100	-1.24561500	-0.99505800
H	3.66478500	-0.54977500	1.80945100
H	4.03454800	0.68094000	-1.73549500
H	2.94792800	1.58919700	2.32087900
H	3.63983400	3.04389400	-2.37022000
H	2.56469000	3.95347500	1.69406300
H	2.92648400	4.69520500	-0.64655500
H	10.57707300	-2.25544800	-0.91239100

VI

C	-2.74294900	-2.48013000	1.53882100
H	-2.87452400	-1.53293200	2.07410200
H	-3.46384700	-3.19825700	1.94827500
H	-1.72901800	-2.85338200	1.74025300
C	-2.90205400	-3.70012300	-0.64313400
H	-1.93040700	-4.17508500	-0.45234100
H	-3.68875600	-4.35223500	-0.24470800
H	-3.03906500	-3.61875100	-1.72837500
C	-2.93317900	-2.32268000	0.02609300
C	-1.83449000	-1.43678700	-0.58818000
C	-1.79252100	-0.00421300	-0.07932800
H	-0.87375500	-1.94061900	-0.39082900
H	-1.95584200	-1.42886000	-1.68346500
H	-2.74626000	0.49955200	-0.29964400
H	-1.67884800	0.00465600	1.01633100
C	-0.65177900	0.79331400	-0.71378900
H	-0.74341300	0.70954900	-1.80948900
C	-0.62652800	2.26866300	-0.35705800
C	0.22139600	3.10665300	-1.08708900
C	-1.38416200	2.81666800	0.67574500
C	0.30505000	4.46092000	-0.79774500
H	0.82286000	2.67771800	-1.89033500
C	-1.30092500	4.17614500	0.96840400
H	-2.05548200	2.18881800	1.25957800

C	-0.45851500	5.00092800	0.23444300
H	0.96772300	5.09930100	-1.37965900
H	-1.90276800	4.58945700	1.77606500
H	-0.39624900	6.06325900	0.46365400
C	0.67901400	0.16589700	-0.40778700
N	1.47553200	-0.31979500	-1.29685400
S	1.22894400	0.04201900	1.28023500
C	2.61451500	-0.84441500	-0.71210800
C	3.66811100	-1.44243700	-1.40762800
C	4.75024500	-1.93196700	-0.69588900
C	4.79560100	-1.83235200	0.70069100
C	3.75971900	-1.24185800	1.41008600
C	2.67157100	-0.75089100	0.69318400
H	3.61482800	-1.50993100	-2.49217200
H	5.57735400	-2.39965000	-1.22646600
H	5.65659500	-2.22302700	1.23990200
H	3.79879200	-1.16446100	2.49474500
C	-4.24451400	-1.70584200	-0.22748200
N	-5.27334200	-1.20597400	-0.42895700

9. References

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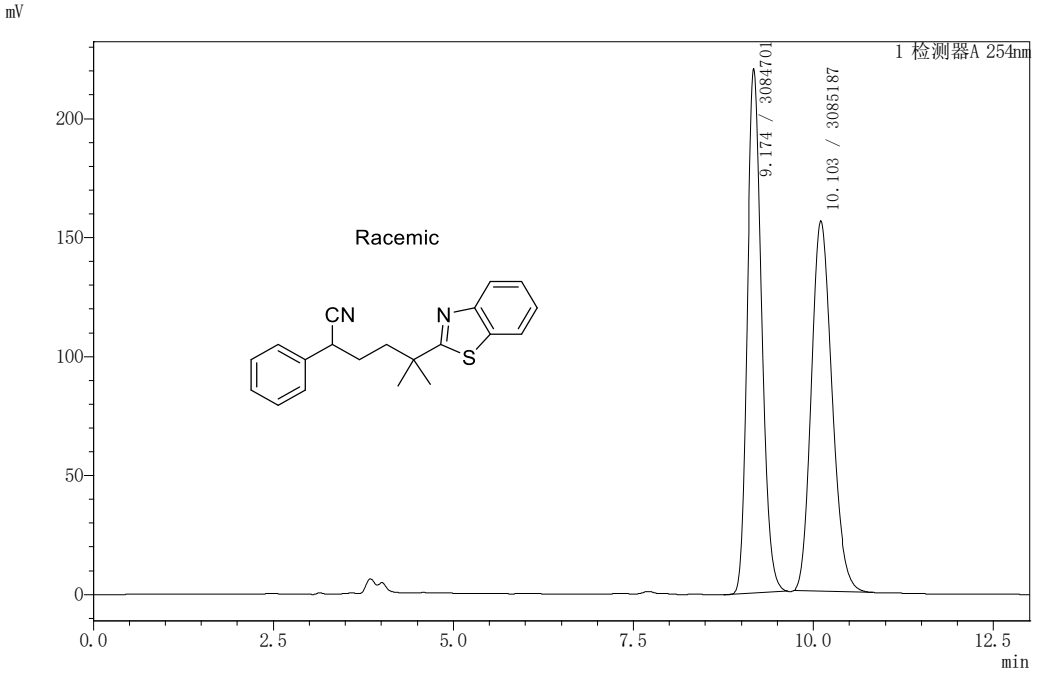
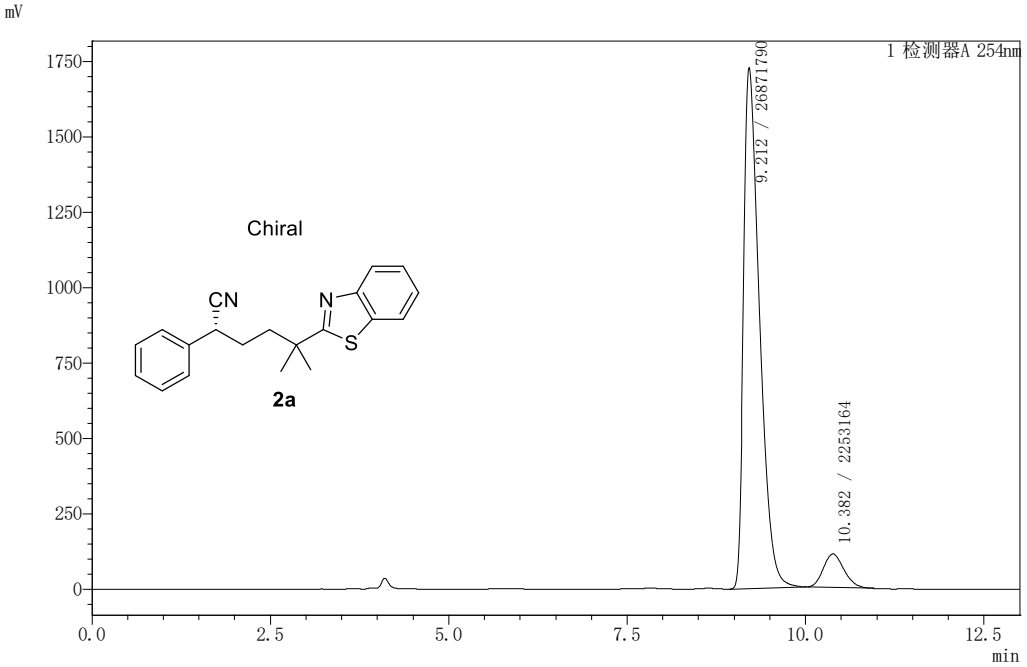
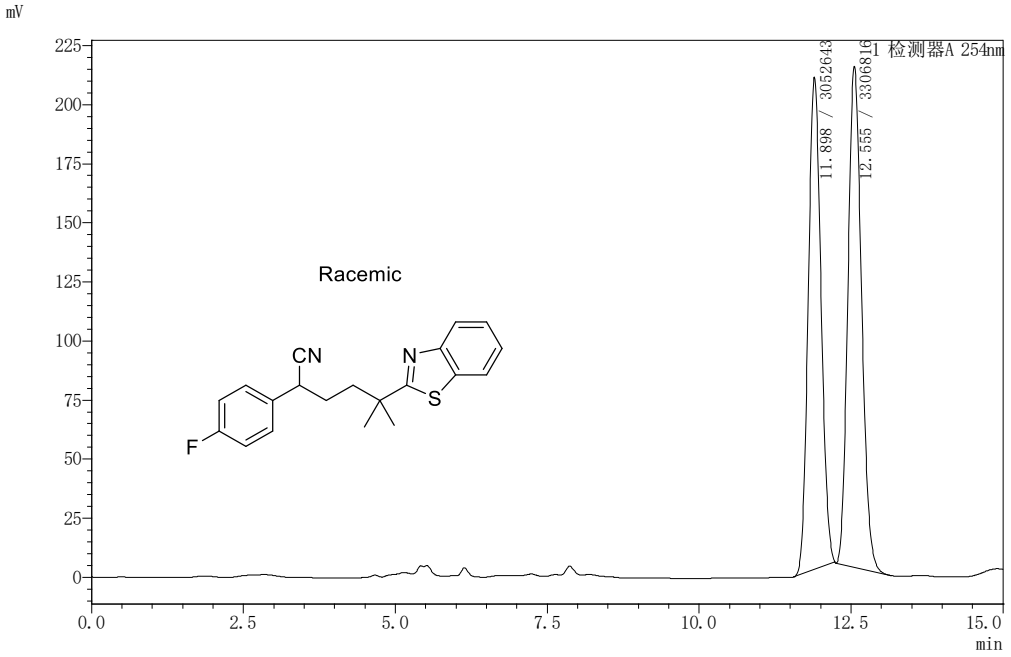
10. HPLC Charts of Products



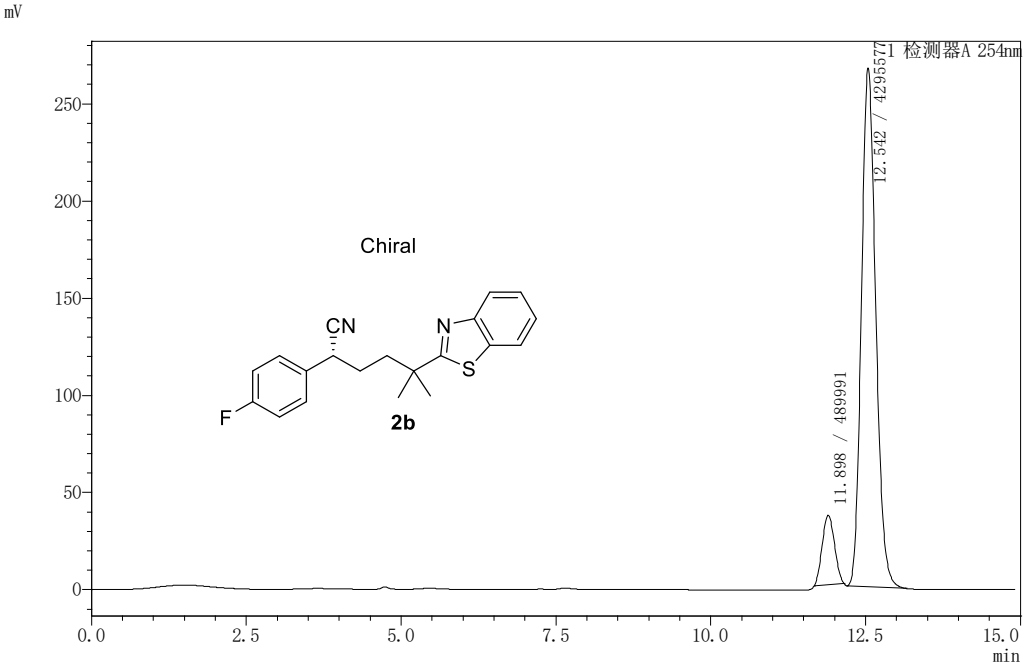
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	9.174	220488	3084701	49.996
2	10.103	155689	3085187	50.004
Total		376177	6169888	100.000



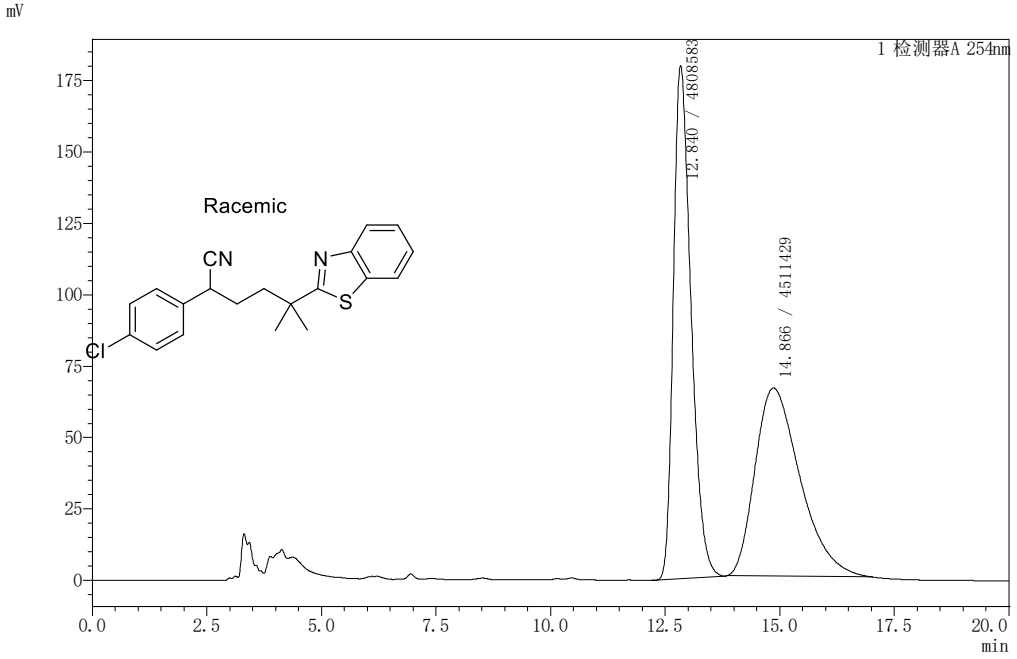
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	9.212	1728175	26871790	92.264
2	10.382	111125	2253164	7.736
Total		1839300	29124955	100.000



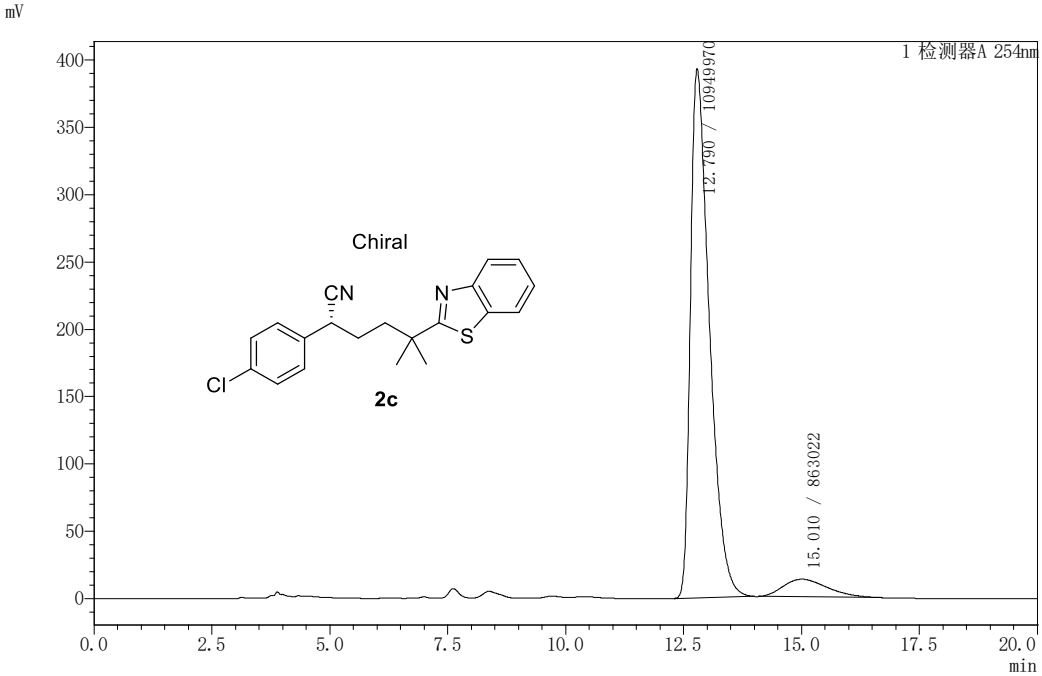
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	11.898	208485	3052643	48.002
2	12.555	212010	3306816	51.998
Total		420495	6359459	100.000



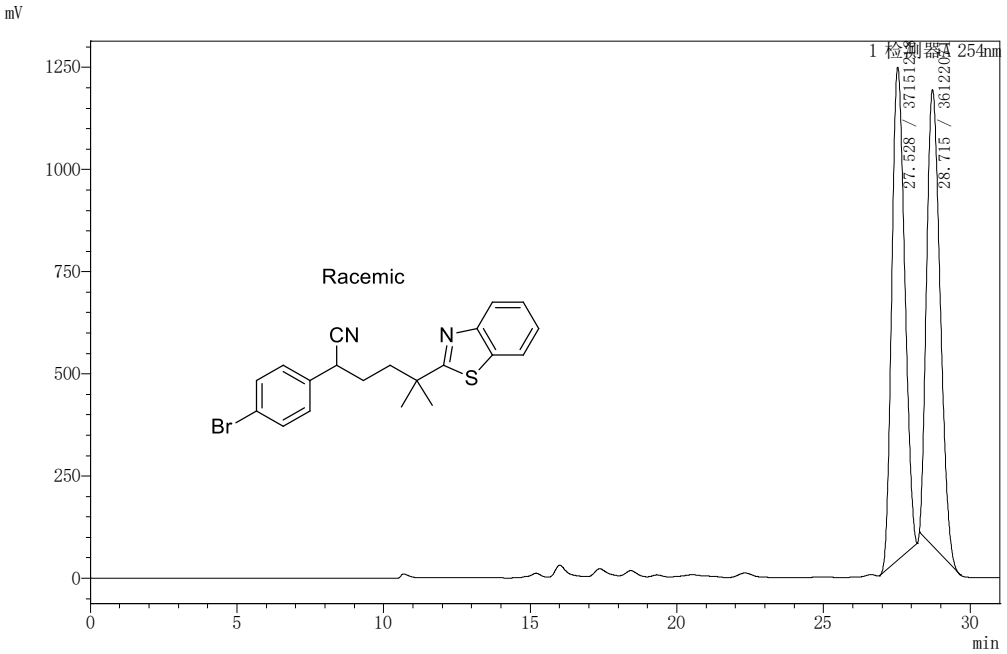
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	11.898	37337	489991	10.239
2	12.542	267130	4295577	89.761
Total		304467	4785568	100.000



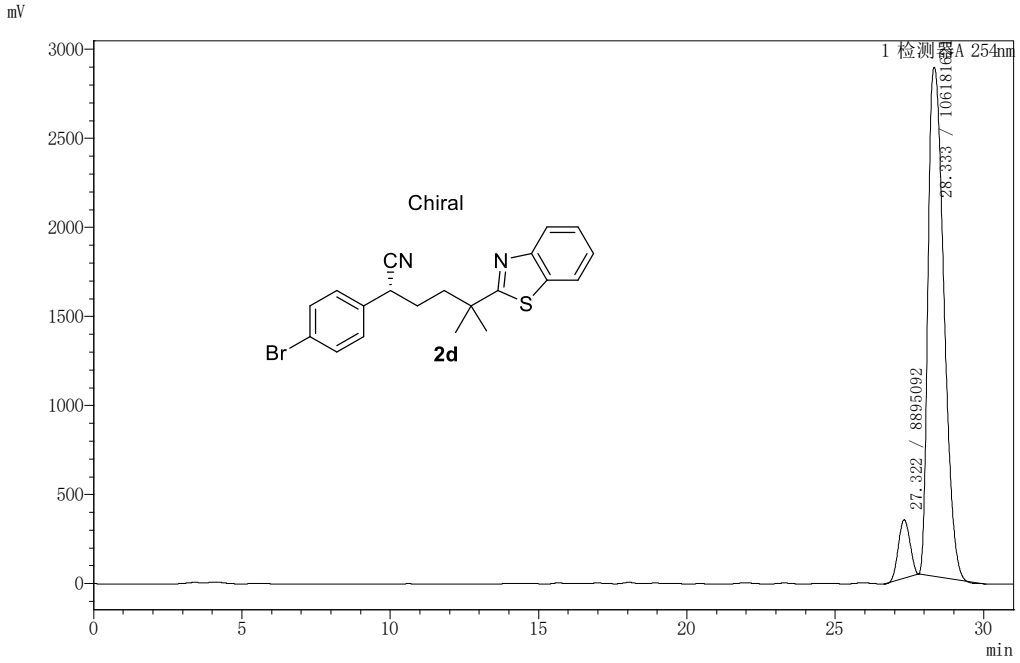
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	12.840	179729	4808583	51.594
2	14.866	65893	4511429	48.406
Total		245623	9320012	100.000



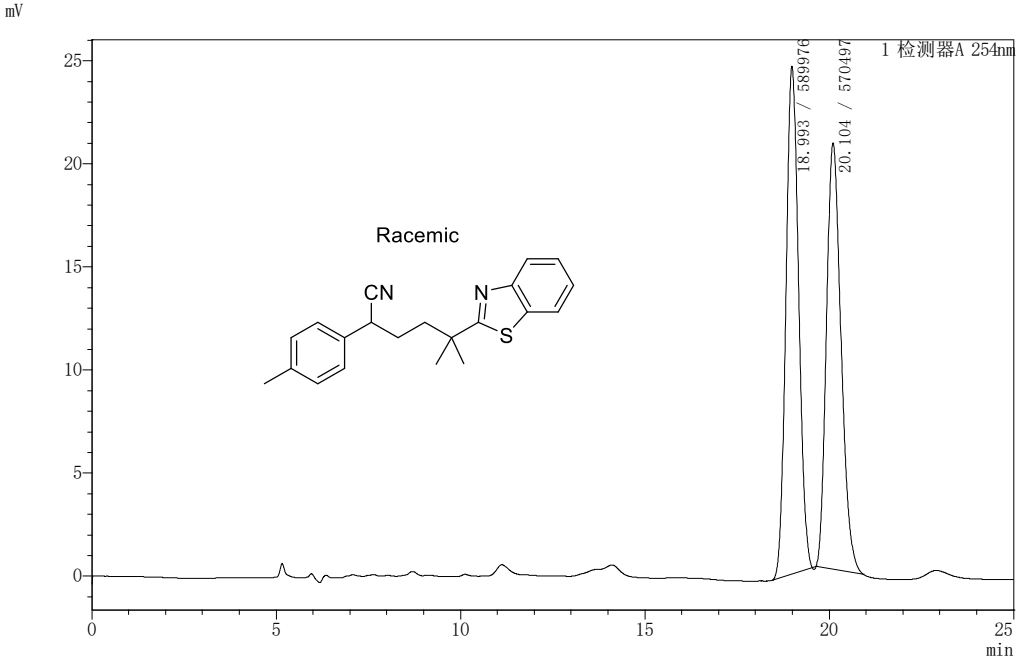
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	12.790	393024	10929525	92.543
2	15.010	13232	880719	7.457
Total		406256	11810244	100.000



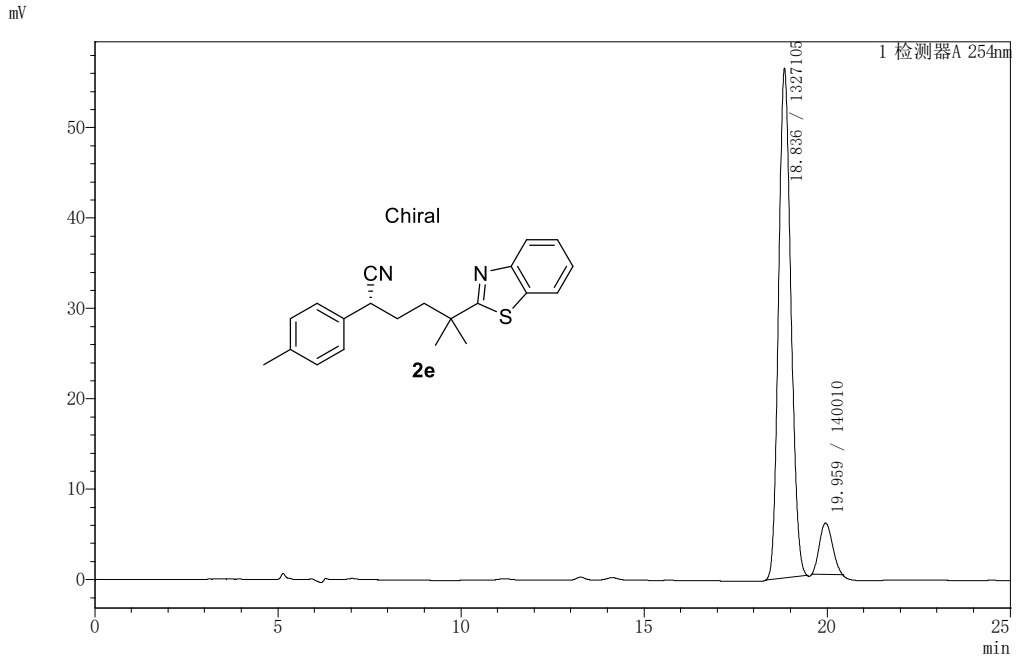
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	27.528	1206332	37151218	50.702
2	28.715	1116886	36122071	49.298
Total		2323218	73273289	100.000



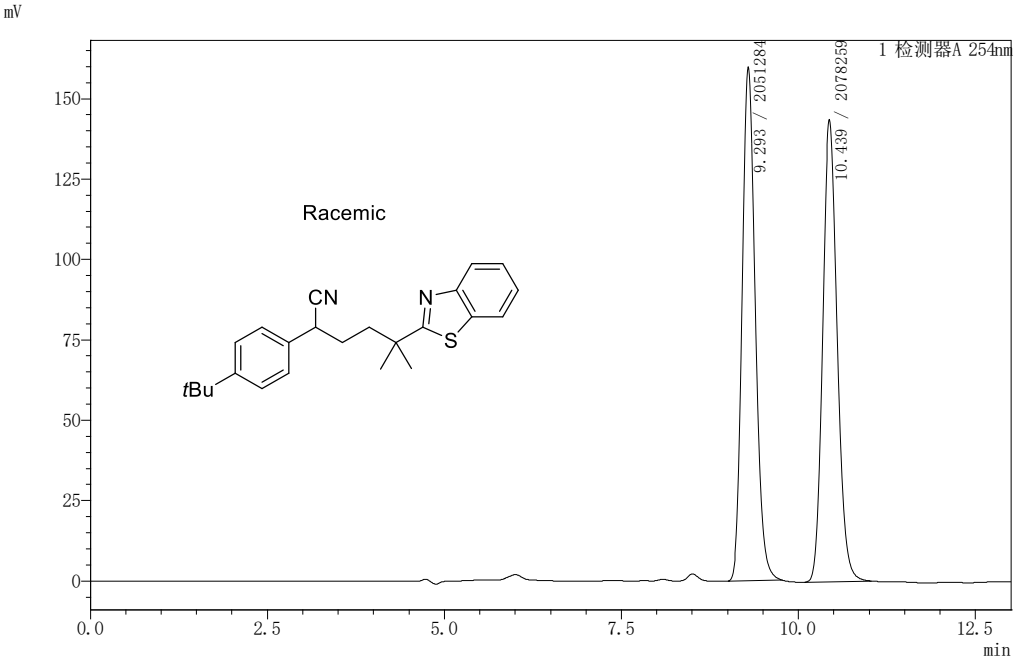
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	27.322	328219	88955092	7.730
2	28.333	28599543	106181612	92.270
Total		3187762	115076713	100.000



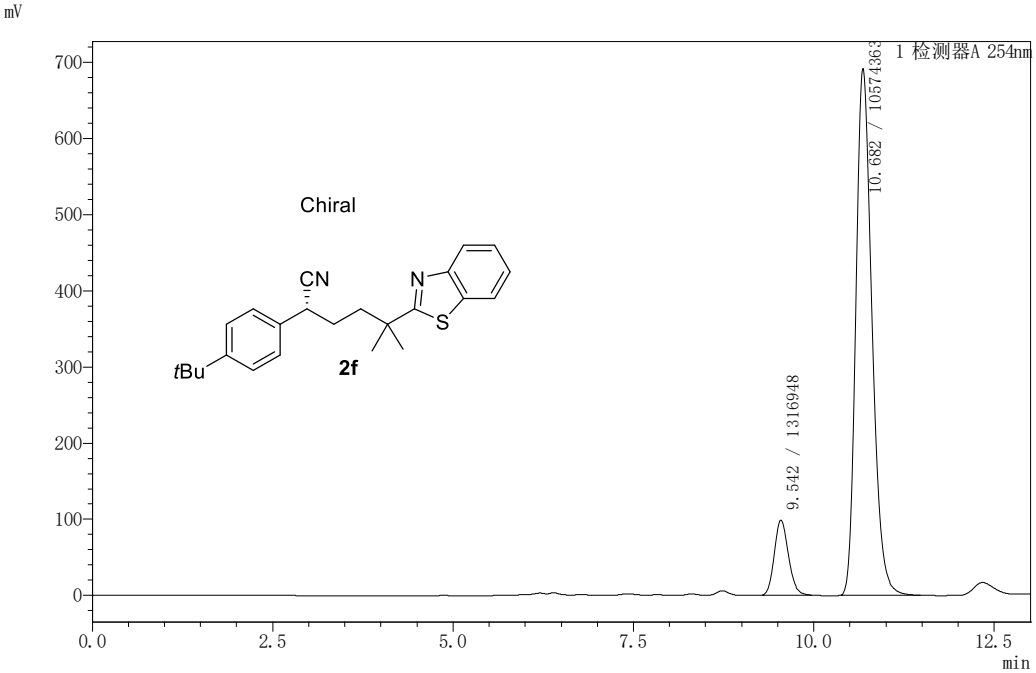
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	18.993	24637	589976	50.839
2	20.104	20688	570497	49.161
Total		45326	1160474	100.000



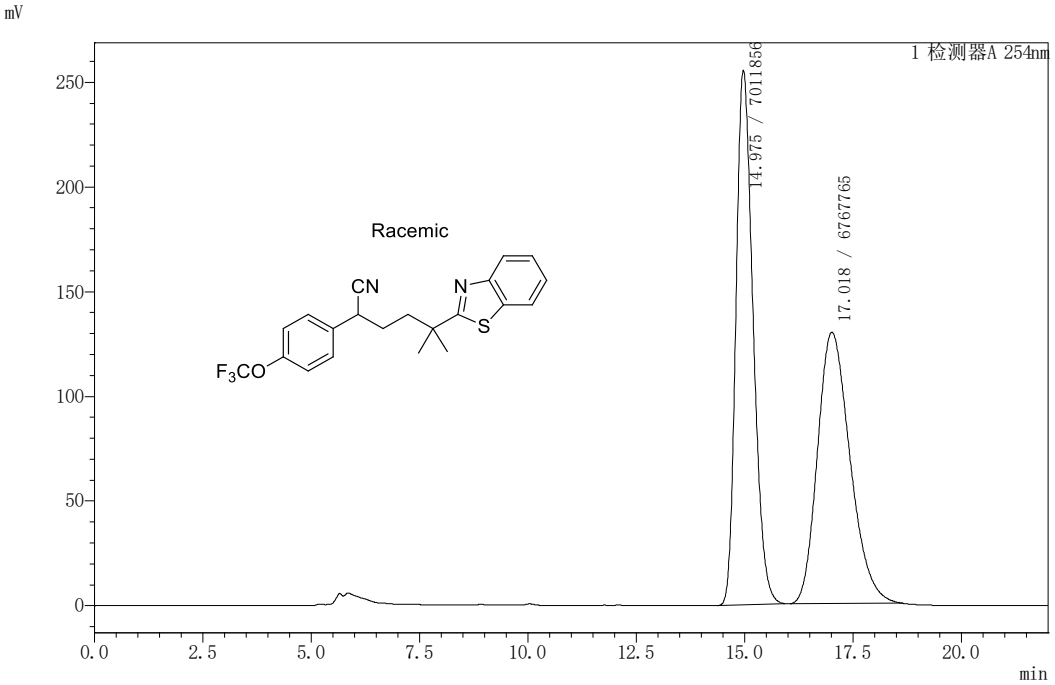
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	18.836	56523	1327105	90.457
2	19.959	5955	140010	9.543
Total		62477	1467115	100.000



No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	9.292	159855	2051284	49.673
2	10.439	143862	2078259	50.327
Total		303717	4129543	100.000



No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	9.542	98622	1316948	11.075
2	10.682	691900	10574363	88.925
Total		790522	11891311	100.000



No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	14.975	255452	7011856	50.886
2	17.018	129520	6767765	49.114
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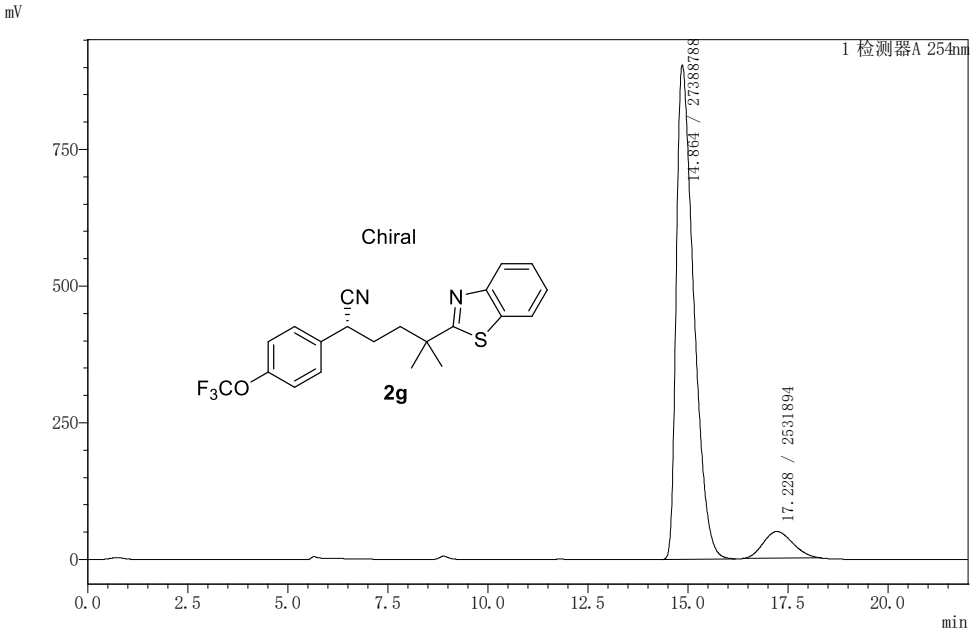

No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	14.864	904752	27388788	91.538
2	17.228	49003	2531894	8.462
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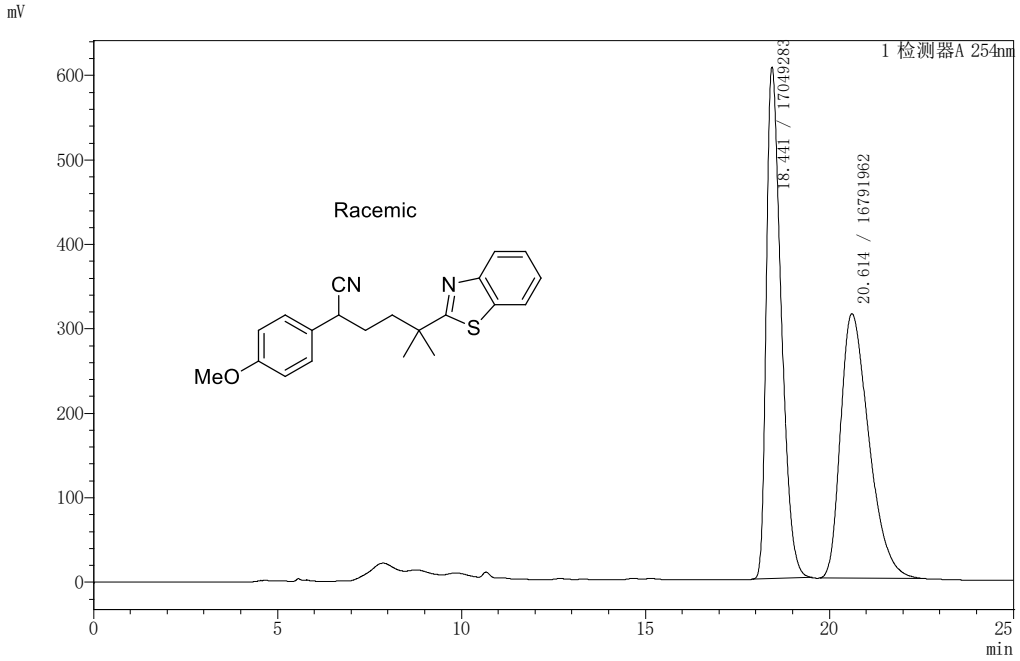

No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	18.441	606115	17049283	50.380
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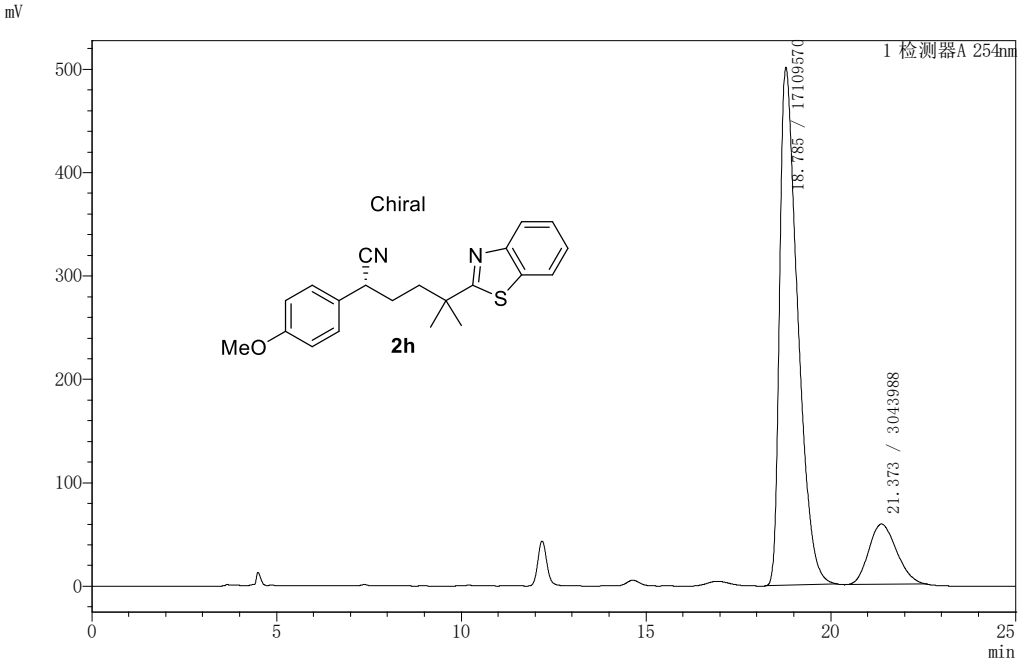
Total		919164	33841245	100.000



No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	18.785	501515	17109570	84.896
2	21.373	58205	3043988	15.104
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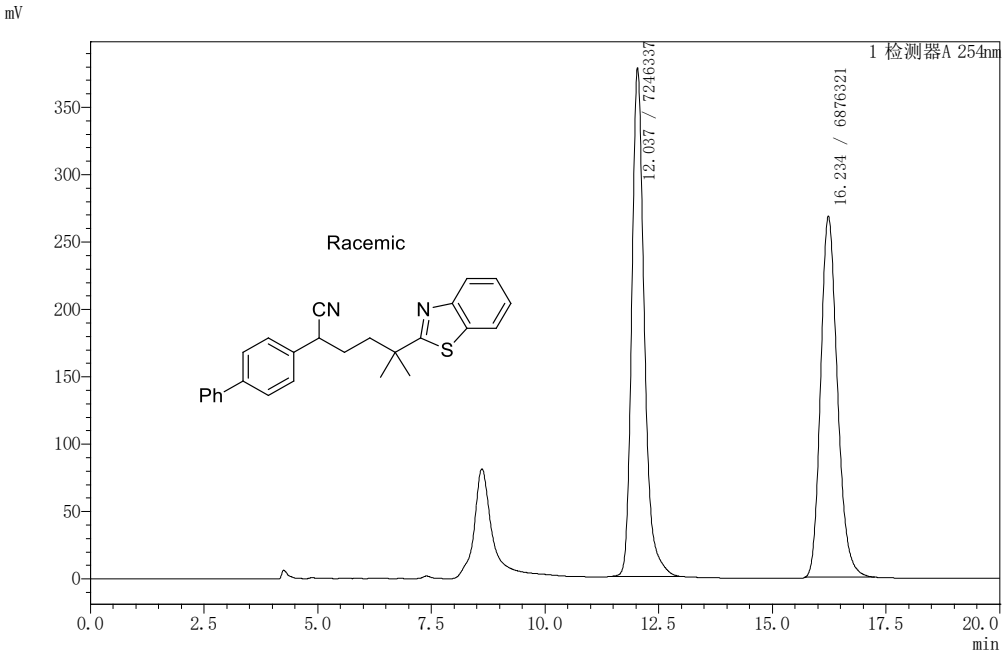

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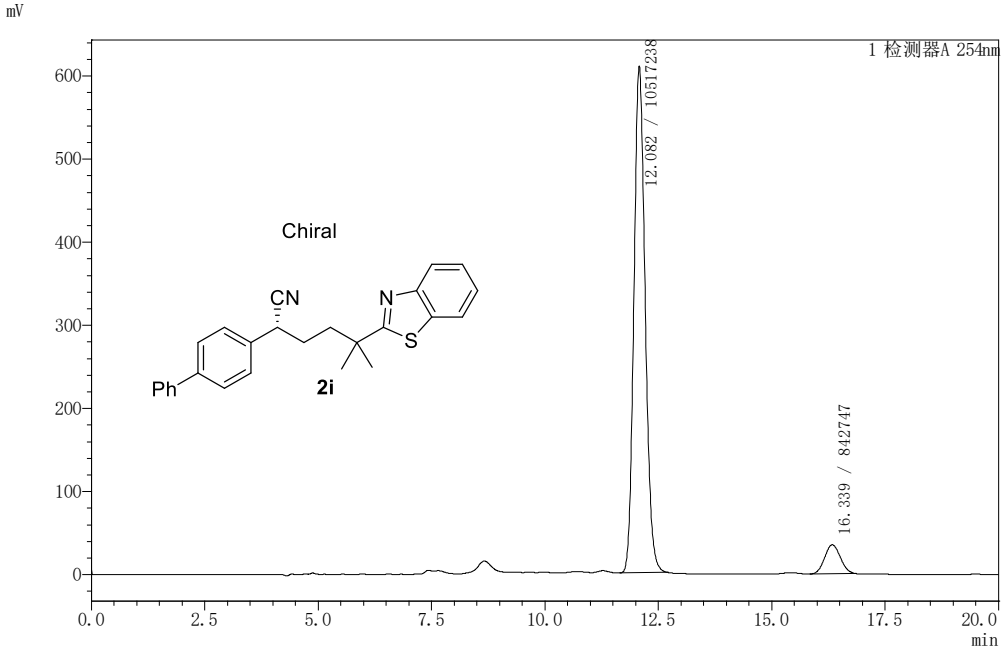
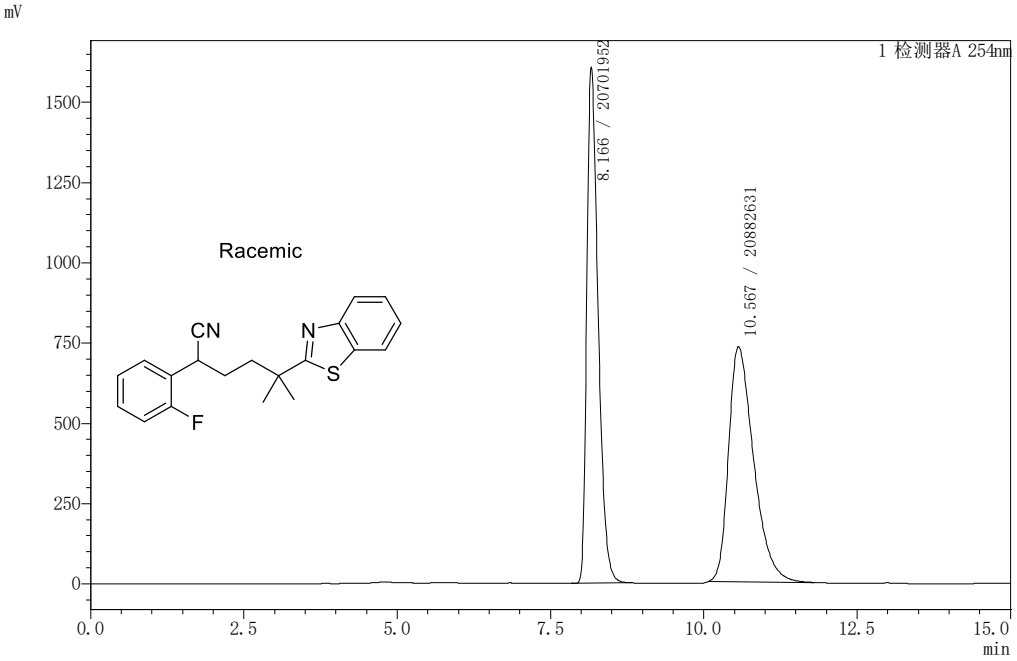
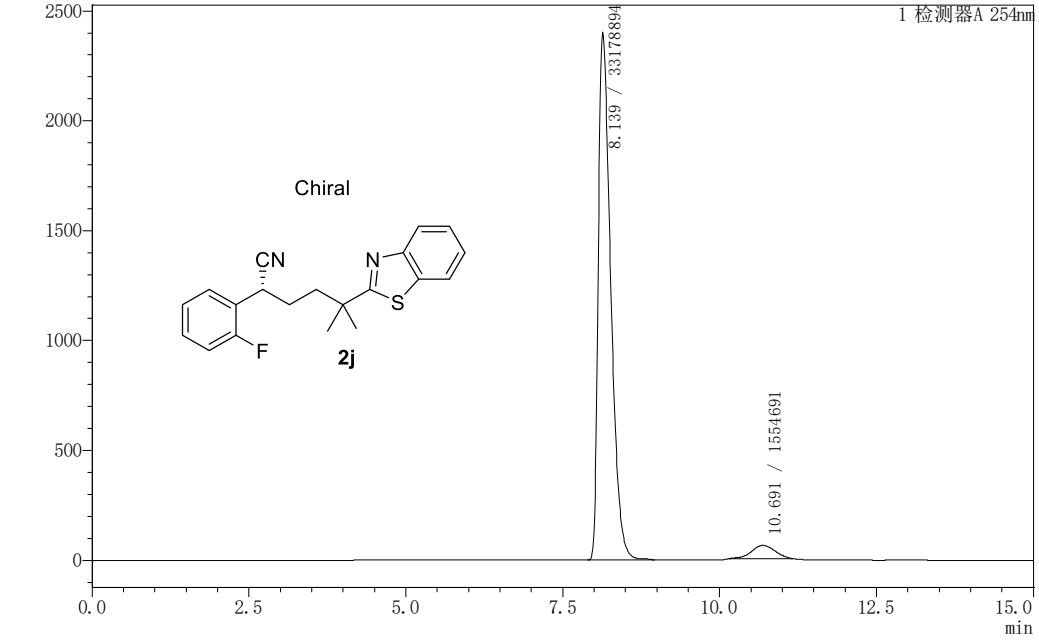
2	16.234	268260	6876321	48.690
Total		645888	14122658	100.000



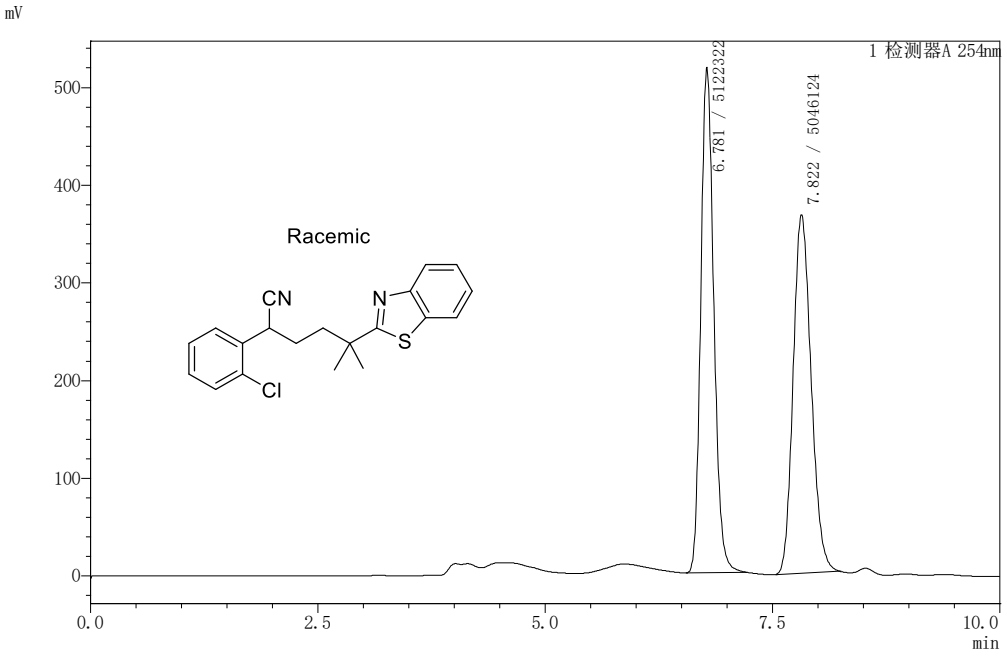
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	12.082	610038	10517238	92.581
2	16.339	34983	842747	7.419
Total		645021	11359985	100.000



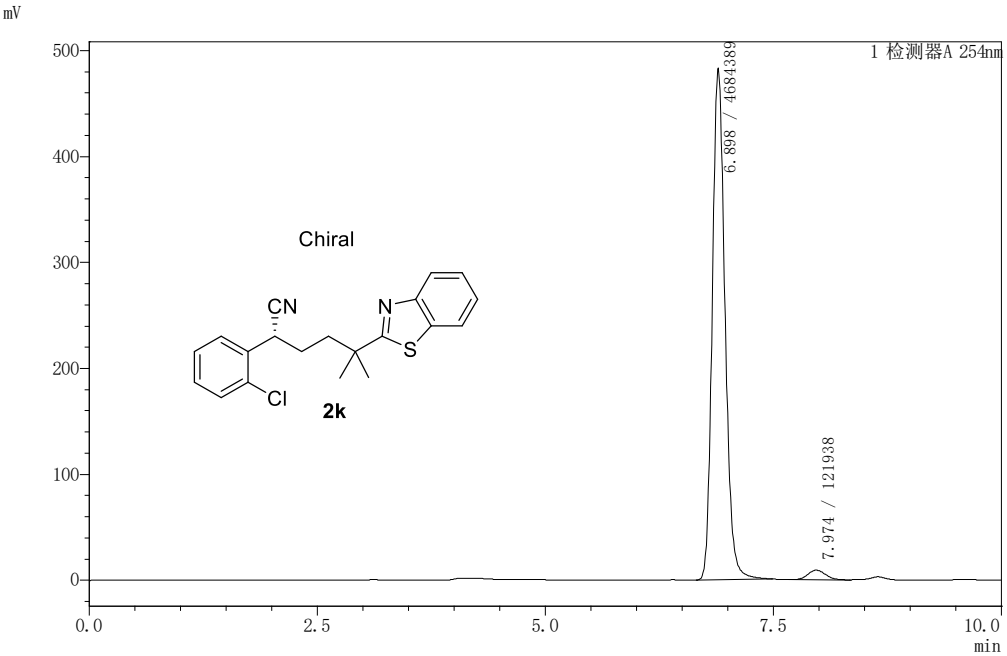
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	8.166	1609084	20701952	49.783
2	10.567	733230	20882631	50.217
Total		2342315	41584583	100.000



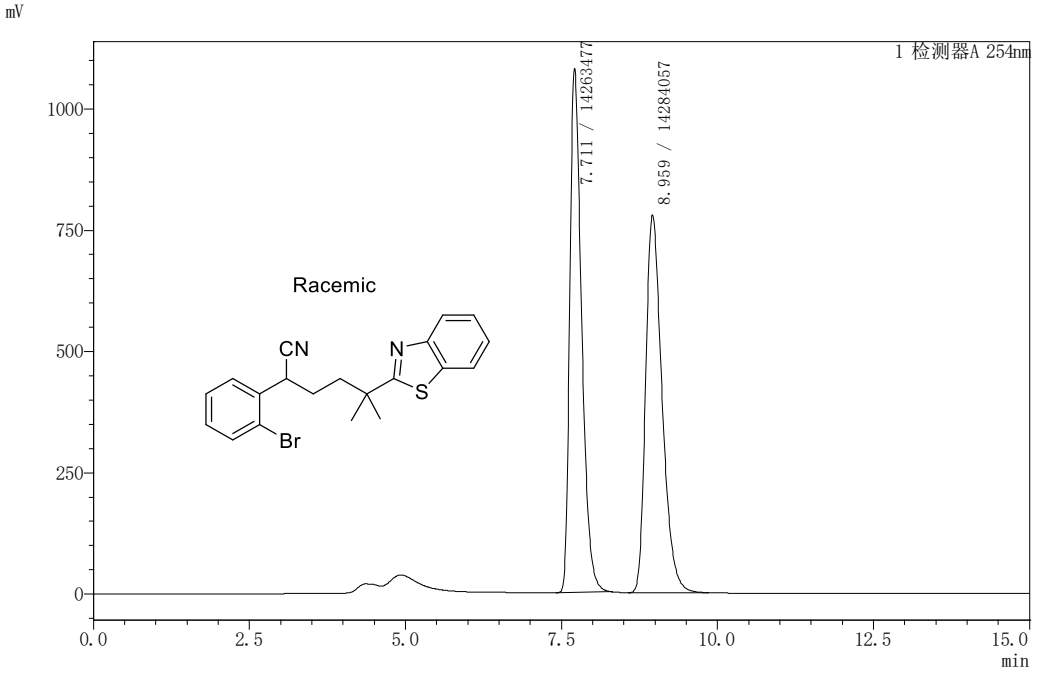
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	8.139	2403499	33178894	95.524
2	10.691	59423	1554691	4.476
Total		2462923	34733585	100.000



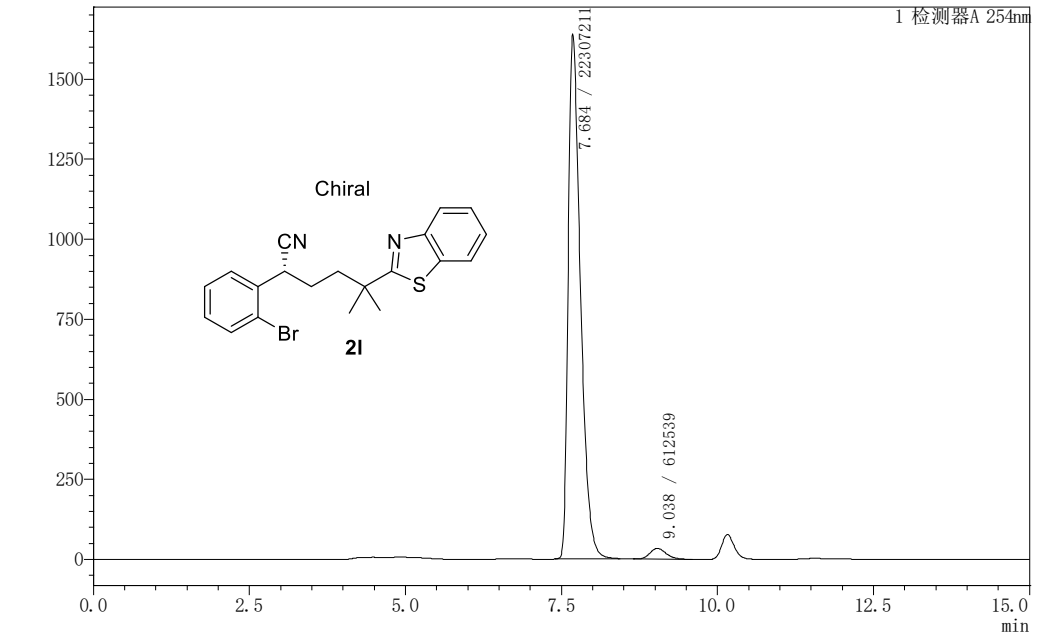
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	6.781	517486	5122322	50.375
2	7.832	366887	5046124	49.625
Total		884372	10168446	100.000



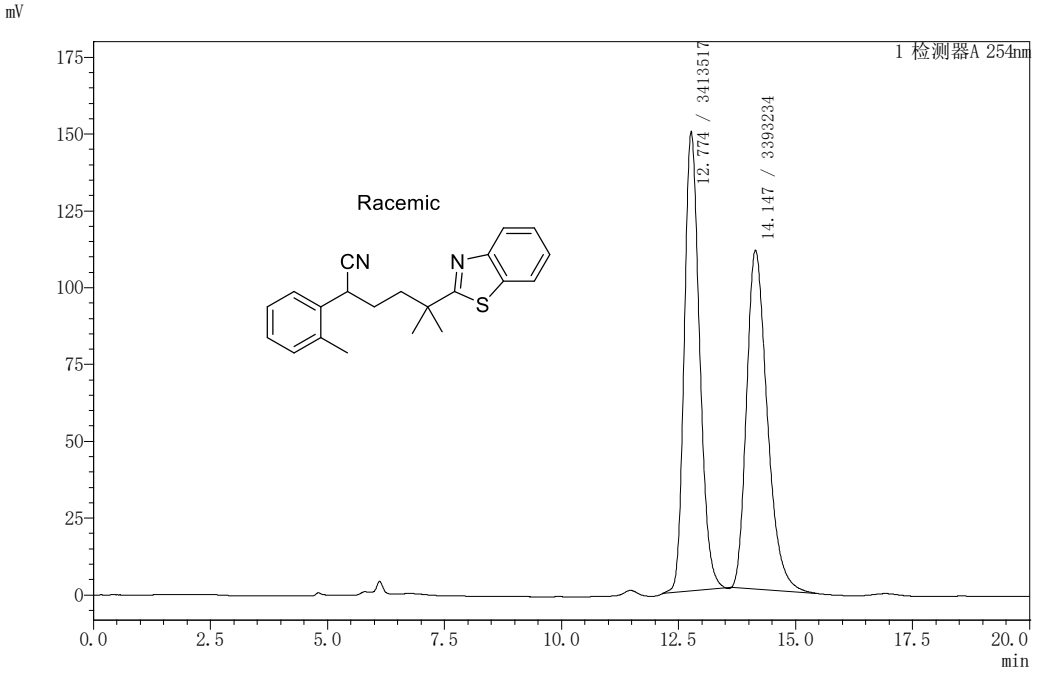
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	6.898	483354	4684389	97.463
2	7.974	9071	121938	2.537
Total		492425	4806327	100.000



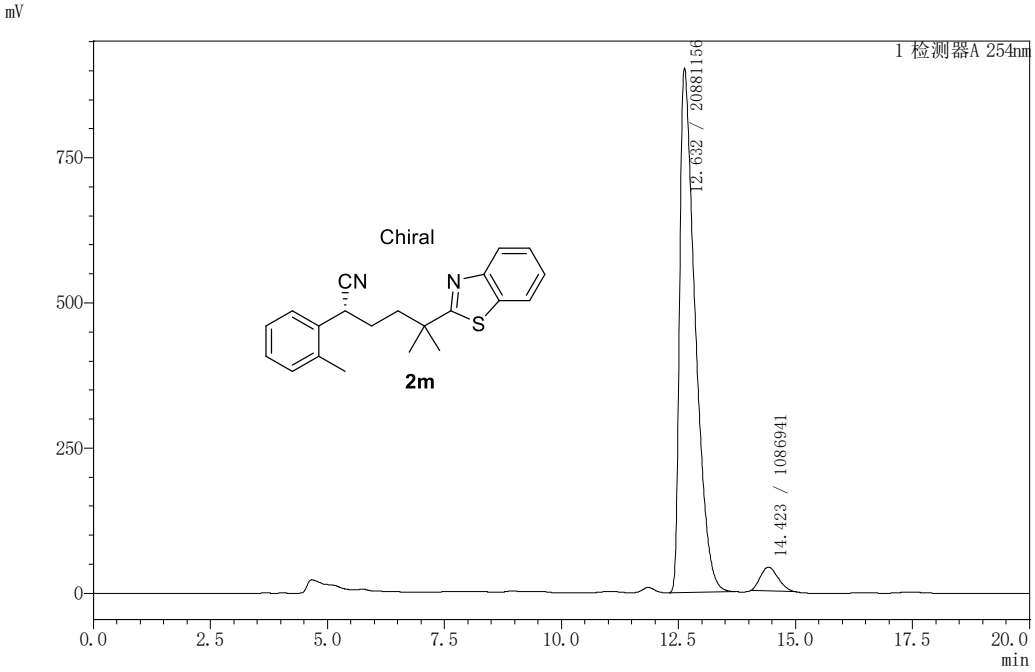
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	7.711	1081093	14263477	49.964
2	8.959	779868	14284057	50.036
Total		1860961	28547534	100.000



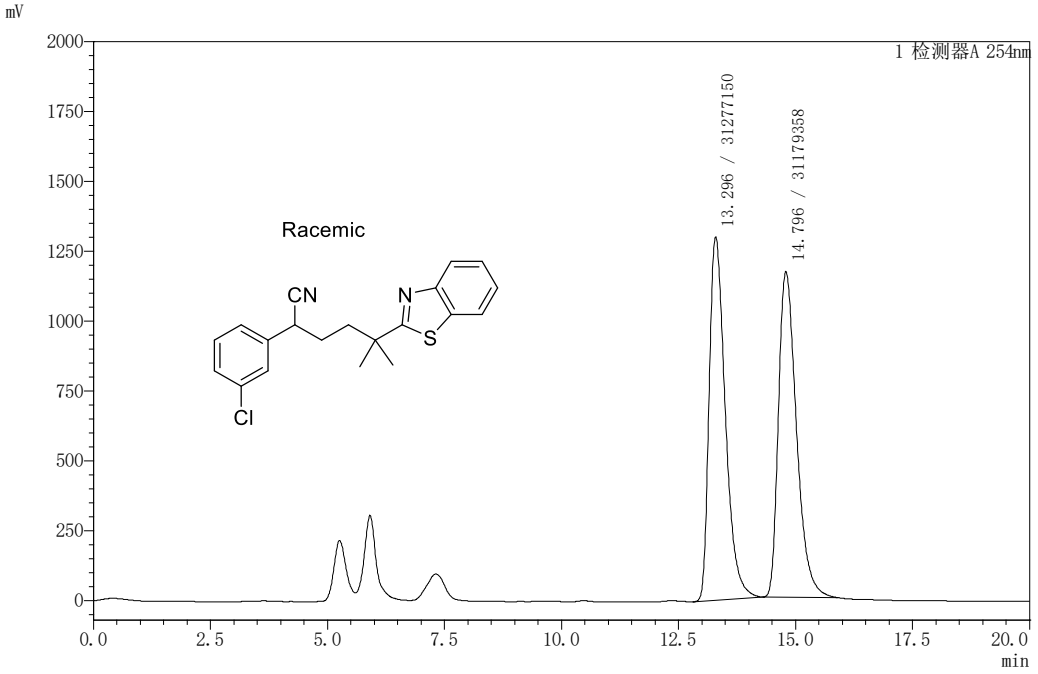
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	7.684	1640361	22307211	97.327
2	9.038	33904	612539	2.673
Total		1674265	22919750	100.000



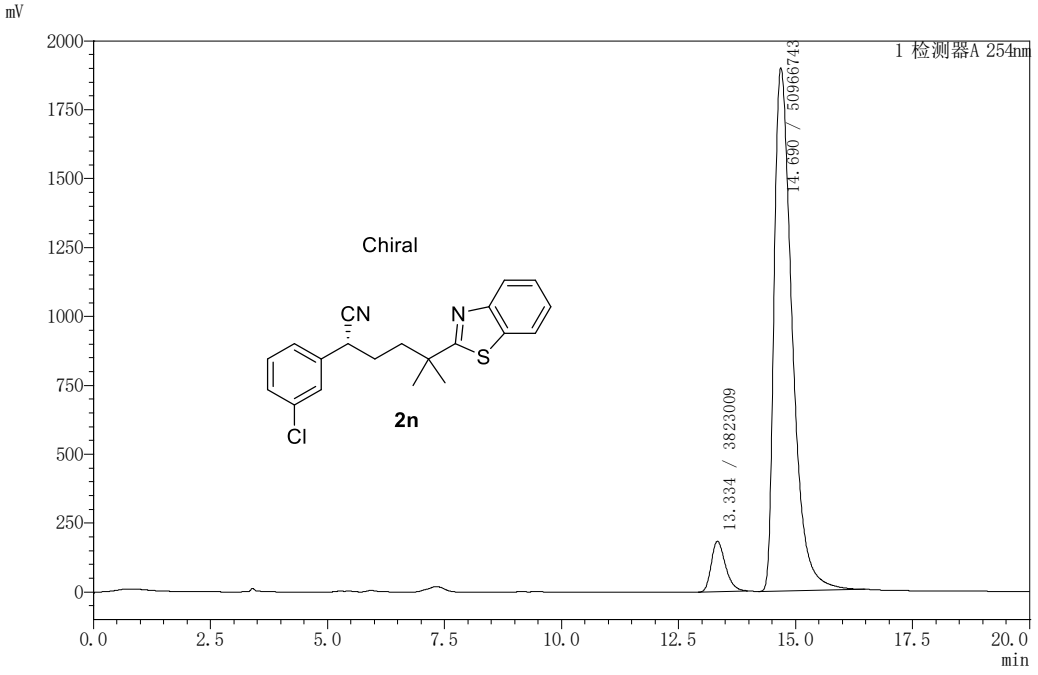
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	12.774	149673	3413517	50.149
2	14.147	110327	3393234	49.851
Total		260000	6806751	100.000



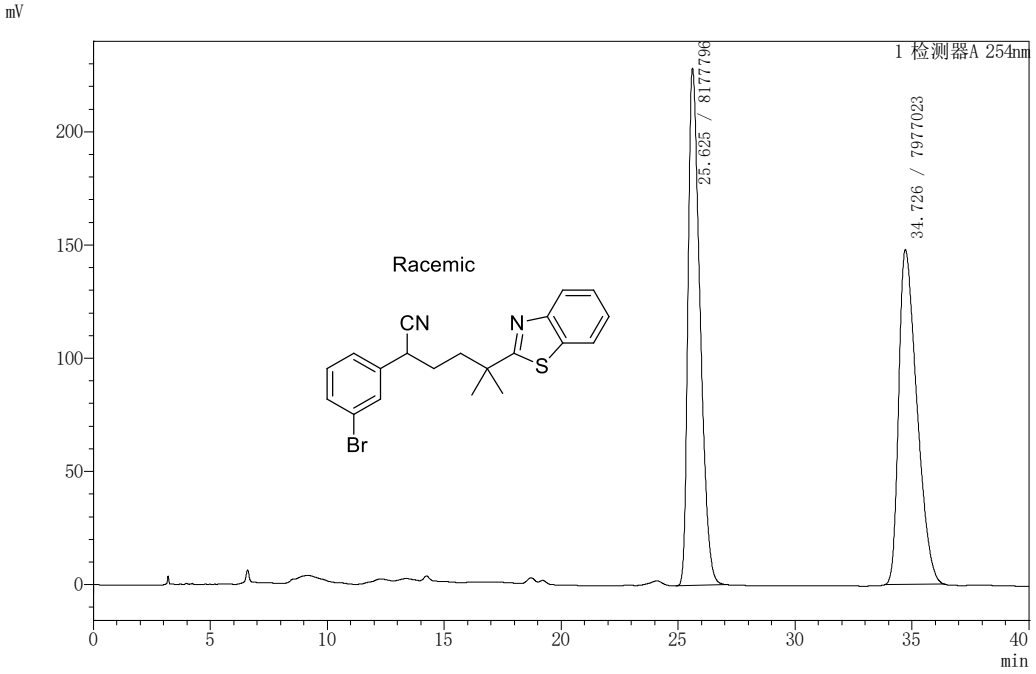
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	12.632	903691	20881156	95.052
2	14.423	41236	1086941	4.948
Total		944927	21968097	100.000



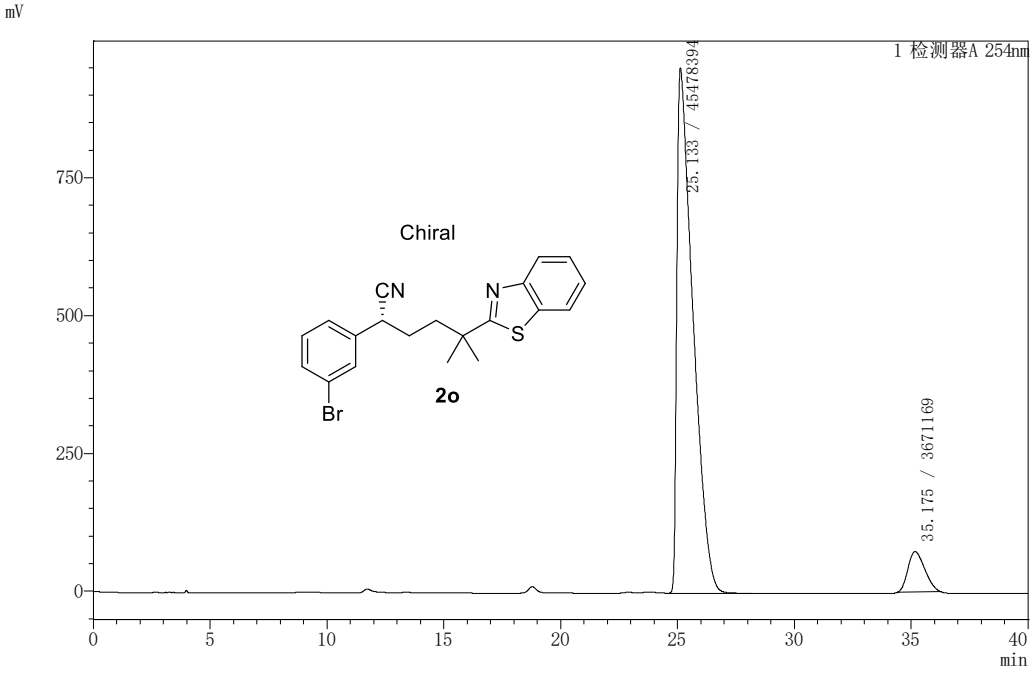
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	13.296	1299940	31277150	50.078
2	14.796	1165456	31179358	49.922
Total		2465396	62456507	100.000



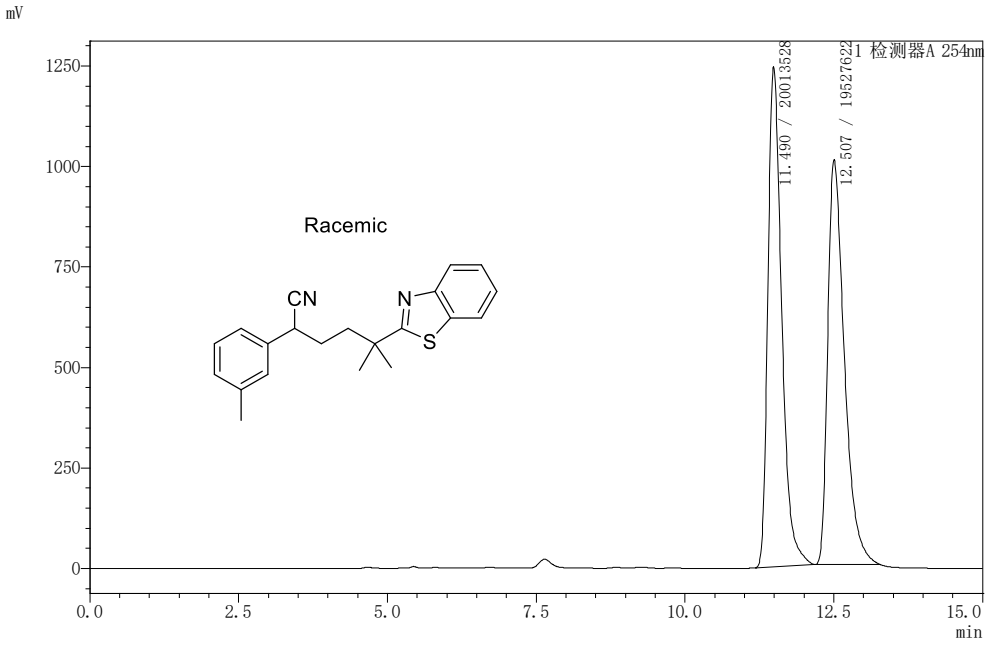
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	13.334	183419	3823009	6.978
2	14.690	1899031	50966743	93.022
Total		2082449	54789751	100.000



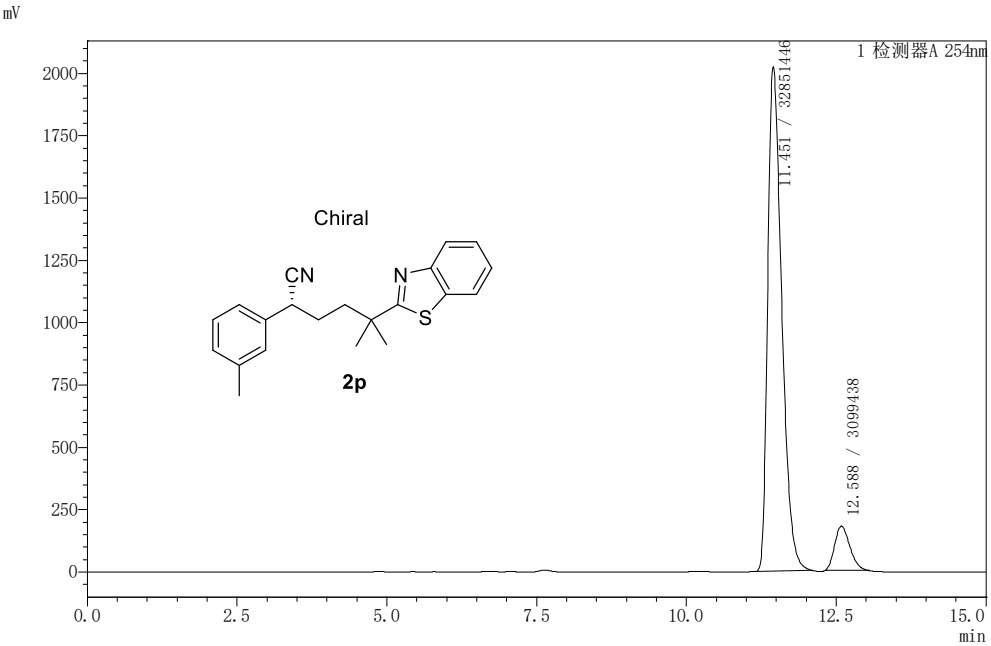
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	26.625	228540	8177796	50.621
2	34.726	147833	7977023	49.379
Total		376374	16154819	100.000



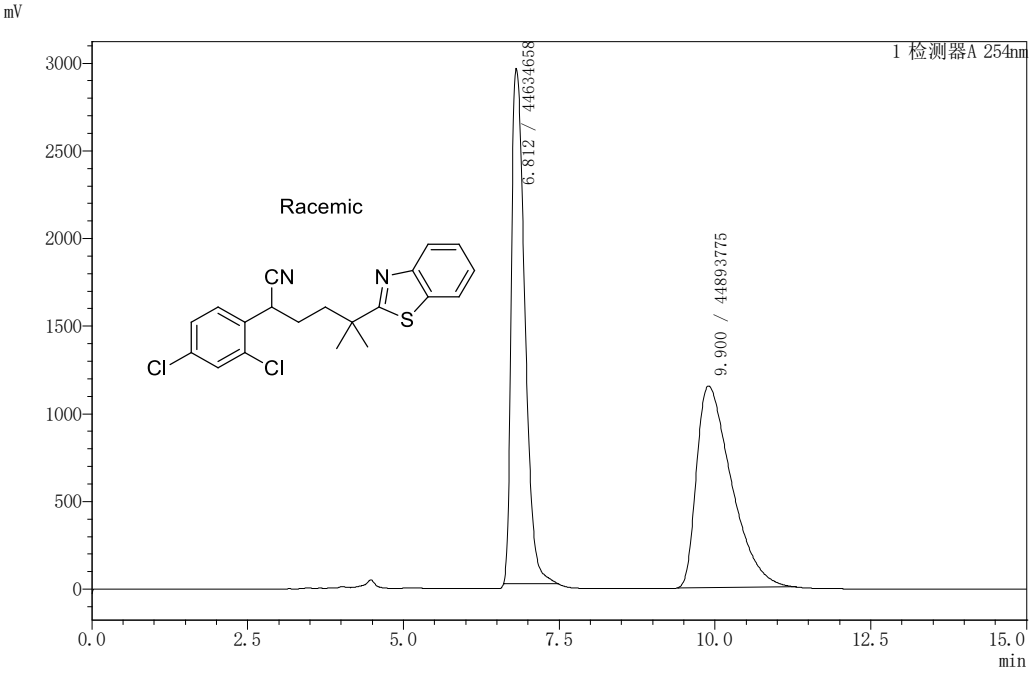
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	25.133	953375	45478394	92.531
2	35.175	73236	3671169	7.469
Total		1026612	49149563	100.000



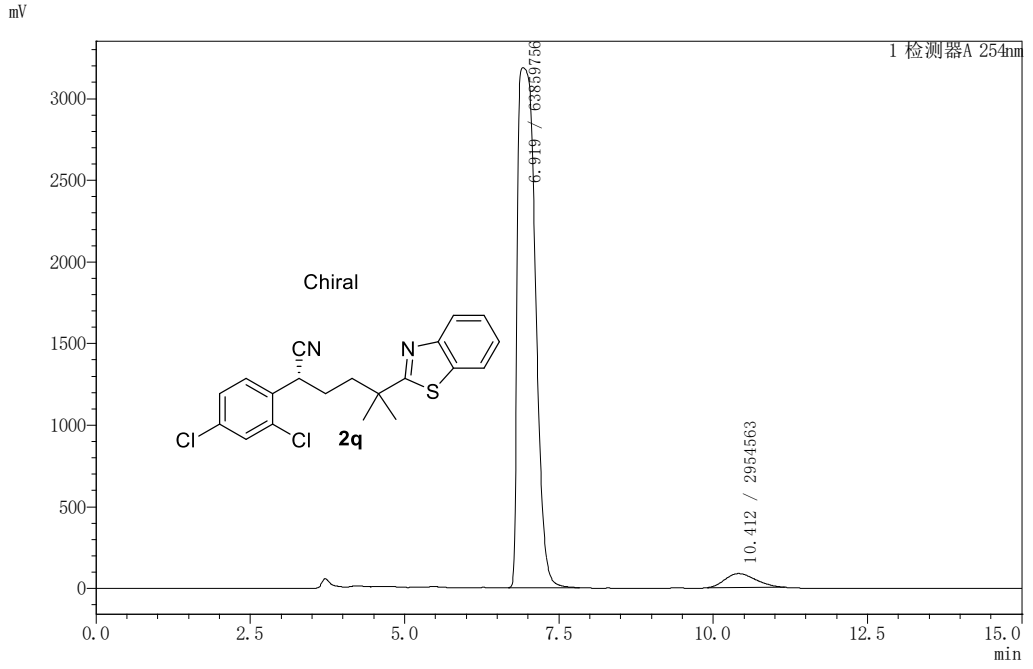
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	11.490	1244991	20013528	50.614
2	12.507	1007620	19527622	49.386
Total		2252611	39541150	100.000



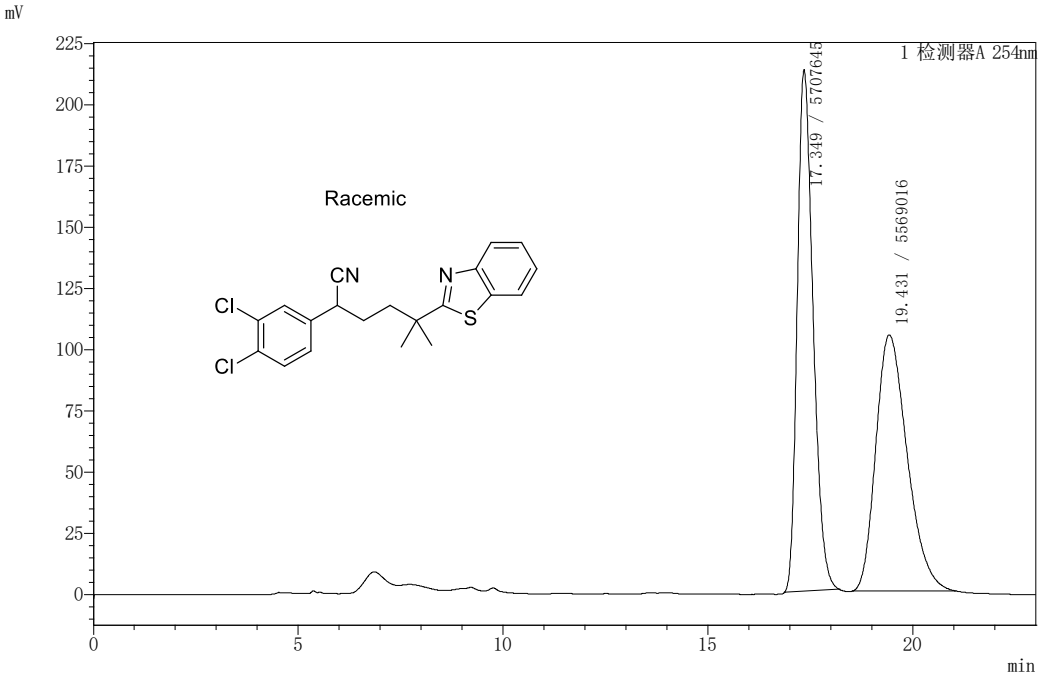
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	11.451	2024366	32851446	91.379
2	12.588	176988	3099438	8.621
Total		2201355	35950884	100.000



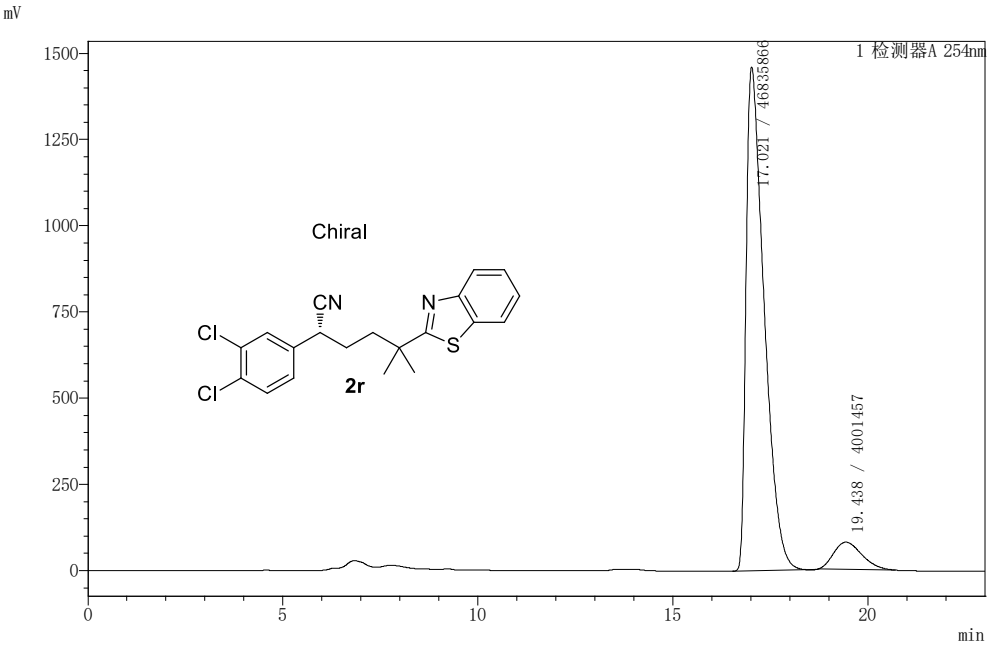
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	6.812	2939493	44634658	49.855
2	9.900	1150969	44893775	50.145
Total		4090462	89528434	100.000



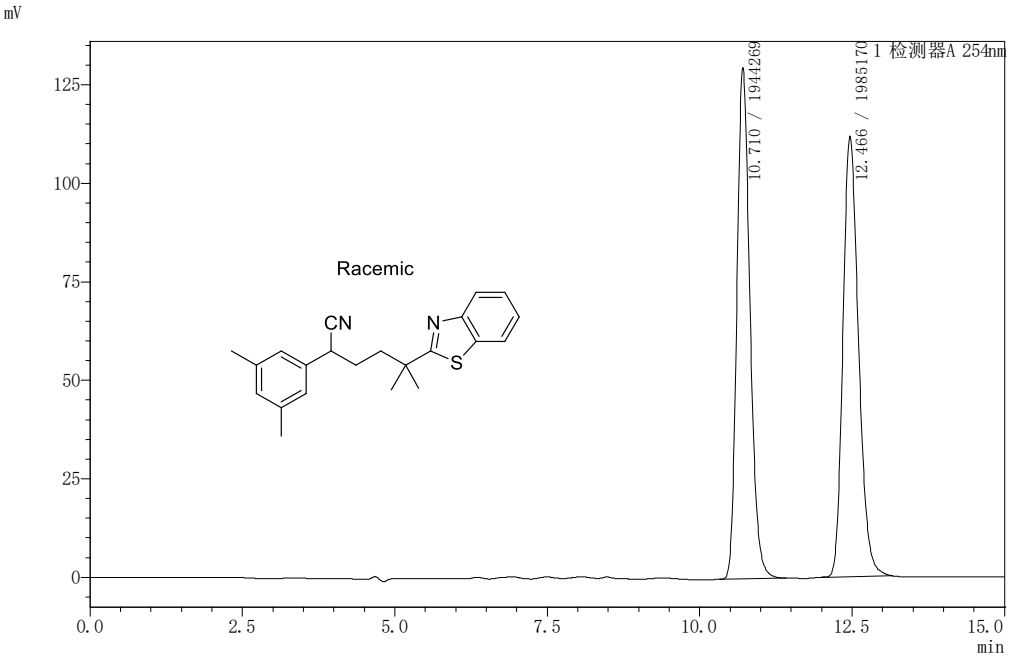
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	6.919	3186116	63859756	95.578
2	10.412	85367	2954563	4.422
Total		3271483	66814319	100.000



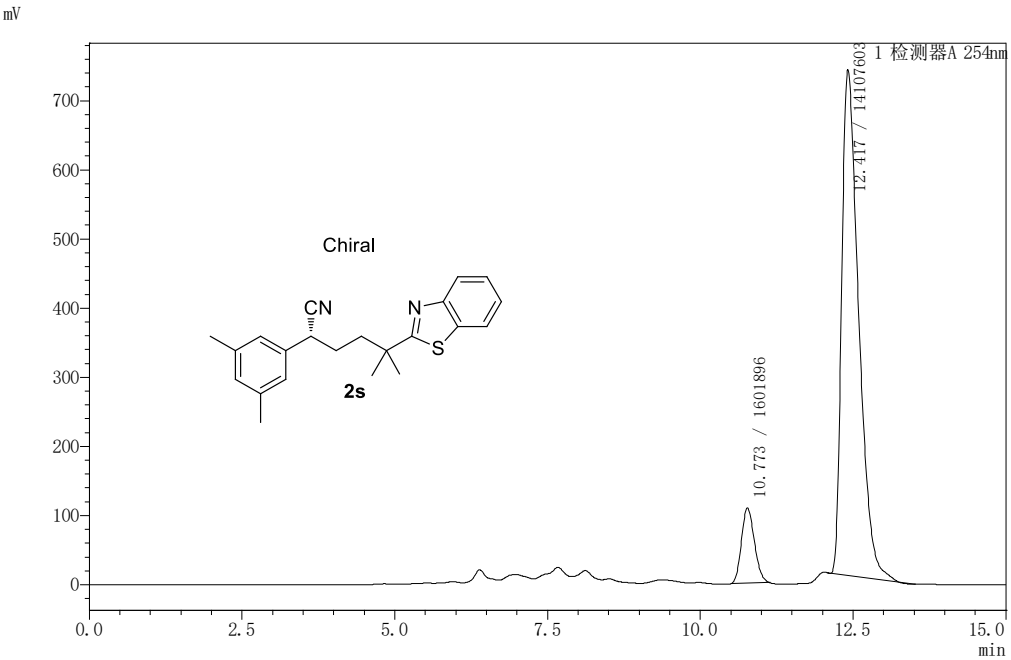
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	17.349	213029	5707645	50.615
2	19.431	104610	5569016	49.385
Total		317638	11276661	100.000



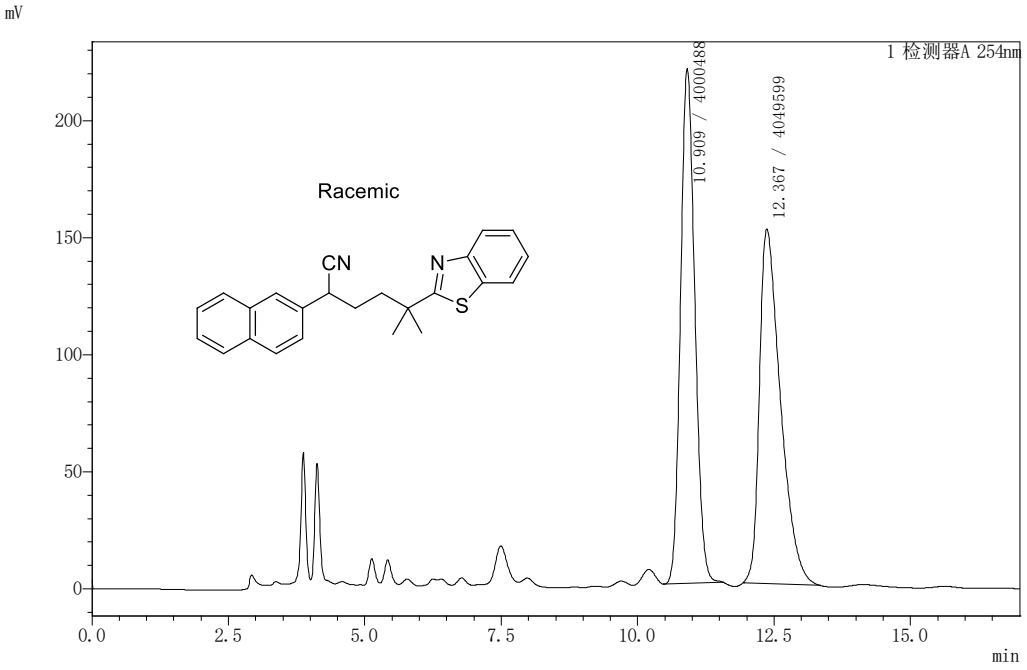
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	17.021	1461020	46835866	92.129
2	19.438	79036	4001457	7.871
Total		1540056	50837323	100.000



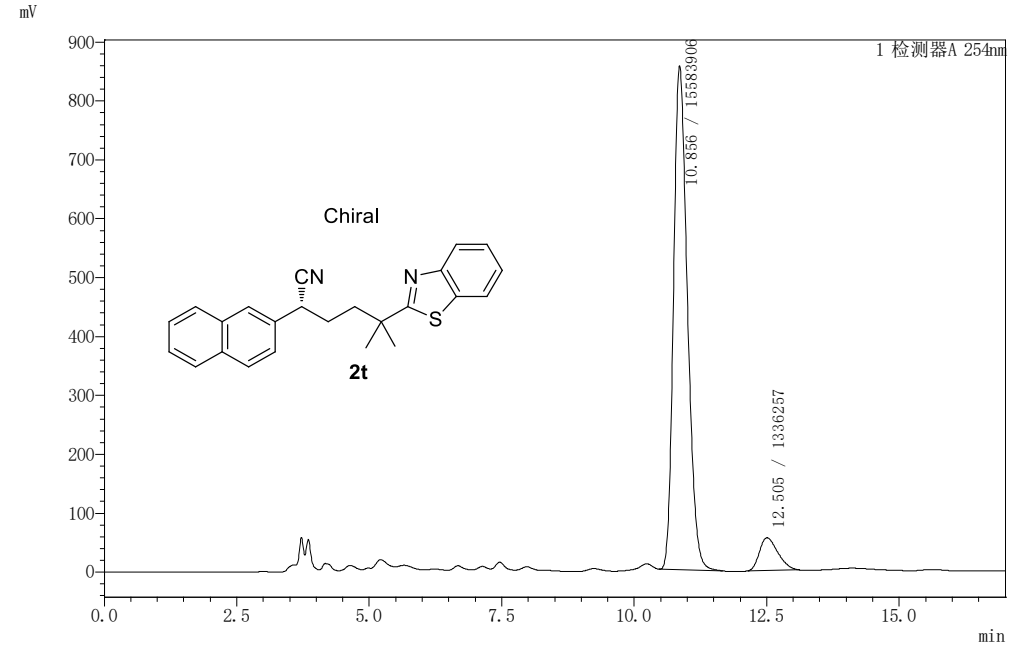
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	10.710	129822	1944269	49.480
2	12.466	111908	1985170	50.520
Total		241730	3929439	100.000



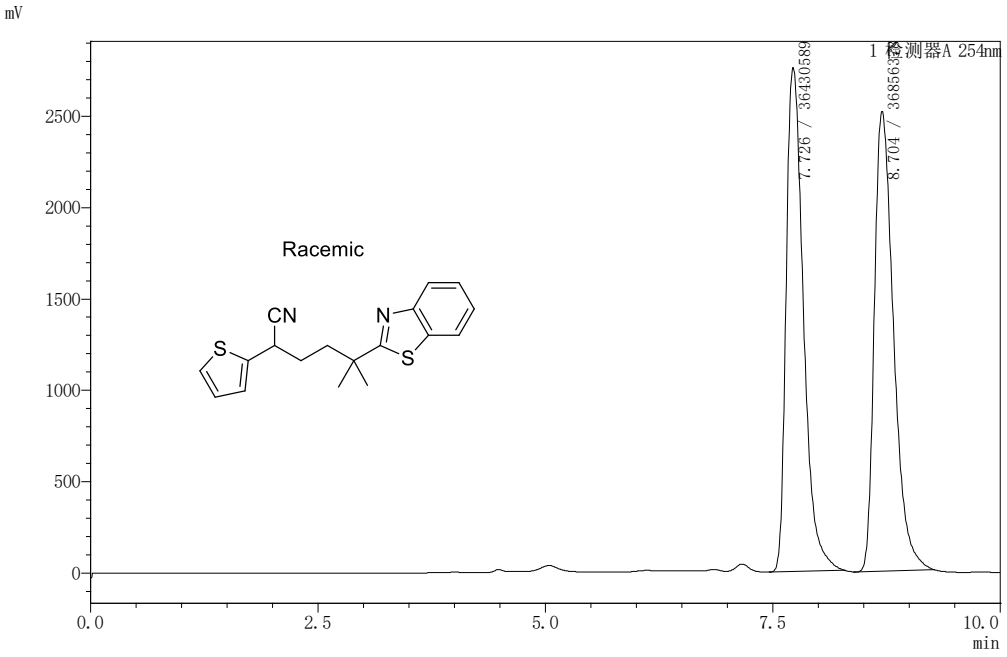
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	10.773	108852	1601896	10.197
2	12.417	732110	14107603	89.803
Total		840961	15709499	100.000



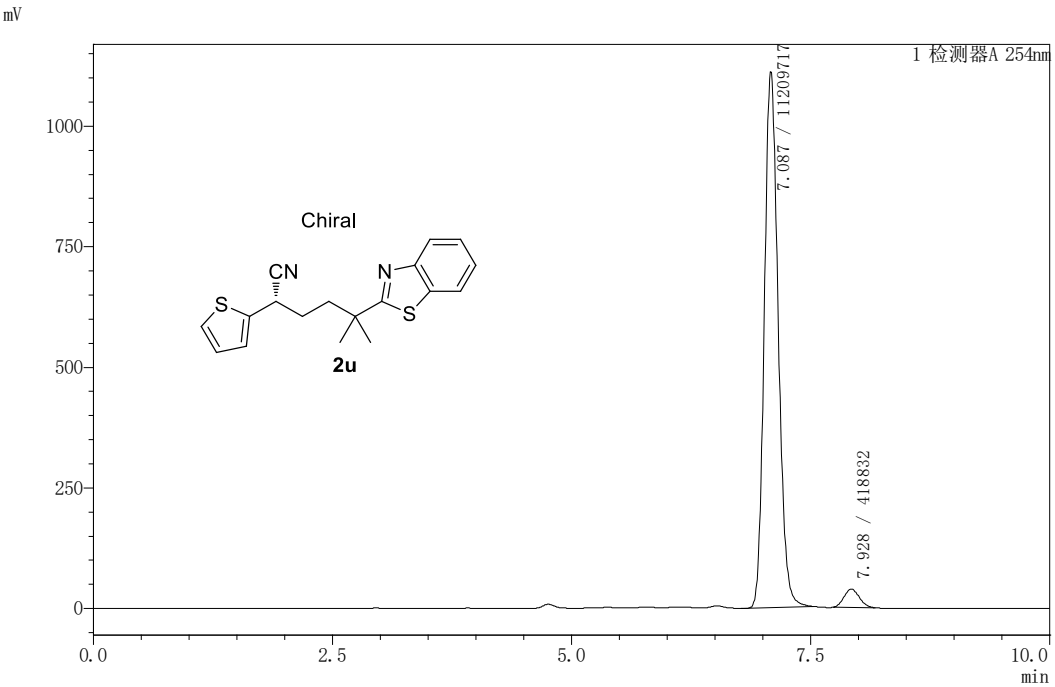
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	10.909	219995	4000488	49.695
2	12.367	151545	4049599	50.305
Total		371540	8050087	100.000



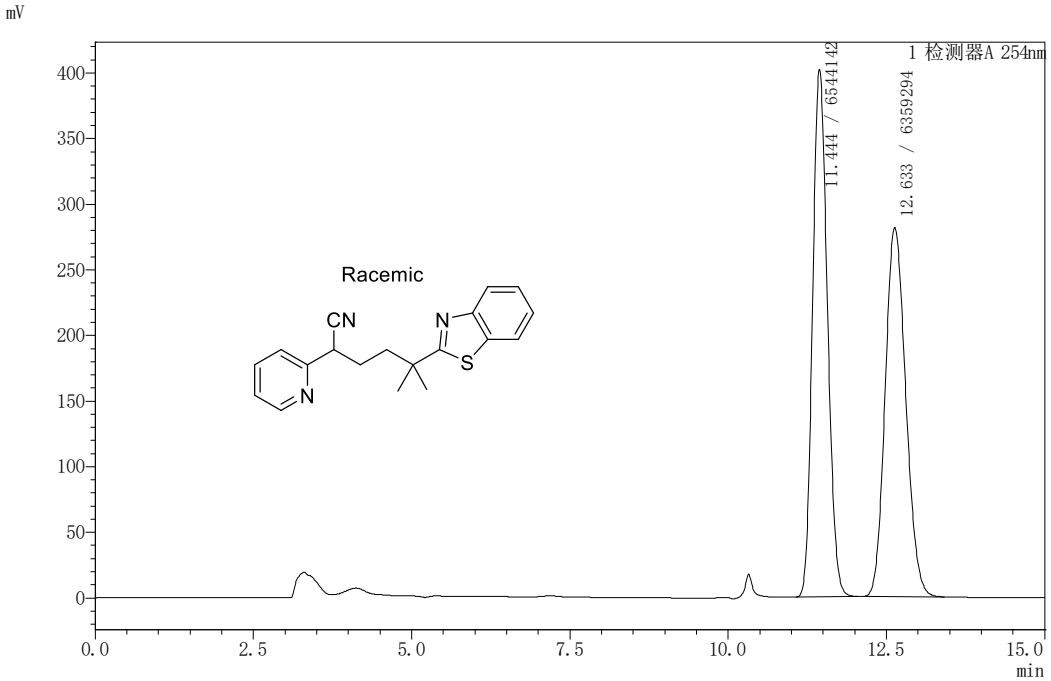
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	10.856	856128	15583906	92.103
2	12.505	55390	1336257	7.897
Total		911518	16920163	100.000



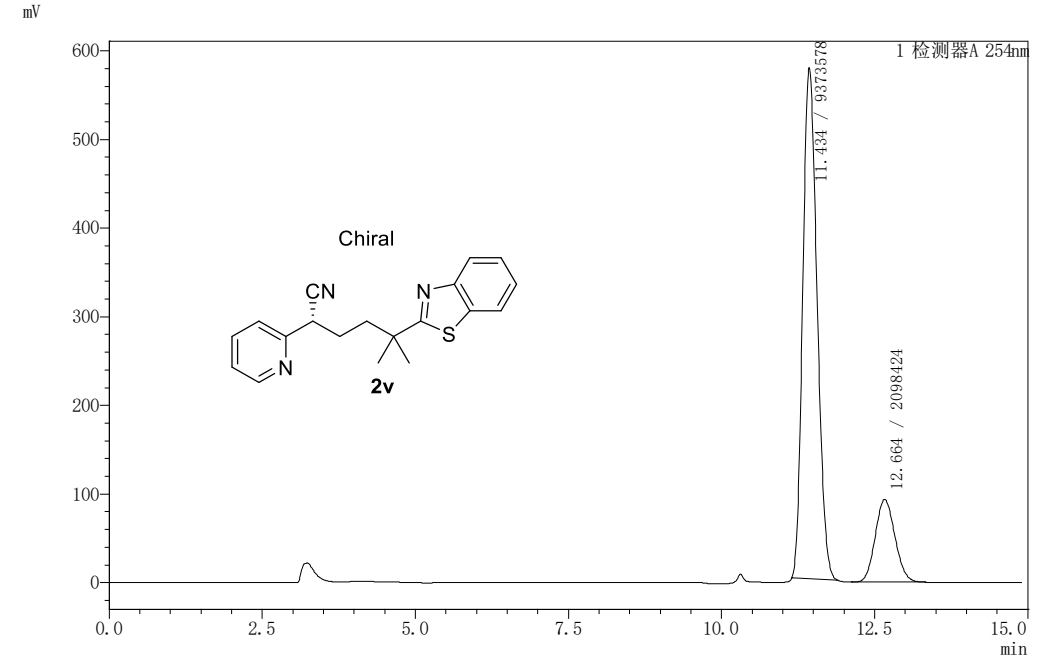
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	7.726	2761338	36430589	49.710
2	8.704	2514568	36856378	50.290
Total		5275906	73286967	100.000



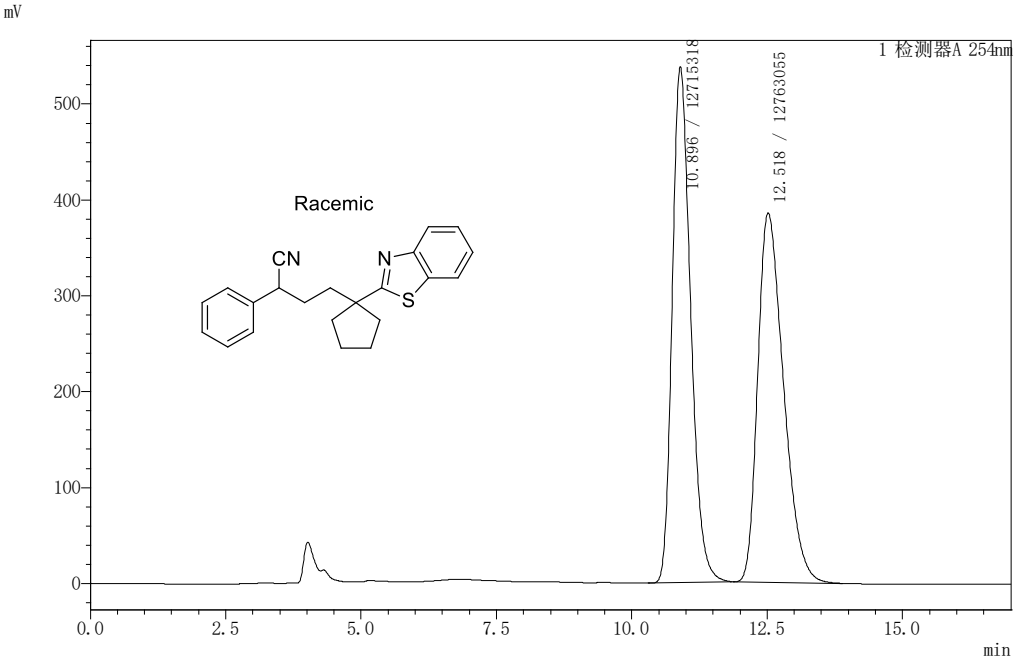
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	7.087	1111144	11209717	96.398
2	7.928	37789	418832	3.602
Total		1148933	11628549	100.000



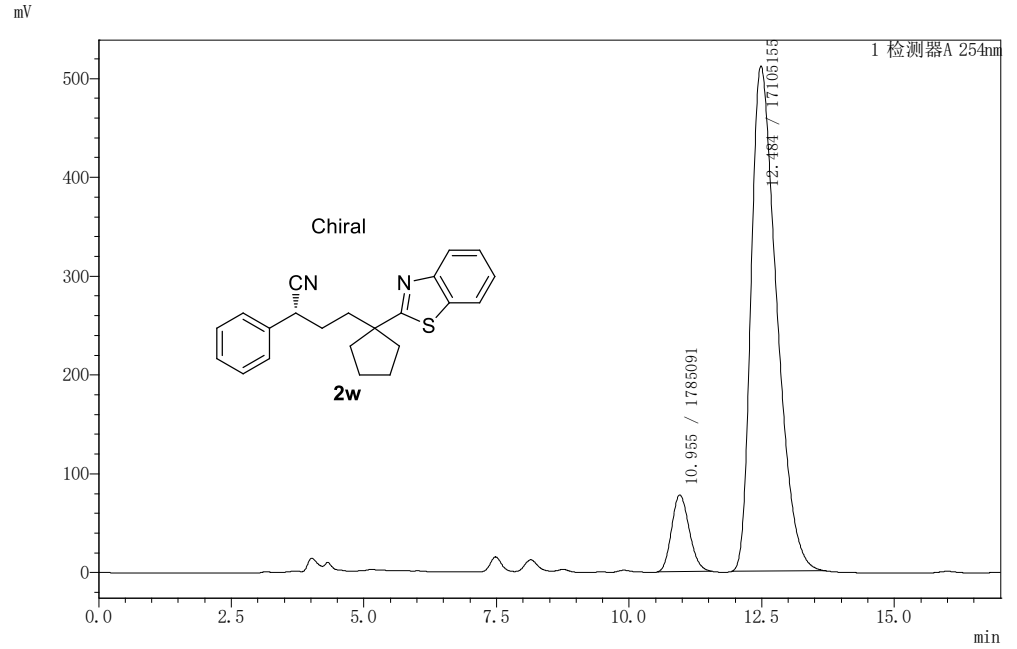
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	11.444	402003	6544142	50.716
2	12.633	281338	6359294	49.284
Total		683341	12903436	100.000



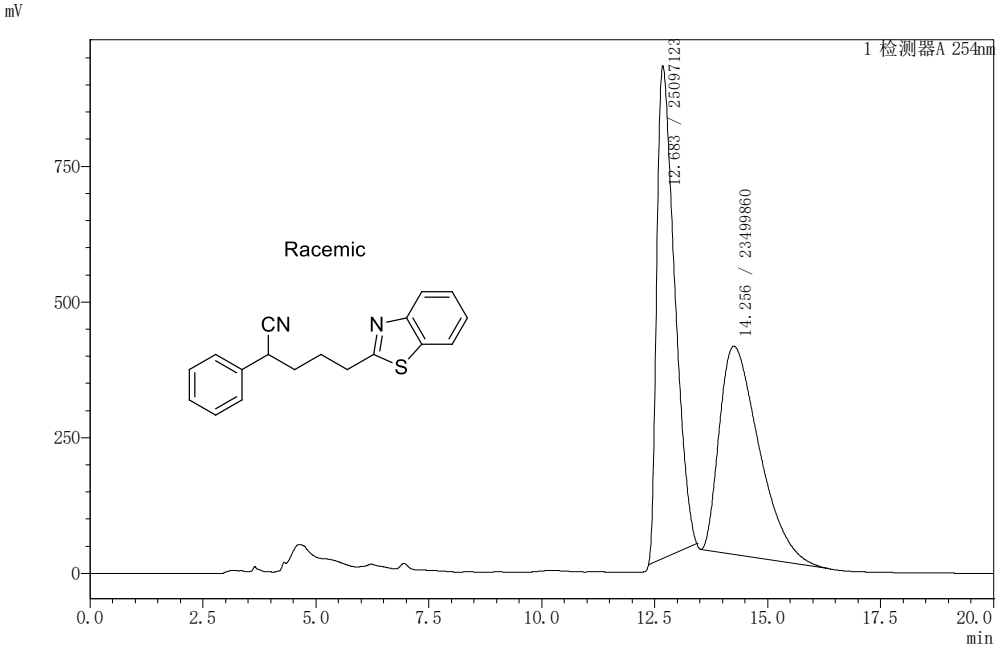
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	11.434	576807	9373578	81.708
2	12.664	93319	2098424	18.292
Total		670126	11472002	100.000



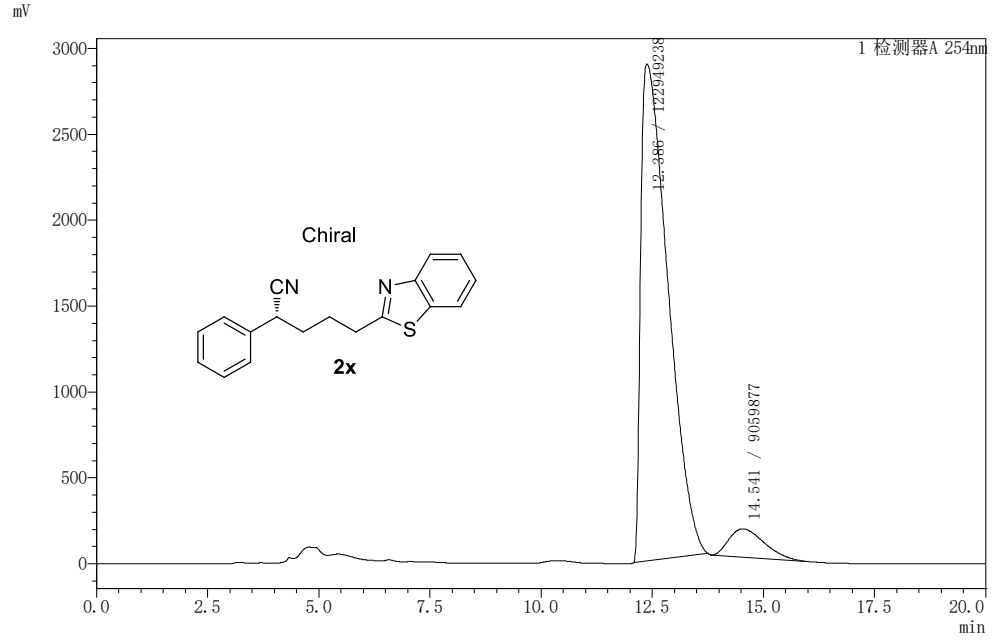
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	10.896	538086	12715318	50.094
2	12.518	384721	12763055	49.906
Total		922807	25478373	100.000



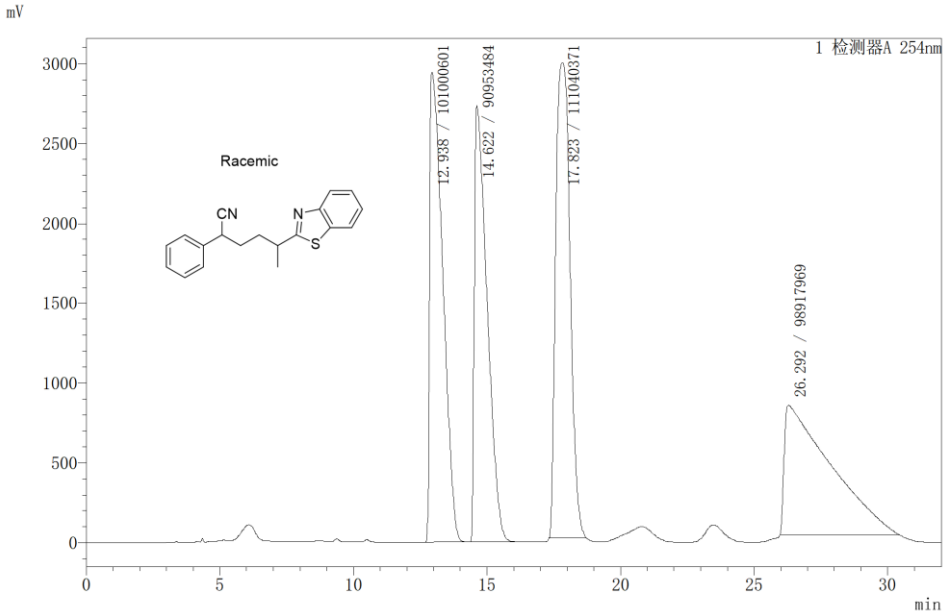
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	10.955	77469	1785091	9.450
2	12.484	511395	17105155	90.550
Total		588864	18890247	100.000



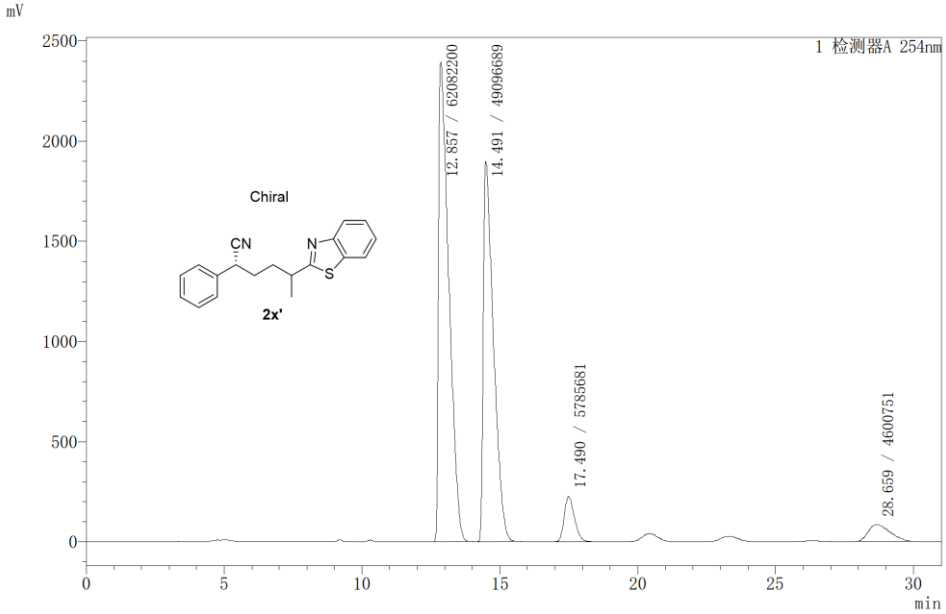
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	12.683	916444	25097123	51.643
2	14.256	379571	23499860	48.357
Total		1296015	48596983	100.000



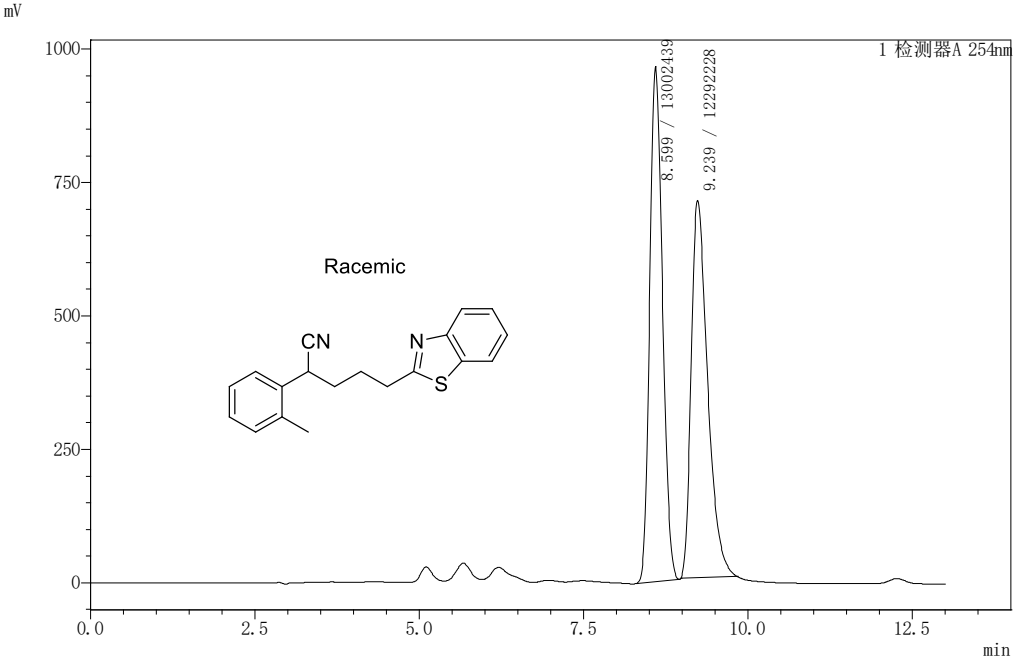
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	12.386	2892007	122949238	93.137
2	14.541	163792	9059877	6.863
Total		3055799	132009115	100.000



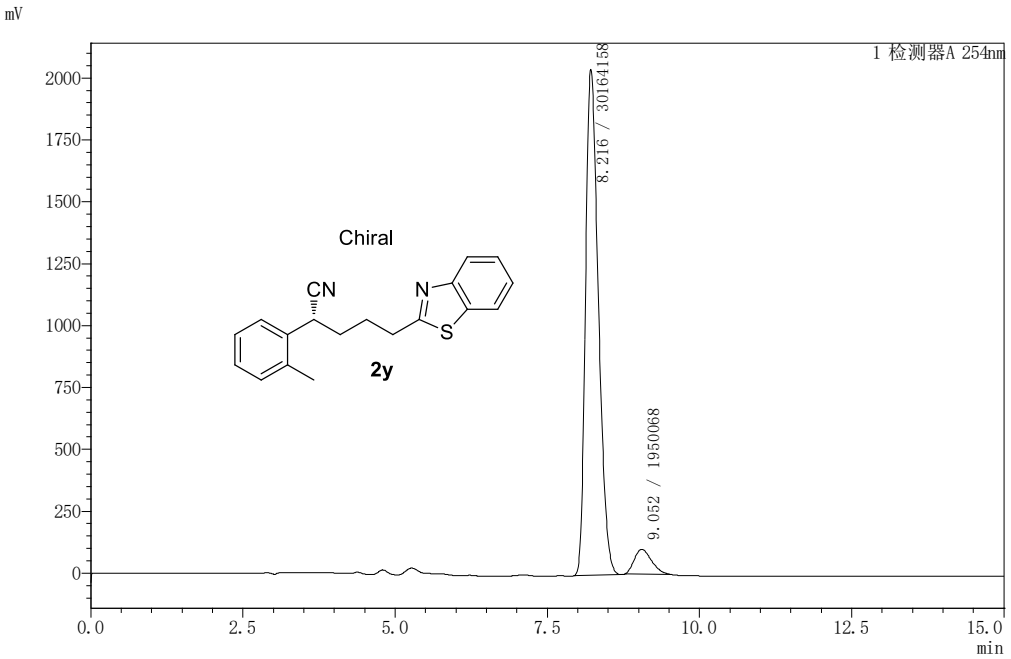
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	12.938	2939494	101000601	25.130
2	14.622	2730020	90953484	22.630
3	17.823	2977086	111040371	27.628
4	26.292	813507	98917969	24.612
Total		9460106	401912426	100.000



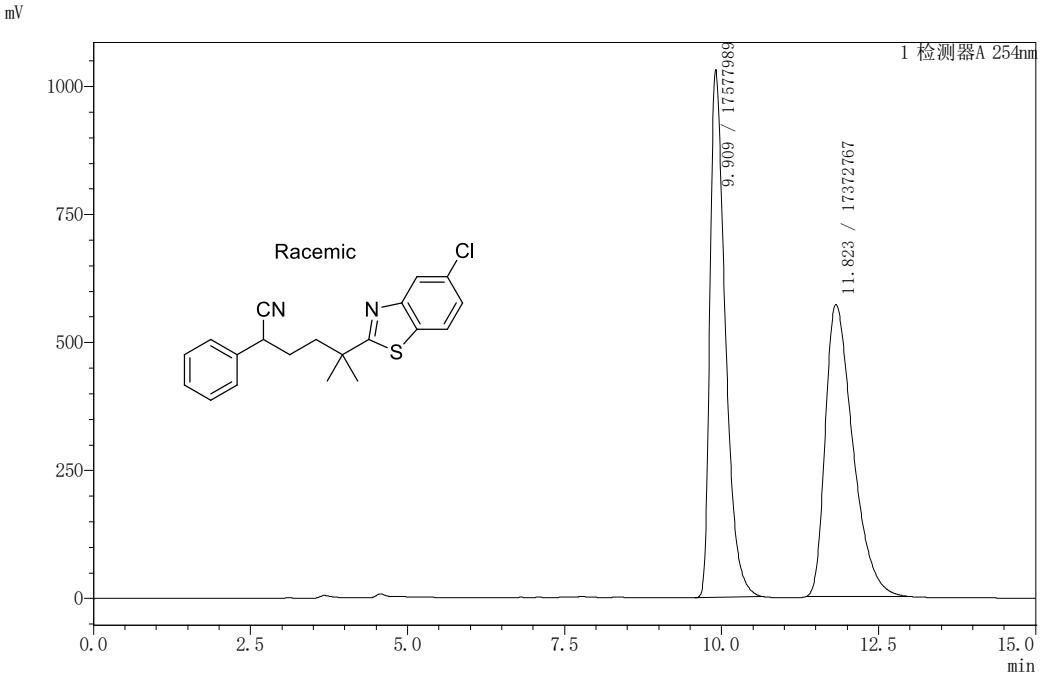
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	12.857	2395301	62082200	51.069
2	14.491	1899815	49096689	40.387
3	17.490	225082	5785681	4.759
4	28.659	84502	4600751	3.785
Total		4604700	121565320	100.000



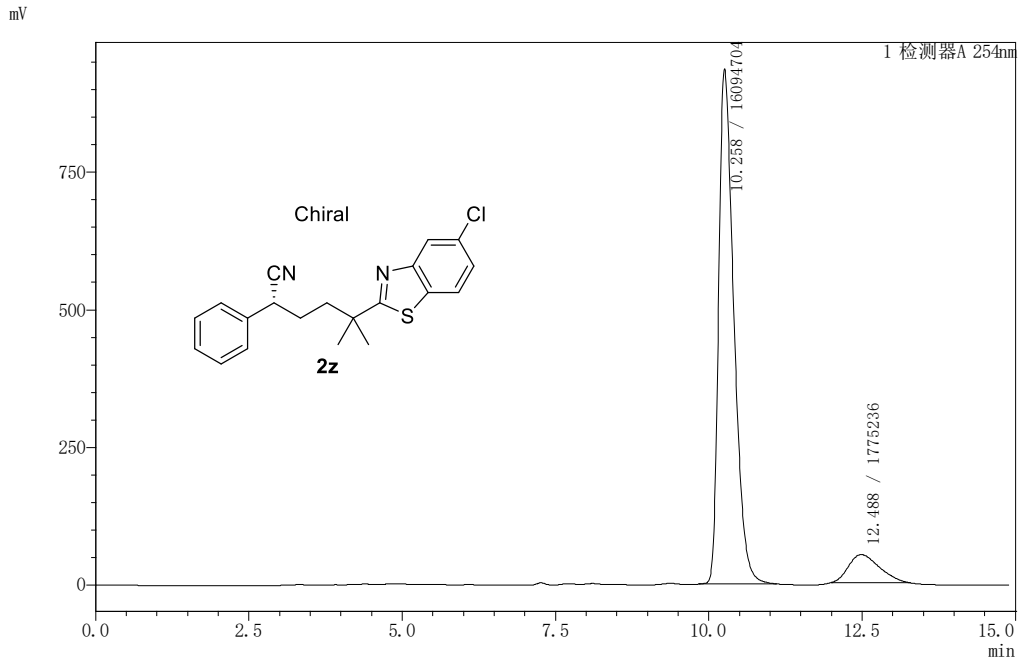
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	8.599	965572	13002439	51.404
2	9.239	706834	12292228	48.596
Total		1672407	25294667	100.000



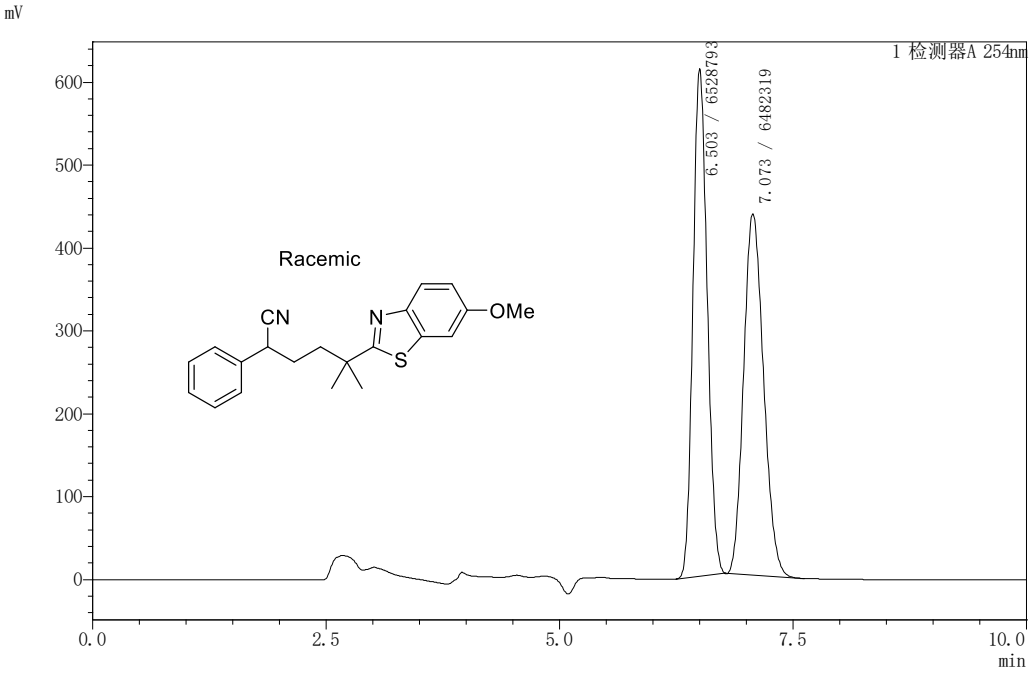
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	8.216	2044744	30164158	93.928
2	9.052	99500	1950068	6.072
Total		2144244	32114227	100.000



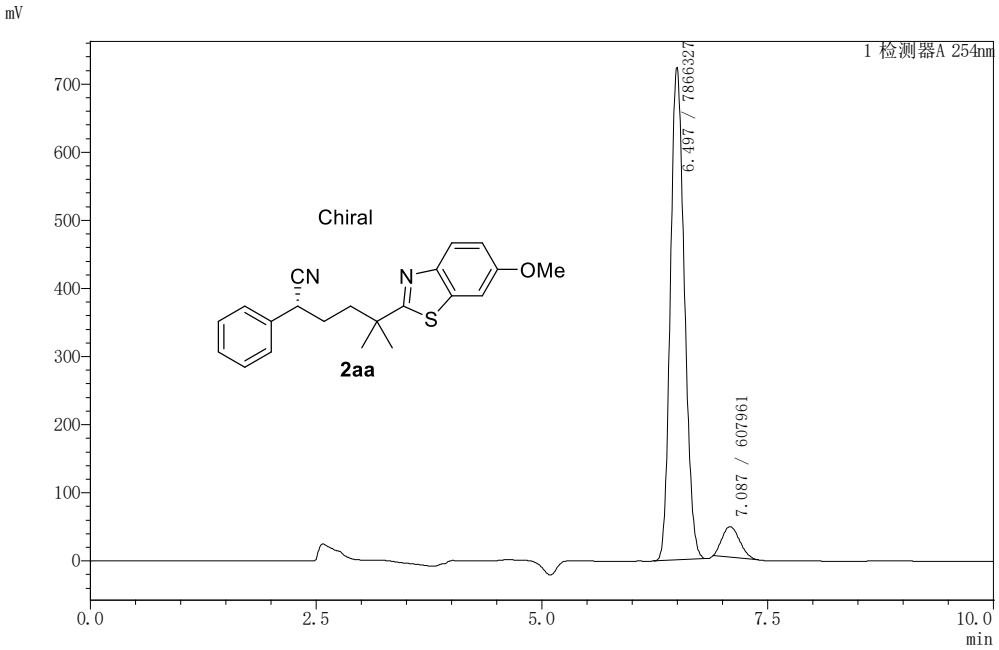
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	9.909	1031504	17577989	50.294
2	11.823	570427	17372767	49.706
Total		1601931	34950756	100.000



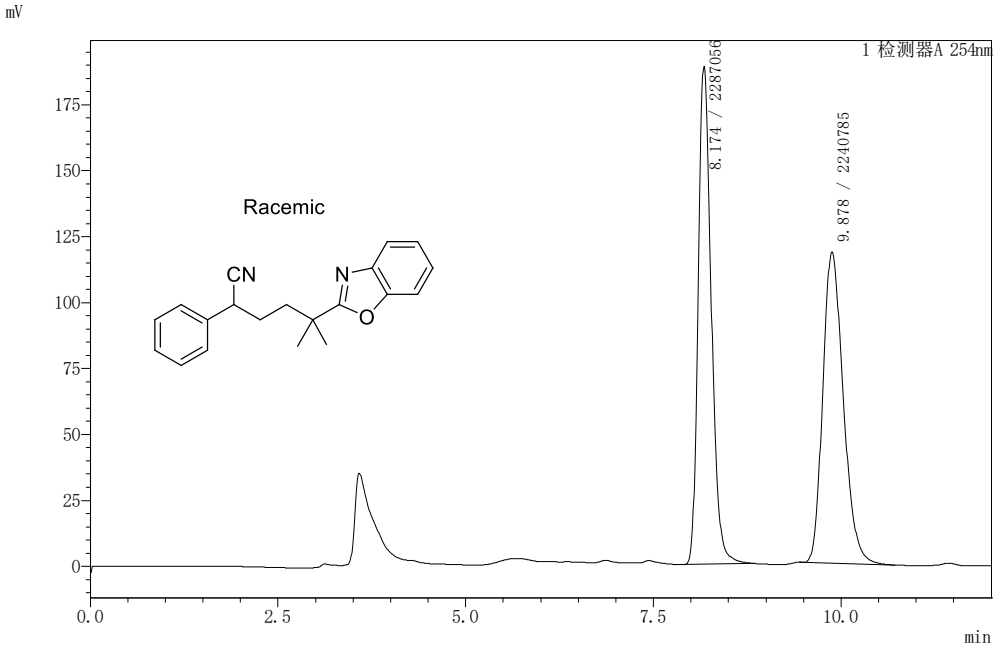
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	10.258	935641	16094704	90.066
2	12.488	53076	1775236	9.934
Total		988717	17869940	100.000



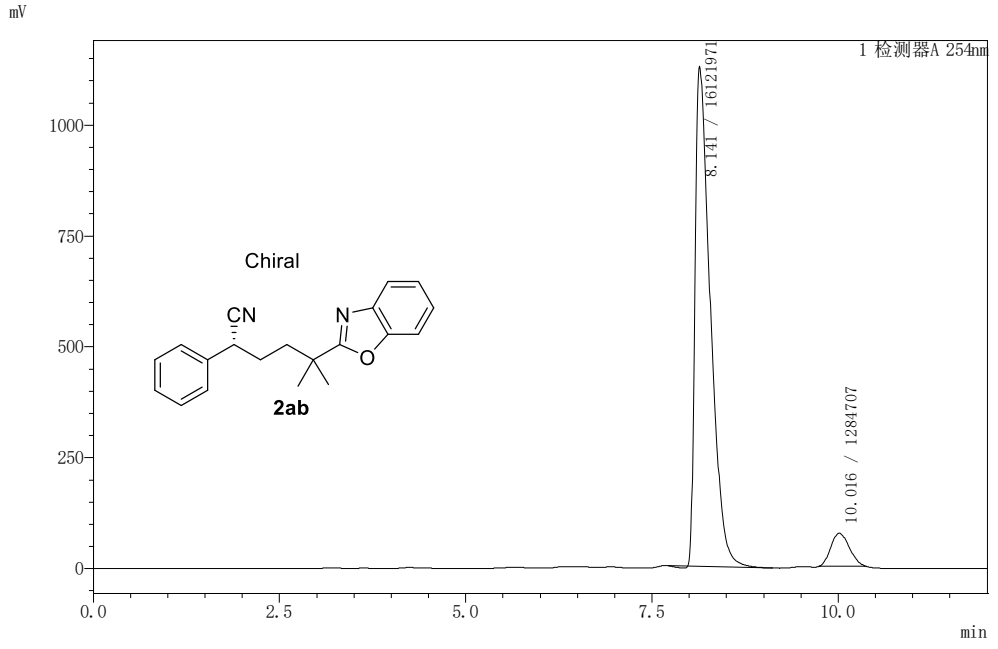
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	6.503	612490	6528793	50.179
2	7.073	435968	6482319	49.821
Total		1048458	13011112	100.000



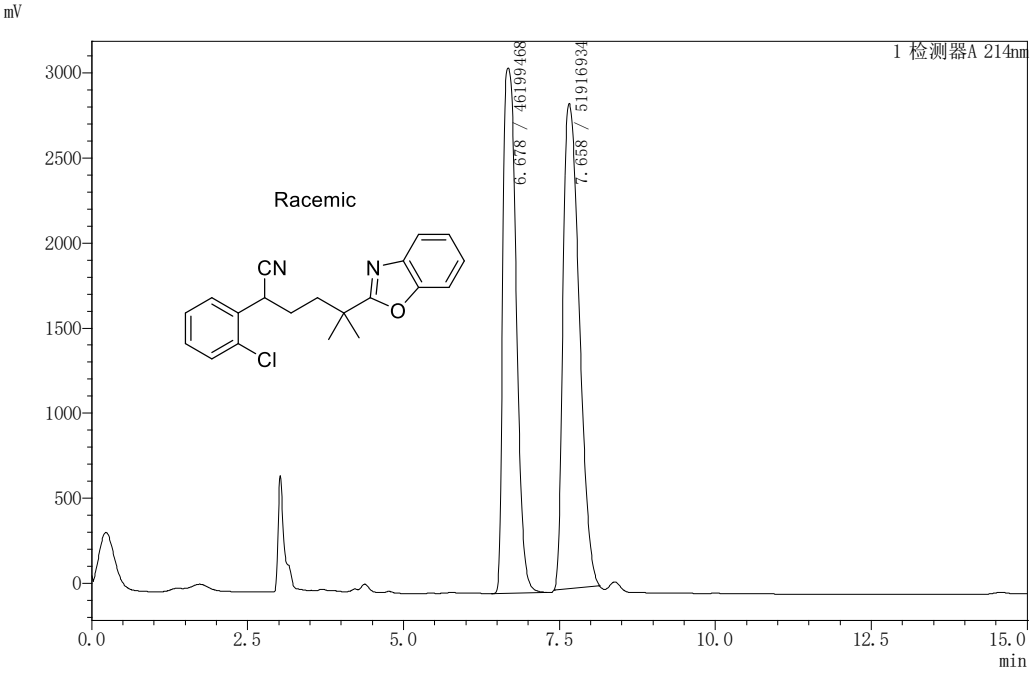
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	6.497	723429	7866327	92.826
2	7.087	44933	607961	7.174
Total		768362	8474287	100.000



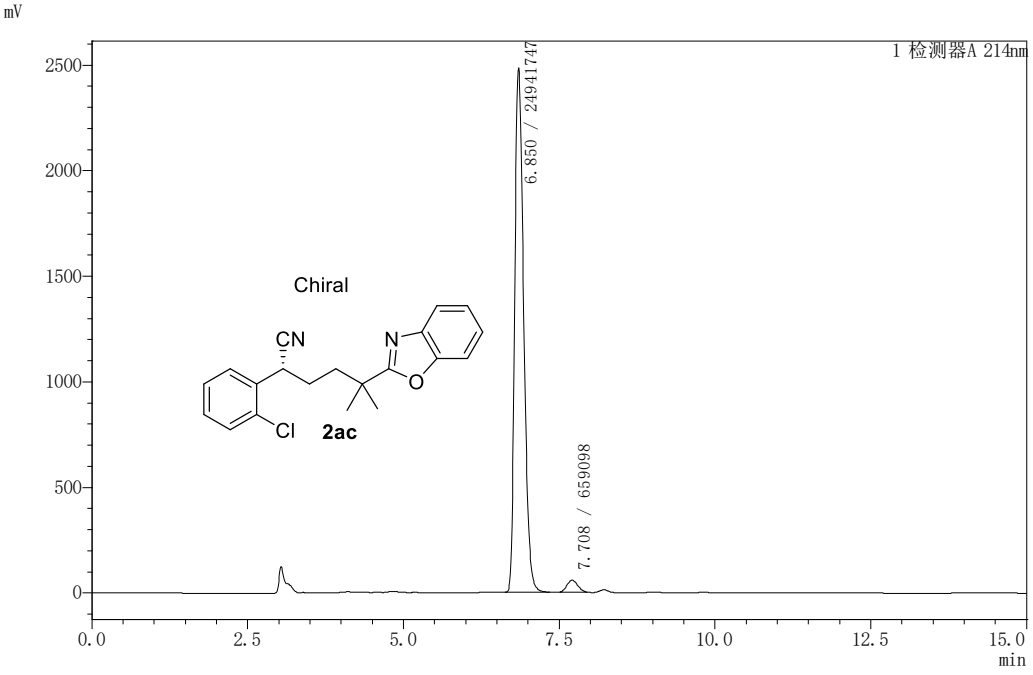
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	8.174	188675	2287056	50.510
2	9.878	117715	2240785	49.490
Total		306391	4527841	100.000



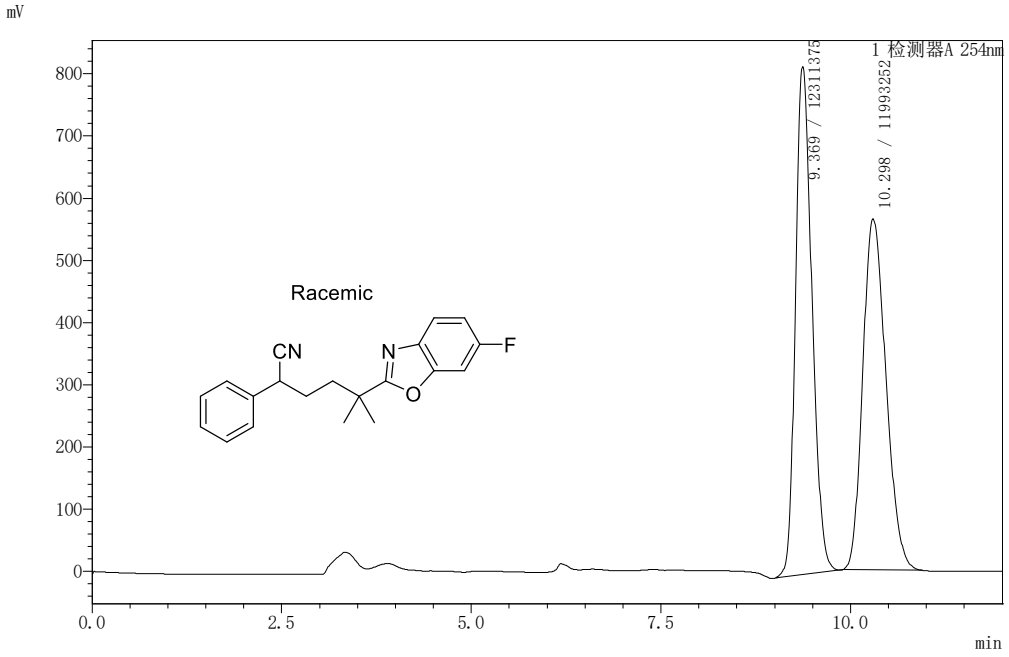
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	8.141	1131729	16121971	92.234
2	10.016	77150	1284707	7.766
Total		1208979	17406678	100.000



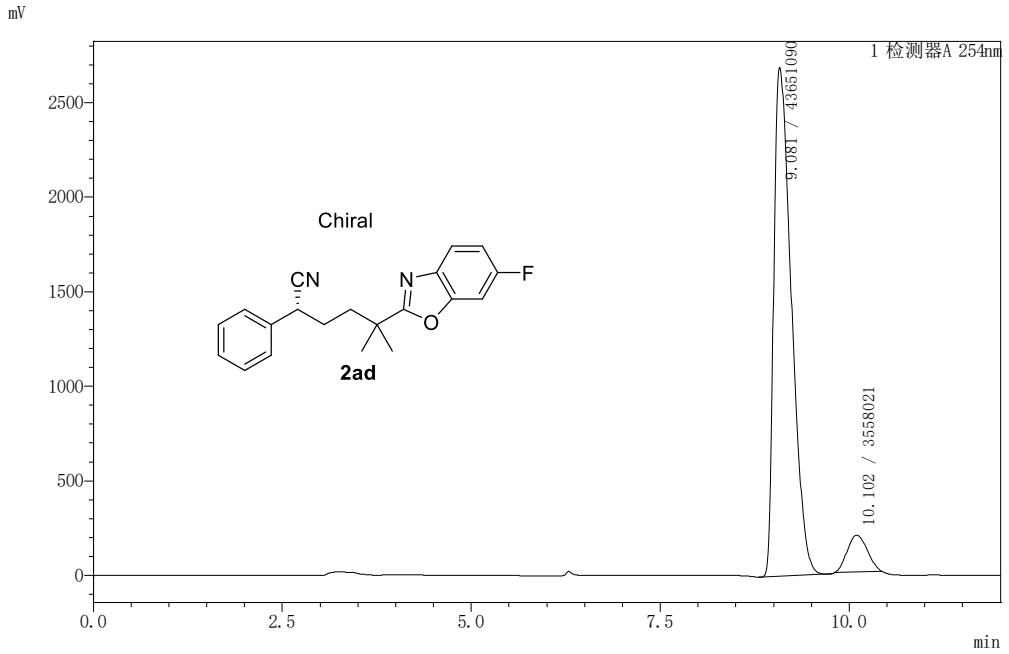
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	6.678	3088965	46199468	47.086
2	7.658	2852303	51916934	52.914
Total		5941268	98166402	100.000



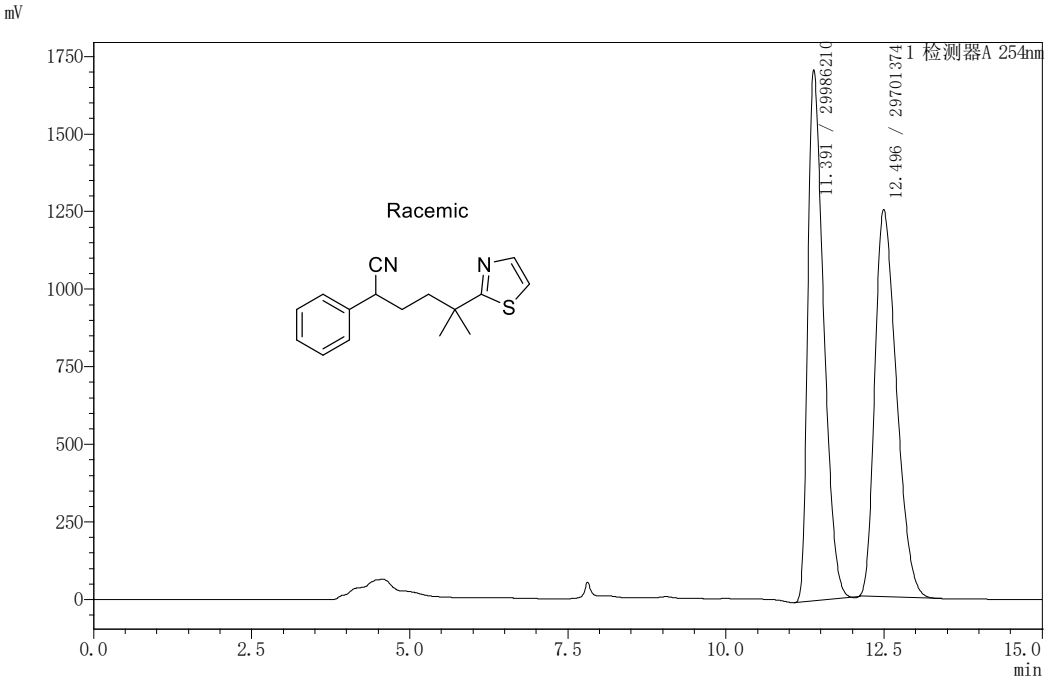
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	6.850	2483961	24941747	97.425
2	7.708	56044	659098	2.575
Total		2540005	25600845	100.000



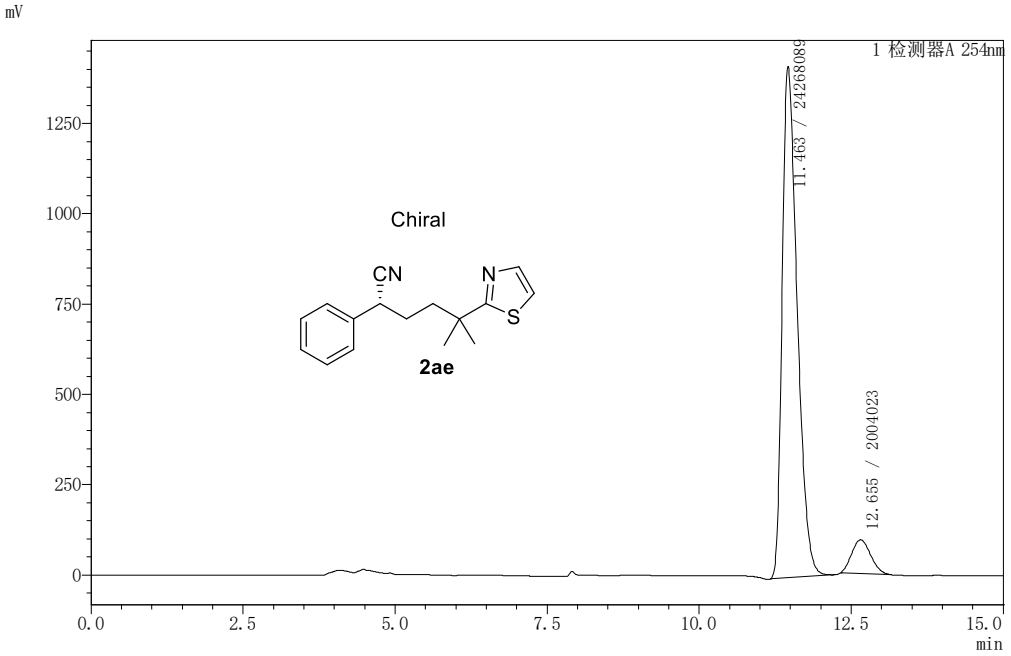
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	9.369	816576	12311375	50.654
2	10.298	564328	11993252	49.346
Total		1380903	24304627	100.000



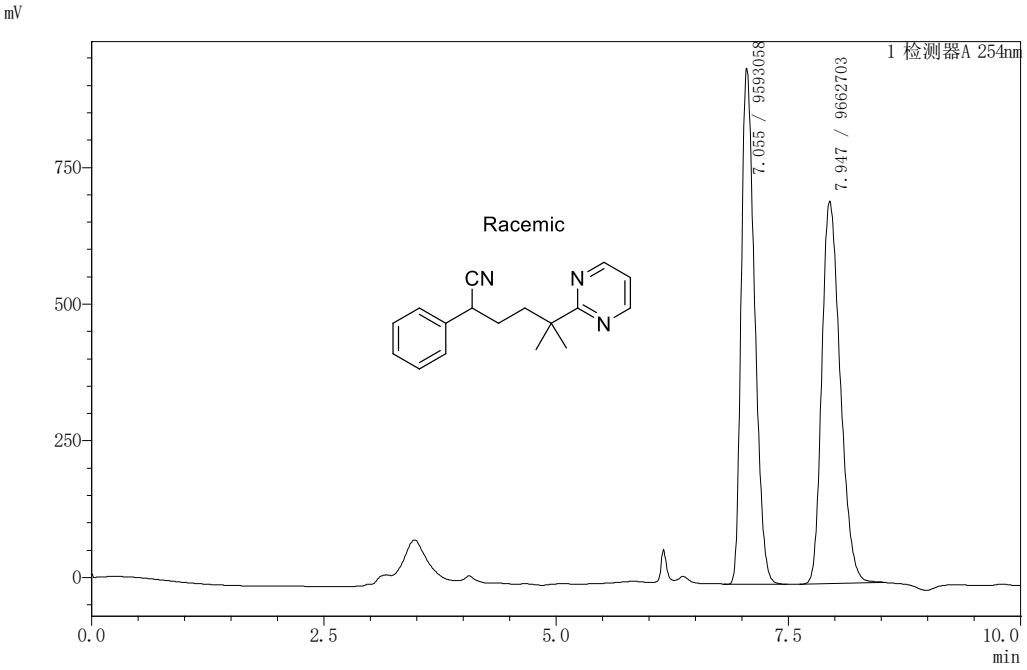
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	9.081	2692149	43651090	92.463
2	10.102	193941	3558021	7.537
Total		2886091	47209111	100.000



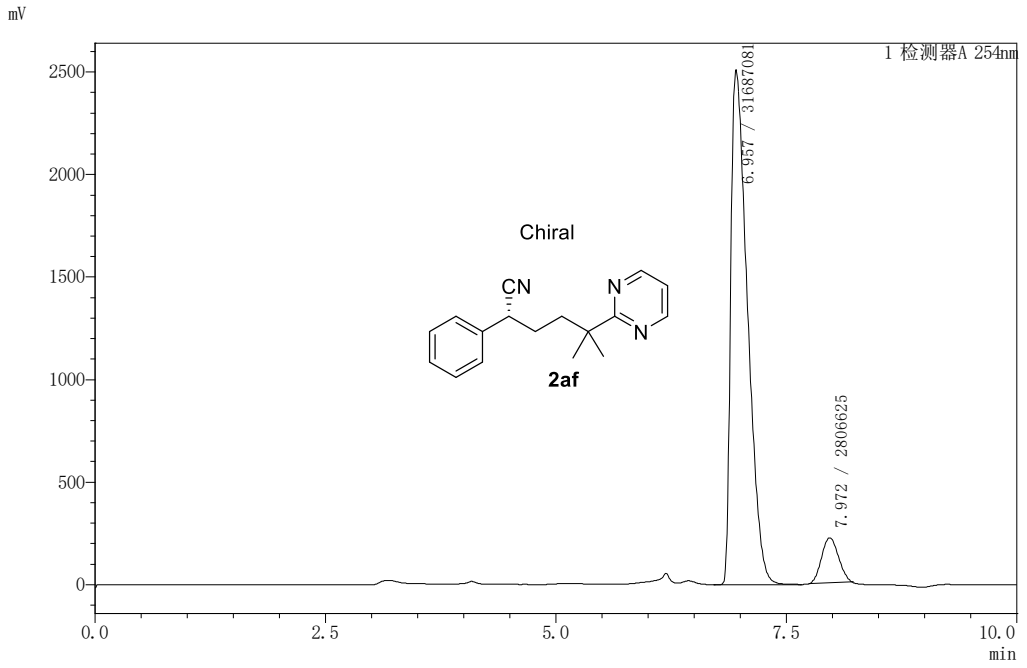
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	11.391	1712706	29986210	50.239
2	12.496	1247200	29701374	49.761
Total		2959906	59687584	100.000



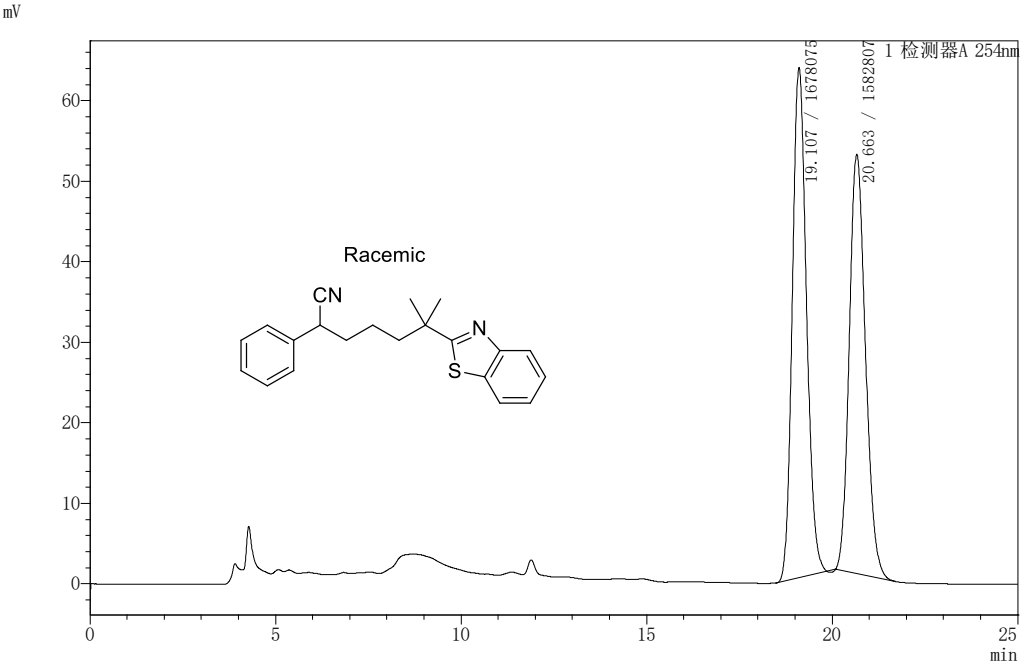
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	11.463	1415706	24268089	92.372
2	12.655	92697	2004023	7.628
Total		1508403	26272113	100.000



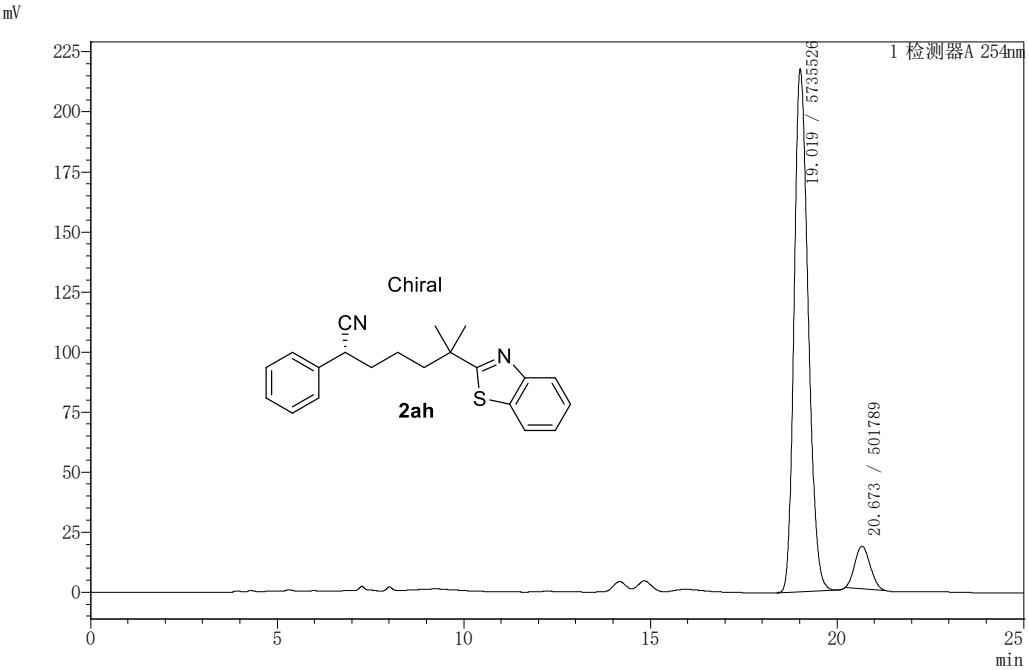
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	7.055	943986	9593058	49.819
2	7.947	699548	9662703	50.181
Total		1643534	19255760	100.000



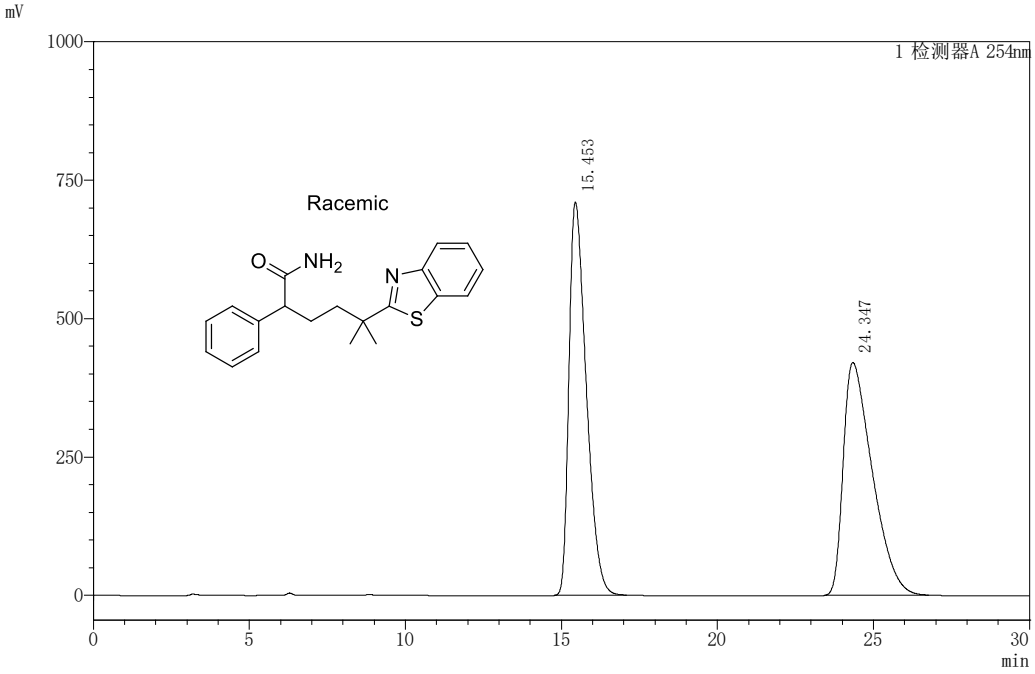
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	6.957	2512310	31687081	91.863
2	7.972	219783	2806625	8.137
Total		2732093	34493705	100.000



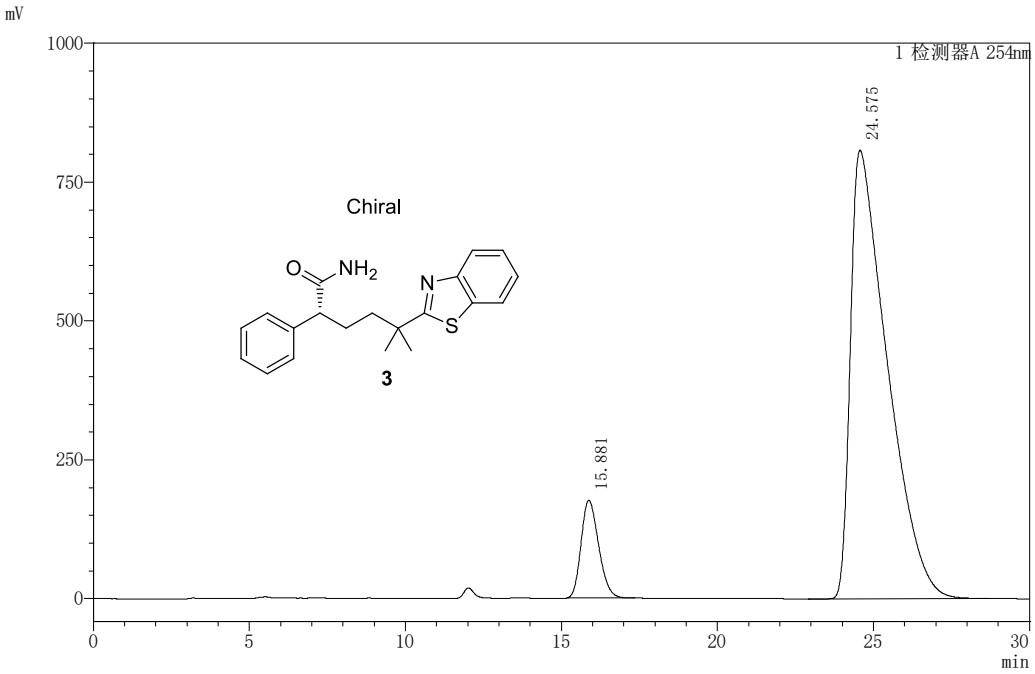
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	19.107	63470	1678075	51.460
2	20.663	52158	1582807	48.540
Total		115628	3260882	100.000



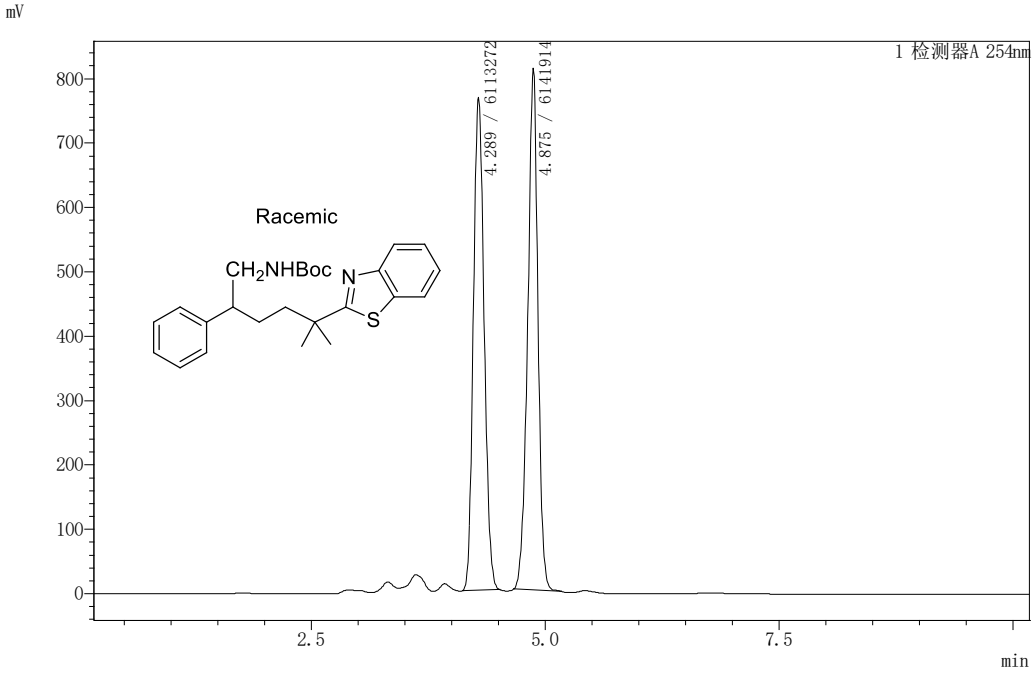
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	19.019	217878	5735526	91.955
2	20.673	18189	501789	8.045
Total		236067	6237315	100.000



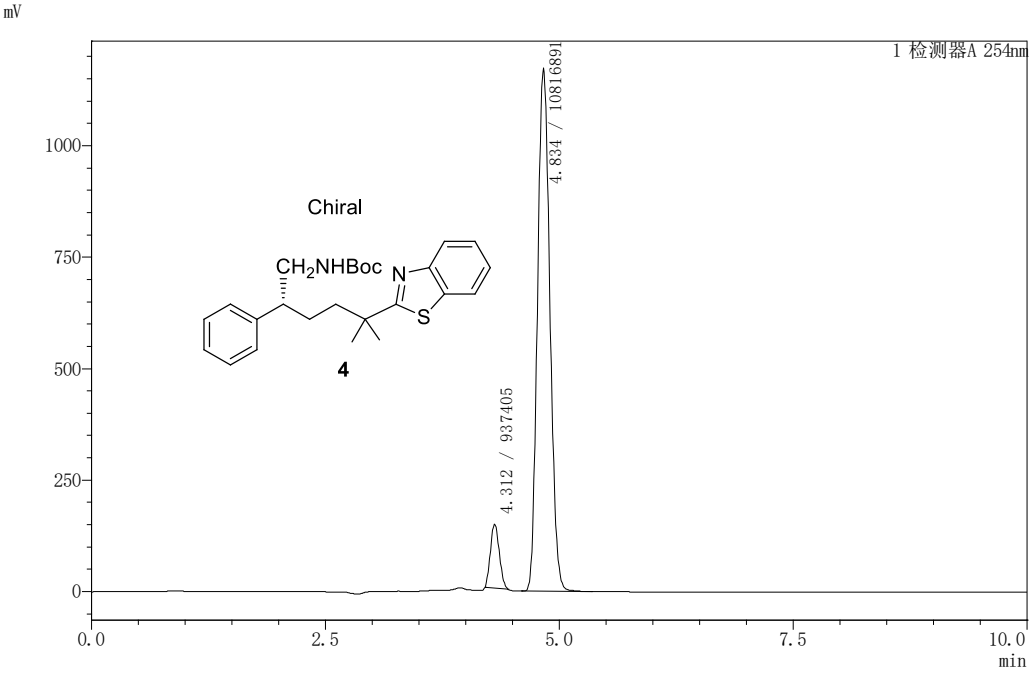
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	15.453	711078	27281128	50.046
2	24.347	420512	27231218	49.954
Total		1131589	54512347	100.000



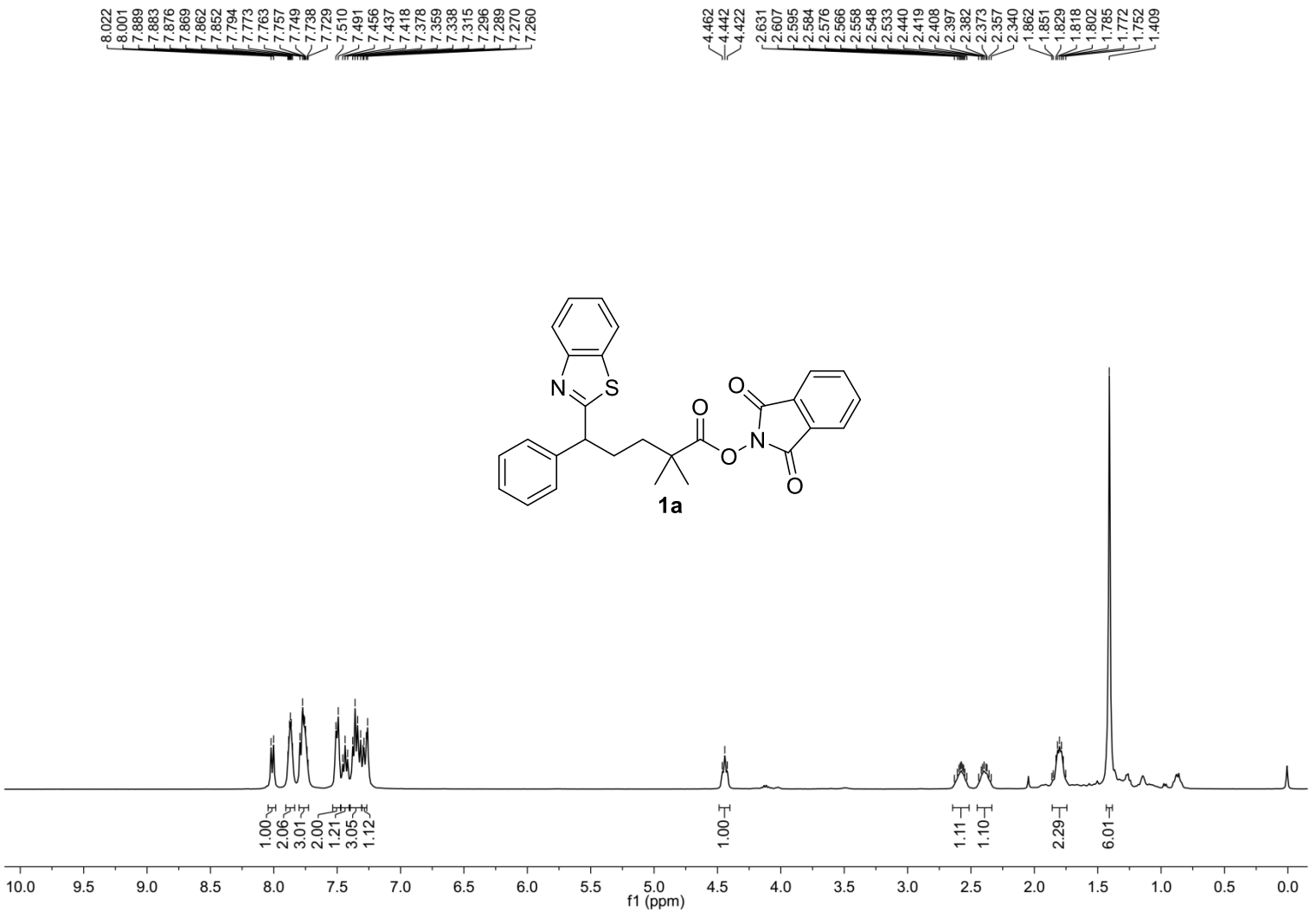
No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	15.881	155583	5428155	9.577
2	24.575	807420	66209938	90.423
Total		963003	71638093	100.000



No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	4.289	765687	6113272	49.883
2	4.875	810988	6141914	50.117
Total		1576675	12255187	100.000



No.	Ret.Time (min)	Height (mAU)	Area(mAU*min)	Rel.Area (%)
1	4.312	410429	937405	7.075
2	4.834	2822969	10816891	92.425
Total		3233398	11779908	100.000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7.738
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7.378
7.359
7.338
7.315
7.296
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7.270
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4.422
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2.584
2.576
2.566
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2.397
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1.802
1.785
1.772
1.752
1.409
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S
O
O
N
O
O
1a
1.00
2.06
3.01
2.00
1.21
3.05
1.12
1.00
1.11
1.10
2.29
6.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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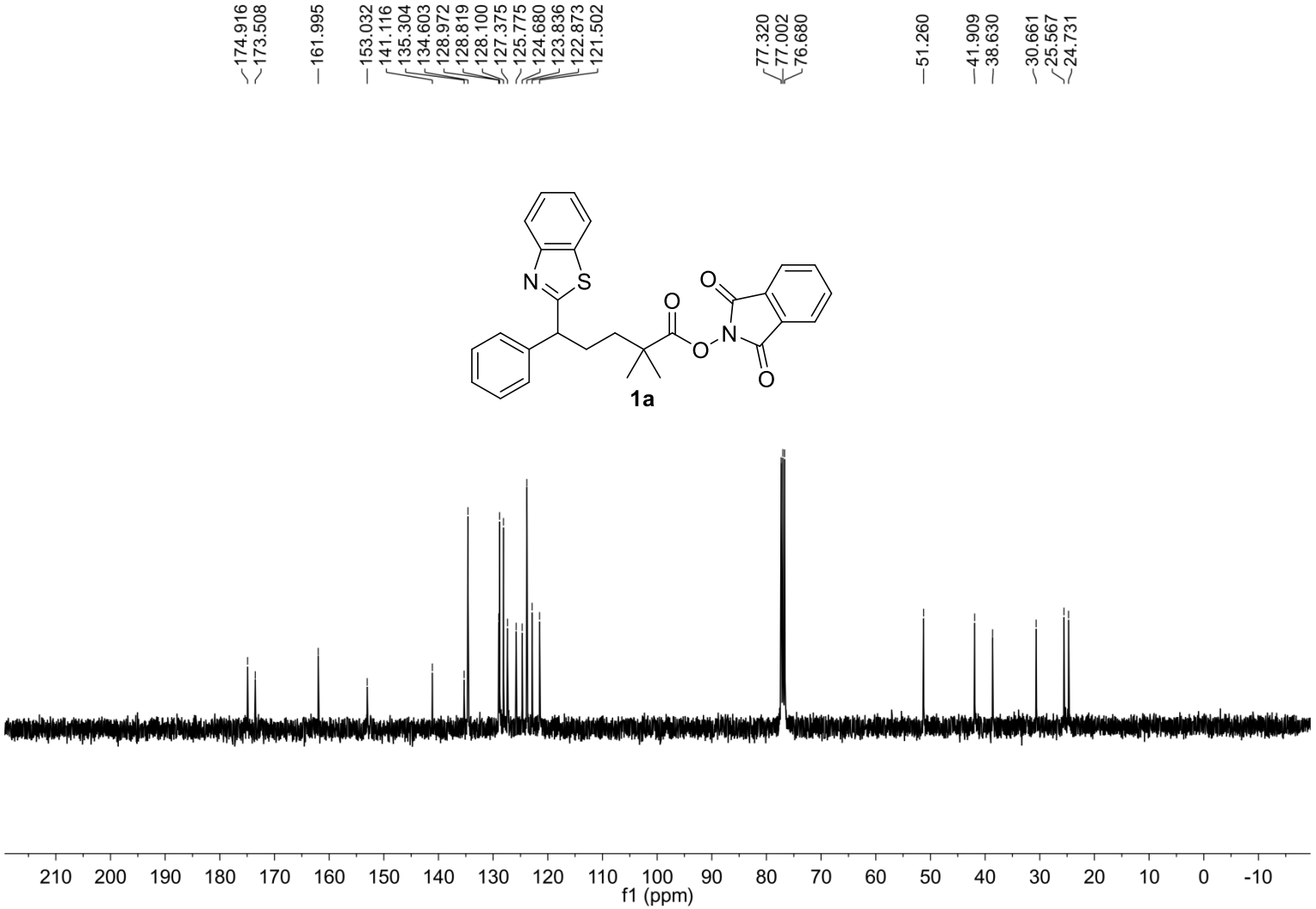
0.0
f1 (ppm)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127.375
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124.680
123.836
122.873
121.502
77.320
77.002
76.680
51.260
41.909
38.630
30.661
25.567
24.731
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S
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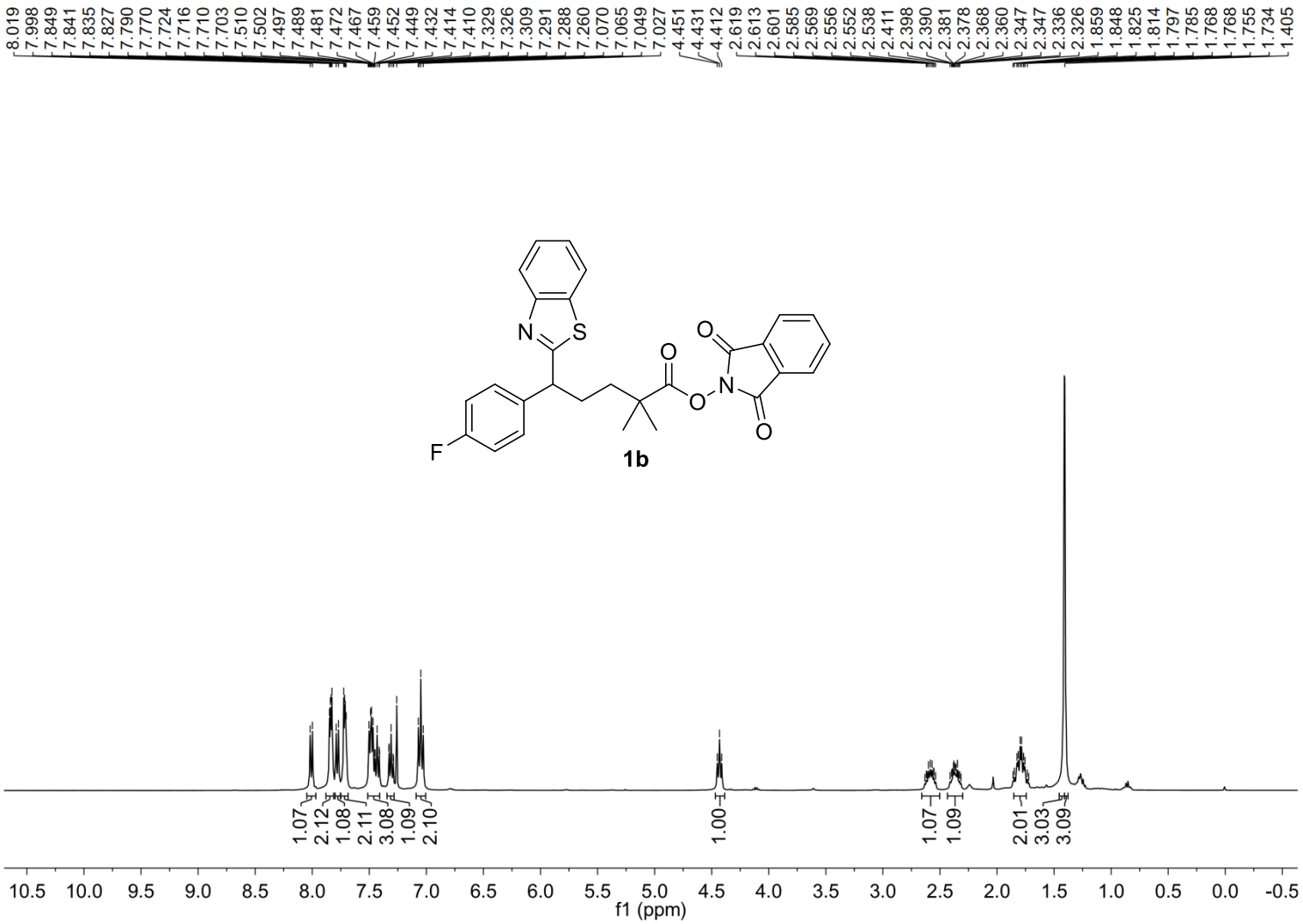
f1 (ppm)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7.489
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7.467
7.459
7.452
7.449
7.432
7.414
7.410
7.329
7.326
7.309
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7.288
7.260
7.070
7.065
7.049
7.027
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4.431
4.412
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2.585
2.569
2.556
2.552
2.538
2.411
2.398
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2.360
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2.347
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1.785
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1.768
1.755
1.734
1.405
N
S
O
O
N
O
O
F
1b
1.07
2.12
1.08
2.11
3.08
1.09
2.10
1.00
1.07
1.09
2.01
3.03
3.09
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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3.0
2.5
2.0
1.5
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0.5
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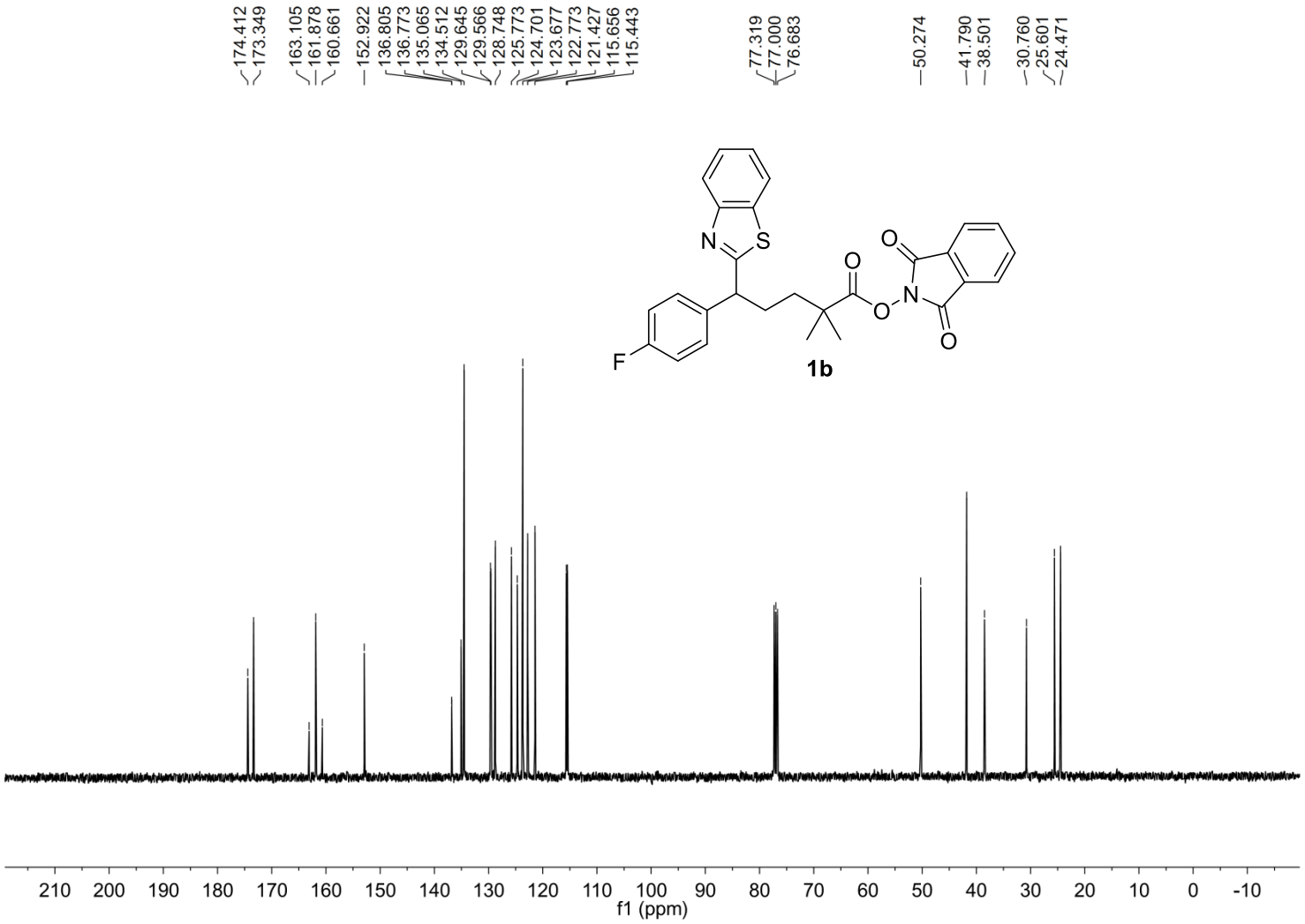
-0.5
f1 (ppm)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128.748
125.773
124.701
123.677
122.773
121.427
115.656
115.443
77.319
77.000
76.683
50.274
41.790
38.501
30.760
25.601
24.471
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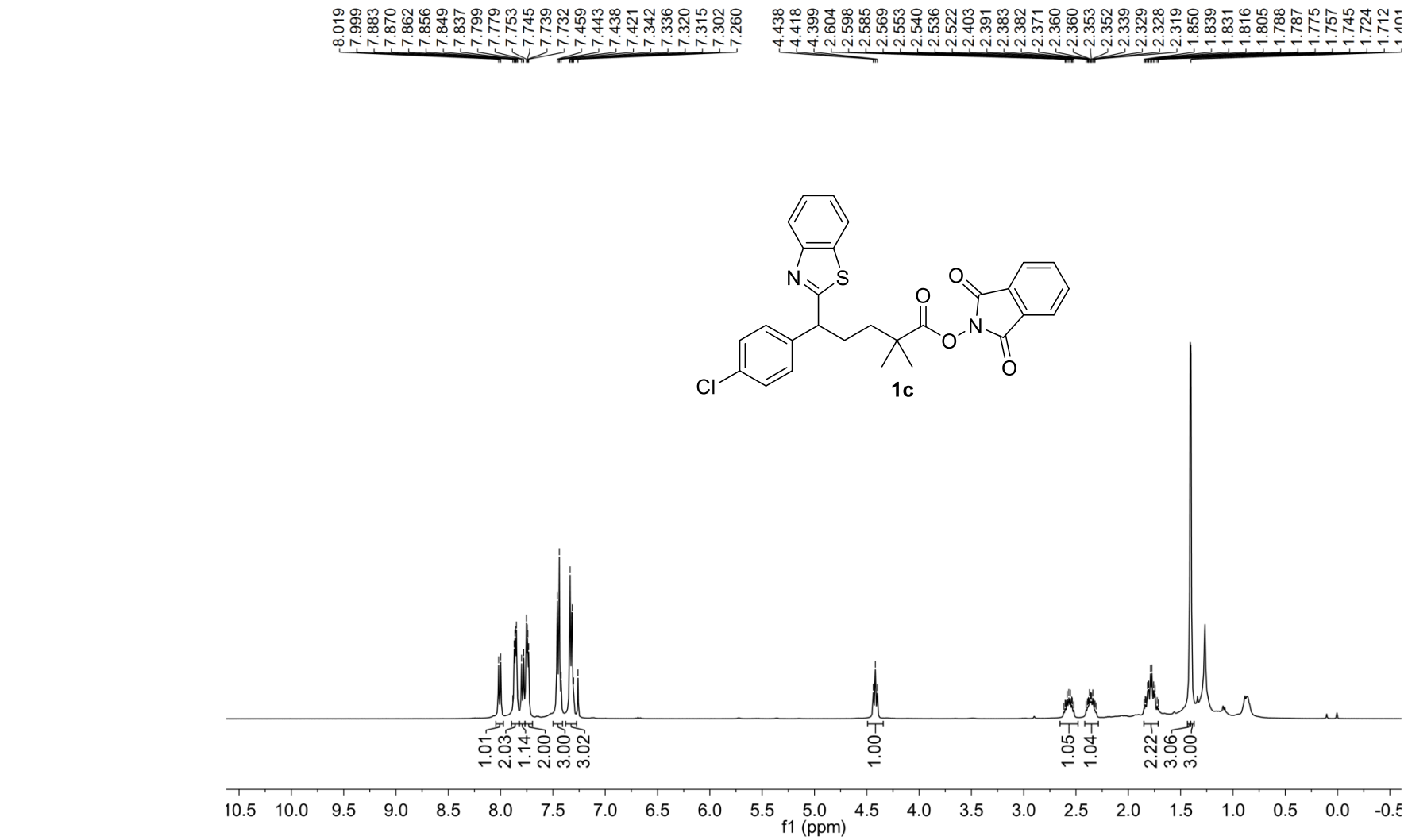
S
O
O
N
O
O
F
1b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.438
7.421
7.342
7.336
7.320
7.315
7.302
7.260
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4.418
4.399
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2.598
2.585
2.569
2.553
2.540
2.536
2.522
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2.382
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2.360
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2.352
2.339
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2.328
2.319
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1.839
1.831
1.816
1.805
1.788
1.787
1.775
1.757
1.745
1.724
1.712
N
S
O
O
N
O
O
O
Cl
1c
1.01
2.03
1.14
2.00
3.00
3.02
1.00
1.05
1.04
2.22
3.06
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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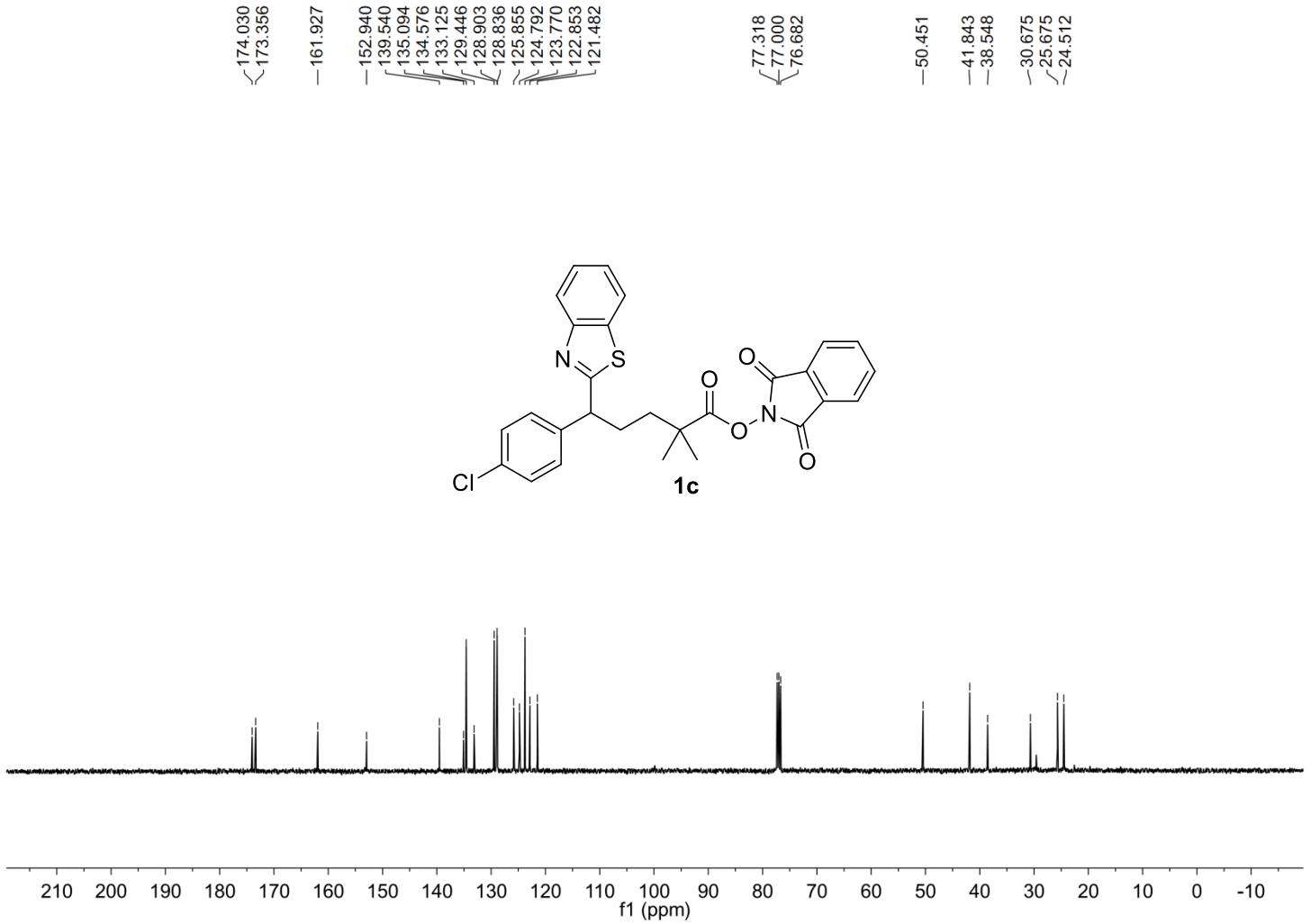
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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123.770
122.853
121.482
77.318
77.000
76.682
50.451
41.843
38.548
30.675
25.675
24.512
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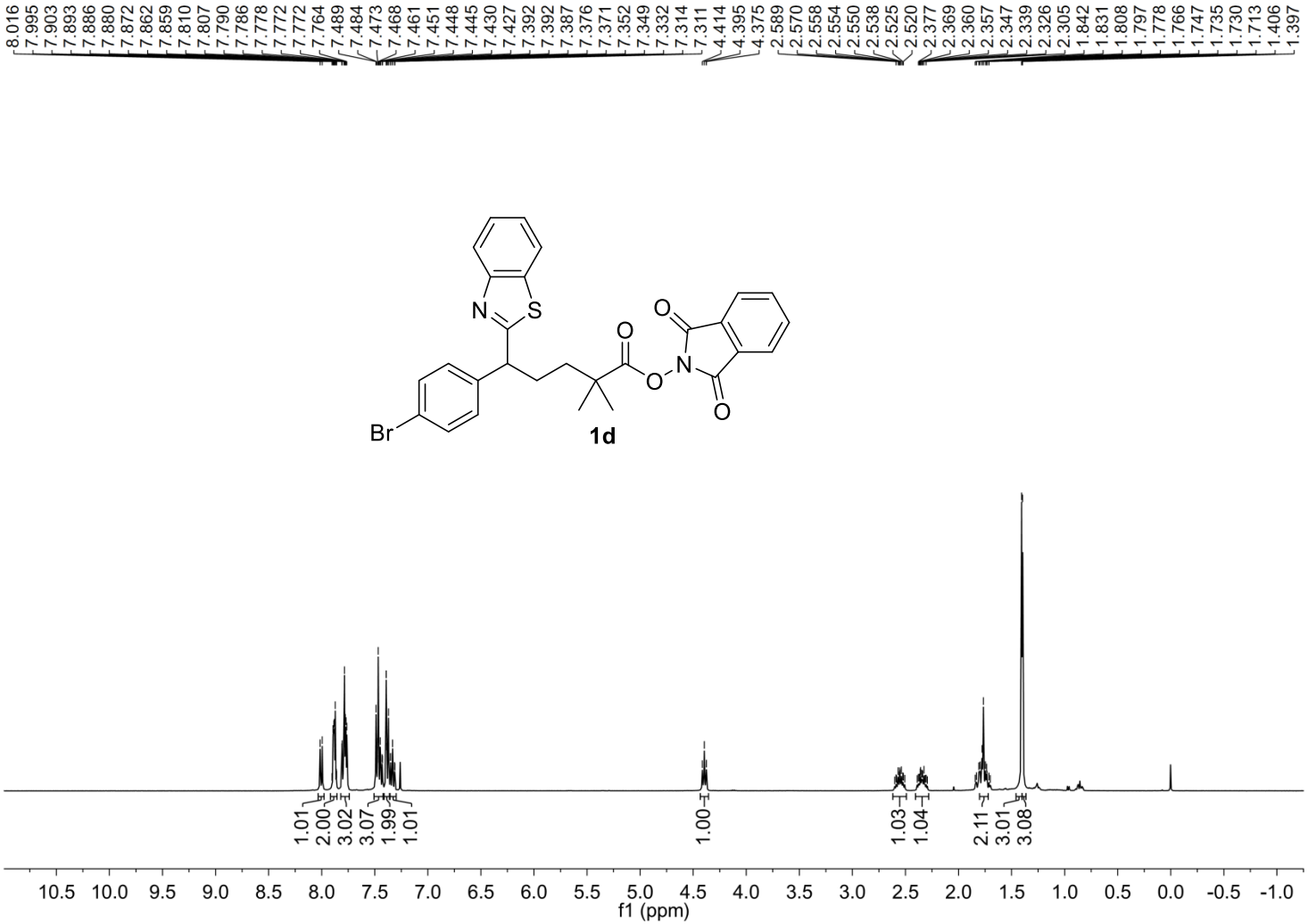
S
O
O
N
O
O
Cl
1c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.772
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7.484
7.473
7.468
7.461
7.451
7.448
7.445
7.430
7.427
7.392
7.392
7.387
7.376
7.371
7.352
7.349
7.332
7.314
7.311
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4.395
4.375
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2.570
2.558
2.554
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2.538
2.525
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2.377
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2.360
2.357
2.347
2.339
2.326
2.305
1.842
1.831
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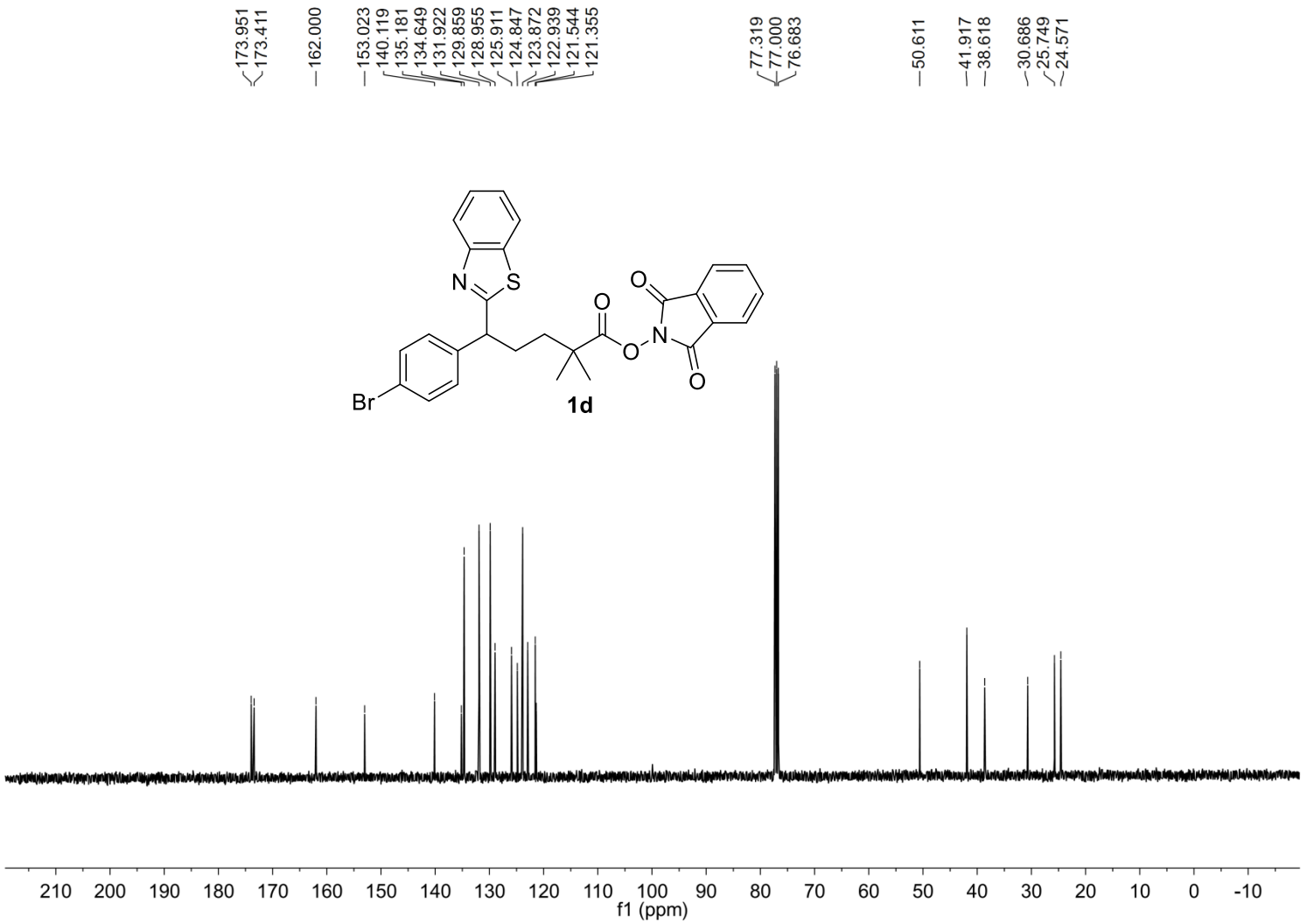
1.797
1.778
1.766
1.747
1.735
1.730
1.713
1.406
1.397
N
S
O
O
N
O
O
Br
1d
1.01
2.00
3.02
3.07
1.99
1.01
1.00
1.03
1.04
2.11
3.01
3.08
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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123.872
122.939
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77.319
77.000
76.683
50.611
41.917
38.618
30.686
25.749
24.571
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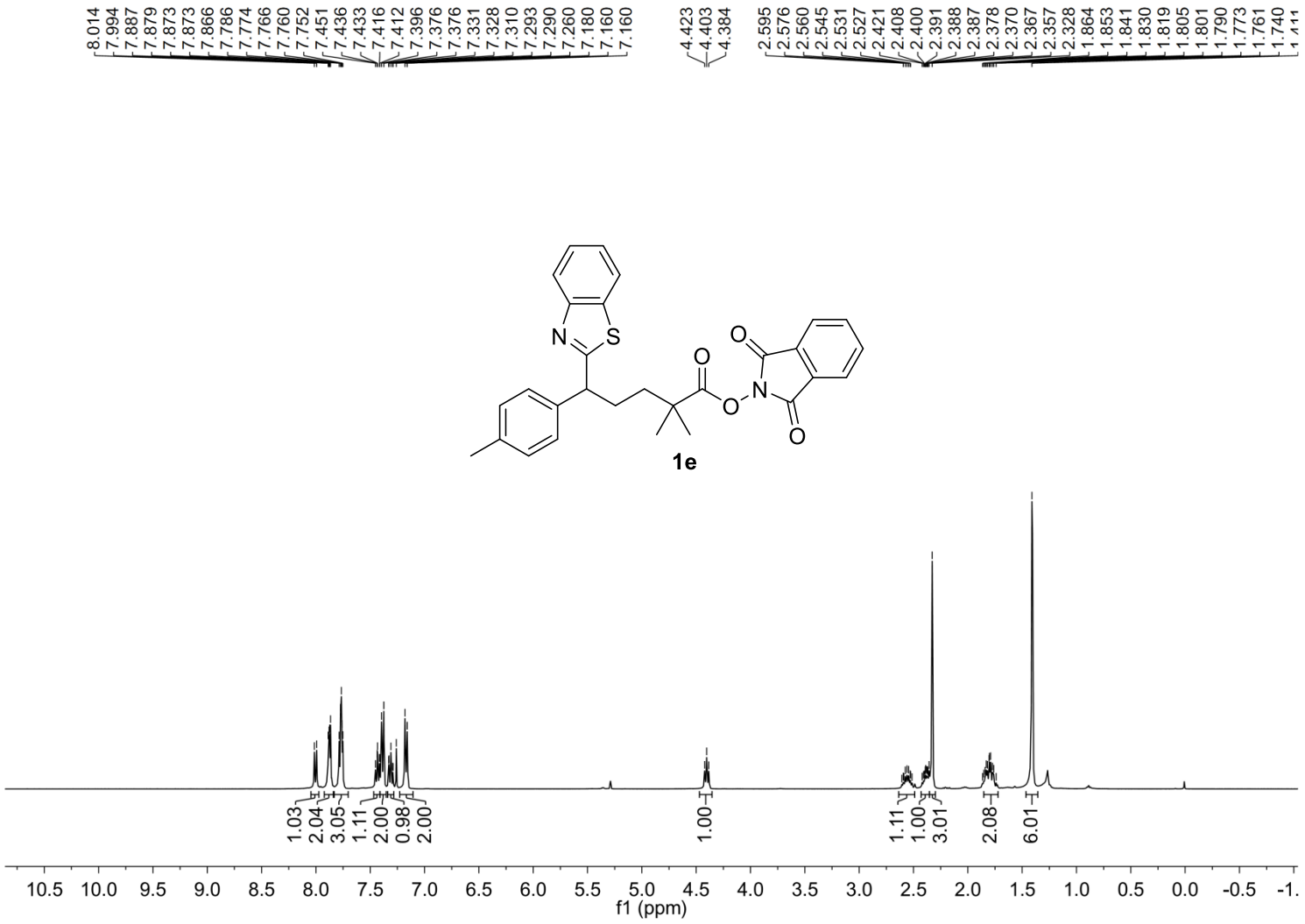
S
O
O
N
O
O
Br
1d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.433
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7.376
7.331
7.328
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7.260
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4.384
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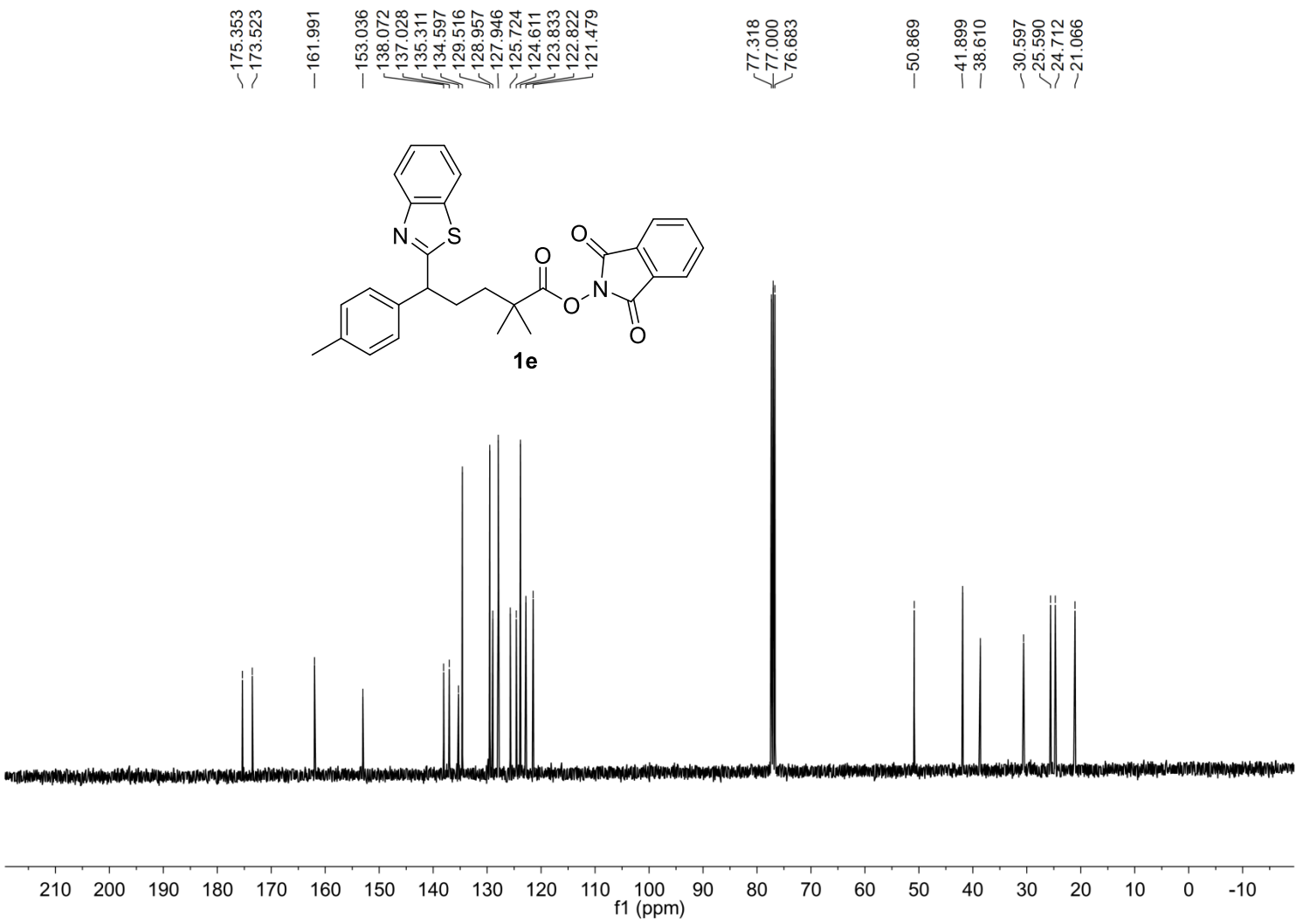
2.576
2.560
2.545
2.531
2.527
2.421
2.408
2.400
2.391
2.388
2.387
2.378
2.370
2.367
2.357
2.328
1.864
1.853
1.841
1.830
1.819
1.805
1.801
1.790
1.773
1.761
1.740
N
S
O
O
N
O
O
1e
1.03
2.04
3.05
1.11
2.00
0.98
2.00
1.00
1.11
1.00
3.01
2.08
6.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)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123.833
122.822
121.479
77.318
77.000
76.683
50.869
41.899
38.610
30.597
25.590
24.712
21.066
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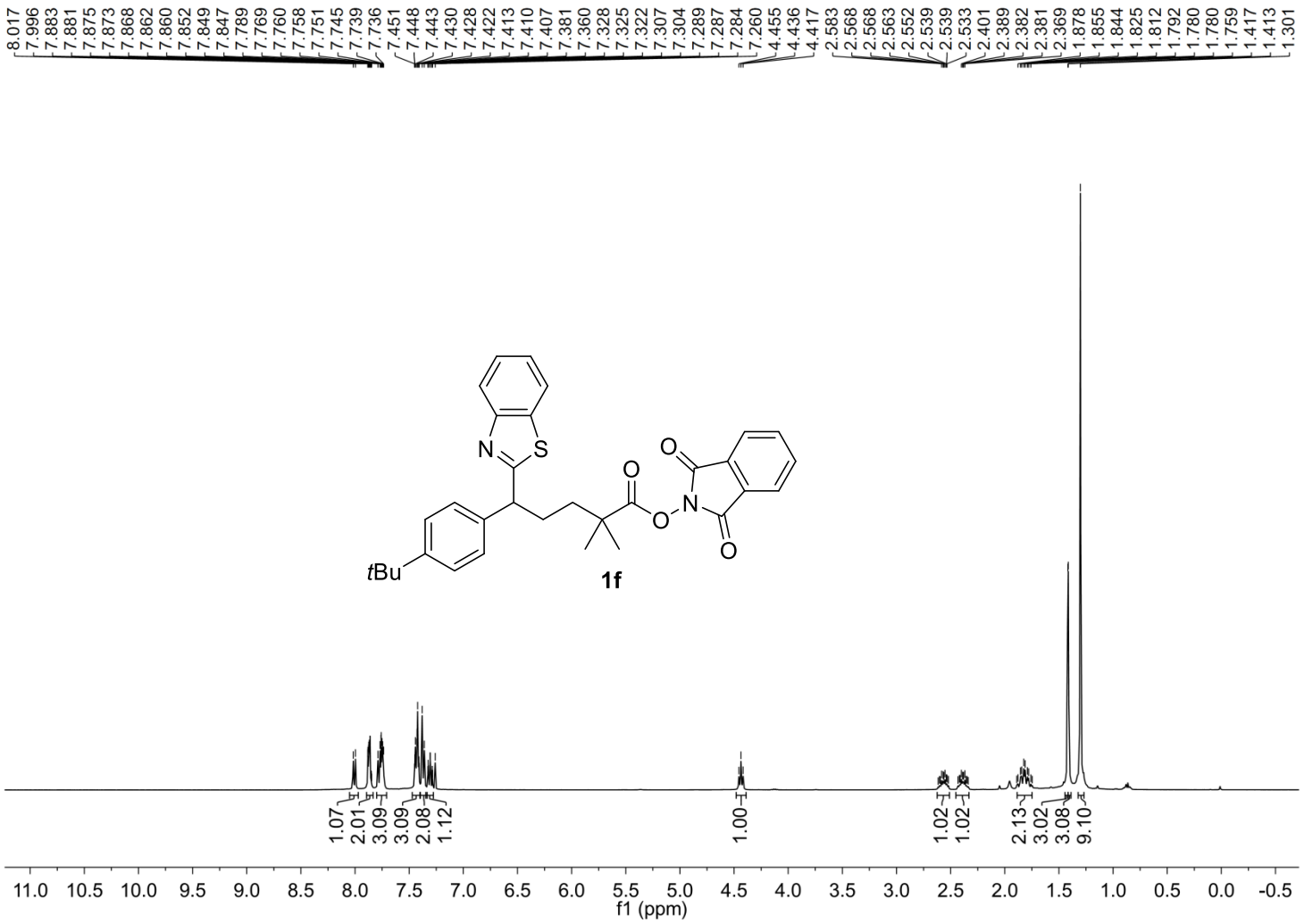
S
O
O
O
N
O
1e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.760
7.758
7.751
7.745
7.739
7.736
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7.448
7.443
7.430
7.428
7.422
7.413
7.410
7.407
7.381
7.360
7.328
7.325
7.322
7.307
7.304
7.289
7.287
7.284
7.260
4.455
4.436
4.417
2.583
2.568
2.568
2.563
2.552
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2.539
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2.401
2.389
2.382
2.381
2.369
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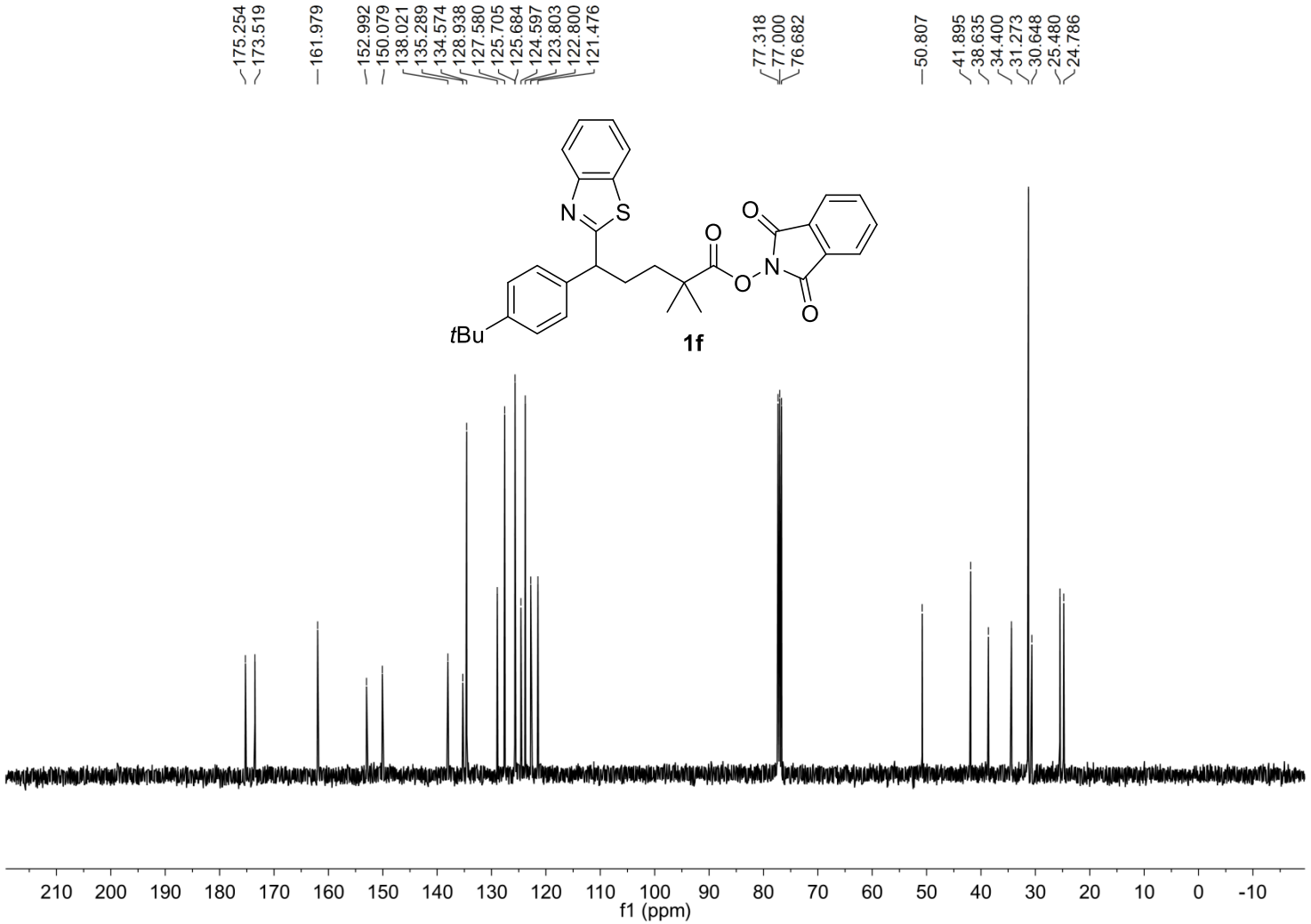
1.855
1.844
1.825
1.812
1.792
1.780
1.780
1.759
1.417
1.413
1.301
N
S
O
O
N
O
O
tBu
1f
1.07
2.01
3.09
3.09
2.08
1.12
1.00
1.02
1.02
2.13
3.02
3.08
9.10
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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134.574
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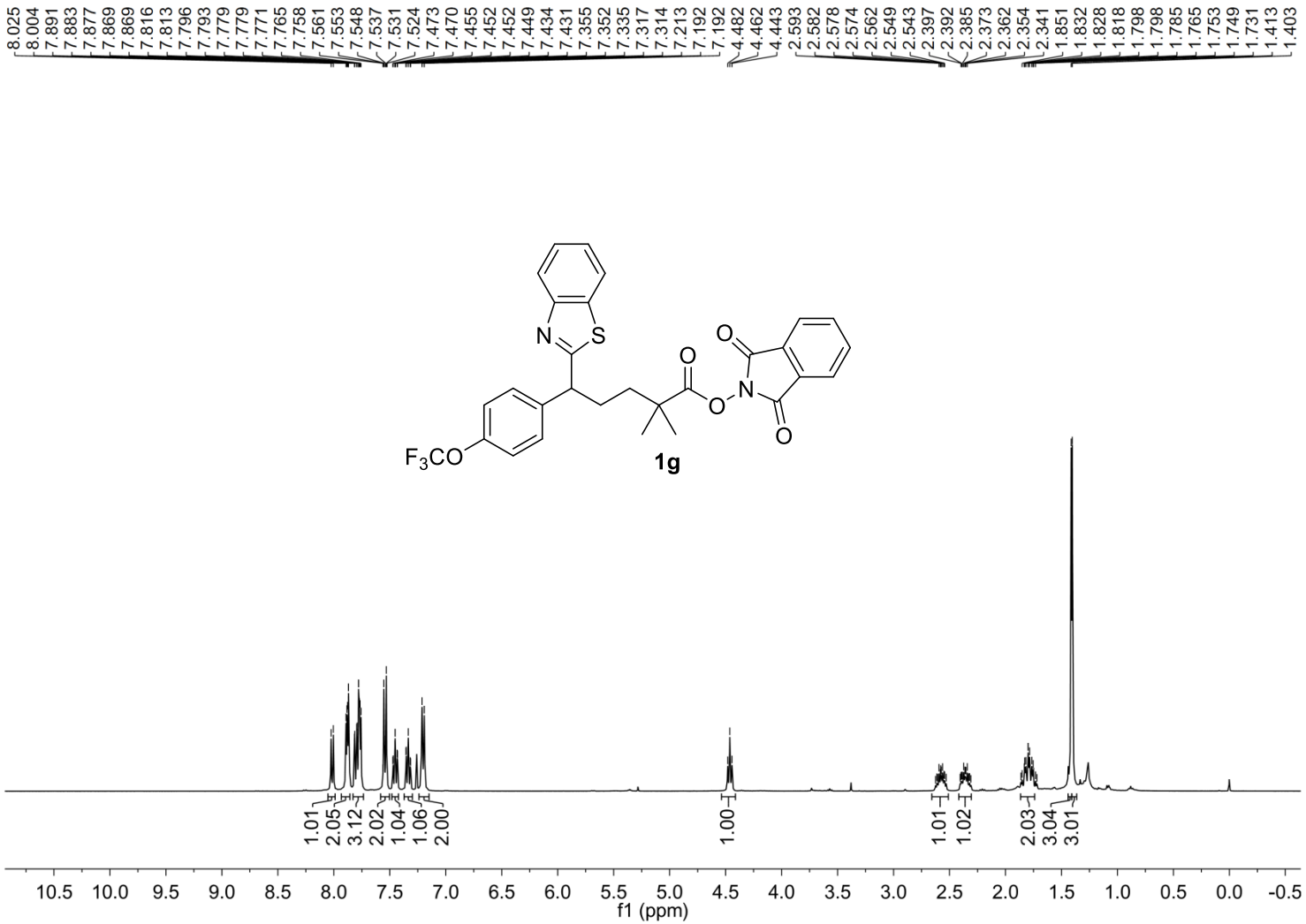
125.705
125.684
124.597
123.803
122.800
121.476
77.318
77.000
76.682
50.807
41.895
38.635
34.400
31.273
30.648
25.480
24.786
N
S
O
O
N
O
O
tBu
1f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.779
7.779
7.771
7.765
7.758
7.561
7.553
7.548
7.537
7.531
7.524
7.473
7.470
7.455
7.452
7.452
7.449
7.434
7.431
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7.335
7.317
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7.213
7.192
7.192
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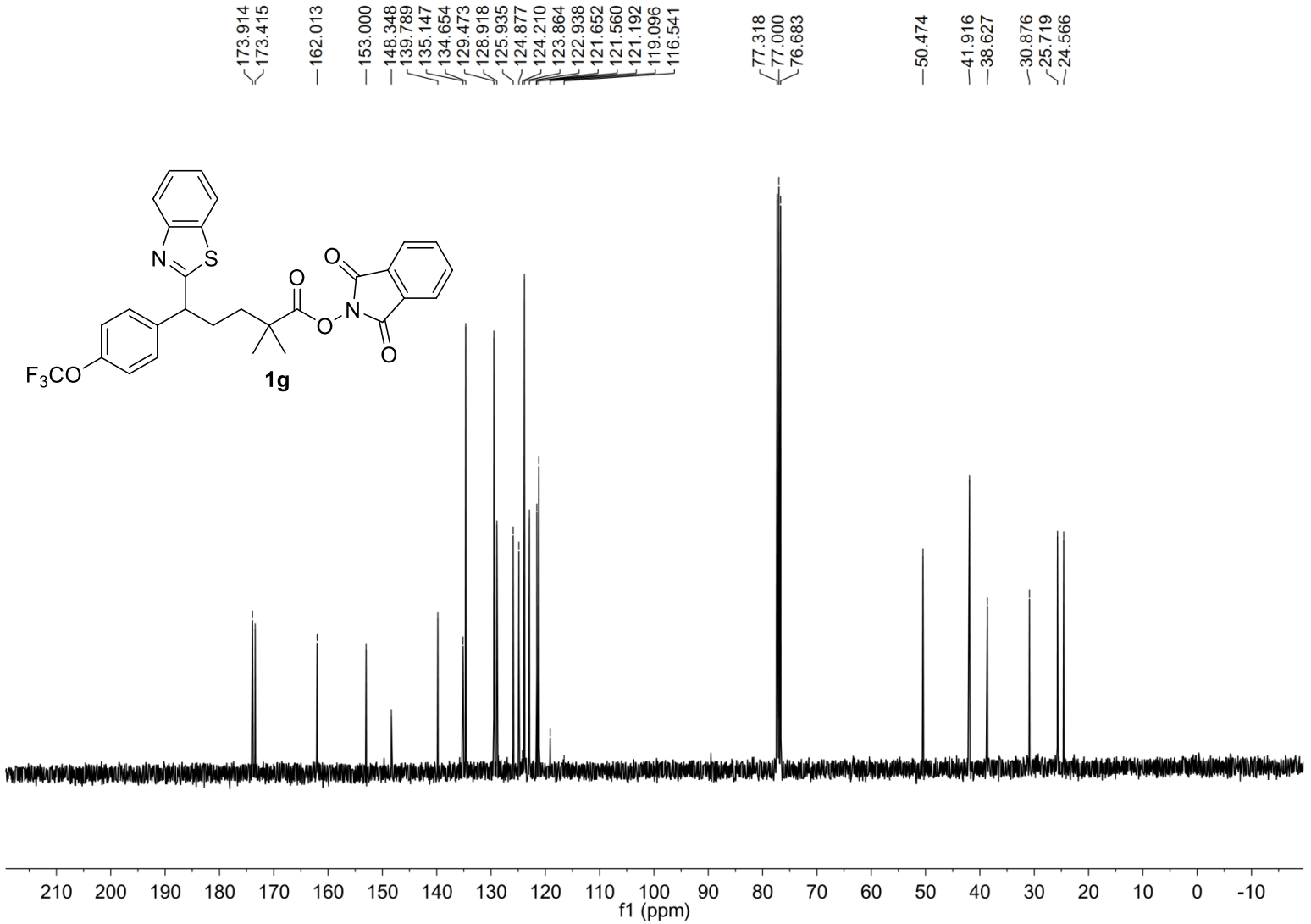
4.462
4.443
2.593
2.582
2.578
2.574
2.562
2.549
2.543
2.397
2.392
2.385
2.373
2.362
2.354
2.341
1.851
1.832
1.828
1.818
1.798
1.798
1.785
1.765
1.753
1.749
1.731
1.413
1.403
N
S
O
O
N
O
O
F3CO
1g
1.01
2.05
3.12
2.02
1.04
1.06
2.00
1.00
1.01
1.02
2.03
3.04
3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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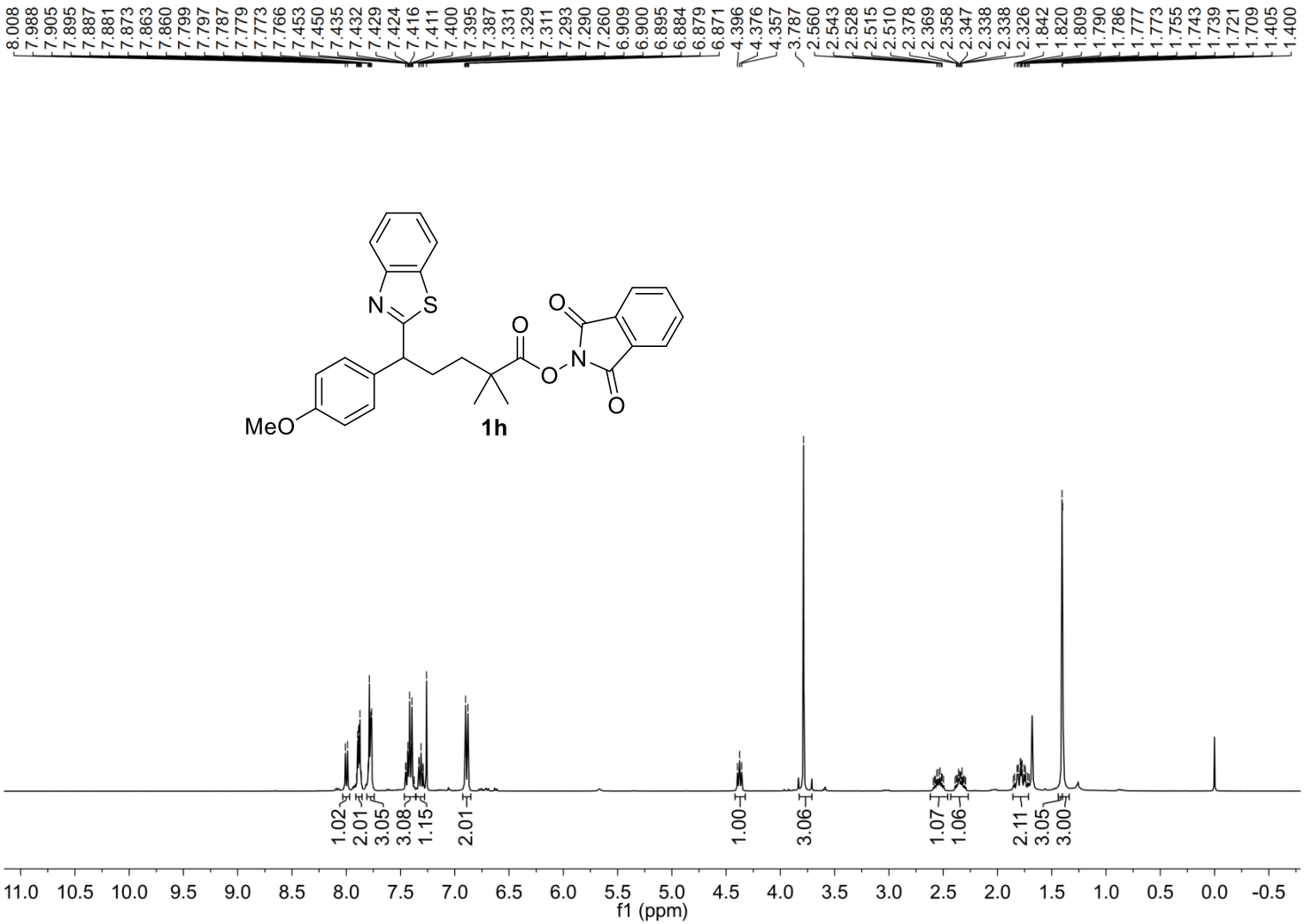
124.877
124.210
123.864
122.938
121.652
121.560
121.192
119.096
116.541
77.318
77.000
76.683
50.474
41.916
38.627
30.876
25.719
24.566
N
S
O
O
N
O
O
O
F3CO
1g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.787
7.779
7.773
7.766
7.453
7.450
7.435
7.432
7.429
7.424
7.416
7.411
7.400
7.395
7.387
7.331
7.329
7.311
7.293
7.290
7.260
6.909
6.900
6.895
6.884
6.879
6.871
4.396
4.376
4.357
3.787
2.560
2.543
2.528
2.515
2.510
2.378
2.369
2.358
2.347
2.338
2.338
2.326
1.842
1.820
1.809
1.790
1.786
1.777
1.773
1.755
1.743
1.739
1.721
1.709
1.405
1.400
N
S
O
O
O
N
O
MeO
1h
1.02
2.01
3.05
3.08
1.15
2.01
1.00
3.06
1.07
1.06
2.11
3.05
3.00
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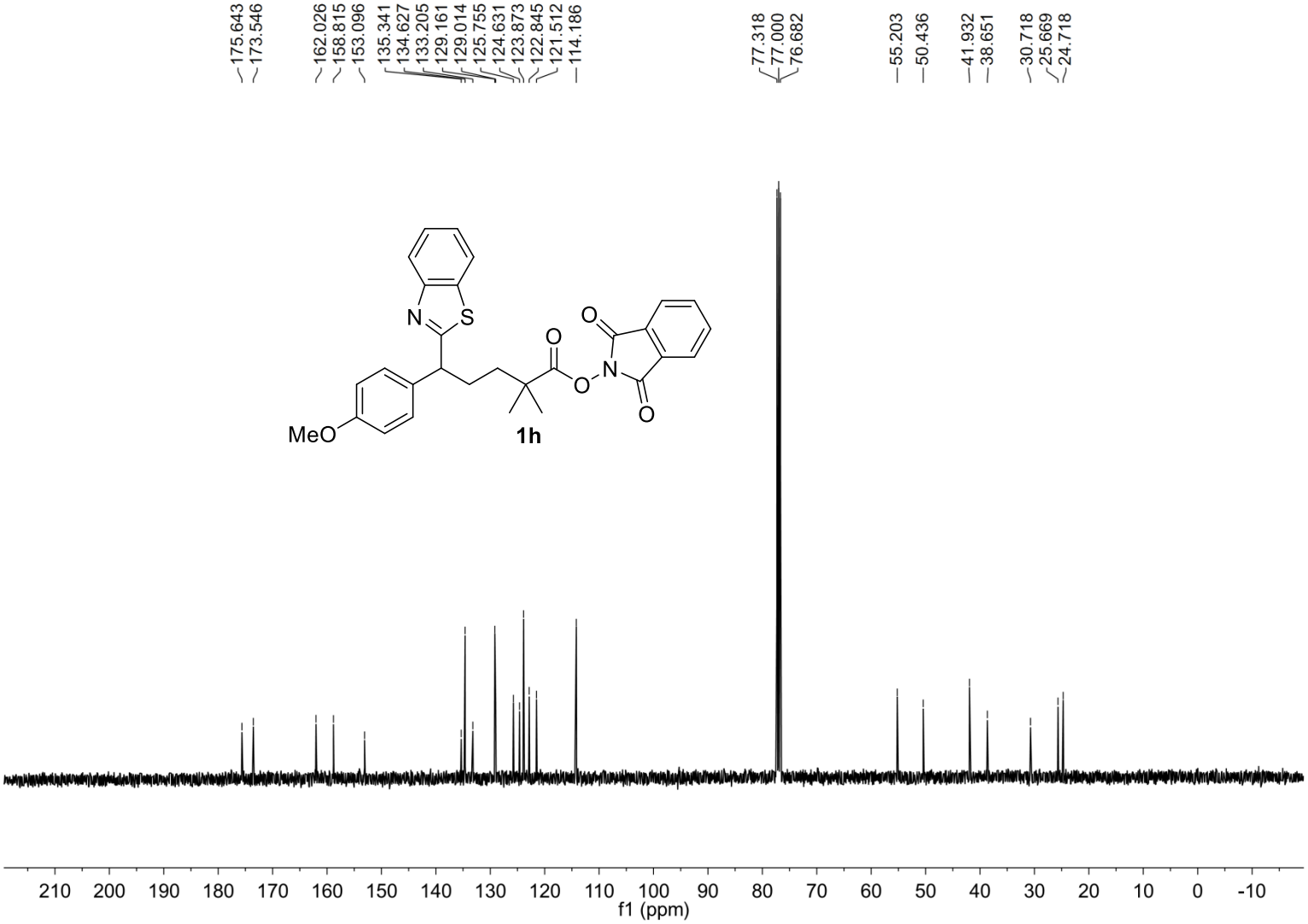
f1 (ppm)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123.873
122.845
121.512
114.186
77.318
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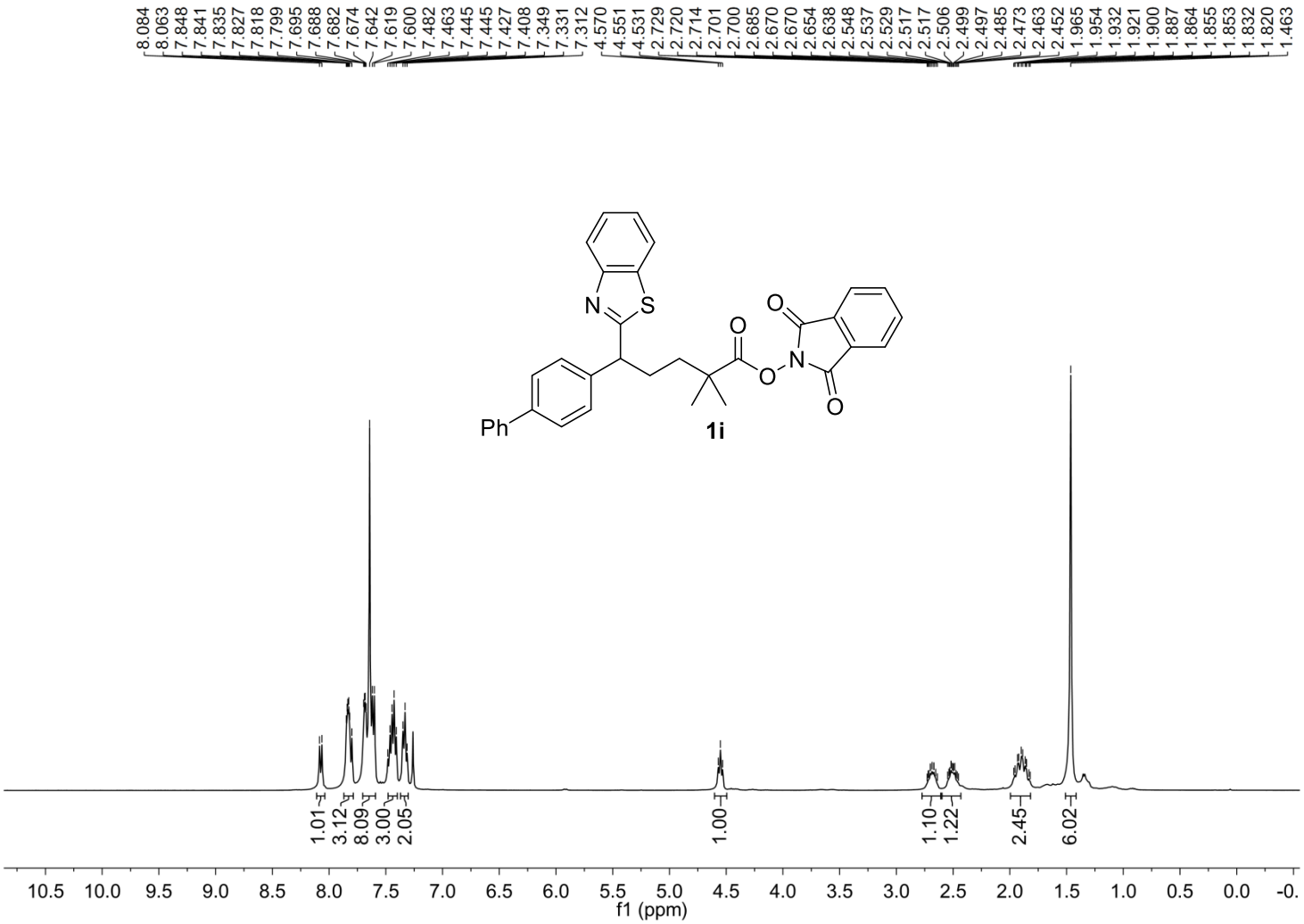
25.669
24.718
MeO
1h
f1 (ppm)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7.688
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7.642
7.619
7.600
7.482
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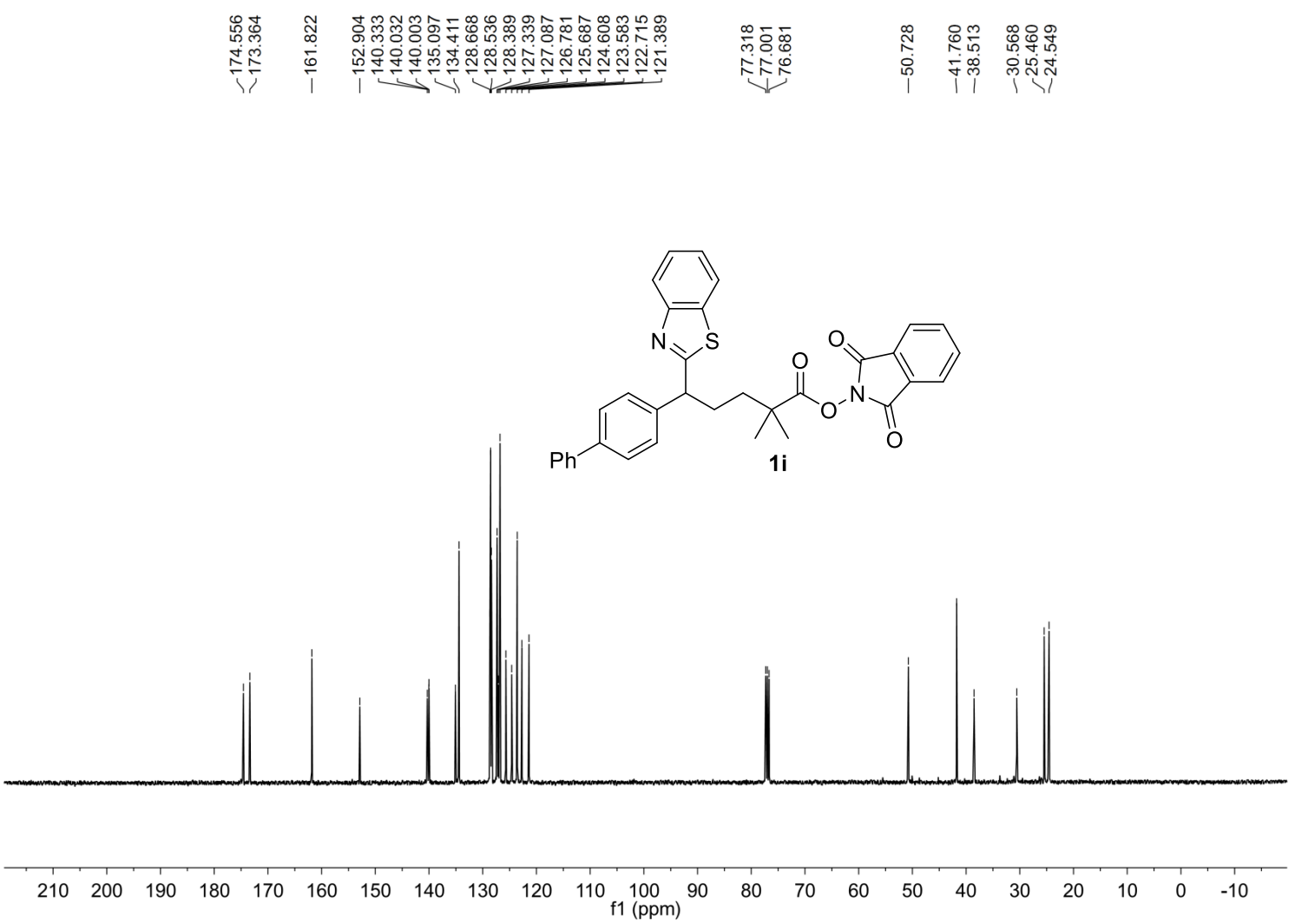
7.445
7.445
7.427
7.408
7.349
7.331
7.312
4.570
4.551
4.531
2.729
2.720
2.714
2.701
2.700
2.685
2.670
2.670
2.654
2.638
2.548
2.537
2.529
2.517
2.517
2.506
2.499
2.497
2.485
2.473
2.463
2.452
1.965
1.954
1.932
1.921
1.900
1.887
1.864
1.855
1.853
1.832
1.820
1.463
N
S
O
O
N
O
O
Ph
1i
1.01
3.12
8.09
3.00
2.05
1.00
1.10
1.22
2.45
6.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)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127.087
126.781
125.687
124.608
123.583
122.715
121.389
77.318
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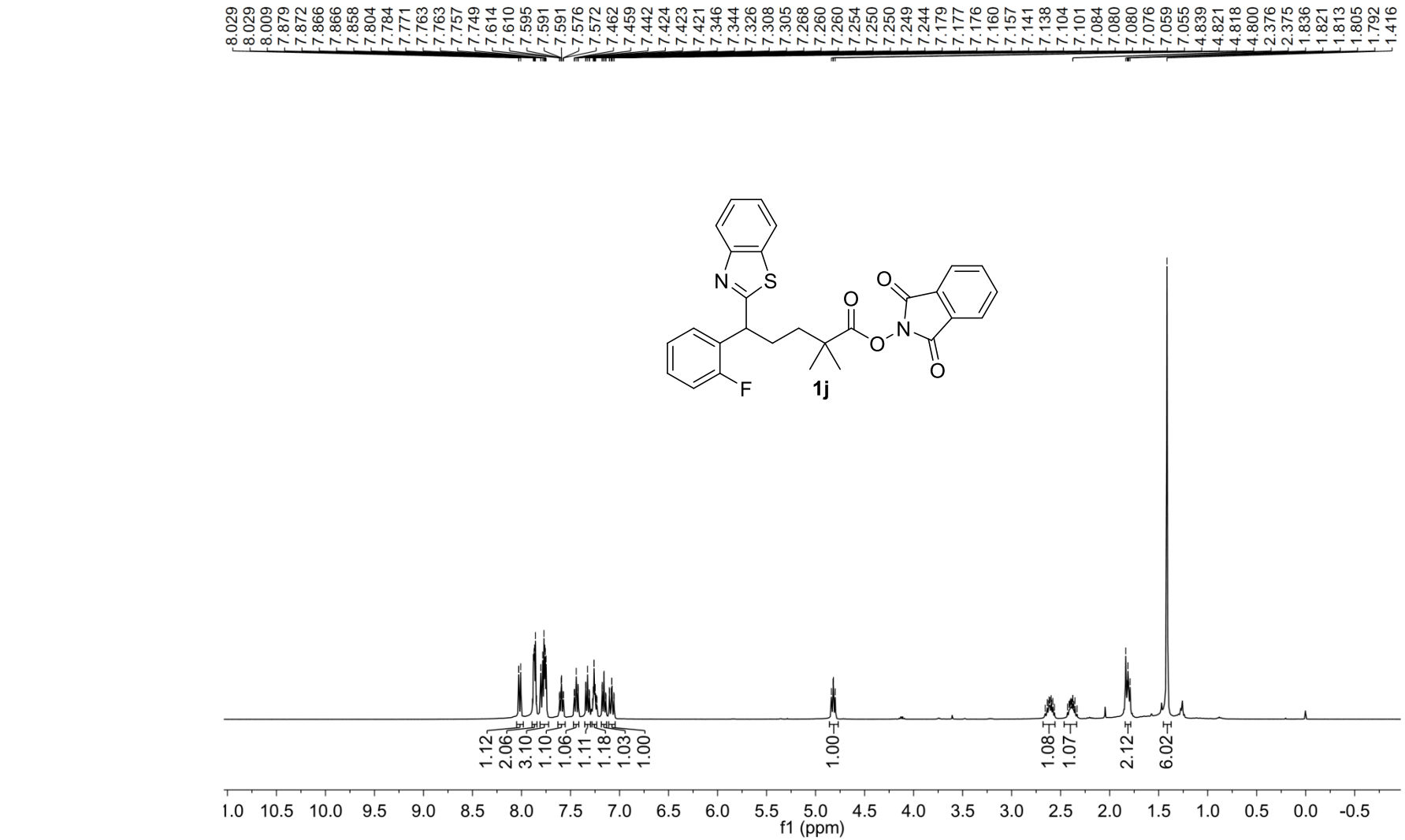
76.681
50.728
41.760
38.513
30.568
25.460
24.549
N
S
O
O
N
O
O
Ph
1i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.260
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7.250
7.250
7.249
7.244
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7.160
7.157
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7.080
7.076
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7.055
4.839
4.821
4.818
4.800
2.376
2.375
1.836
1.821
1.813
1.805
1.792
1.416
N
S
O
O
N
O
O
F
1j
1.12
2.06
3.10
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1.06
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1.00
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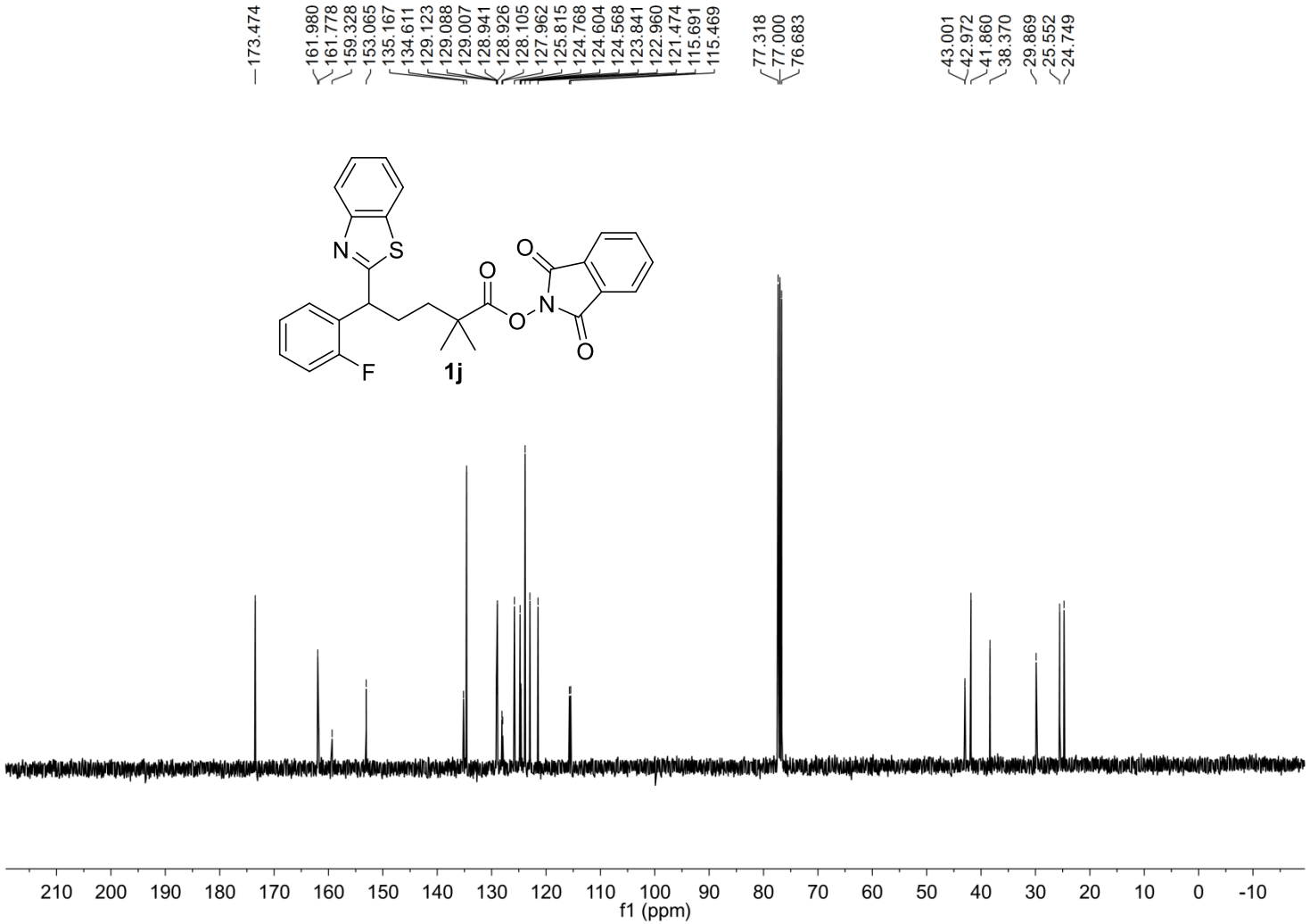
1.07
2.12
6.02
f1 (ppm)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128.105
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125.815
124.768
124.604
124.568
123.841
122.960
121.474
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115.469
77.318
77.000
76.683
43.001
42.972
41.860
38.370
29.869
25.552
24.749
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S
O
O
N
O
O
F
1j
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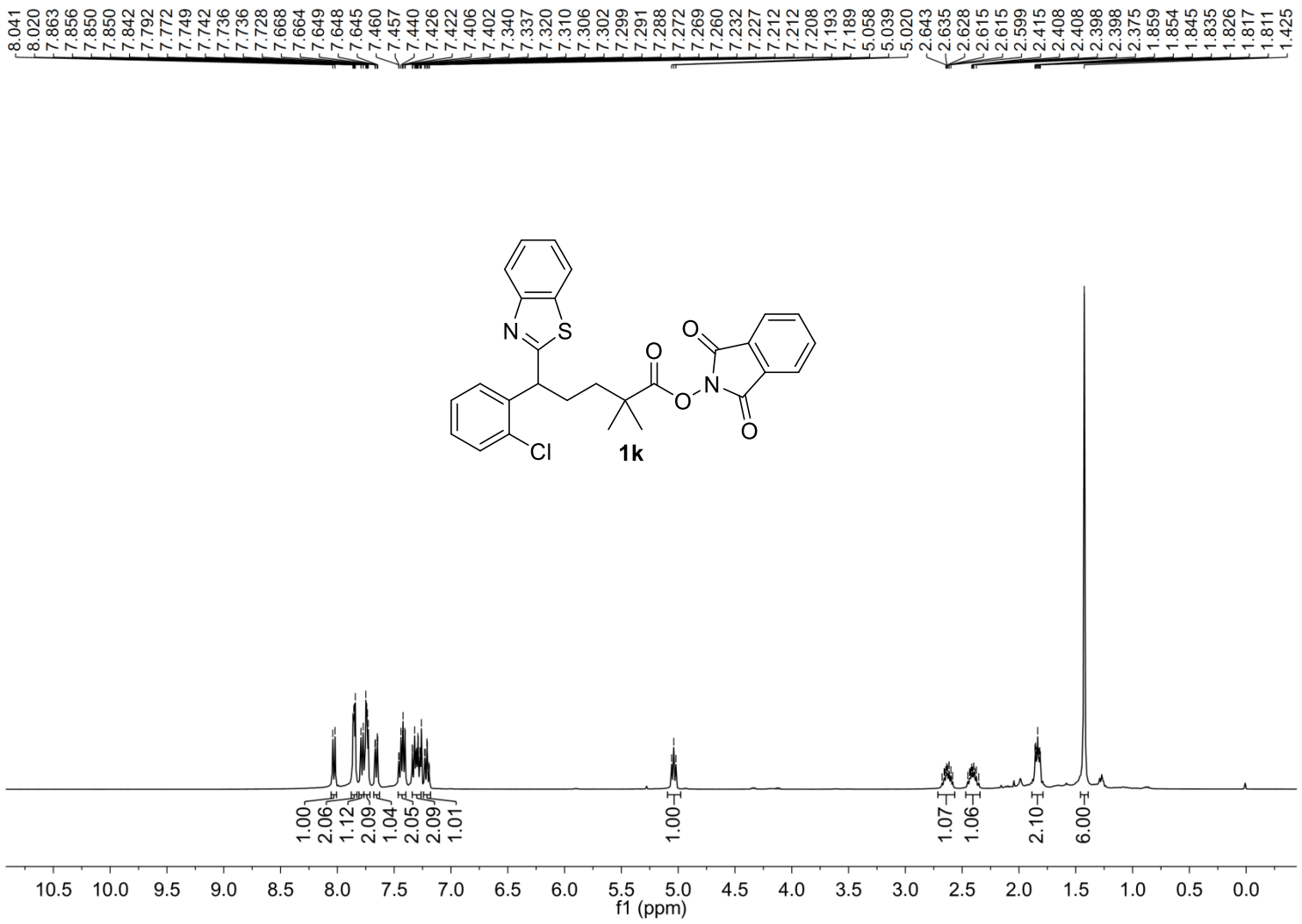
f1 (ppm)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7.648
7.645
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7.422
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7.227
7.212
7.212
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5.039
5.020
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2.615
2.615
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2.408
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2.398
2.375
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1.854
1.845
1.835
1.826
1.817
1.811
1.425
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S
O
O
N
O
O
Cl
1k
1.00
2.06
1.12
2.09
1.04
2.05
2.09
1.01
1.00
1.07
1.06
2.10
6.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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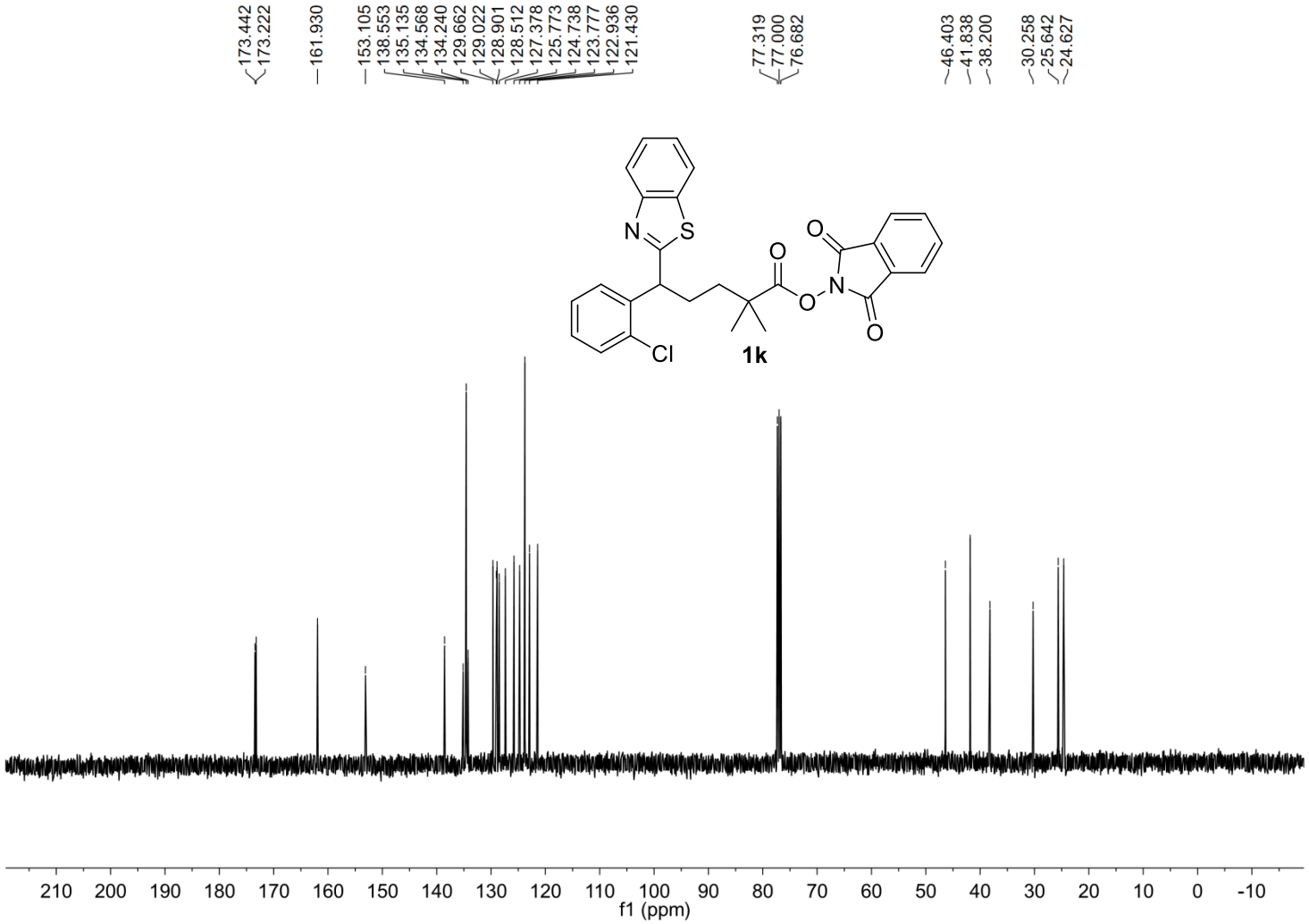
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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127.378
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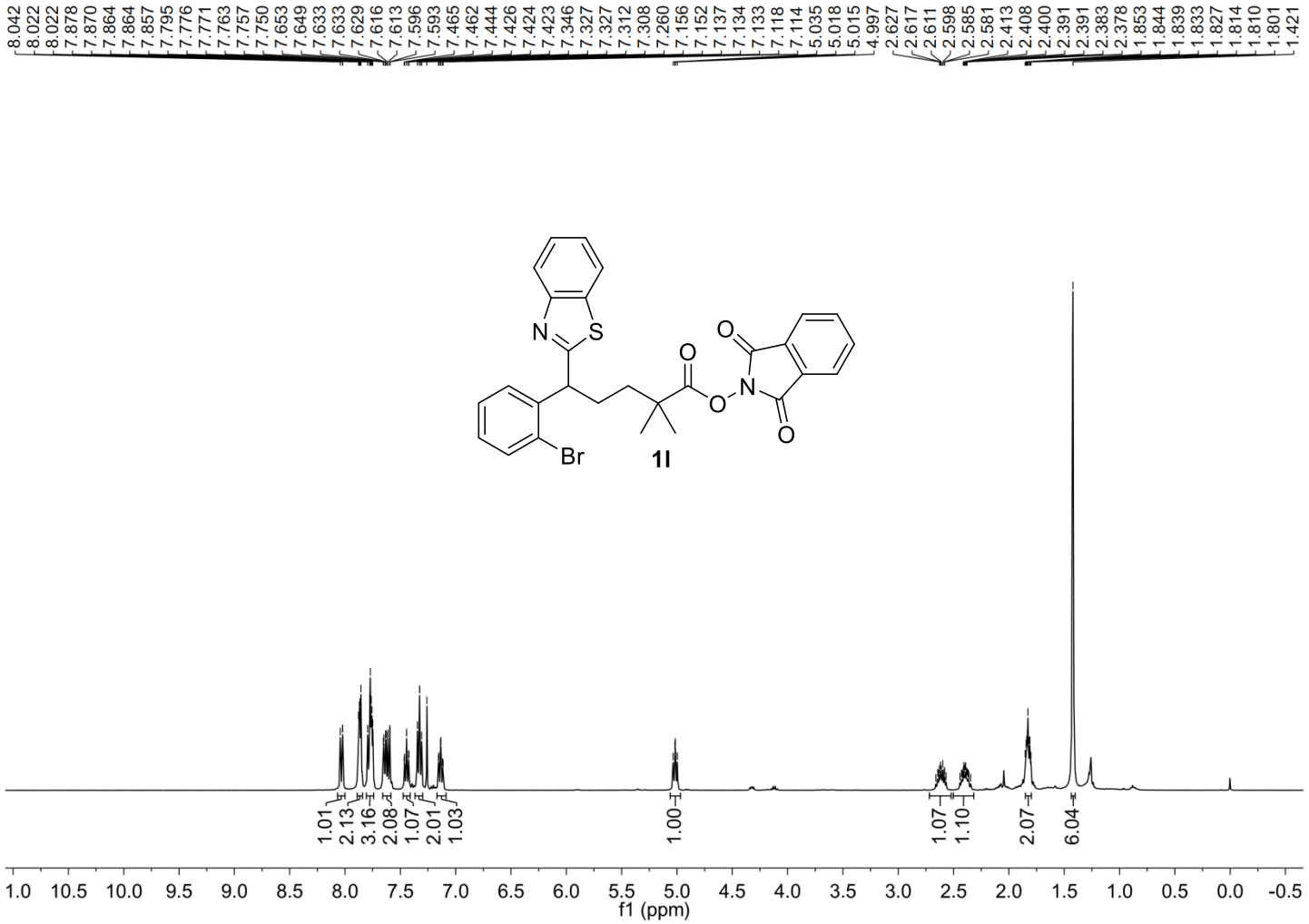
124.738
123.777
122.936
121.430
77.319
77.000
76.682
46.403
41.838
38.200
30.258
25.642
24.627
N
S
O
O
N
O
O
Cl
1k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.633
7.629
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7.613
7.596
7.593
7.465
7.462
7.444
7.426
7.424
7.423
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7.327
7.312
7.308
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7.133
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5.018
5.015
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2.611
2.598
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2.581
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2.378
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1.844
1.839
1.833
1.827
1.814
1.810
1.801
1.421
N
S
O
O
N
O
O
Br
1l
1.01
2.13
3.16
2.08
1.07
2.01
1.03
1.00
1.07
1.10
2.07
6.04
1.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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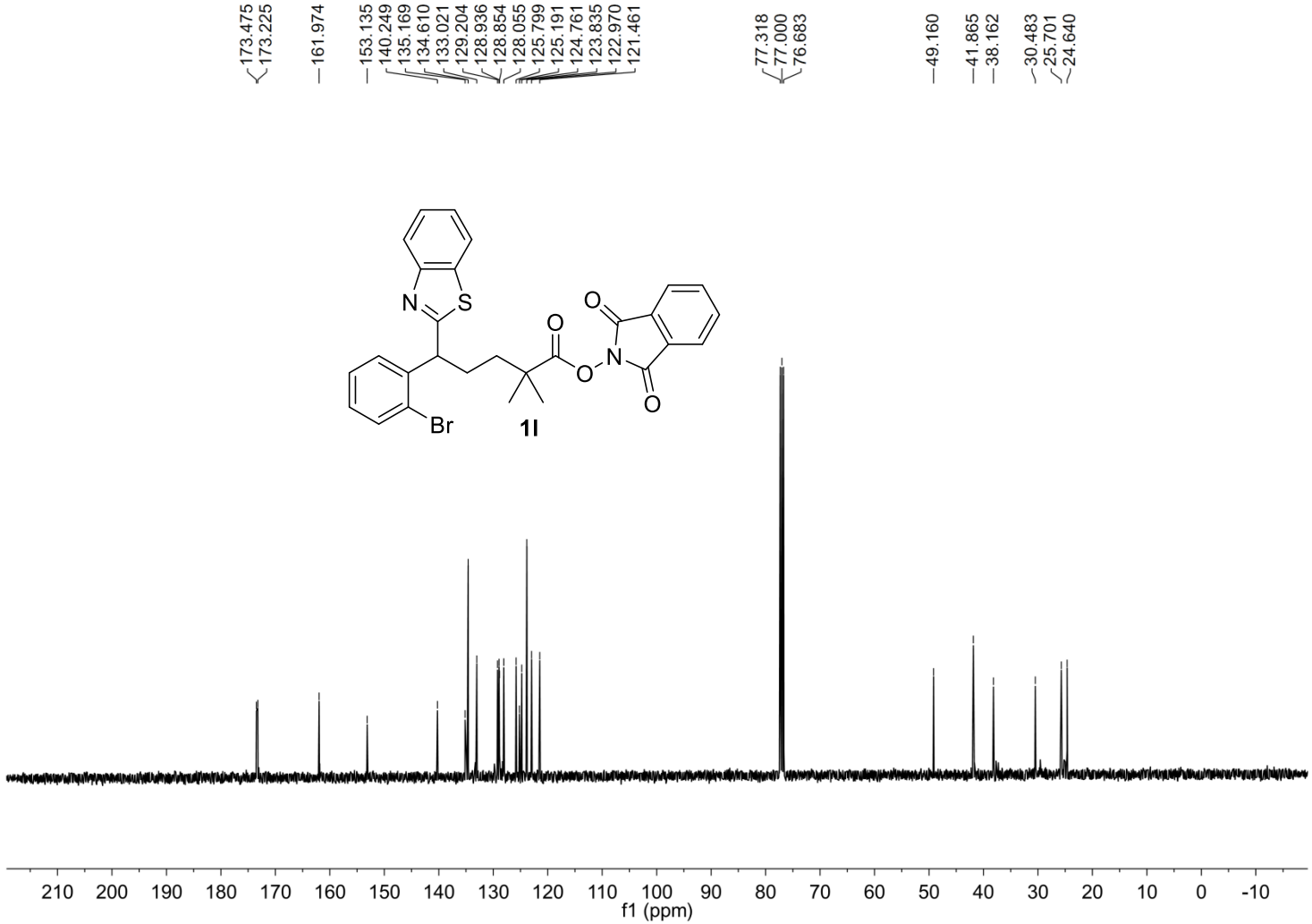
-0.5
f1 (ppm)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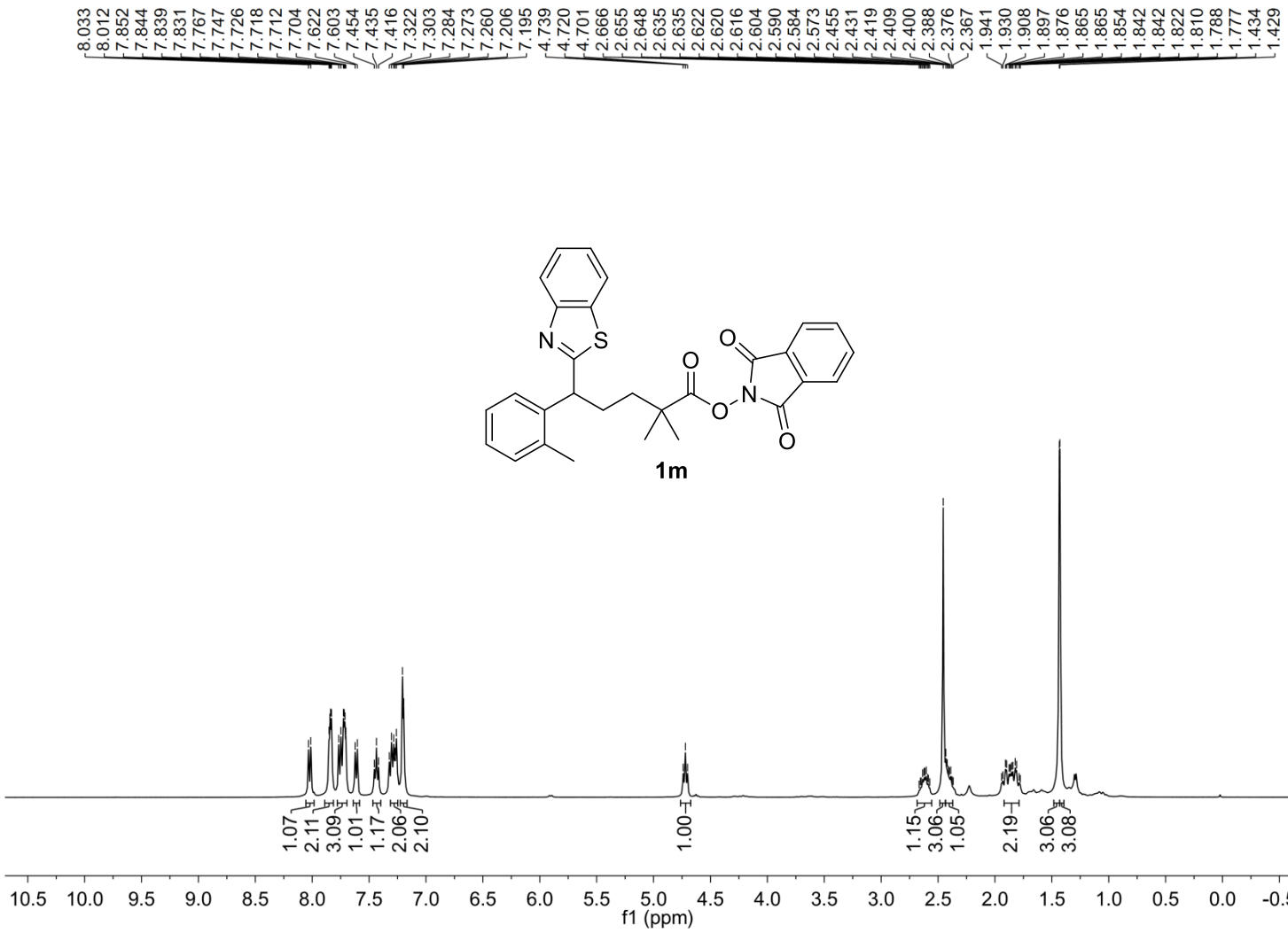
125.799
125.191
124.761
123.835
122.970
121.461
77.318
77.000
76.683
49.160
41.865
38.162
30.483
25.701
24.640
N
S
O
O
O
N
O
Br
1l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.603
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7.303
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7.273
7.260
7.206
7.195
4.739
4.720
4.701
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2.655
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2.620
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1.842
1.842
1.822
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1.777
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1.429
N
S
O
O
N
O
O
1m
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3.09
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1.17
2.06
2.10
1.00
1.15
3.06
1.05
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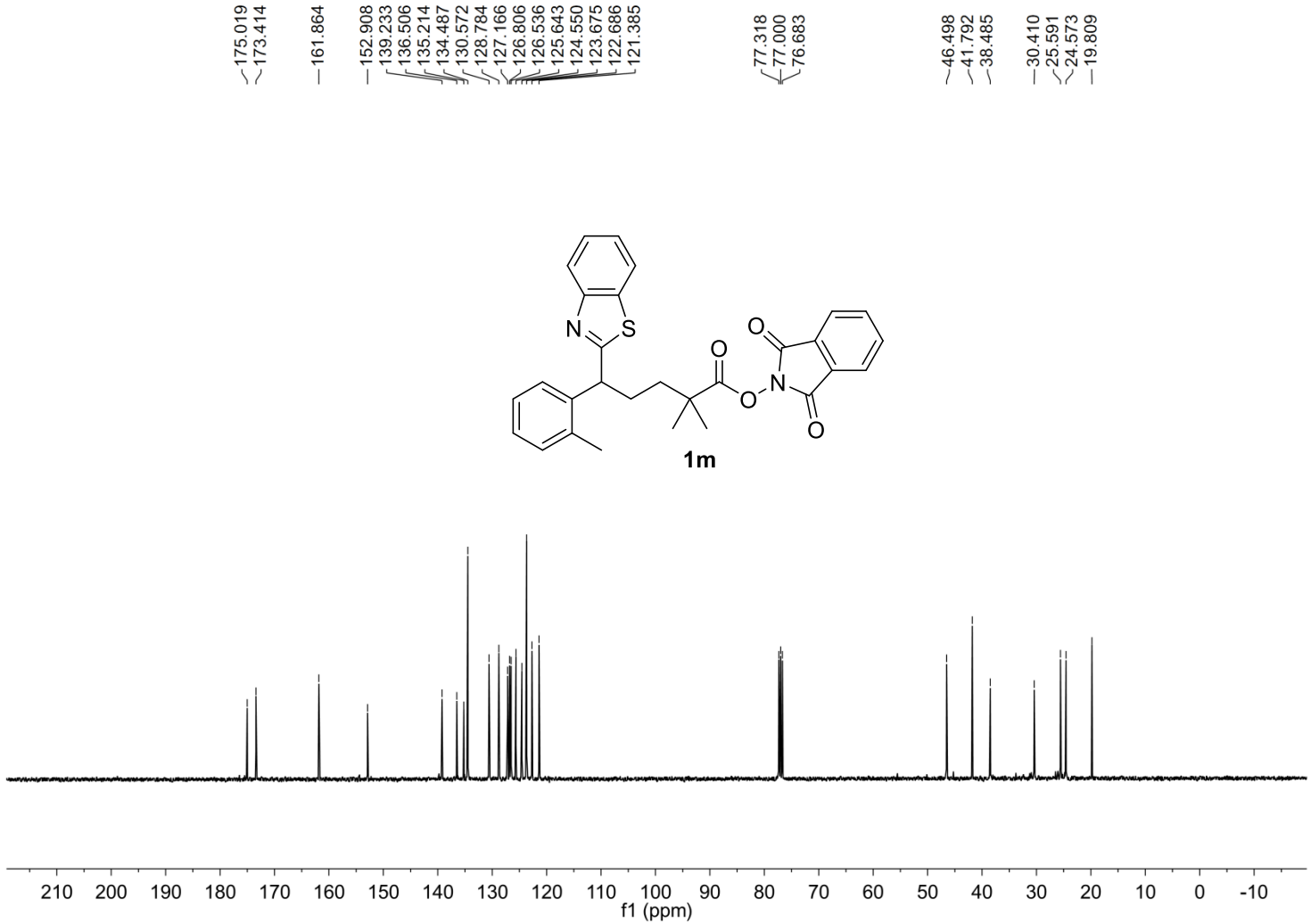
f1 (ppm)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134.487
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126.806
126.536
125.643
124.550
123.675
122.686
121.385
77.318
77.000
76.683
46.498
41.792
38.485
30.410
25.591
24.573
19.809
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S
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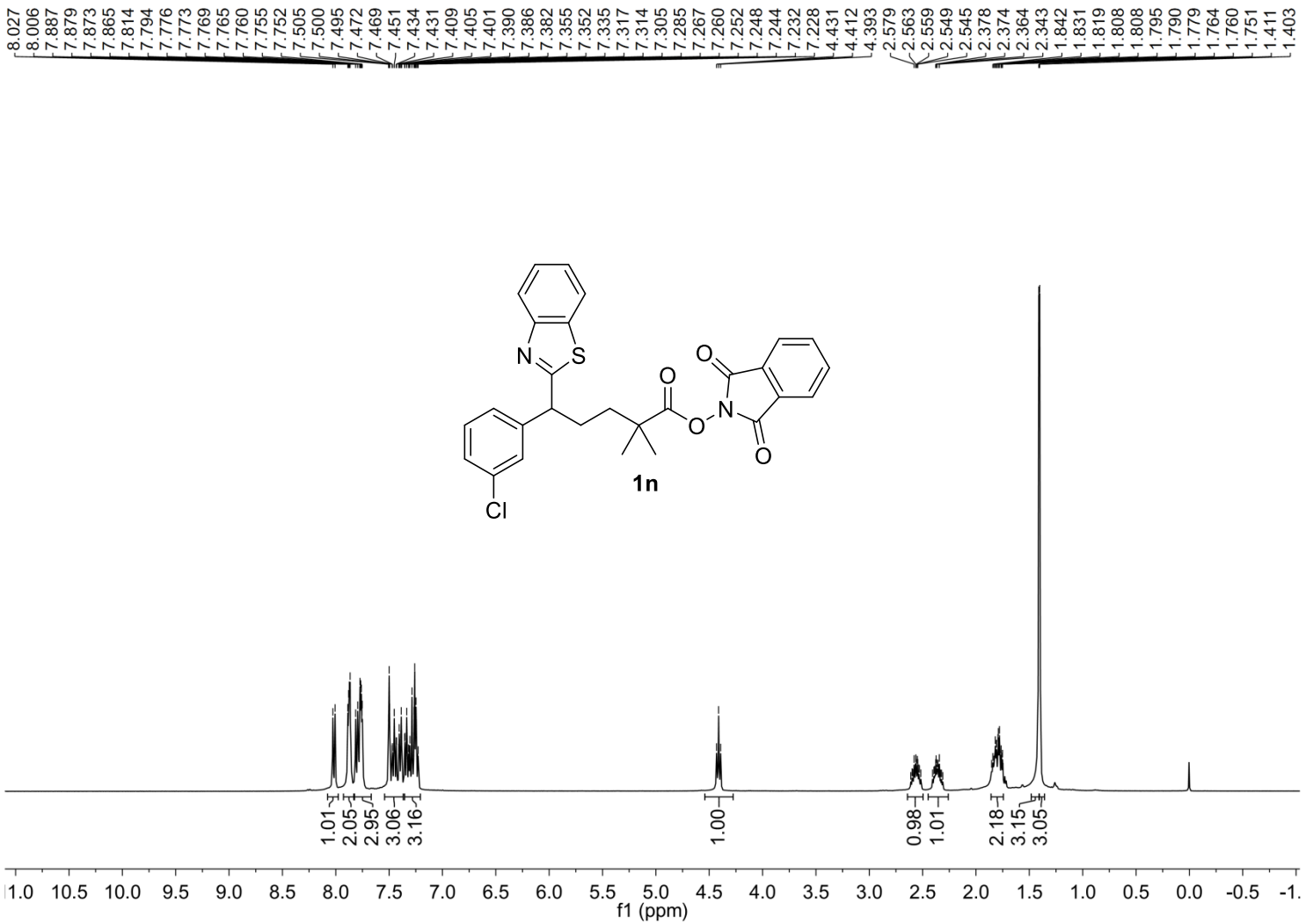
O
N
O
O
1m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.760
7.755
7.752
7.505
7.500
7.495
7.472
7.469
7.451
7.434
7.431
7.409
7.405
7.401
7.390
7.386
7.382
7.355
7.352
7.335
7.317
7.314
7.305
7.285
7.267
7.260
7.252
7.248
7.244
7.232
7.228
4.431
4.412
4.393
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2.563
2.559
2.549
2.545
2.378
2.374
2.364
2.343
1.842
1.831
1.819
1.808
1.808
1.795
1.790
1.779
1.764
1.760
1.751
1.411
1.403
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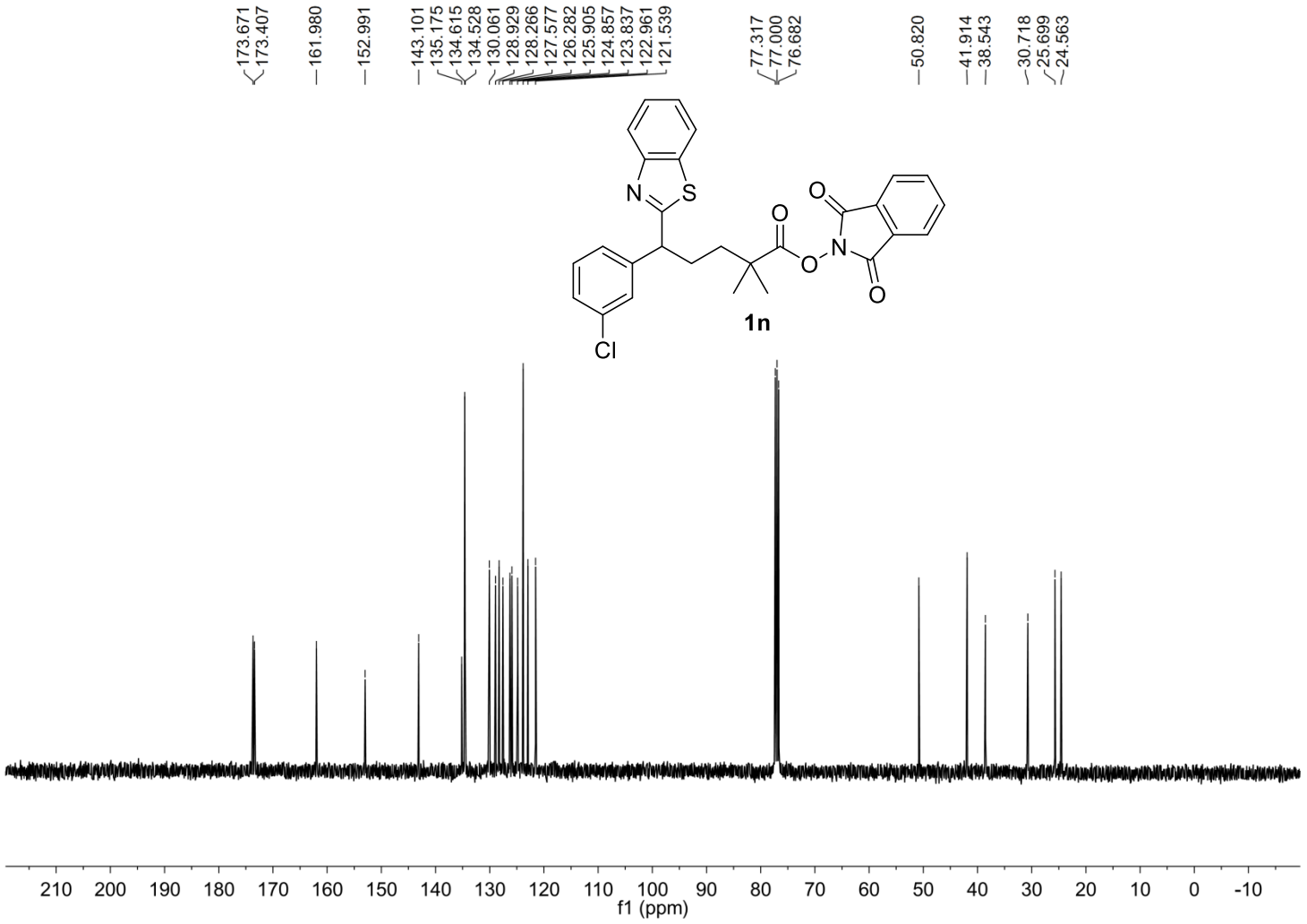
S
O
O
N
O
O
Cl
1n
1.01
2.05
2.95
3.06
3.16
1.00
0.98
1.01
2.18
3.15
3.05
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)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125.905
124.857
123.837
122.961
121.539
77.317
77.000
76.682
50.820
41.914
38.543
30.718
25.699
24.563
N
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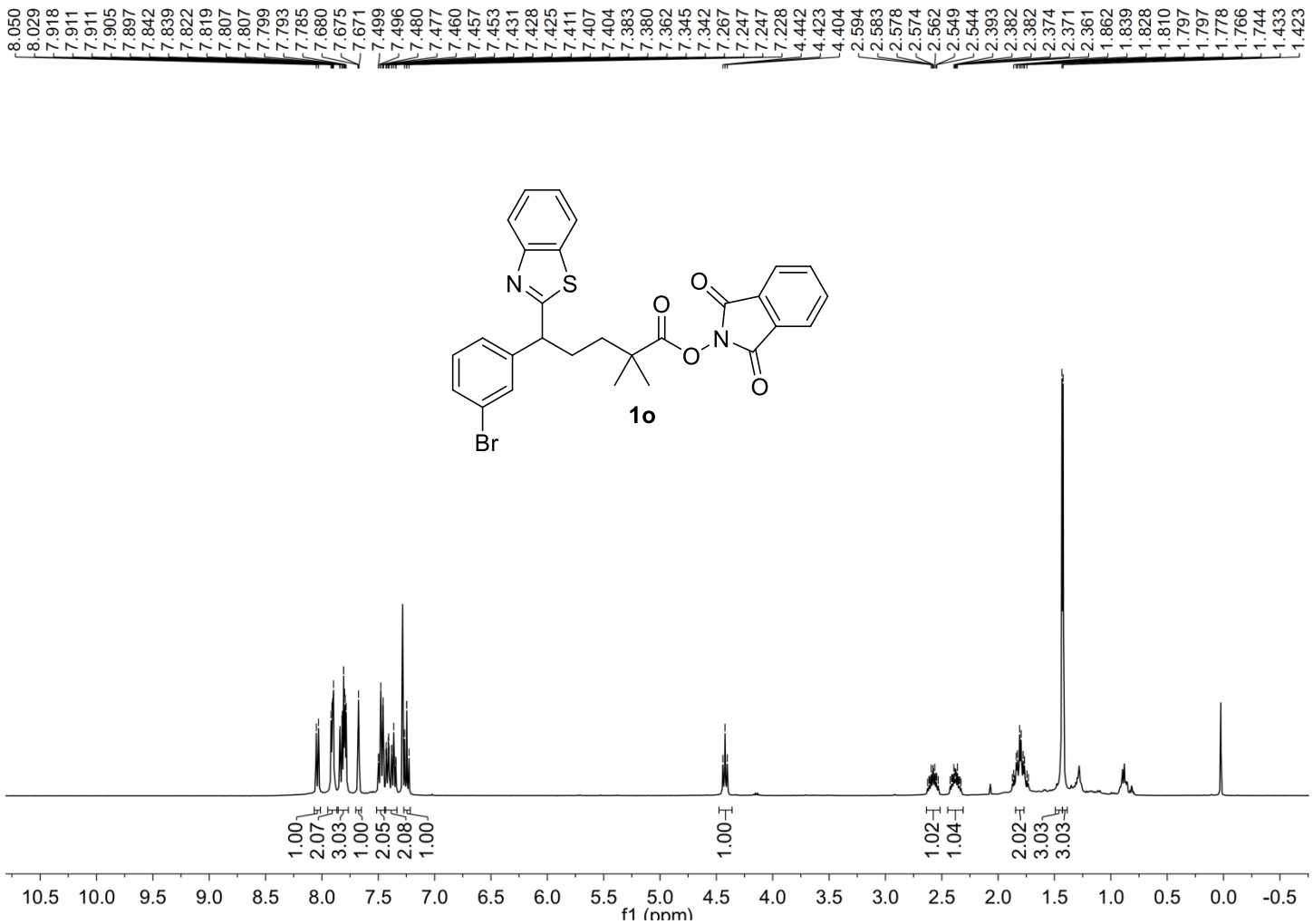
O
O
O
N
O
Cl
1n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.807
7.799
7.793
7.785
7.680
7.675
7.671
7.499
7.496
7.480
7.477
7.460
7.457
7.453
7.431
7.428
7.425
7.411
7.407
7.404
7.383
7.380
7.362
7.345
7.342
7.267
7.247
7.247
7.228
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4.423
4.404
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2.583
2.578
2.574
2.562
2.549
2.544
2.393
2.382
2.382
2.374
2.371
2.361
1.862
1.839
1.828
1.810
1.797
1.797
1.778
1.766
1.744
1.433
1.423
N
S
O
O
N
O
O
Br
1o
1.00
2.07
3.03
1.00
2.05
2.08
1.00
1.00
1.02
1.04
2.02
3.03
3.03
10.5
10.0
9.5
9.0
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8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
2.5
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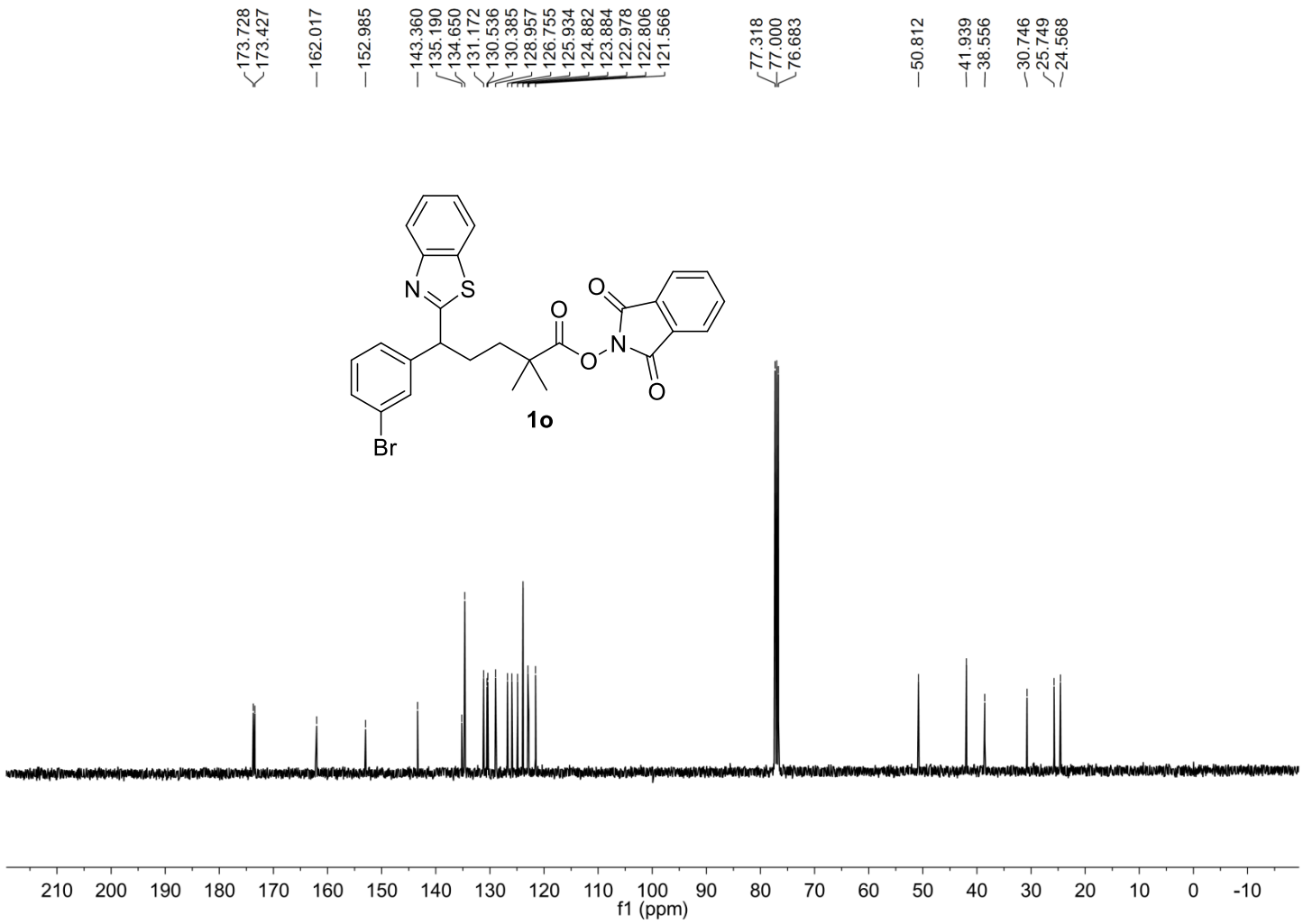
-0.5
f1 (ppm)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123.884
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122.806
121.566
77.318
77.000
76.683
50.812
41.939
38.556
30.746
25.749
24.568
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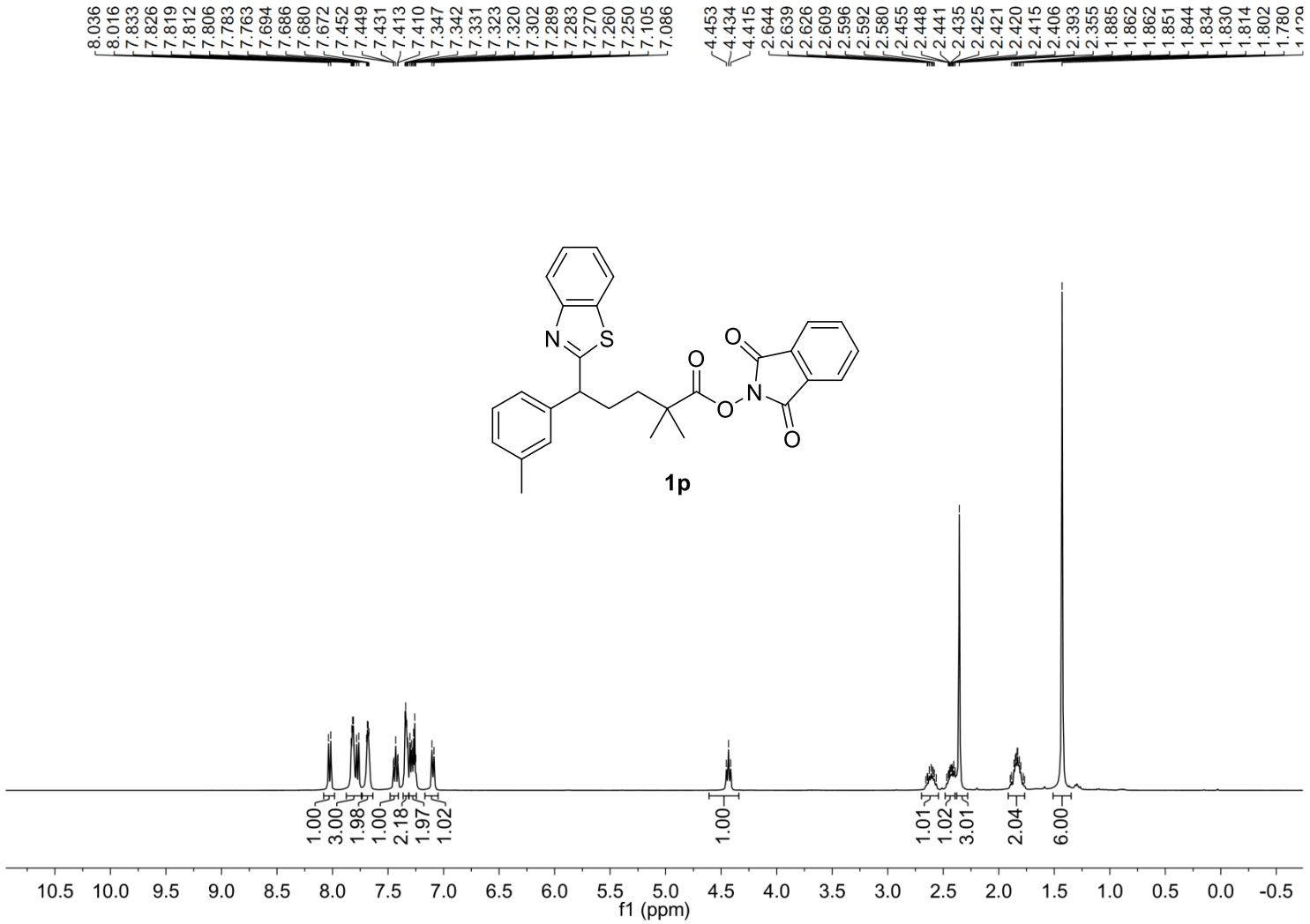
O
O
N
O
O
Br
1o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.680
7.672
7.452
7.449
7.431
7.413
7.410
7.347
7.342
7.331
7.323
7.320
7.302
7.289
7.283
7.270
7.260
7.250
7.105
7.086
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4.434
4.415
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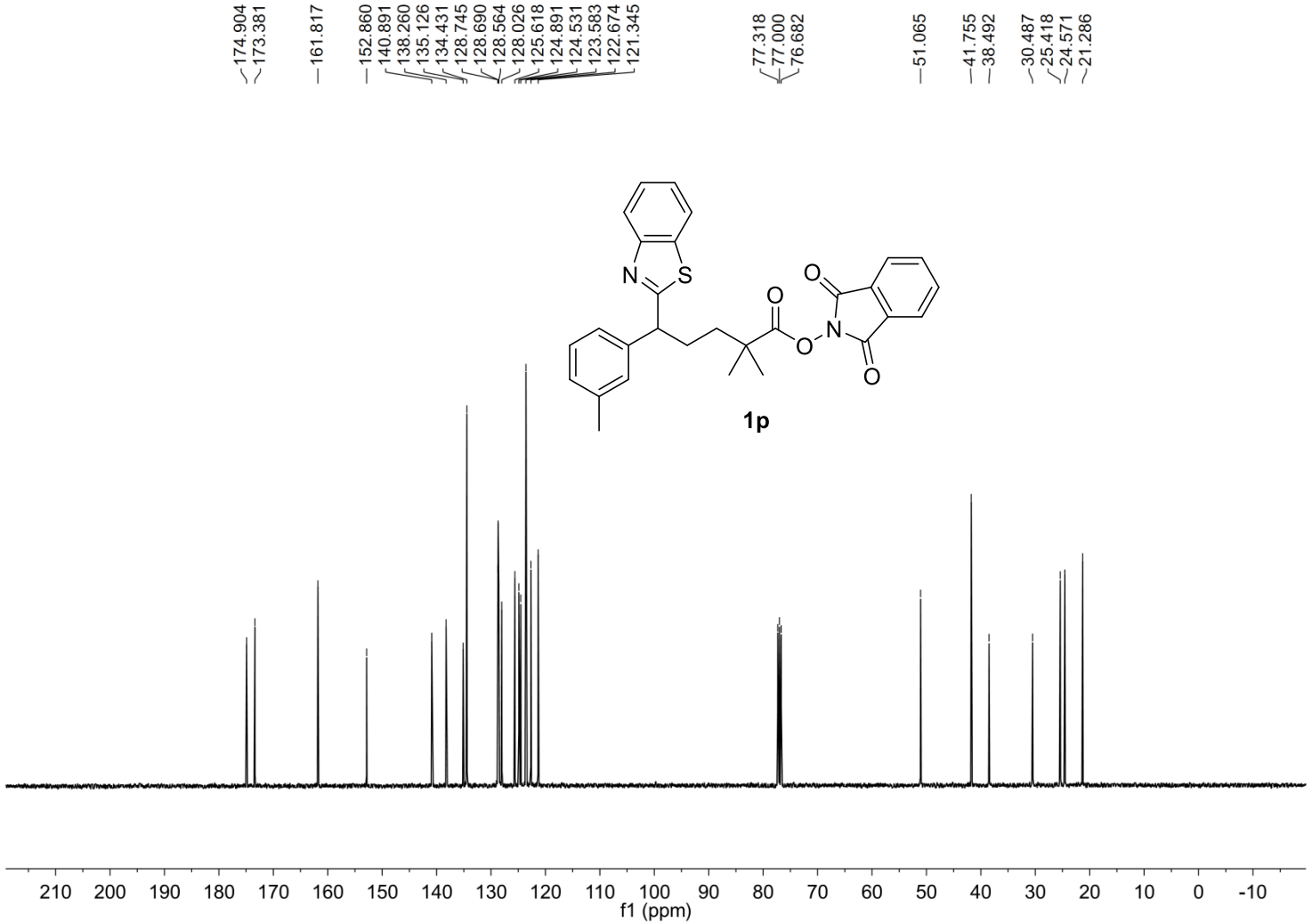
2.639
2.626
2.609
2.596
2.592
2.580
2.455
2.448
2.441
2.435
2.425
2.421
2.420
2.415
2.406
2.393
2.355
1.885
1.862
1.862
1.851
1.844
1.834
1.830
1.814
1.802
1.780
N
S
O
O
N
O
O
1p
1.00
3.00
1.98
1.00
2.18
1.97
1.02
1.00
1.01
1.02
3.01
2.04
6.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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134.431
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128.026
125.618
124.891
124.531
123.583
122.674
121.345
77.318
77.000
76.682
51.065
41.755
38.492
30.487
25.418
24.571
21.286
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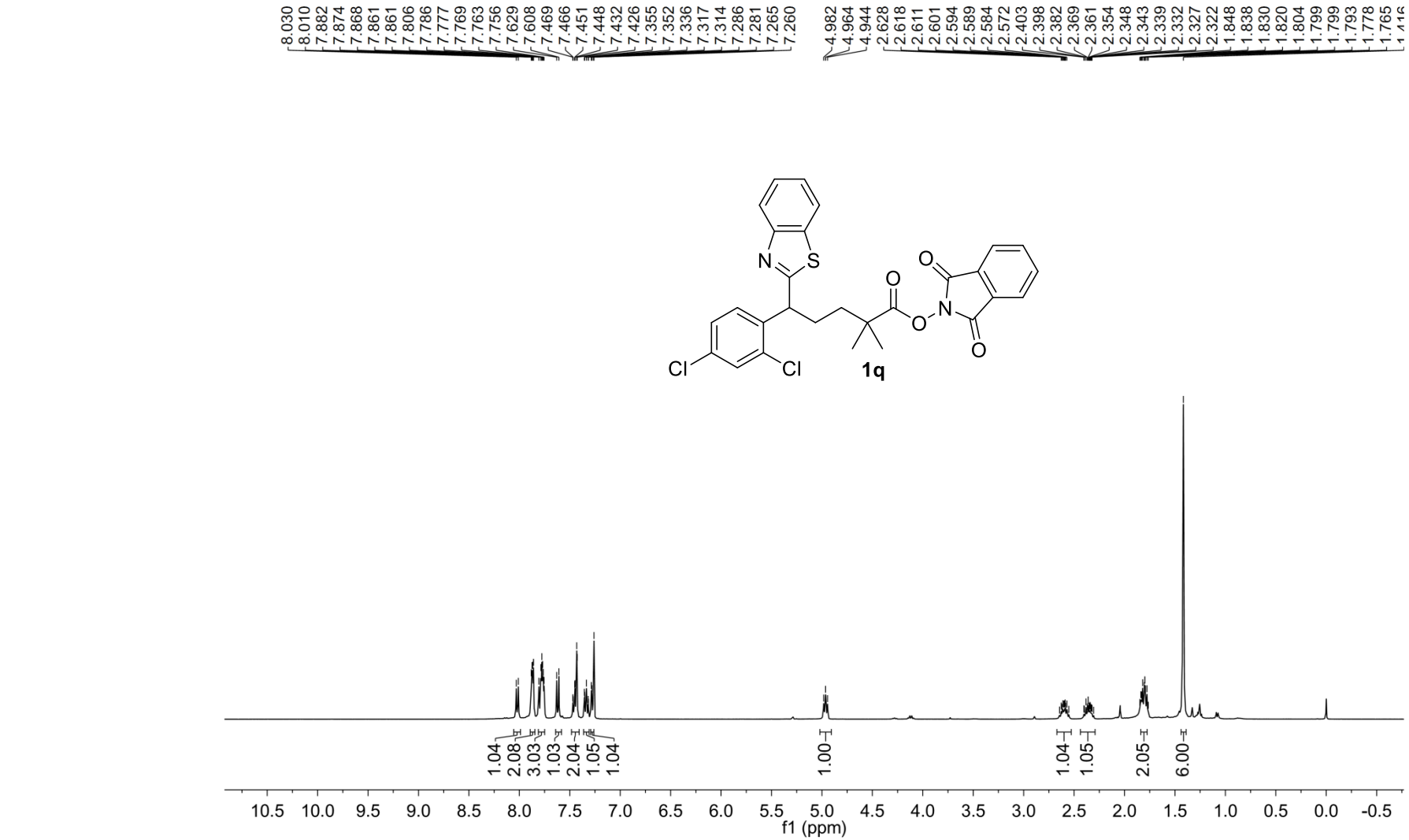
O
O
O
N
O
1p
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.763
7.756
7.629
7.608
7.469
7.466
7.451
7.448
7.432
7.426
7.355
7.352
7.336
7.317
7.314
7.286
7.281
7.265
7.260
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4.964
4.944
2.628
2.618
2.611
2.601
2.594
2.589
2.584
2.572
2.403
2.398
2.382
2.369
2.361
2.354
2.348
2.343
2.339
2.332
2.327
2.322
1.848
1.838
1.830
1.820
1.804
1.799
1.799
1.793
1.778
1.765
N
S
O
O
O
N
O
Cl
Cl
1q
1.04
2.08
3.03
1.03
2.04
1.05
1.04
1.00
1.04
1.05
2.05
6.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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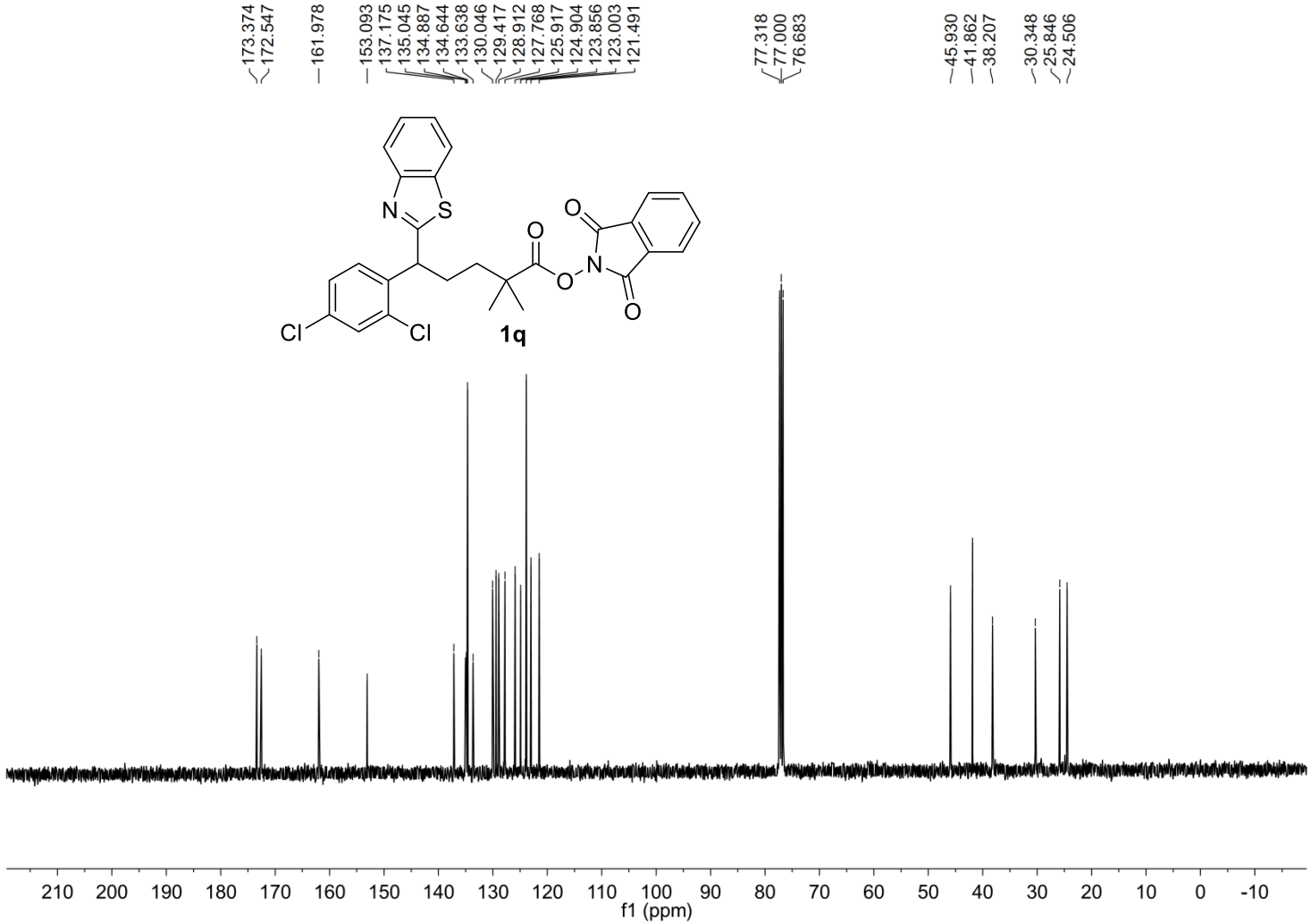
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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123.856
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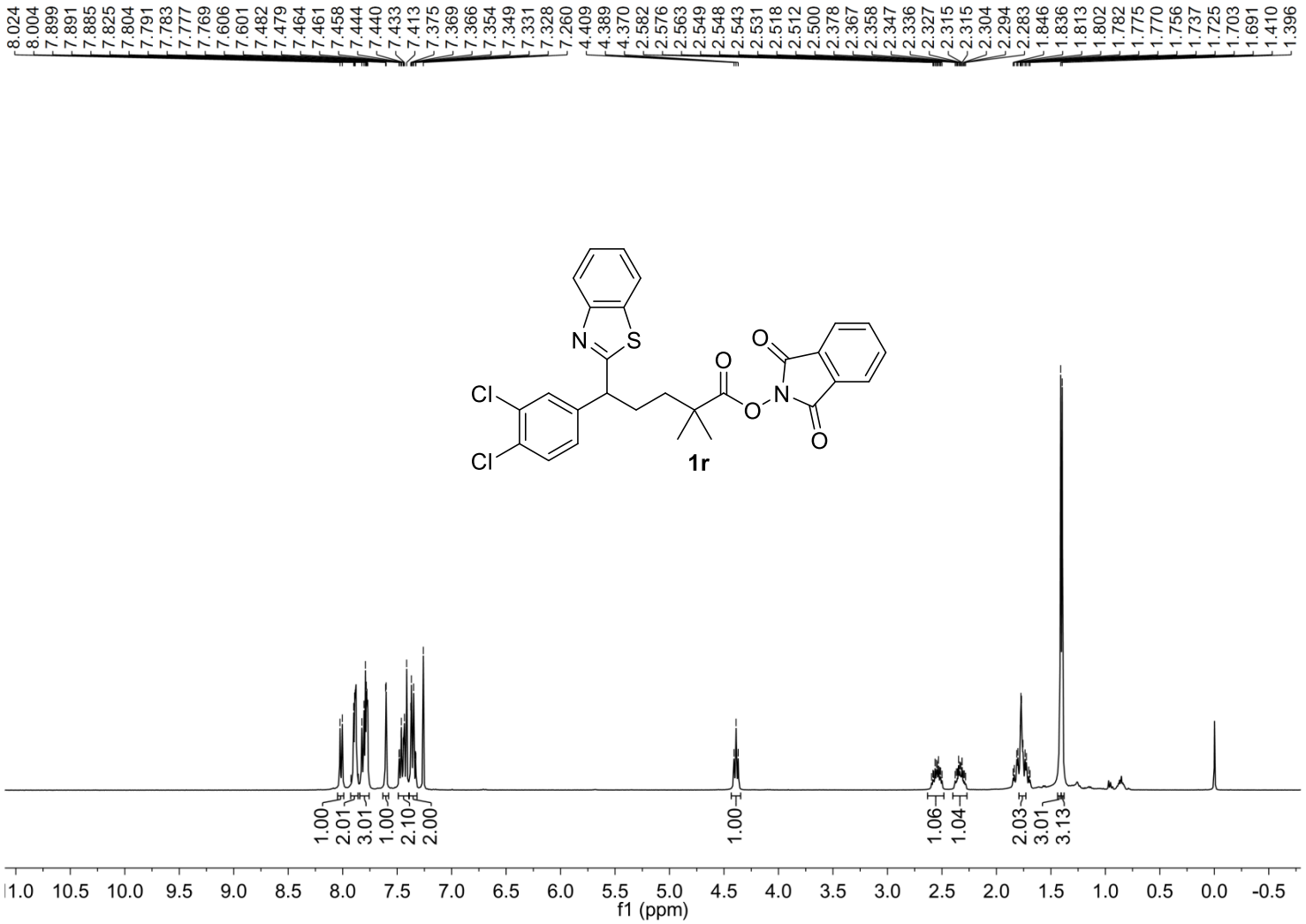
41.862
38.207
30.348
25.846
24.506
N
S
O
O
N
O
O
Cl
Cl
1q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.458
7.444
7.440
7.433
7.413
7.375
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7.366
7.354
7.349
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7.260
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2.518
2.512
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2.336
2.327
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2.315
2.304
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1.813
1.802
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1.775
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1.756
1.737
1.725
1.703
1.691
1.410
1.396
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S
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O
N
O
O
Cl
Cl
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3.01
1.00
2.10
2.00
1.00
1.06
1.04
2.03
3.01
3.13
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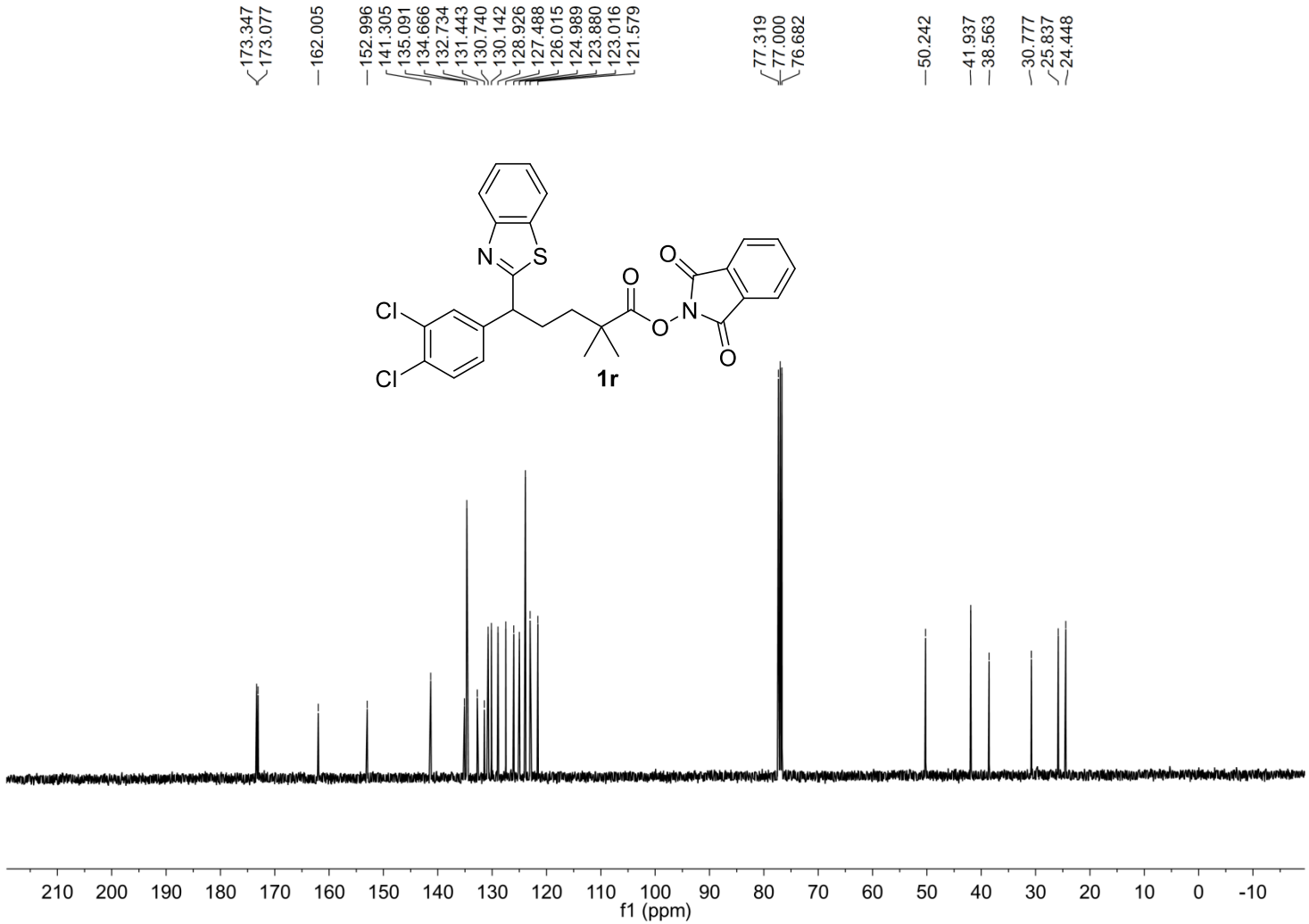
f1 (ppm)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126.015
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123.880
123.016
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77.319
77.000
76.682
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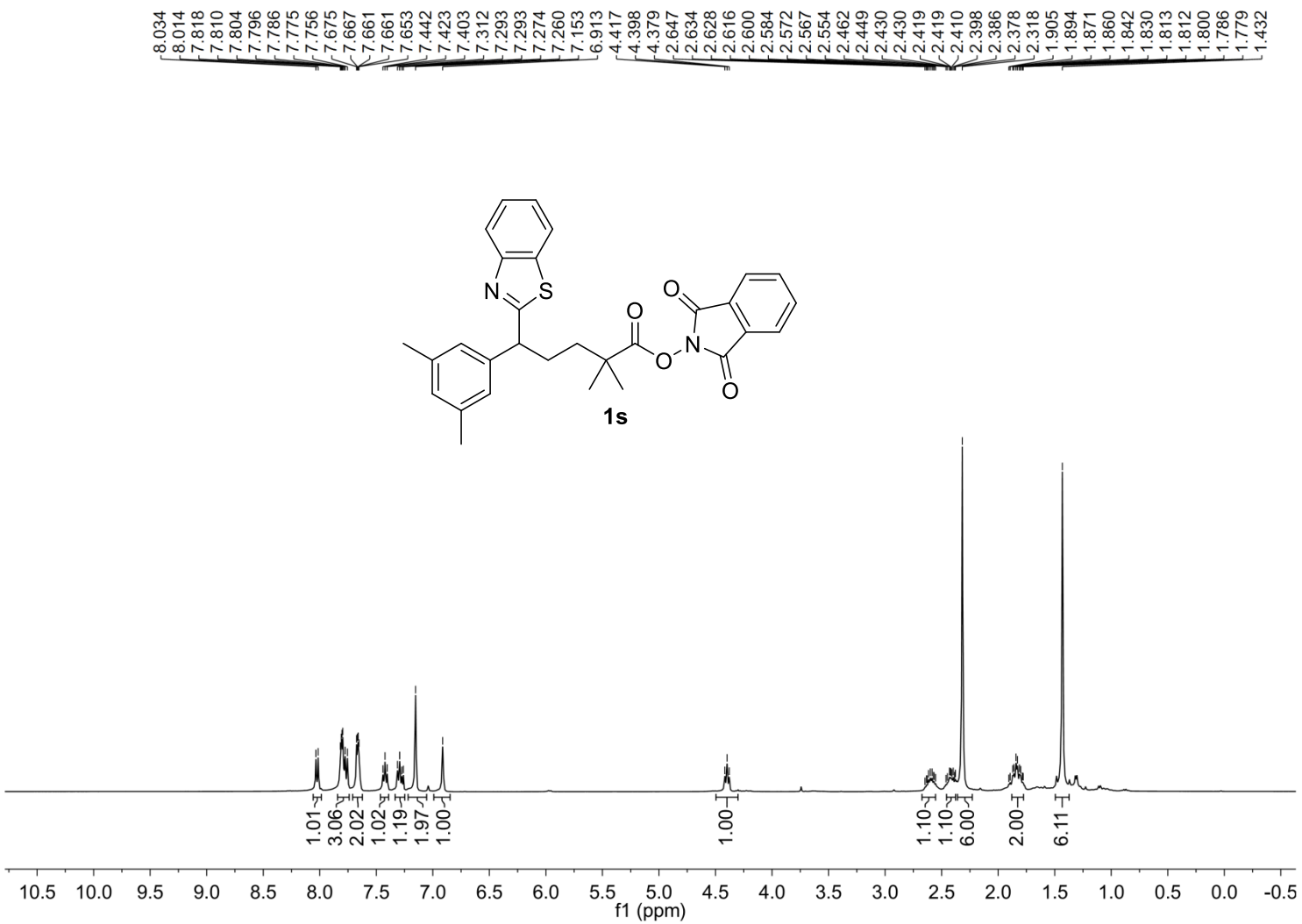
41.937
38.563
30.777
25.837
24.448
N
S
O
O
N
O
O
Cl
Cl
1r
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.661
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7.423
7.403
7.312
7.293
7.293
7.274
7.260
7.153
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4.417
4.398
4.379
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2.600
2.584
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2.567
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2.462
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1.871
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1.830
1.813
1.812
1.800
1.786
1.779
1.432
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S
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O
N
O
O
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3.06
2.02
1.02
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1.00
1.00
1.10
1.10
6.00
2.00
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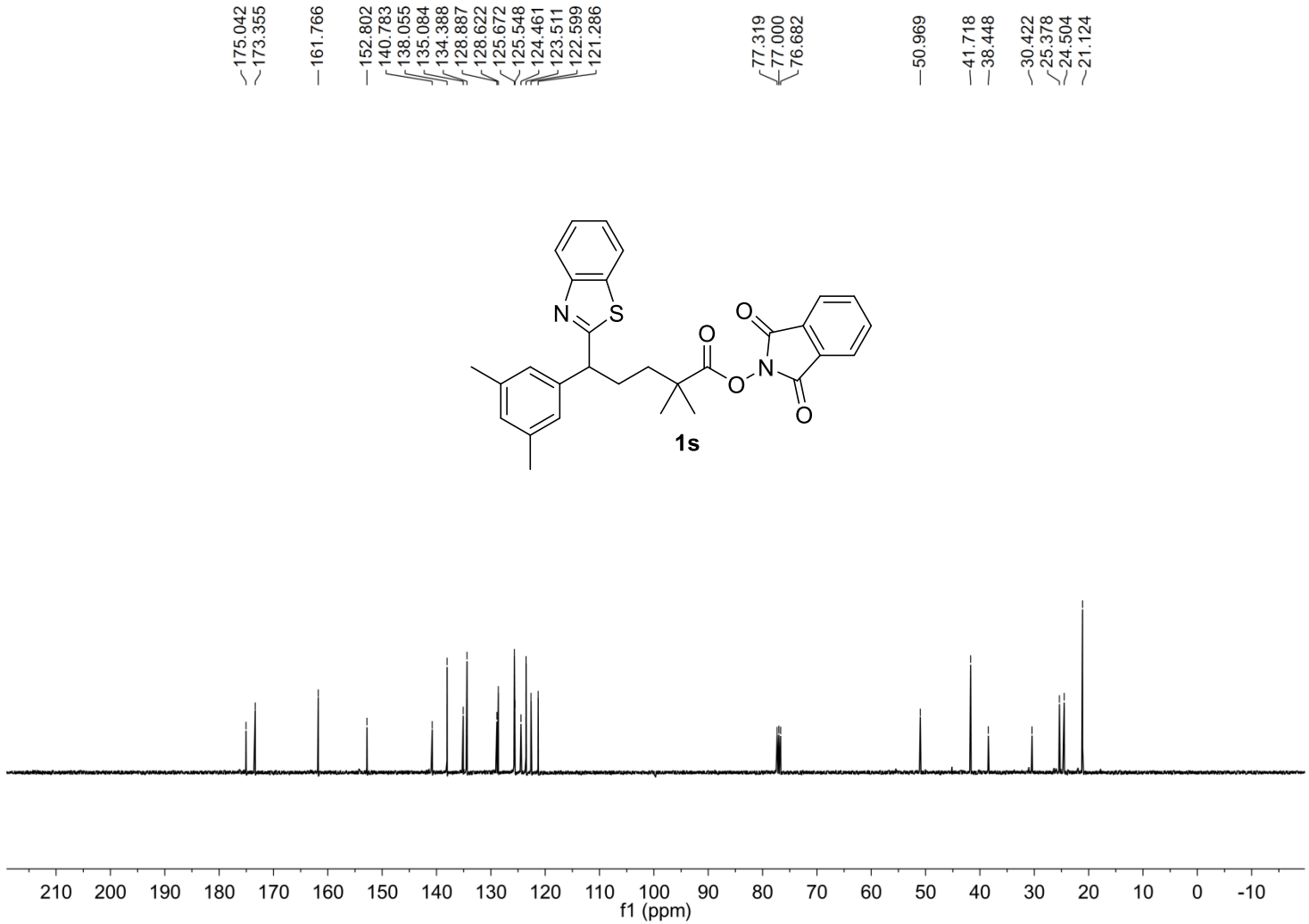
f1 (ppm)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125.548
124.461
123.511
122.599
121.286
77.319
77.000
76.682
50.969
41.718
38.448
30.422
25.378
24.504
21.124
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S
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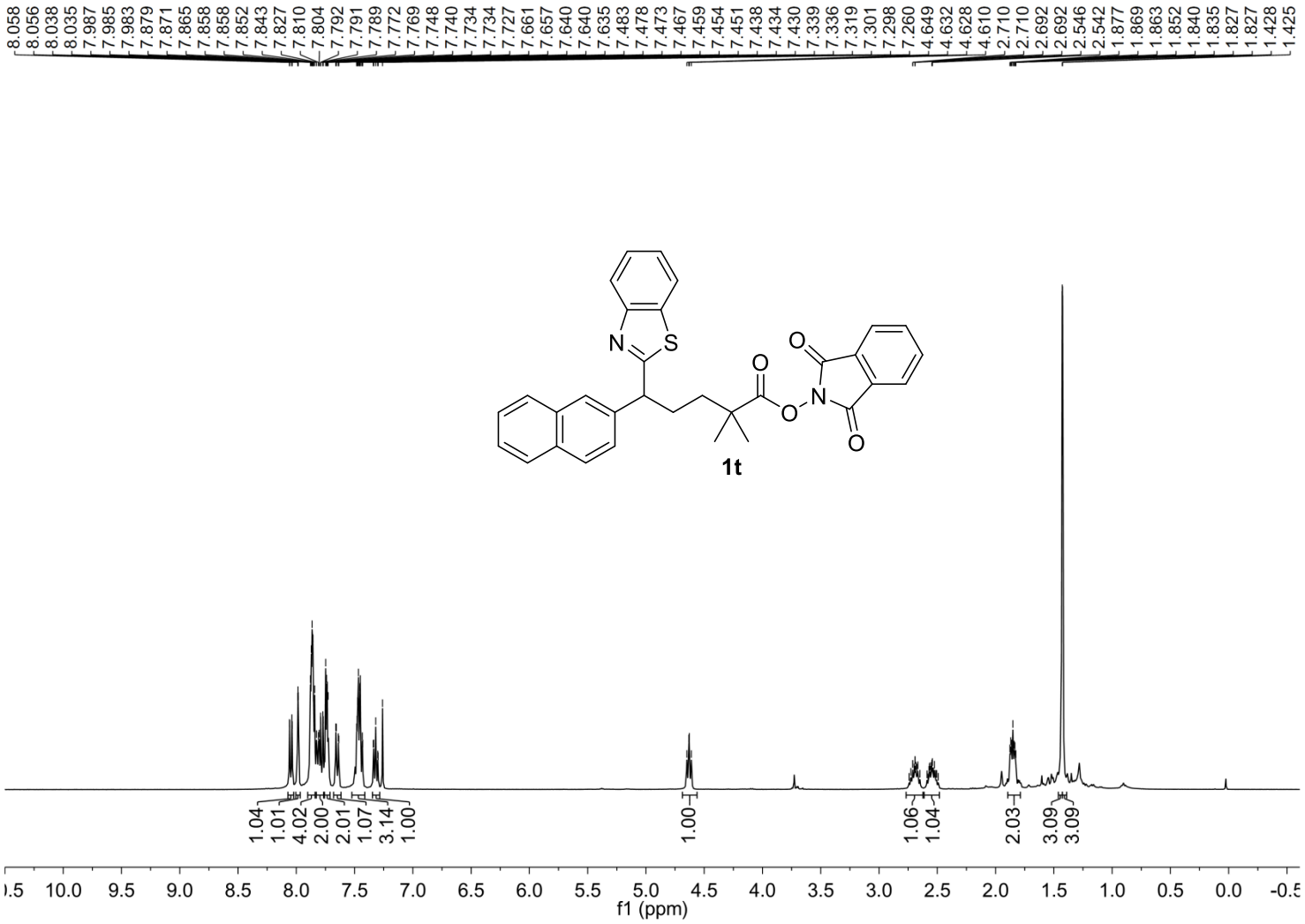
O
N
O
O
1s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.843
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7.789
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7.769
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7.434
7.430
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7.336
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2.692
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S
O
O
N
O
O
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4.02
2.00
2.01
1.07
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1.00
1.00
1.06
1.04
2.03
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3.09
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9.0
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7.5
7.0
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6.0
5.5
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2.5
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1.0
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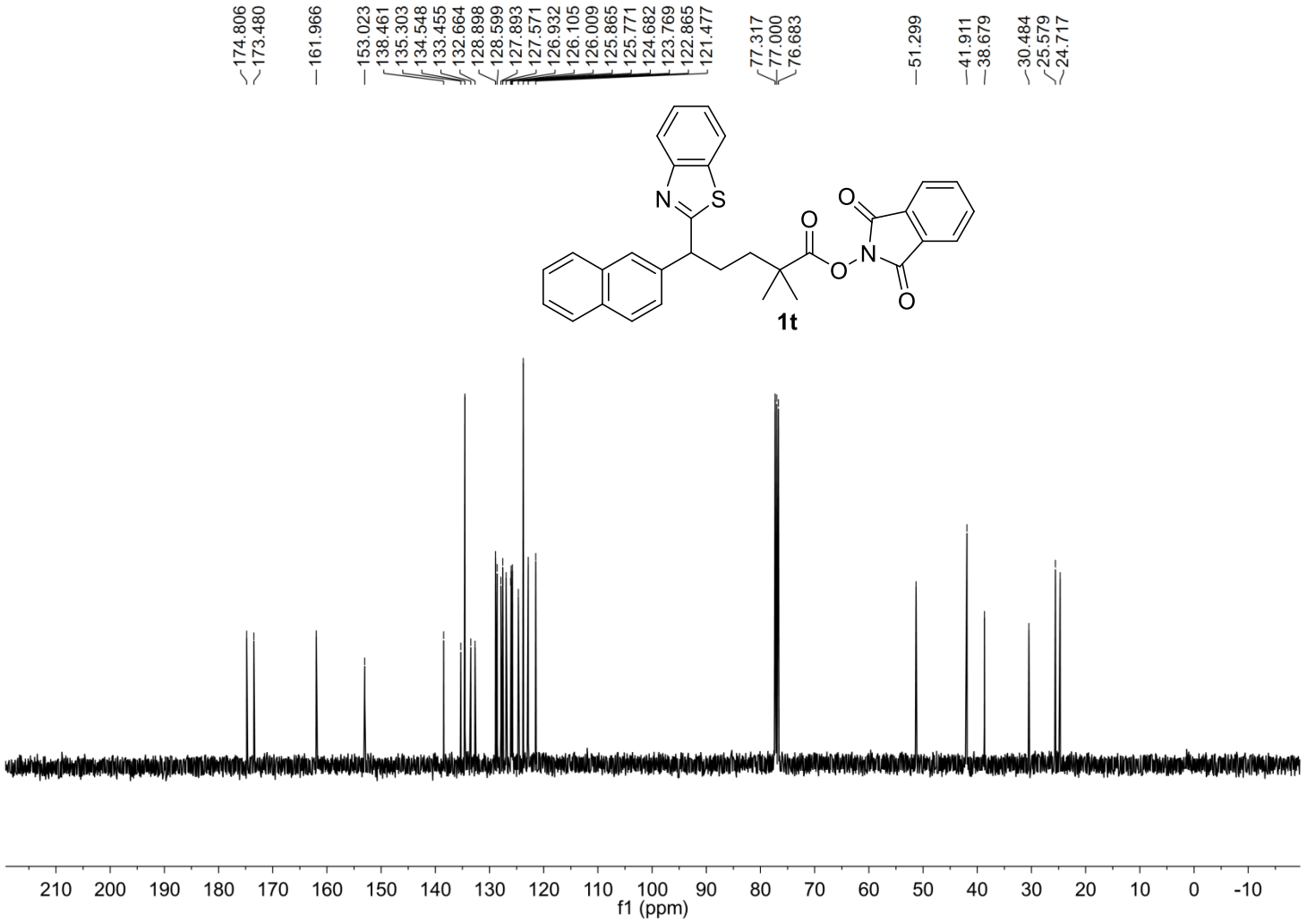
0.0
f1 (ppm)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127.571
126.932
126.105
126.009
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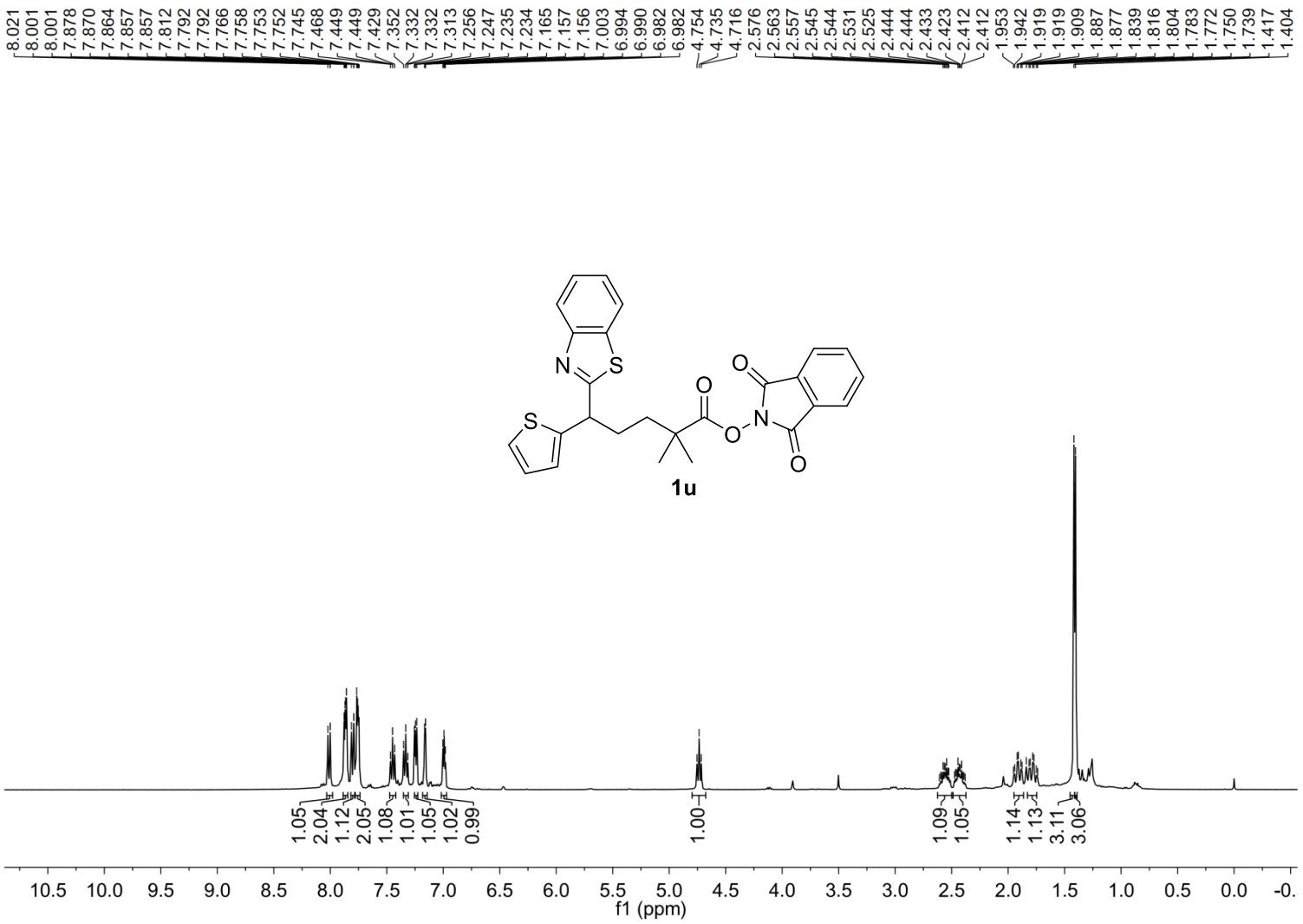
125.771
124.682
123.769
122.865
121.477
77.317
77.000
76.683
51.299
41.911
38.679
30.484
25.579
24.717
N
S
O
O
O
N
O
1t
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.332
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1.919
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7.5
7.0
6.5
6.0
5.5
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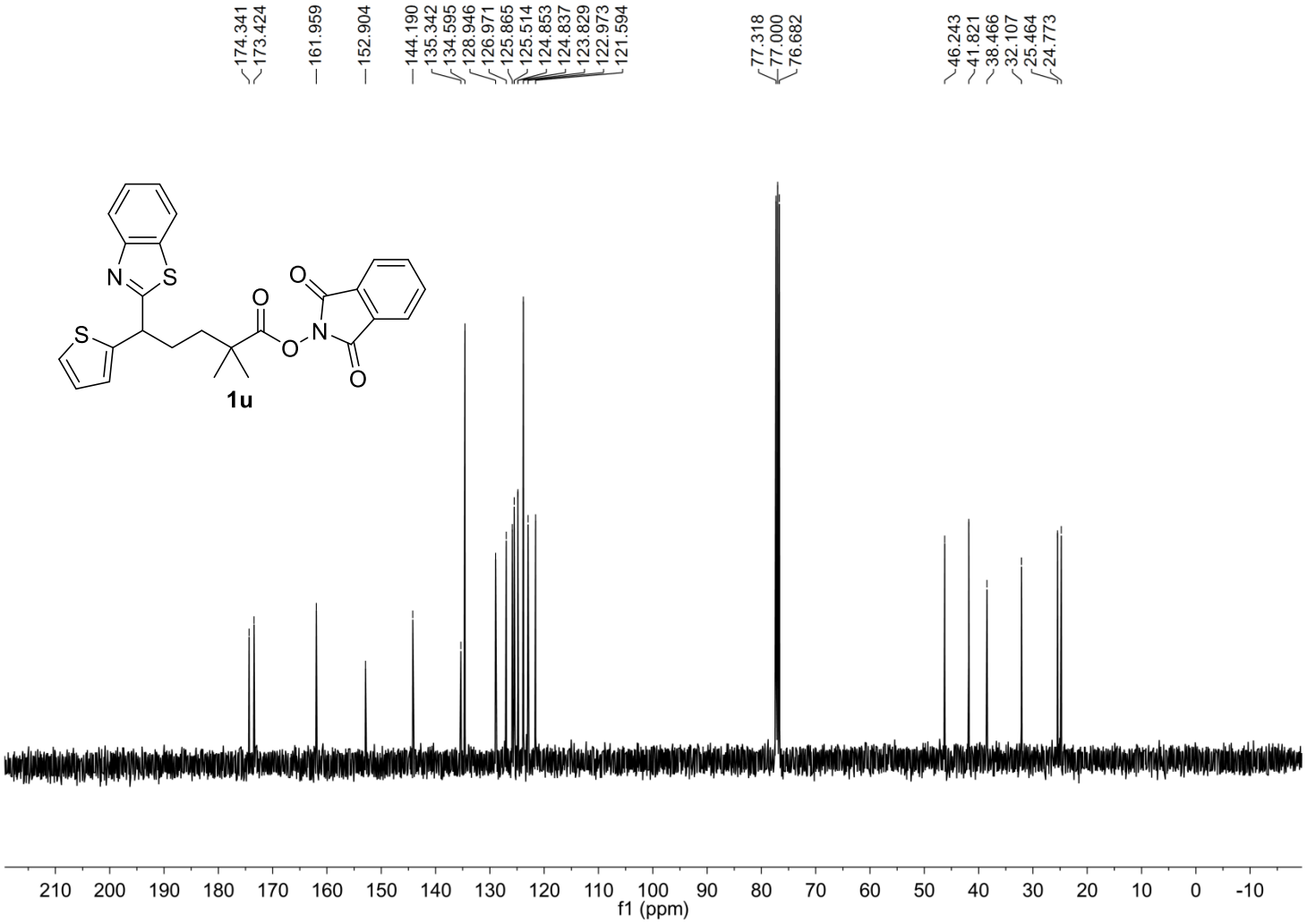
-0.
f1 (ppm)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128.946
126.971
125.865
125.514
124.853
124.837
123.829
122.973
121.594
77.318
77.000
76.682
46.243
41.821
38.466
32.107
25.464
24.773
1u
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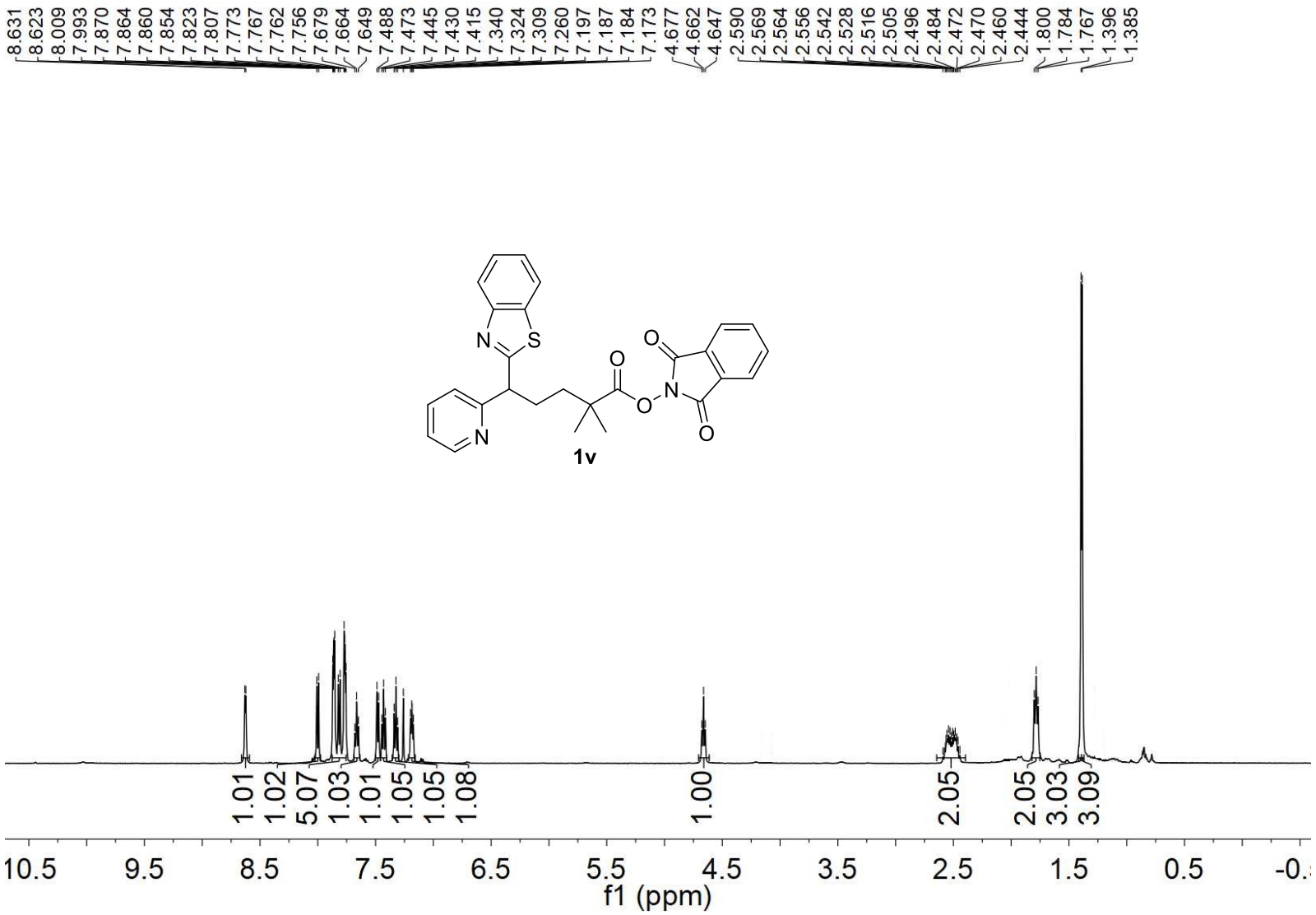
f1 (ppm)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7.767
7.762
7.756
7.679
7.664
7.649
7.488
7.473
7.445
7.430
7.415
7.340
7.324
7.309
7.260
7.197
7.187
7.184
7.173
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4.662
4.647
2.590
2.569
2.564
2.556
2.542
2.528
2.516
2.505
2.496
2.484
2.472
2.470
2.460
2.444
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1.784
1.767
1.396
1.385
1.01
1.02
5.07
1.03
1.01
1.05
1.05
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1.00
2.05
2.05
3.03
3.09
10.5
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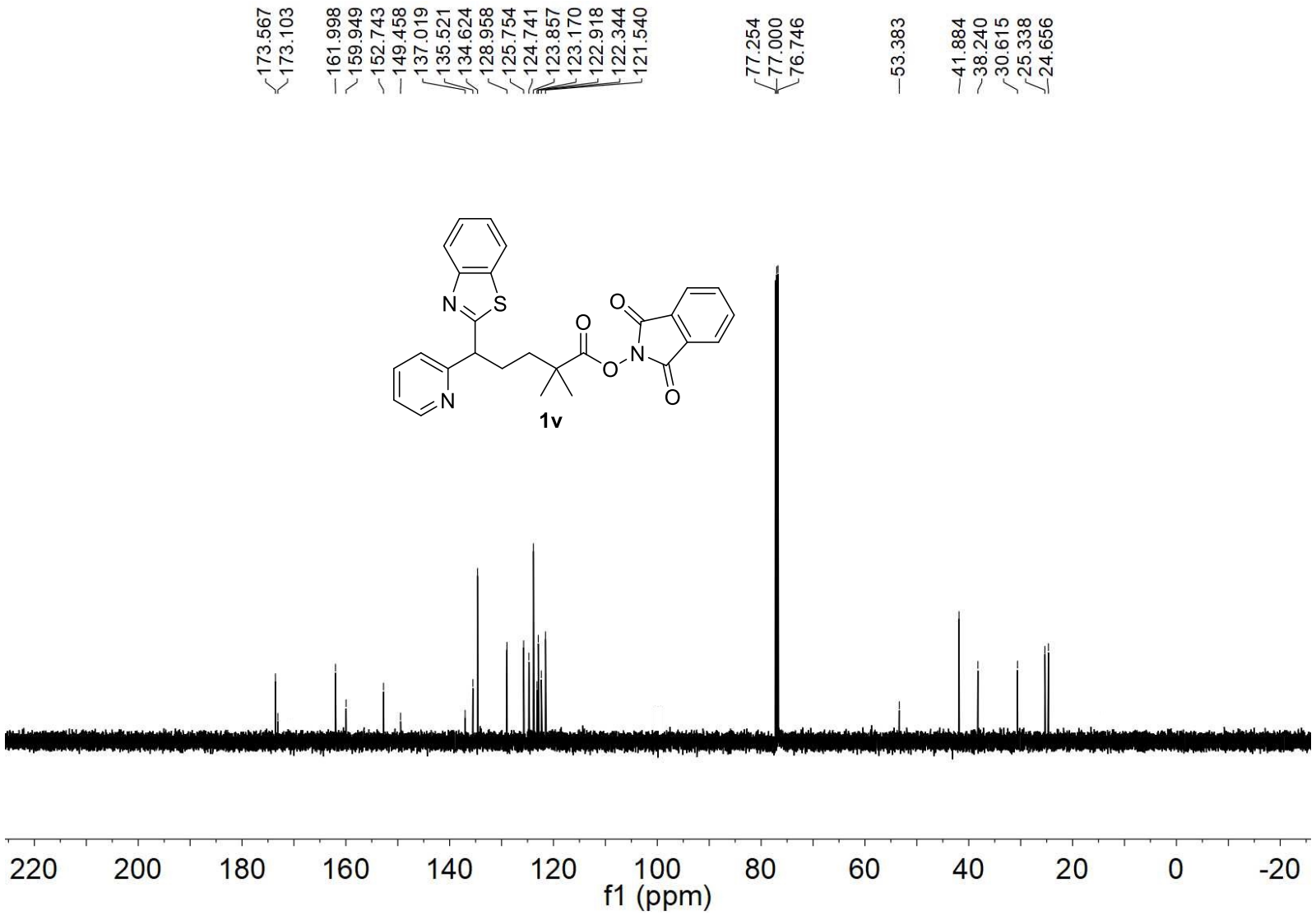
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

1v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123.170
122.918
122.344
121.540
77.254
77.000
76.746
53.383
41.884
38.240
30.615
25.338
24.656
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220
200
180
160
140
120
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80
60
40
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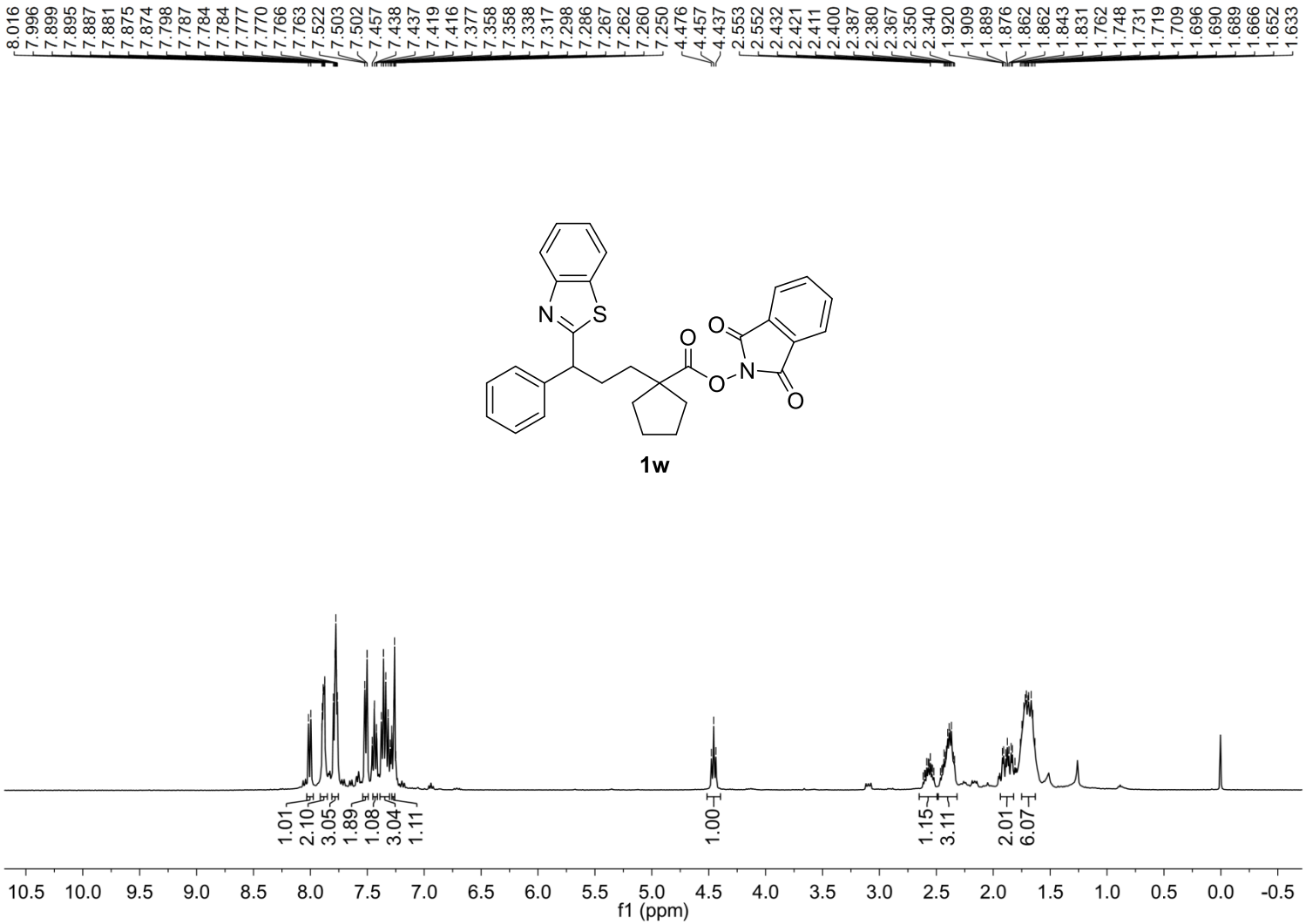
-20
f1 (ppm)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7.784
7.777
7.770
7.766
7.763
7.522
7.503
7.502
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7.438
7.437
7.419
7.416
7.377
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7.358
7.338
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7.298
7.286
7.267
7.262
7.260
7.250
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4.457
4.437
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2.552
2.432
2.421
2.411
2.400
2.387
2.380
2.367
2.350
2.340
1.920
1.909
1.889
1.876
1.862
1.862
1.843
1.831
1.762
1.748
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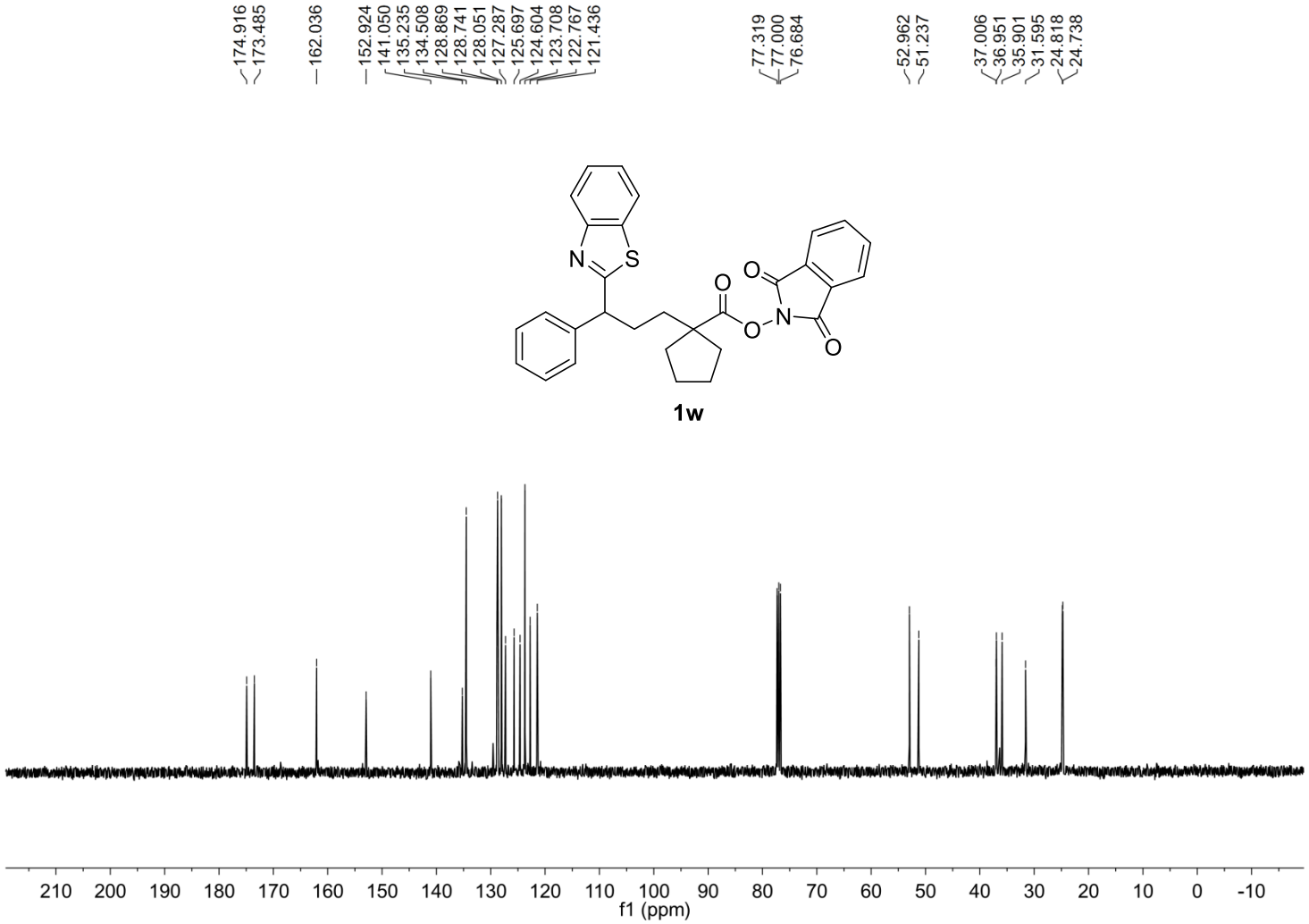
1.719
1.709
1.696
1.690
1.689
1.666
1.652
1.633
N
S
O
O
N
O
1w
1.01
2.10
3.05
1.89
1.08
3.04
1.11
1.00
1.15
3.11
2.01
6.07
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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123.708
122.767
121.436
77.319
77.000
76.684
52.962
51.237
37.006
36.951
35.901
31.595
24.818
24.738
N
S
O
O
N
O
O
1w
210
200
190
180
170
160
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140
130
120
110
100
90
80
70
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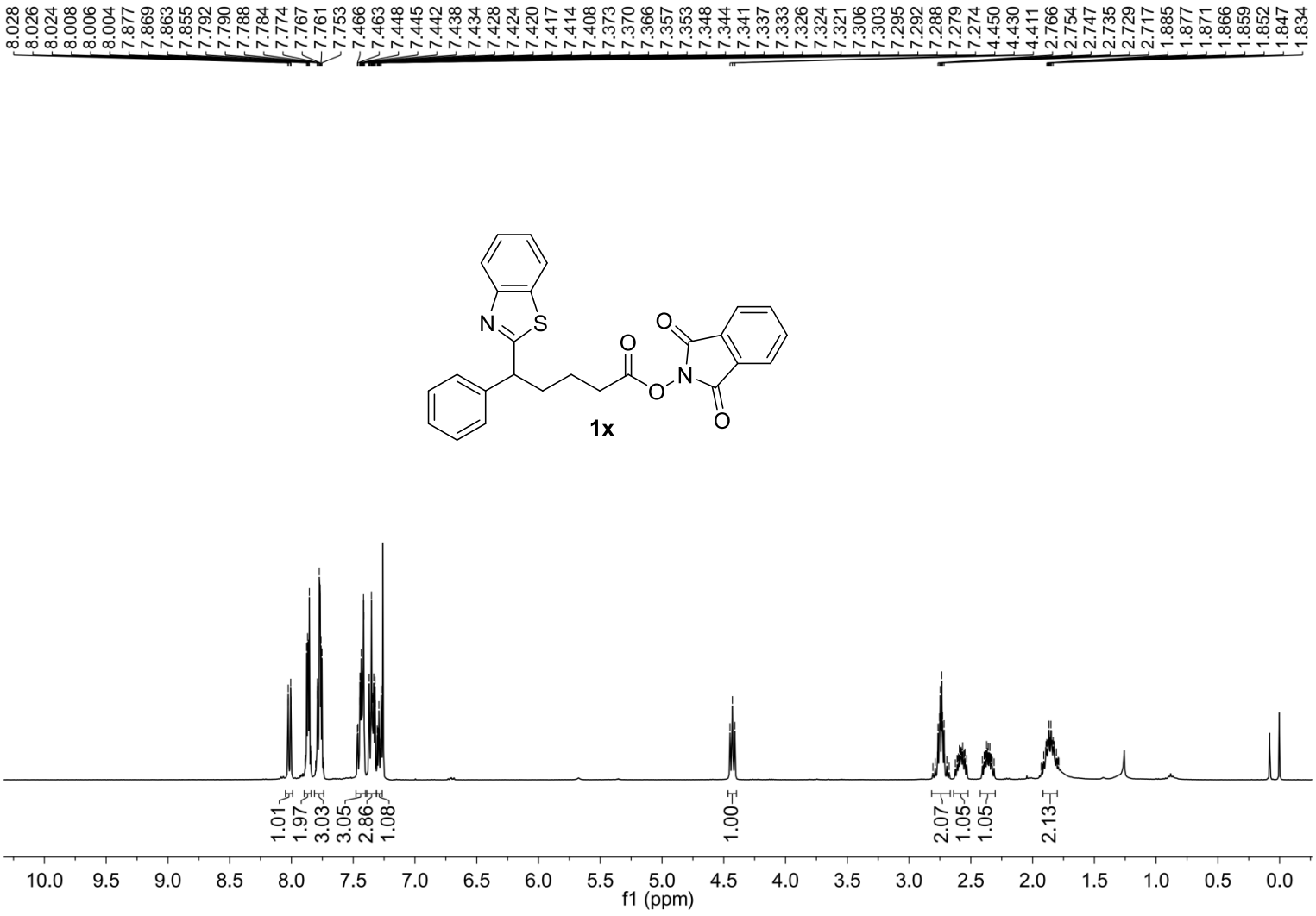
50
40
30
20
10
0
-10
f1 (ppm)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7.788
7.784
7.774
7.767
7.761
7.753
7.466
7.463
7.448
7.445
7.442
7.438
7.434
7.428
7.424
7.420
7.417
7.414
7.408
7.373
7.370
7.366
7.357
7.353
7.348
7.344
7.341
7.337
7.333
7.326
7.324
7.321
7.306
7.303
7.295
7.292
7.288
7.279
7.274
4.450
4.430
4.411
2.766
2.754
2.747
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2.729
2.717
1.885
1.877
1.871
1.866
1.859
1.852
1.847
1.834
N
S
O
O
N
O
O
1x
1.01
1.97
3.03
3.05
2.86
1.08
1.00
2.07
1.05
1.05
2.13
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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2.5
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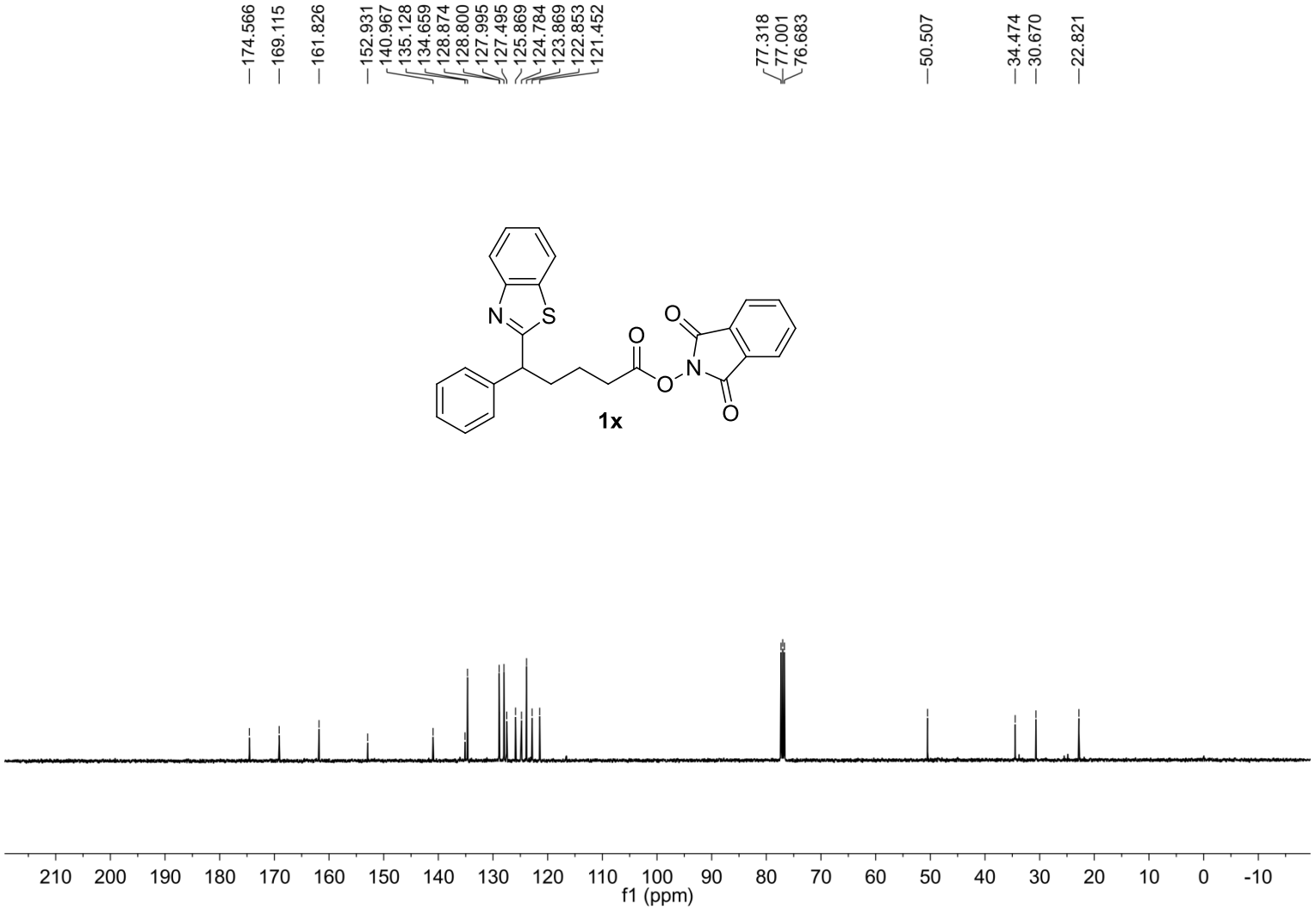
1.0
0.5
0.0
f1 (ppm)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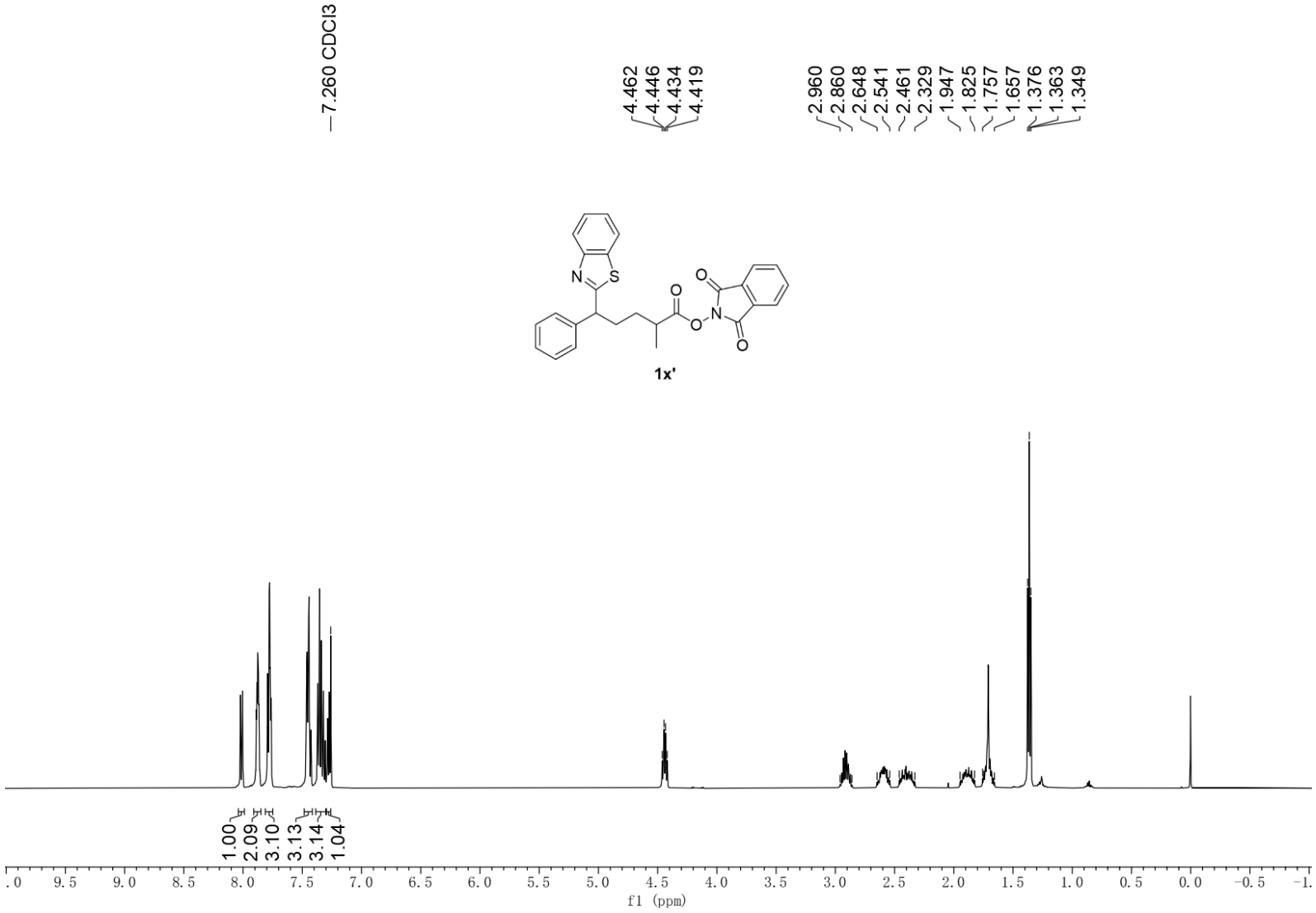
134.659
128.874
128.800
127.995
127.495
125.869
124.784
123.869
122.853
121.452
77.318
77.001
76.683
50.507
34.474
30.670
22.821
N
S
O
O
N
O
O
1x
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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2.329
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1.825
1.757
1.657
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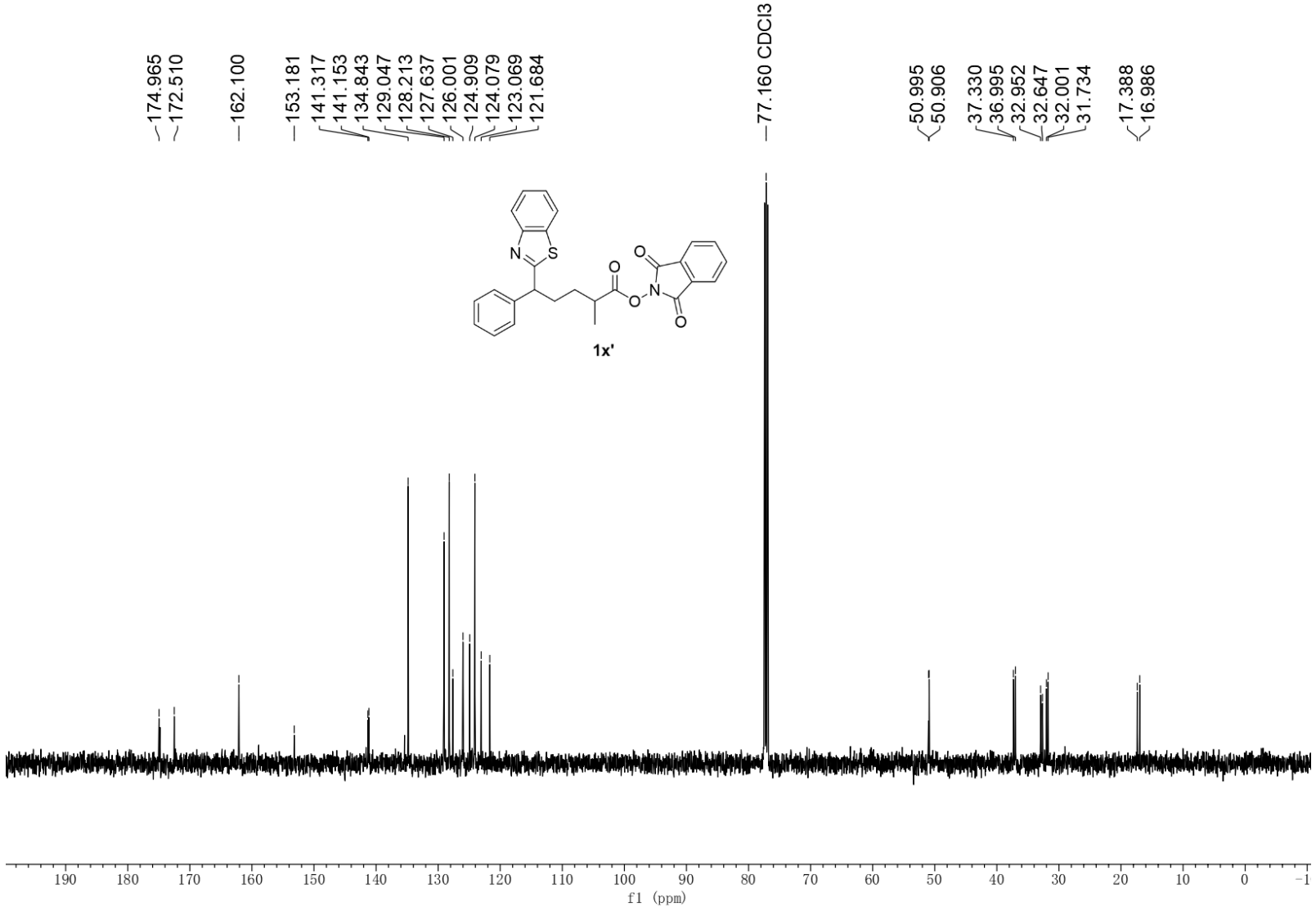
1.349
1.00
2.09
3.10
3.13
3.14
1.04
f1 (ppm)

1x'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129.047
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127.637
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124.909
124.079
123.069
121.684
77.160 CDCl3
50.995
50.906
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36.995
32.952
32.647
32.001
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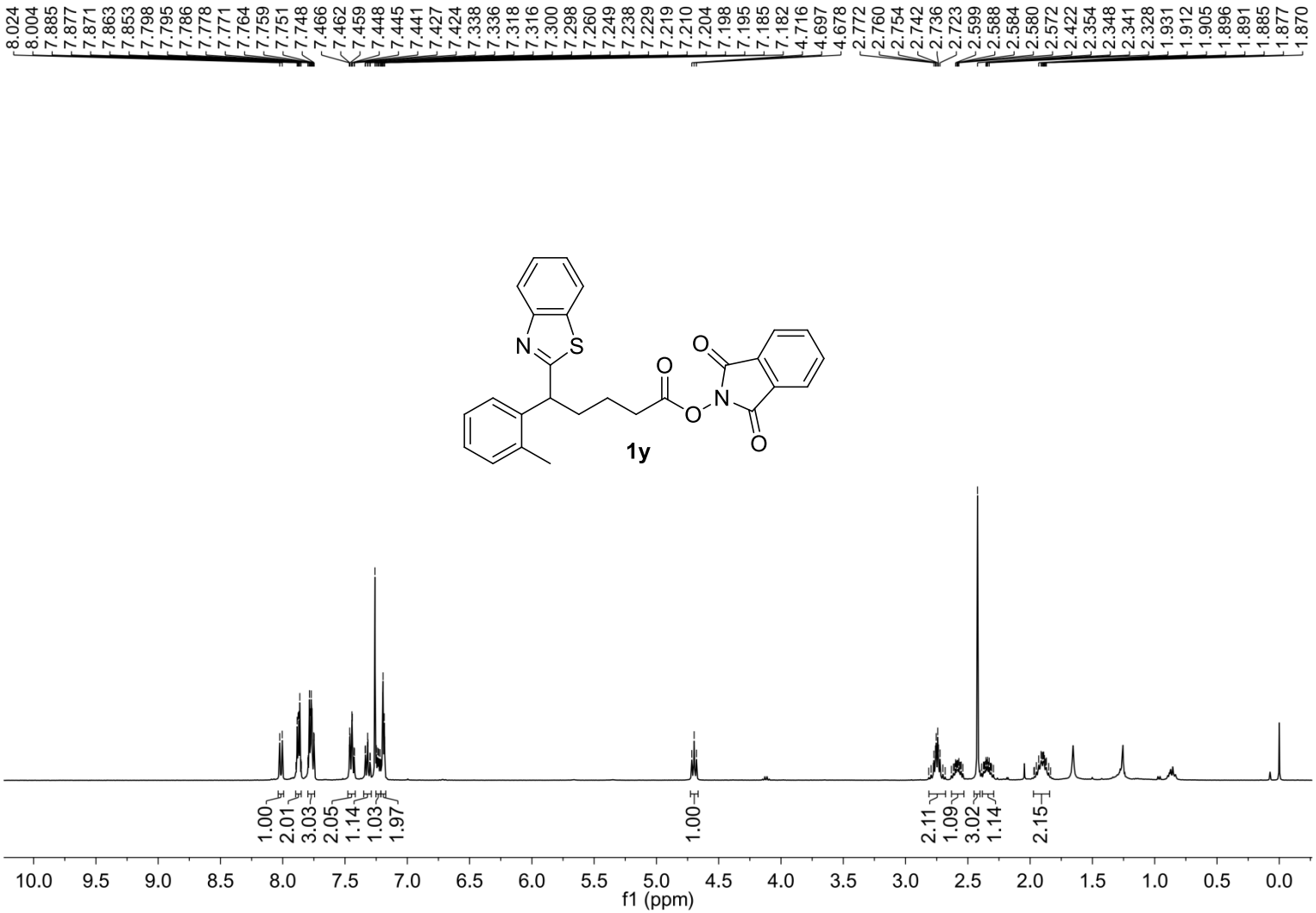
17.388
16.986
1x'
f1 (ppm)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7.786
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7.771
7.764
7.759
7.751
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7.466
7.462
7.459
7.448
7.445
7.441
7.427
7.424
7.338
7.336
7.318
7.316
7.300
7.298
7.260
7.249
7.238
7.229
7.219
7.210
7.204
7.198
7.195
7.185
7.182
4.716
4.697
4.678
2.772
2.760
2.754
2.742
2.736
2.723
2.599
2.588
2.584
2.580
2.572
2.422
2.354
2.348
2.341
2.328
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1.912
1.905
1.896
1.891
1.885
1.877
1.870
N
S
O
O
N
O
O
1y
1.00
2.01
3.03
2.05
1.14
1.03
1.97
1.00
2.11
1.09
3.02
1.14
2.15
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.5
3.0
2.5
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1.0
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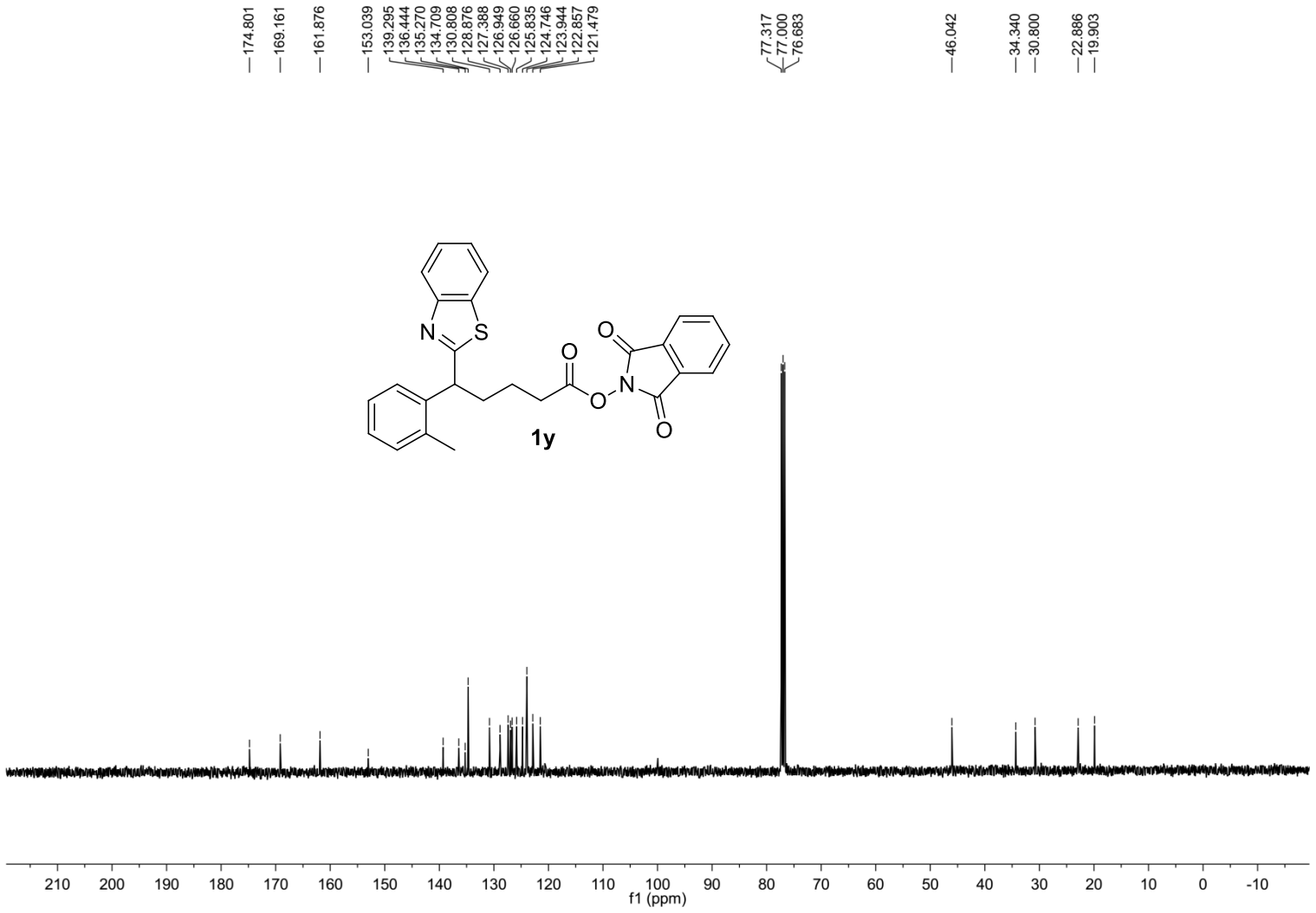
0.0
f1 (ppm)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126.660
125.835
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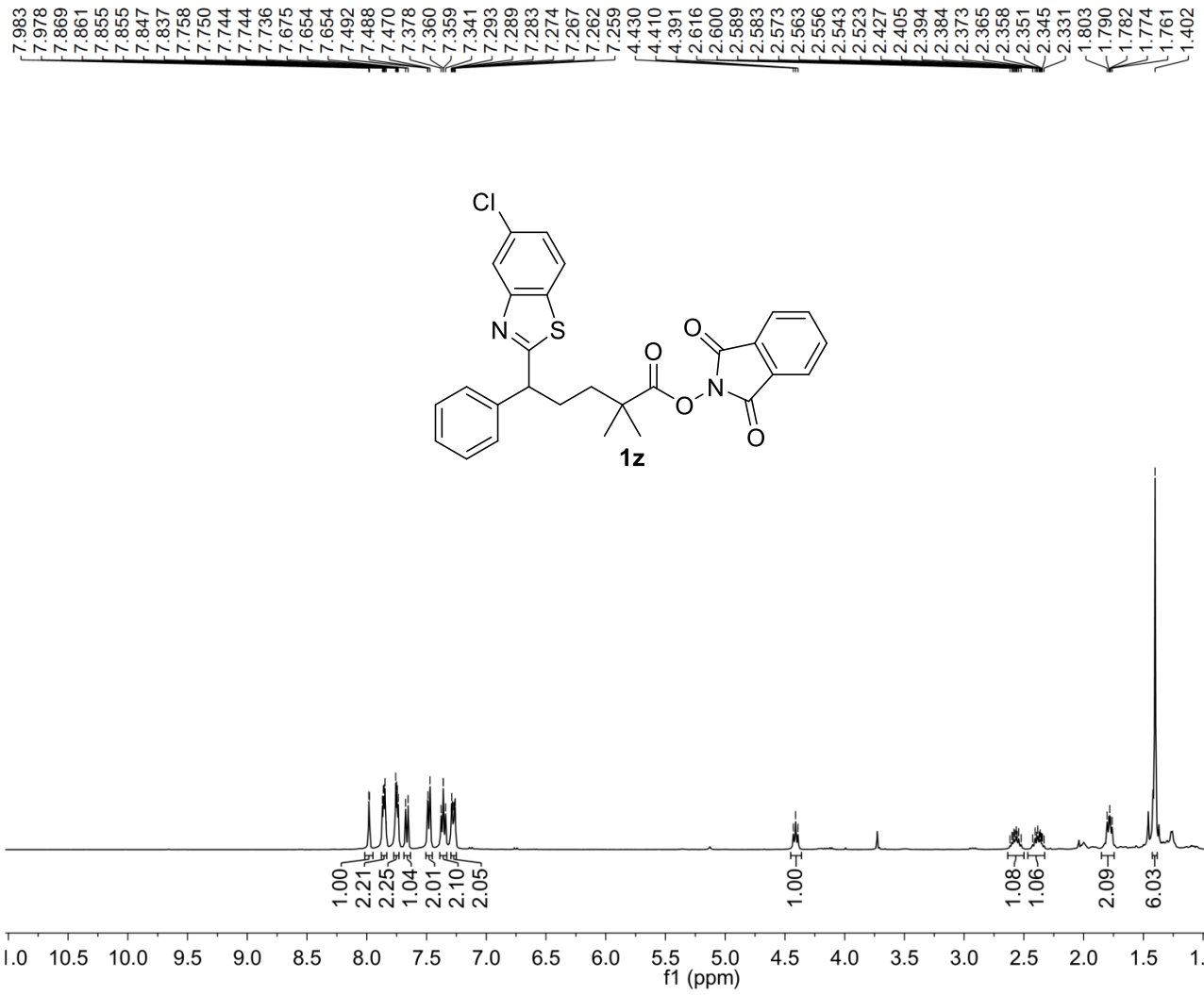
123.944
122.857
121.479
77.317
77.000
76.683
46.042
34.340
30.800
22.886
19.903
N
S
O
O
N
O
O
1y
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.654
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7.488
7.470
7.378
7.360
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7.283
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7.267
7.262
7.259
4.430
4.410
4.391
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2.600
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2.583
2.573
2.563
2.556
2.543
2.523
2.427
2.405
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2.373
2.365
2.358
2.351
2.345
2.331
1.803
1.790
1.782
1.774
1.761
1.402
Cl
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S
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O
N
O
O
1z
1.00
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2.25
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2.05
1.00
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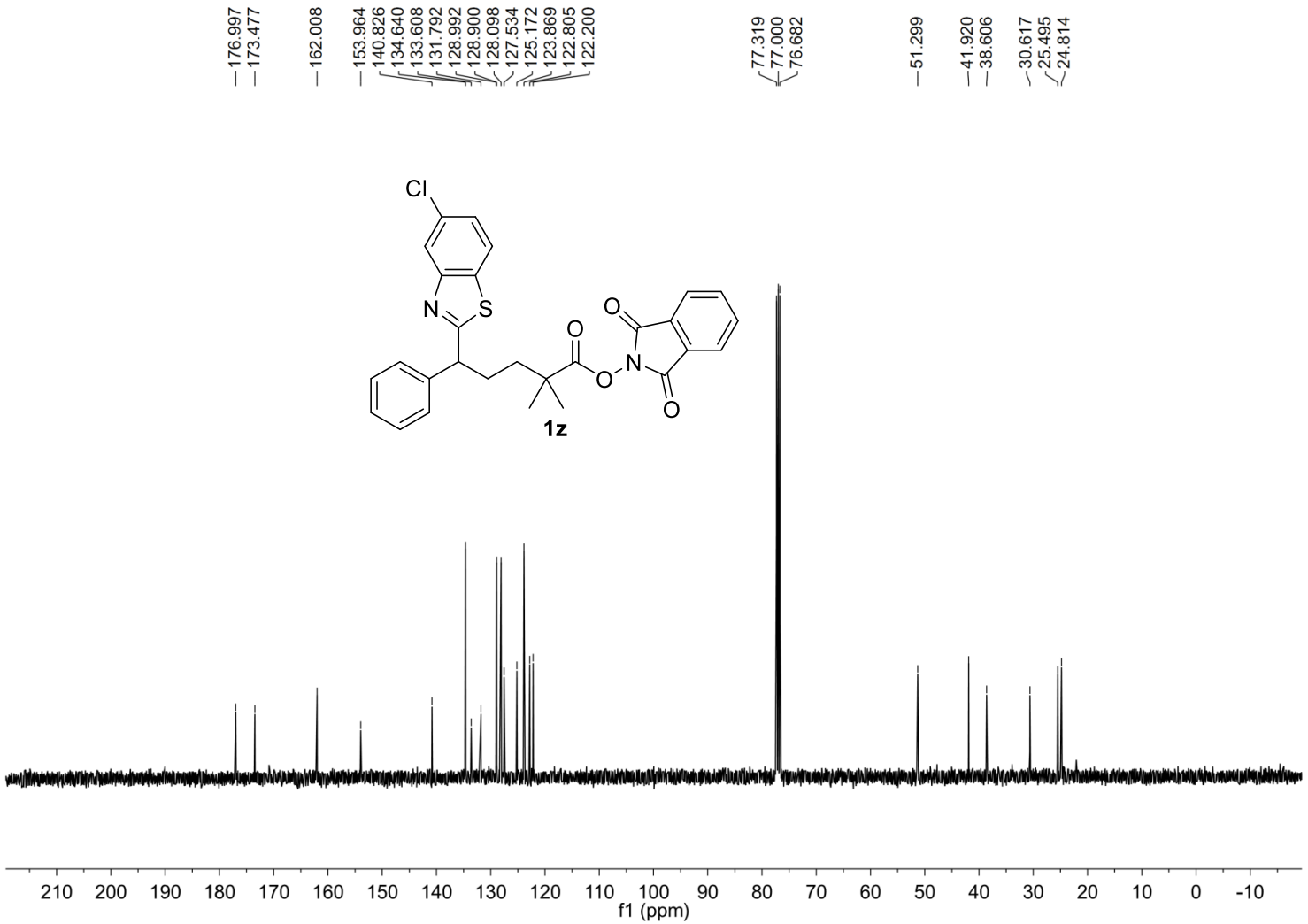
1.06
2.09
6.03
f1 (ppm)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123.869
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77.319
77.000
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51.299
41.920
38.606
30.617
25.495
24.814
Cl
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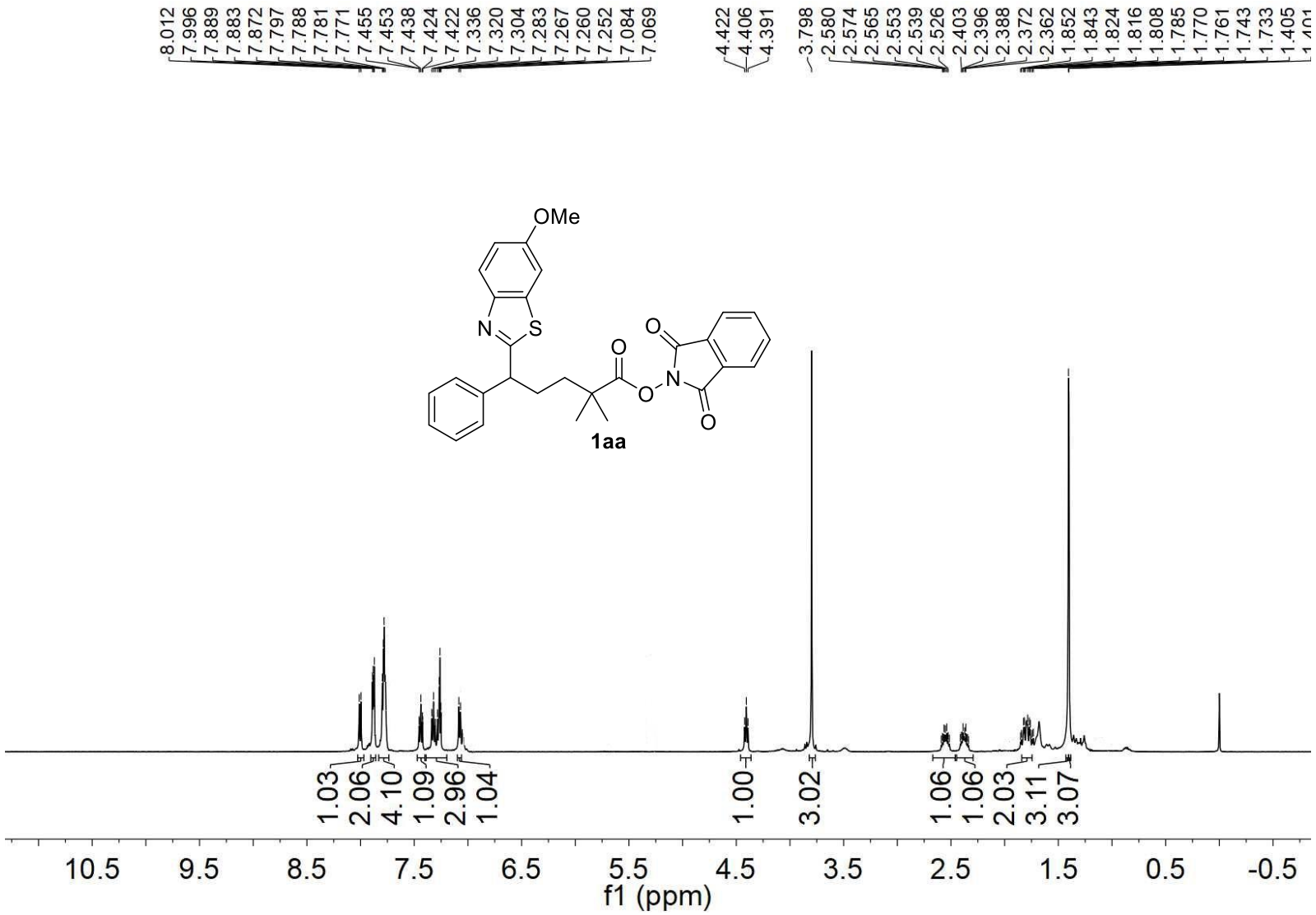
O
N
O
O
1z
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.422
7.336
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7.304
7.283
7.267
7.260
7.252
7.084
7.069
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2.574
2.565
2.553
2.539
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2.403
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2.388
2.372
2.362
1.852
1.843
1.824
1.816
1.808
1.785
1.770
1.761
1.743
1.733
1.405
OMe
N
S
O
O
N
O
O
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2.06
4.10
1.09
2.96
1.04
1.00
3.02
1.06
1.06
2.03
3.11
3.07
10.5
9.5
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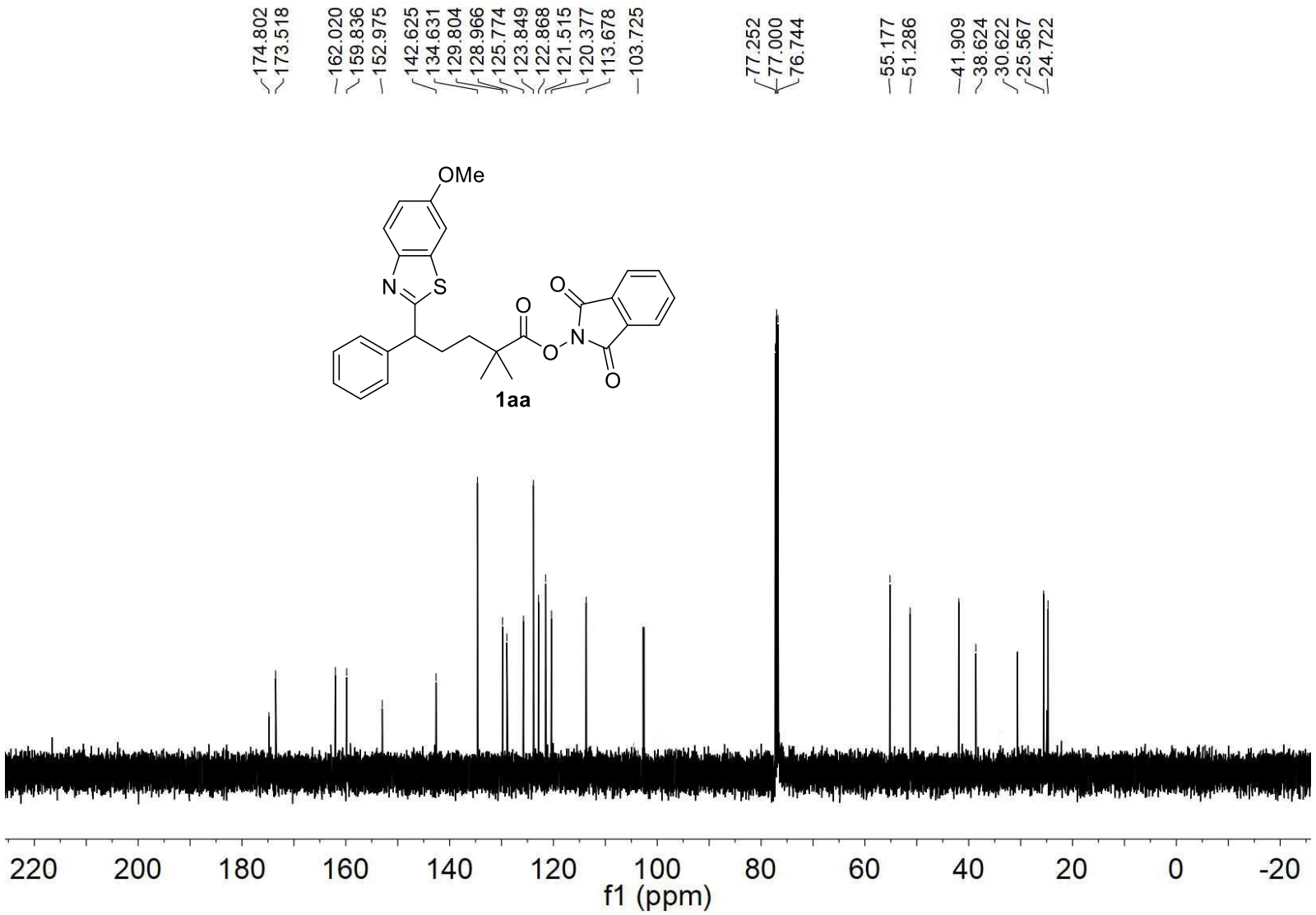
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)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125.774
123.849
122.868
121.515
120.377
113.678
103.725
77.252
77.000
76.744
55.177
51.286
41.909
38.624
30.622
25.567
24.722
OMe
N
S
O
O
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O
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220
200
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120
100
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60
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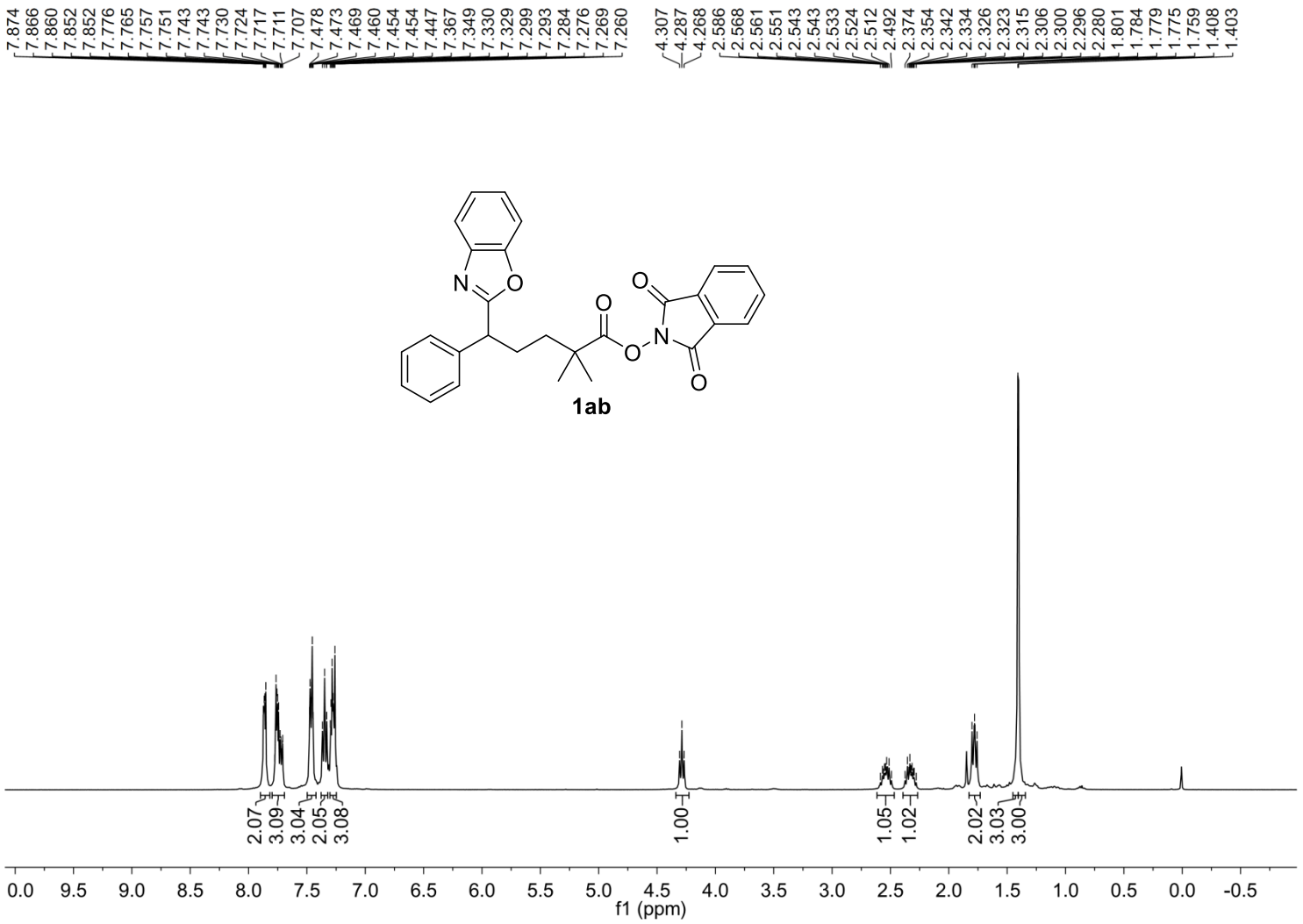
f1 (ppm)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7.717
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7.707
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O
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3.09
3.04
2.05
3.08
1.00
1.05
1.02
2.02
3.03
3.00
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9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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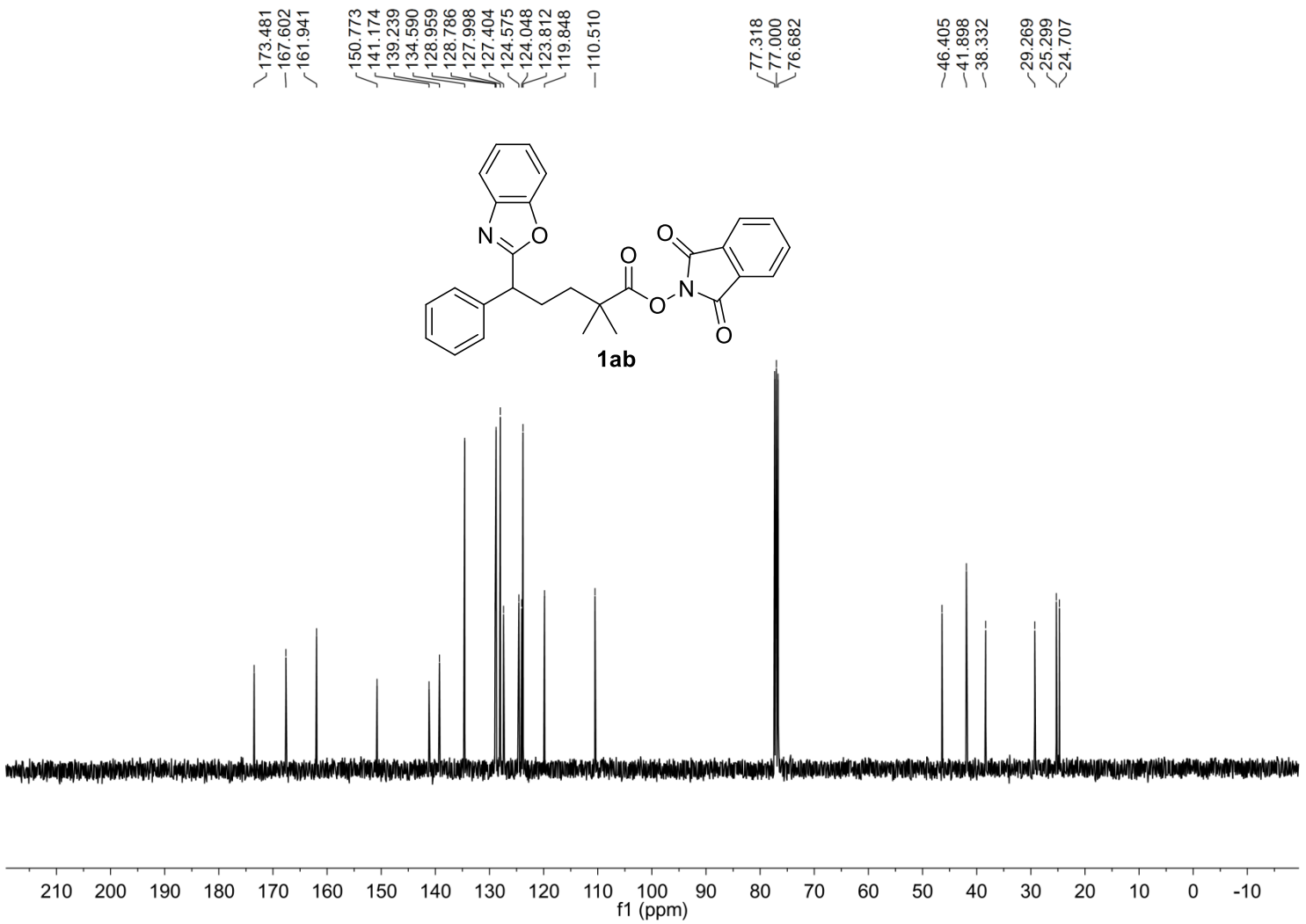
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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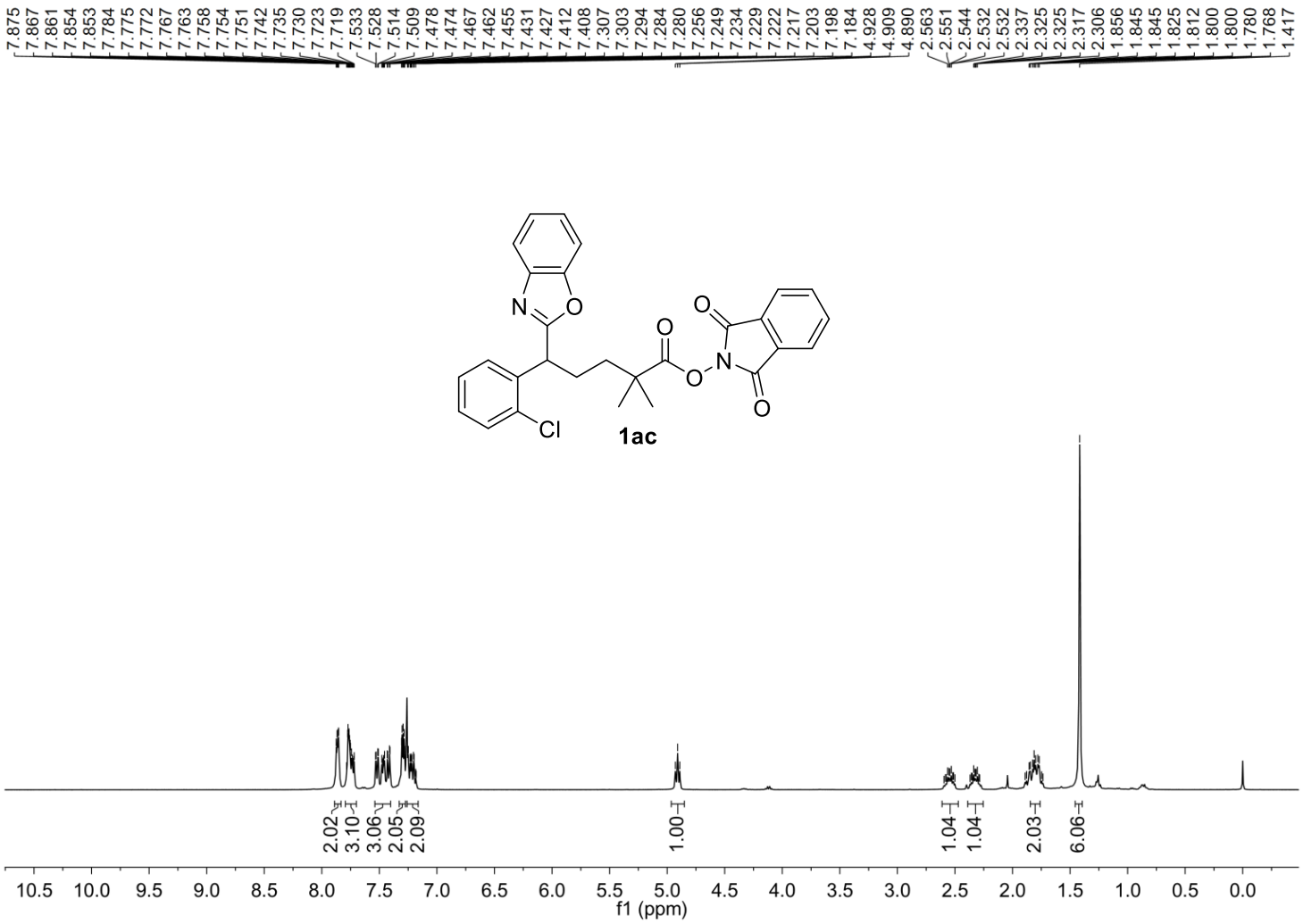
127.404
124.575
124.048
123.812
119.848
110.510
77.318
77.000
76.682
46.405
41.898
38.332
29.269
25.299
24.707
1ab
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.509
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2.532
2.337
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2.325
2.317
2.306
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1.845
1.825
1.812
1.800
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1.768
1.417
N
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O
O
N
O
O
Cl
1ac
2.02
3.10
3.06
2.05
2.09
1.00
1.04
1.04
2.03
6.06
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.5
3.0
2.5
2.0
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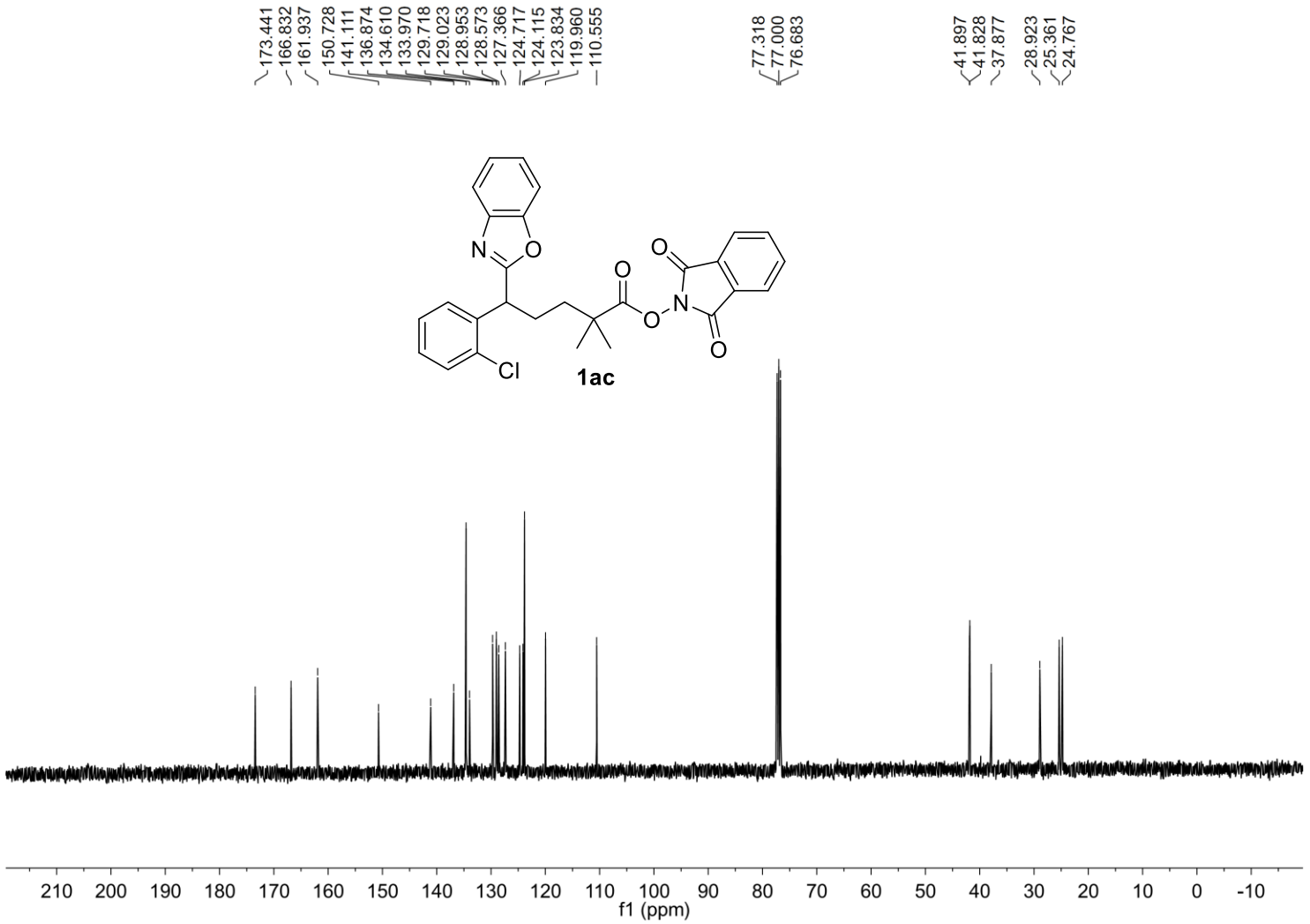
1.0
0.5
0.0
f1 (ppm)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128.953
128.573
127.366
124.717
124.115
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77.318
77.000
76.683
41.897
41.828
37.877
28.923
25.361
24.767
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O
O
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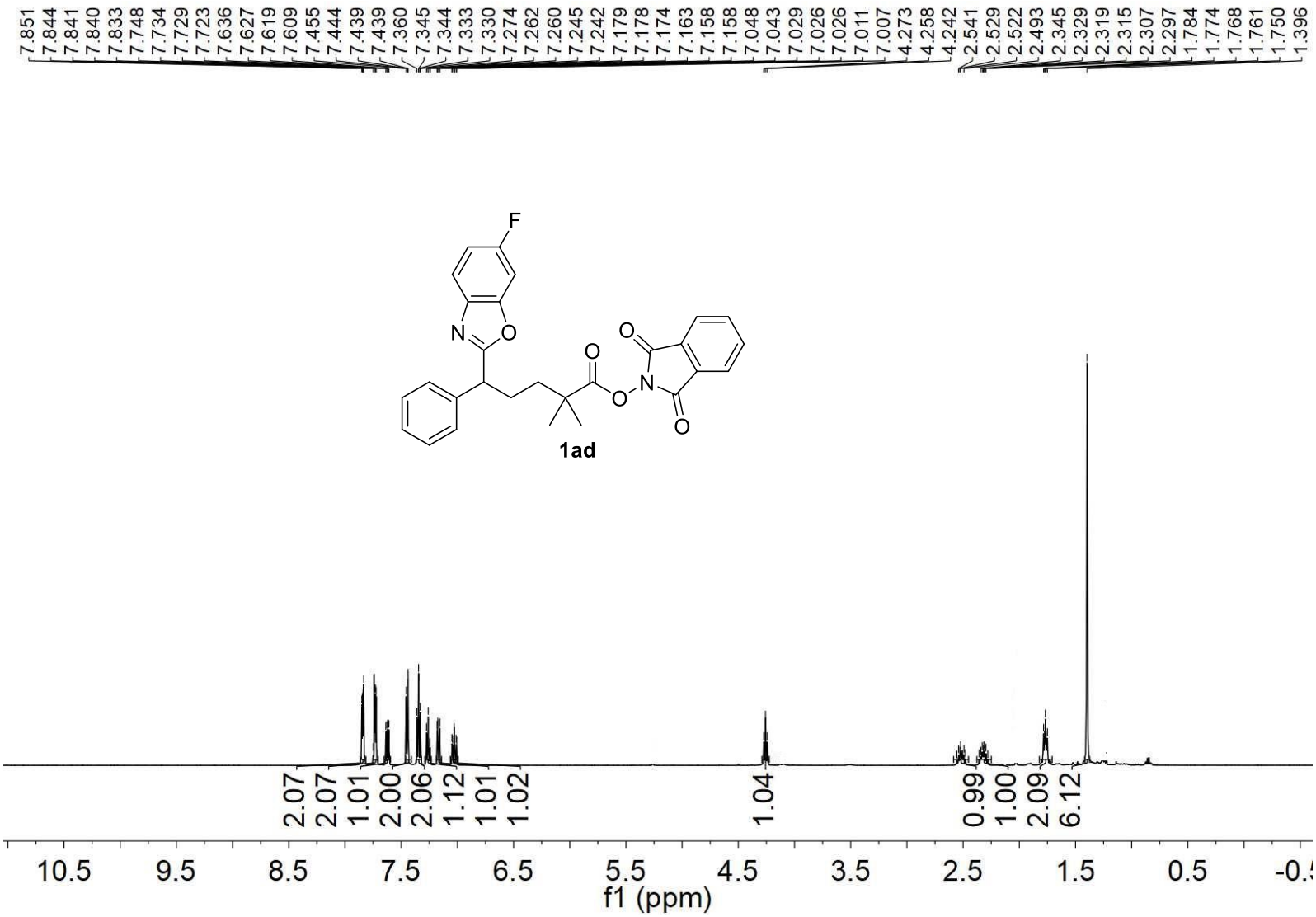
f1 (ppm)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7.609
7.455
7.444
7.439
7.439
7.360
7.345
7.344
7.333
7.330
7.274
7.262
7.260
7.245
7.242
7.179
7.178
7.174
7.163
7.158
7.158
7.048
7.043
7.029
7.026
7.026
7.011
7.007
4.273
4.258
4.242
2.541
2.529
2.522
2.493
2.345
2.329
2.319
2.315
2.307
2.297
1.784
1.774
1.768
1.761
1.750
1.396
F
N
O
O
O
N
O
O
1ad
2.07
2.07
1.01
2.00
2.06
1.12
1.01
1.02
1.04
0.99
1.00
2.09
6.12
10.5
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5.5
4.5
3.5
2.5
1.5
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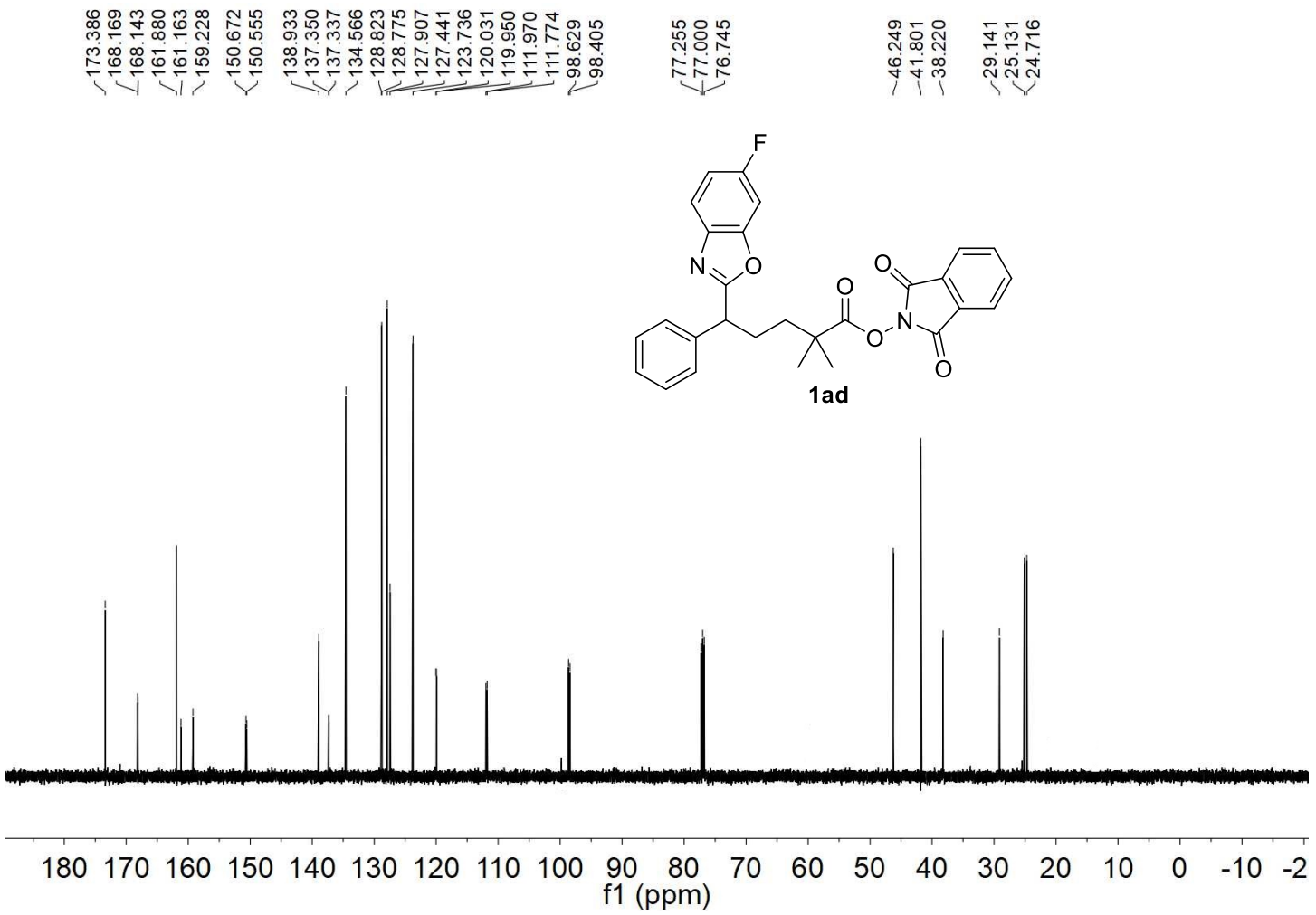
f1 (ppm)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150.555
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134.566
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128.775
127.907
127.441
123.736
120.031
119.950
111.970
111.774
98.629
98.405
77.255
77.000
76.745
46.249
41.801
38.220
29.141
25.131
24.716
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O
O
N
O
1ad
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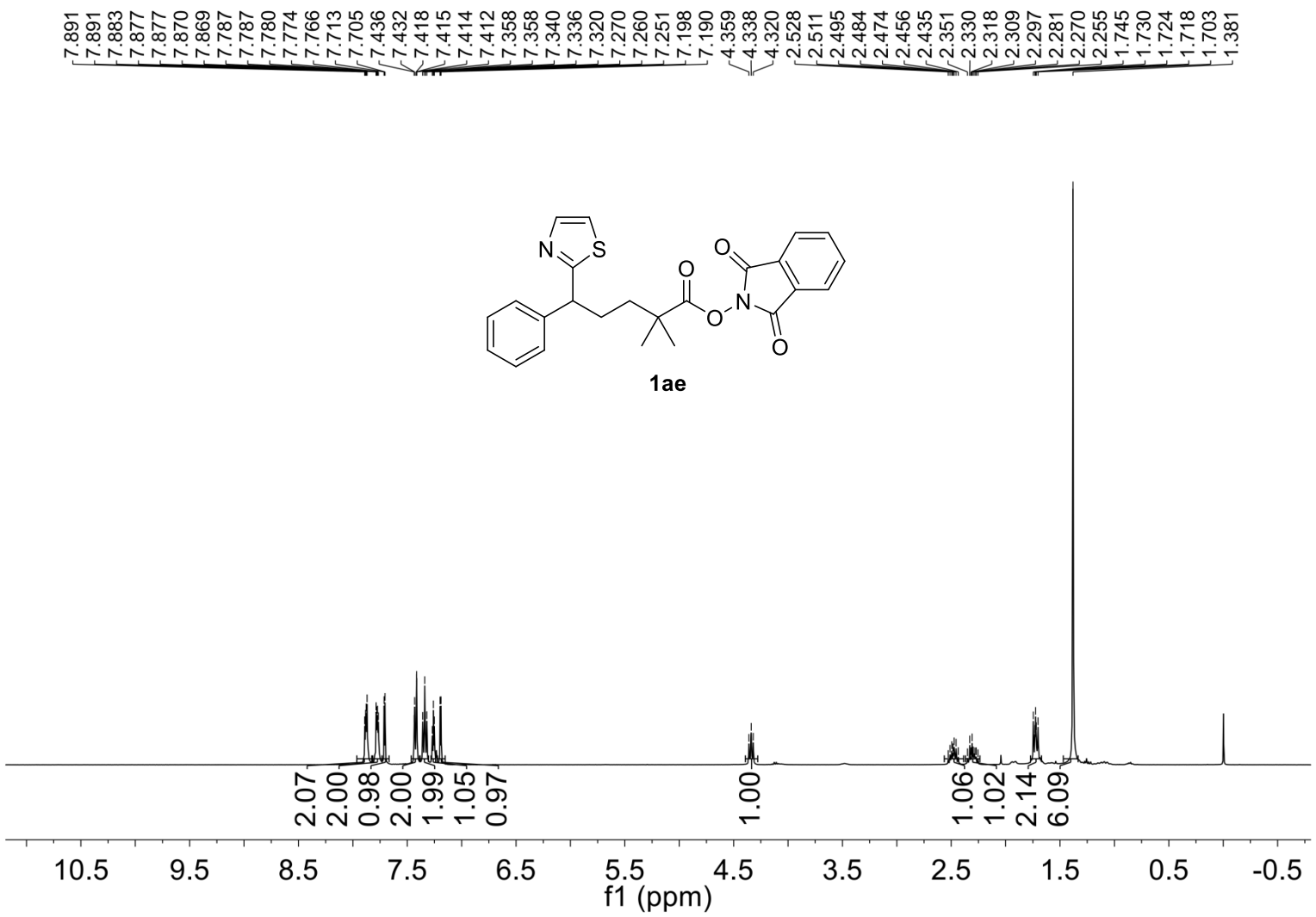
f1 (ppm)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7.787
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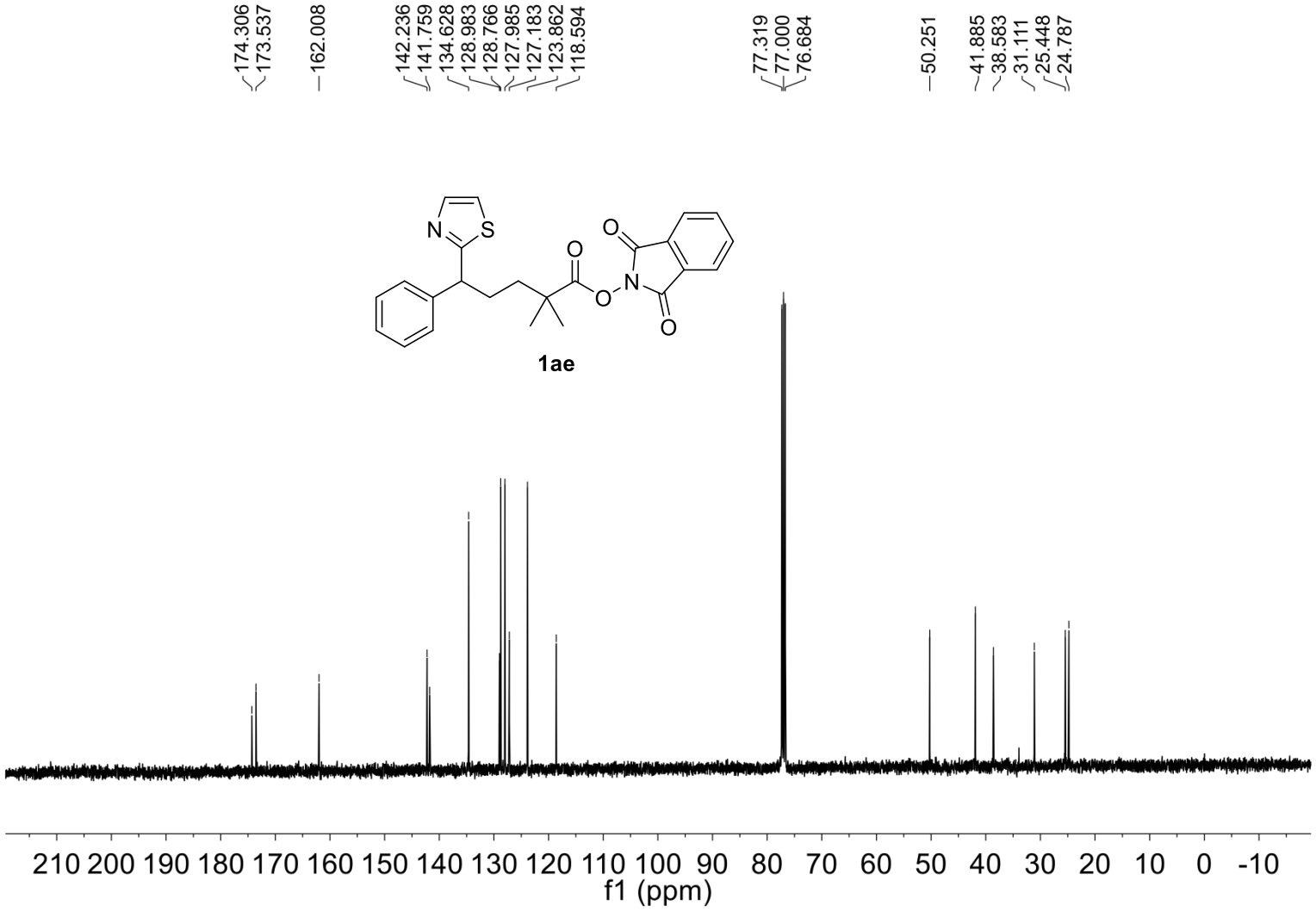
7.713
7.705
7.436
7.432
7.418
7.415
7.414
7.412
7.358
7.358
7.340
7.336
7.320
7.270
7.260
7.251
7.198
7.190
4.359
4.338
4.320
2.528
2.511
2.495
2.484
2.474
2.456
2.435
2.351
2.330
2.318
2.309
2.297
2.281
2.270
2.255
1.745
1.730
1.724
1.718
1.703
1.381
N
S
O
O
N
O
O
1ae
2.07
2.00
0.98
2.00
1.99
1.05
0.97
1.00
1.06
1.02
2.14
6.09
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)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77.000
76.684
50.251
41.885
38.583
31.111
25.448
24.787
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O
N
O
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1ae
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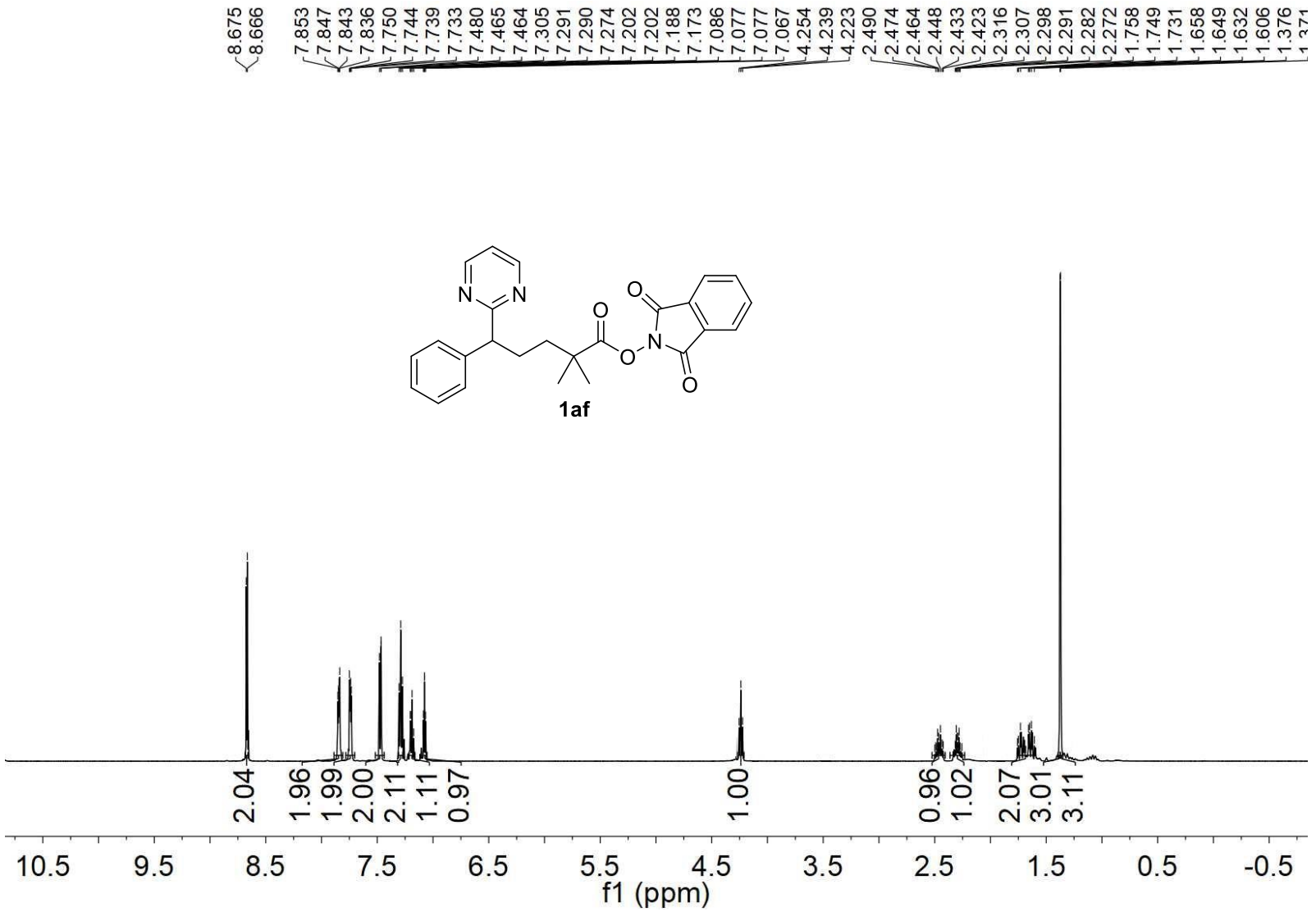
f1 (ppm)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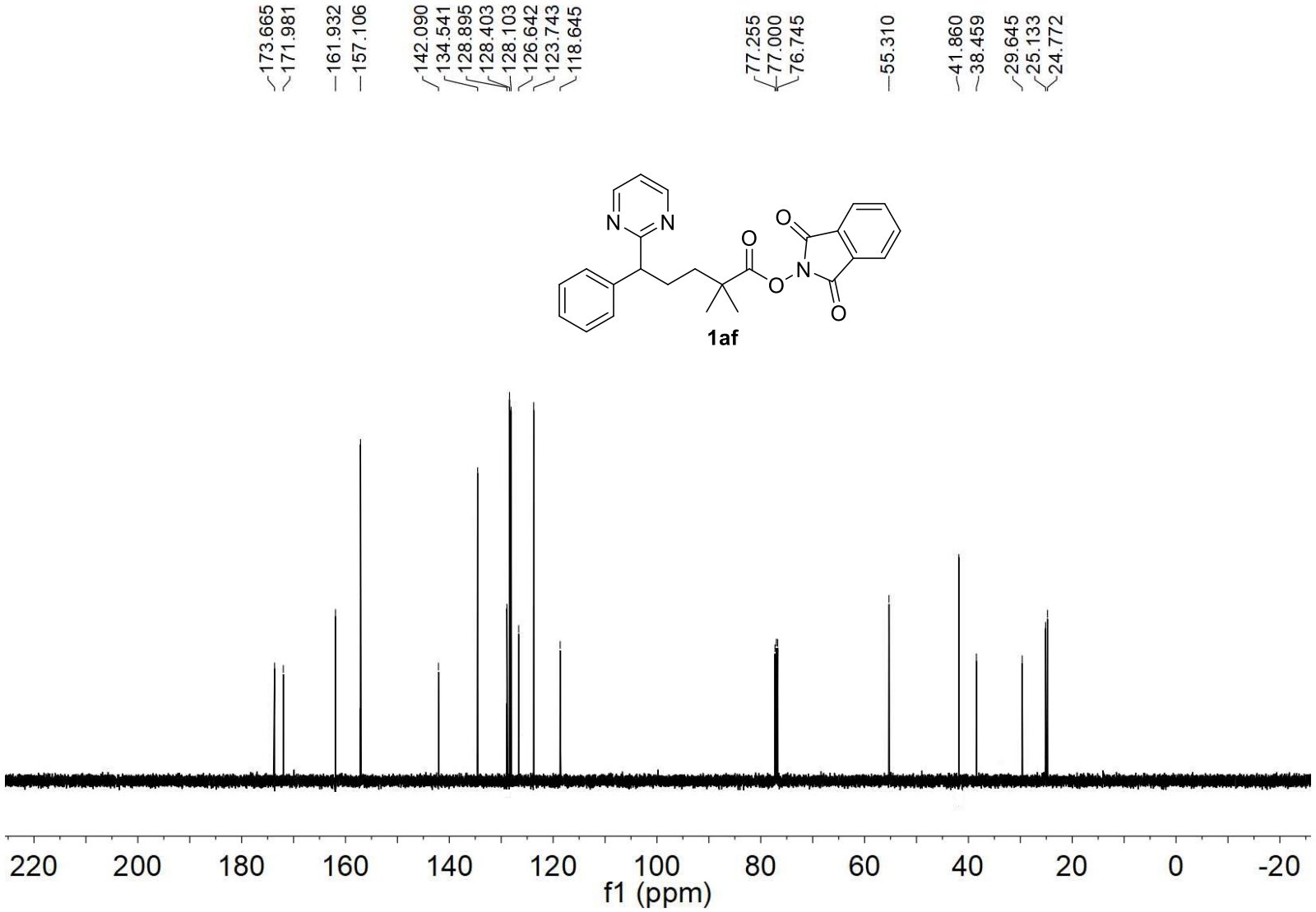
7.464
7.305
7.291
7.290
7.274
7.202
7.202
7.188
7.173
7.086
7.077
7.077
7.067
4.254
4.239
4.223
2.490
2.474
2.464
2.448
2.433
2.423
2.316
2.307
2.298
2.291
2.282
2.272
1.758
1.749
1.731
1.658
1.649
1.632
1.606
1.376
N
N
O
O
O
N
O
O
1af
2.04
1.96
1.99
2.00
2.11
1.11
0.97
1.00
0.96
1.02
2.07
3.01
3.11
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)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77.255
77.000
76.745
55.310
41.860
38.459
29.645
25.133
24.772
N
N
O
O
O
N
O
O
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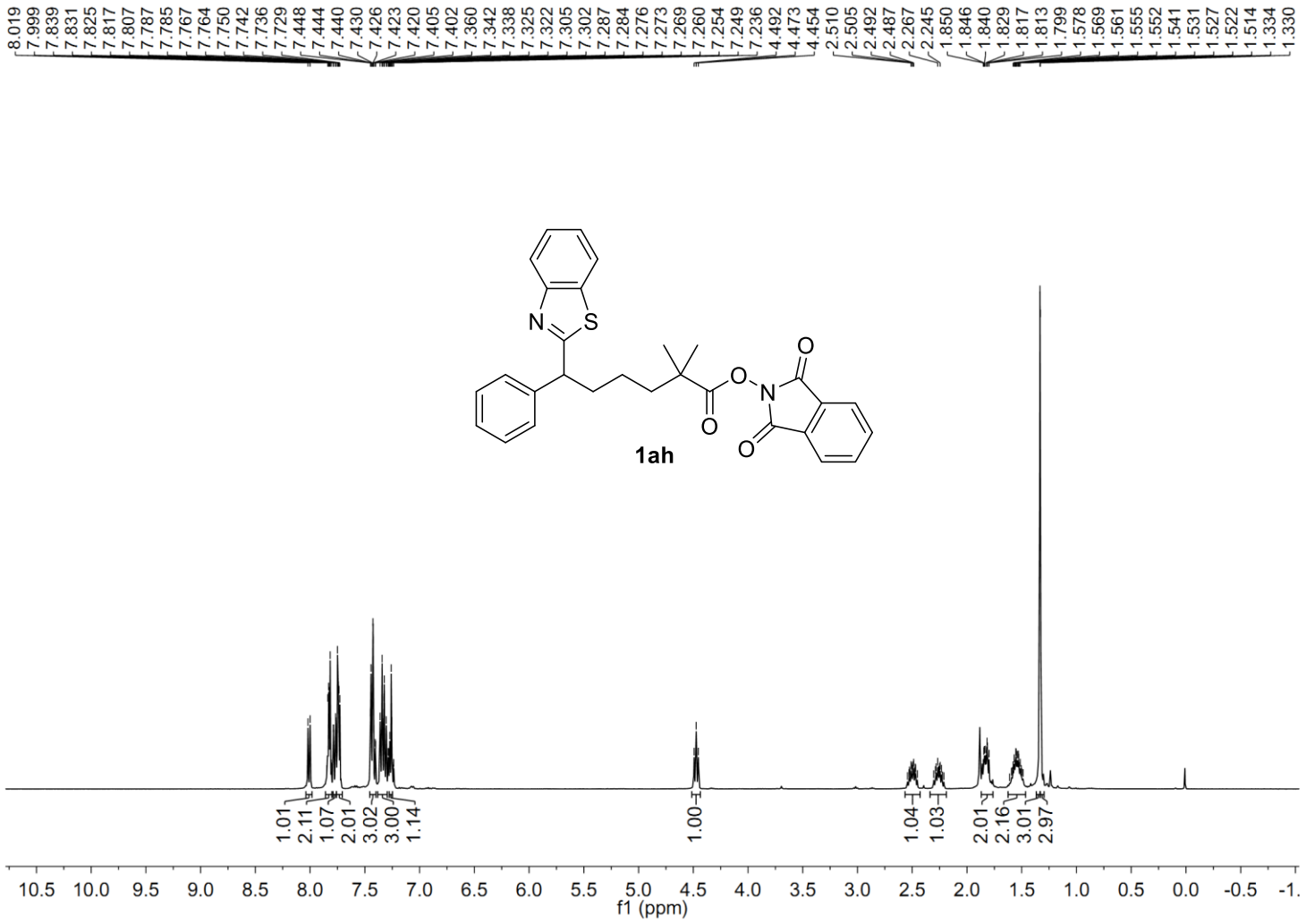
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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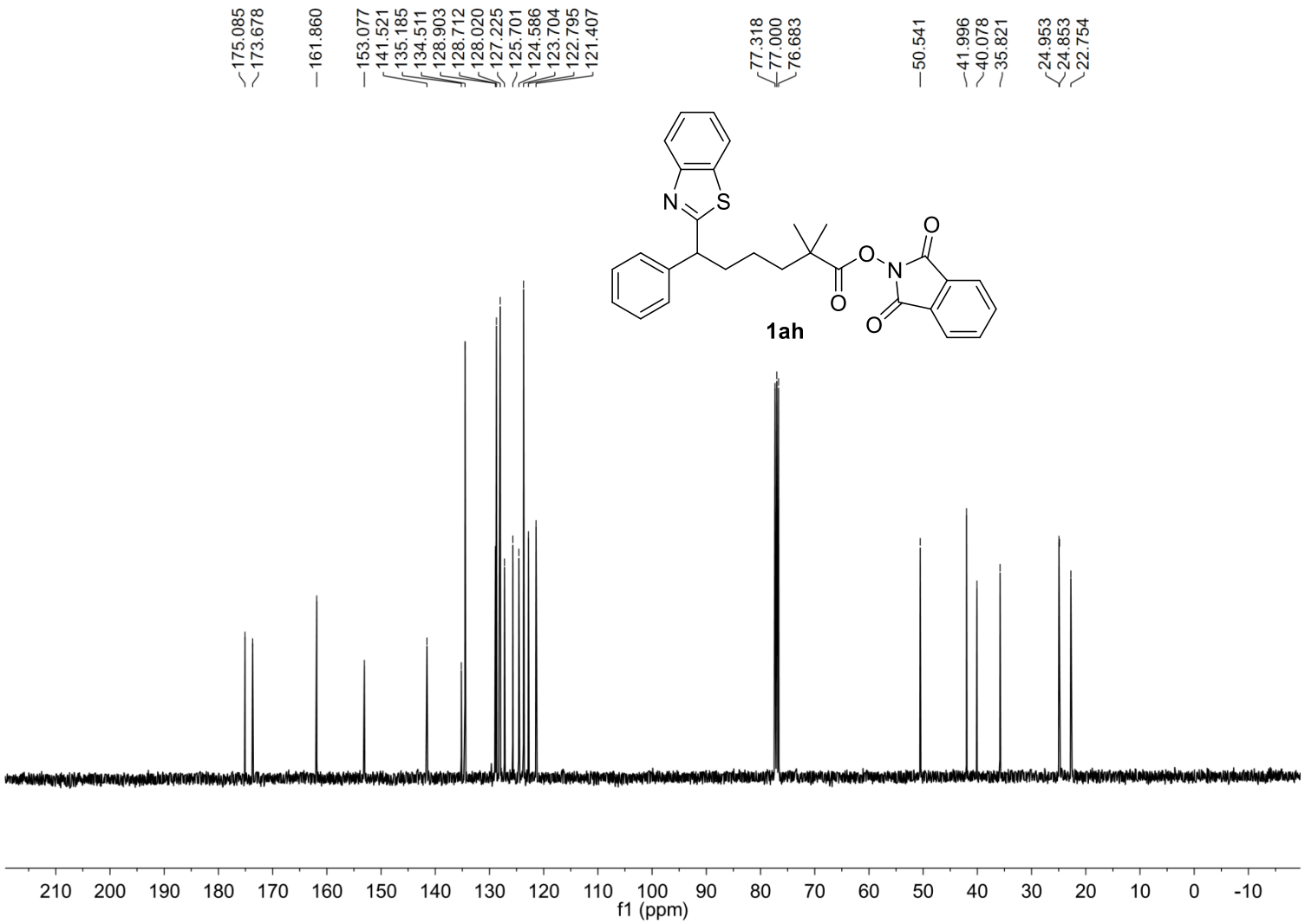
7.750
7.742
7.736
7.729
7.448
7.444
7.440
7.430
7.426
7.423
7.420
7.405
7.402
7.360
7.342
7.338
7.325
7.322
7.305
7.302
7.287
7.284
7.276
7.273
7.269
7.260
7.254
7.249
7.236
4.492
4.473
4.454
2.510
2.505
2.492
2.487
2.267
2.245
1.850
1.846
1.840
1.829
1.817
1.813
1.799
1.578
1.569
1.561
1.555
1.552
1.541
1.531
1.527
1.522
1.514
1.334
1.330
N
S
O
O
N
O
O
1ah
1.01
2.11
1.07
2.01
3.02
3.00
1.14
1.00
1.04
1.03
2.01
2.16
3.01
2.97
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)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127.225
125.701
124.586
123.704
122.795
121.407
77.318
77.000
76.683
50.541
41.996
40.078
35.821
24.953
24.853
22.754
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S
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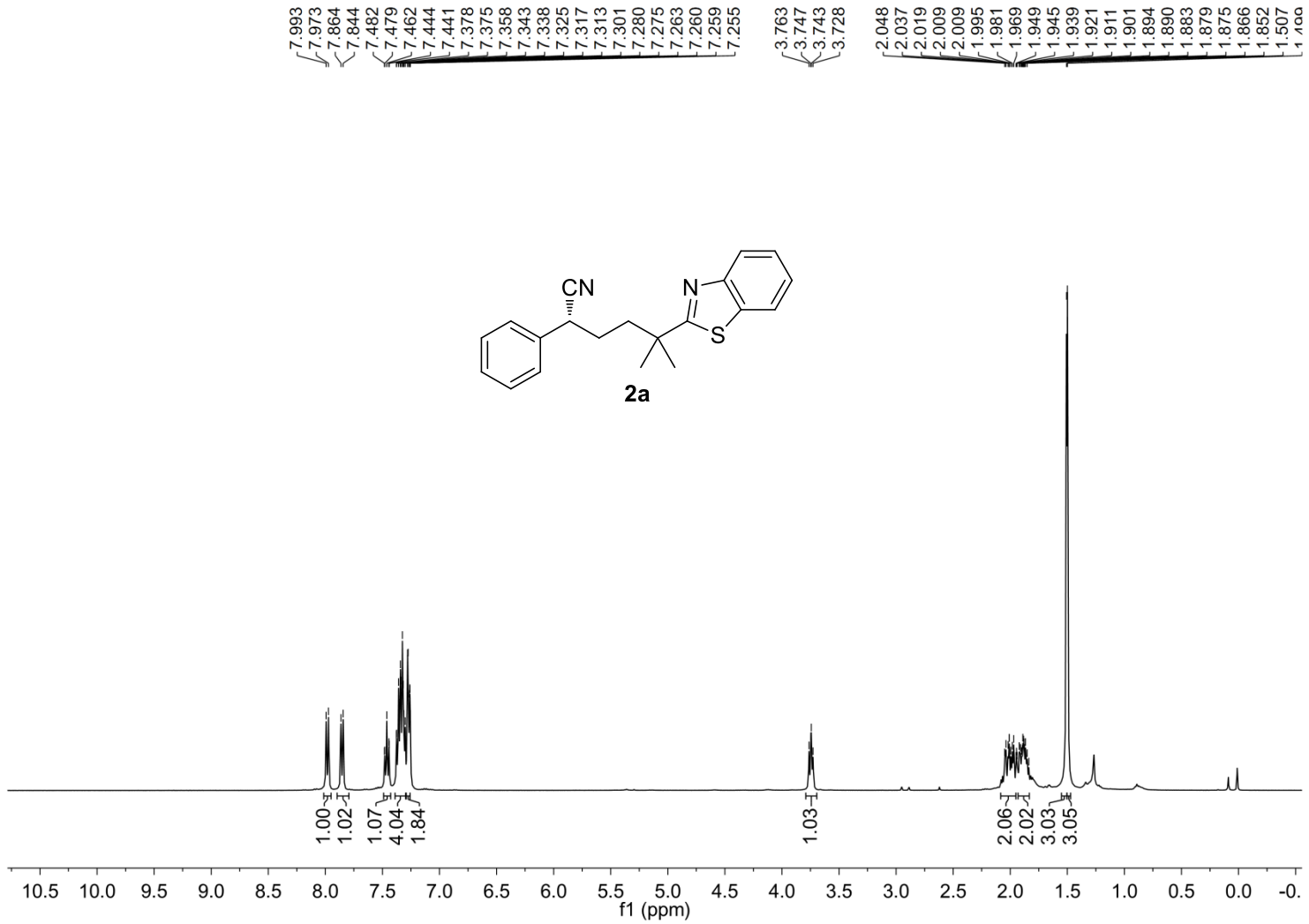
O
N
O
O
1ah
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.444
7.441
7.378
7.375
7.358
7.343
7.338
7.325
7.317
7.313
7.301
7.280
7.275
7.263
7.260
7.259
7.255
3.763
3.747
3.743
3.728
2.048
2.037
2.019
2.009
2.009
1.995
1.981
1.969
1.949
1.945
1.939
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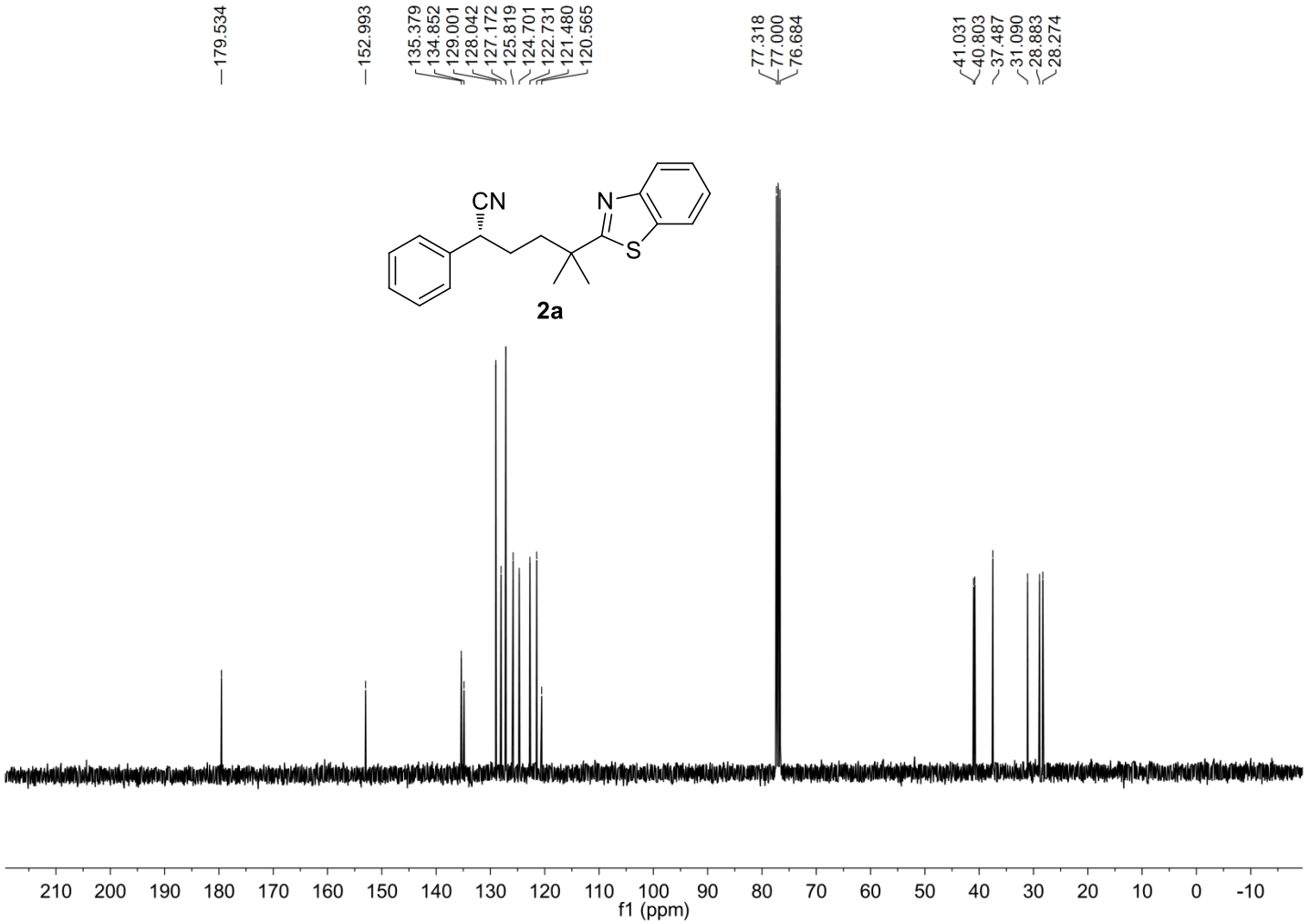
1.911
1.901
1.894
1.890
1.883
1.879
1.875
1.866
1.852
1.507
CN
N
S
2a
1.00
1.02
1.07
4.04
1.84
1.03
2.06
2.02
3.03
3.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)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77.000
76.684
41.031
40.803
37.487
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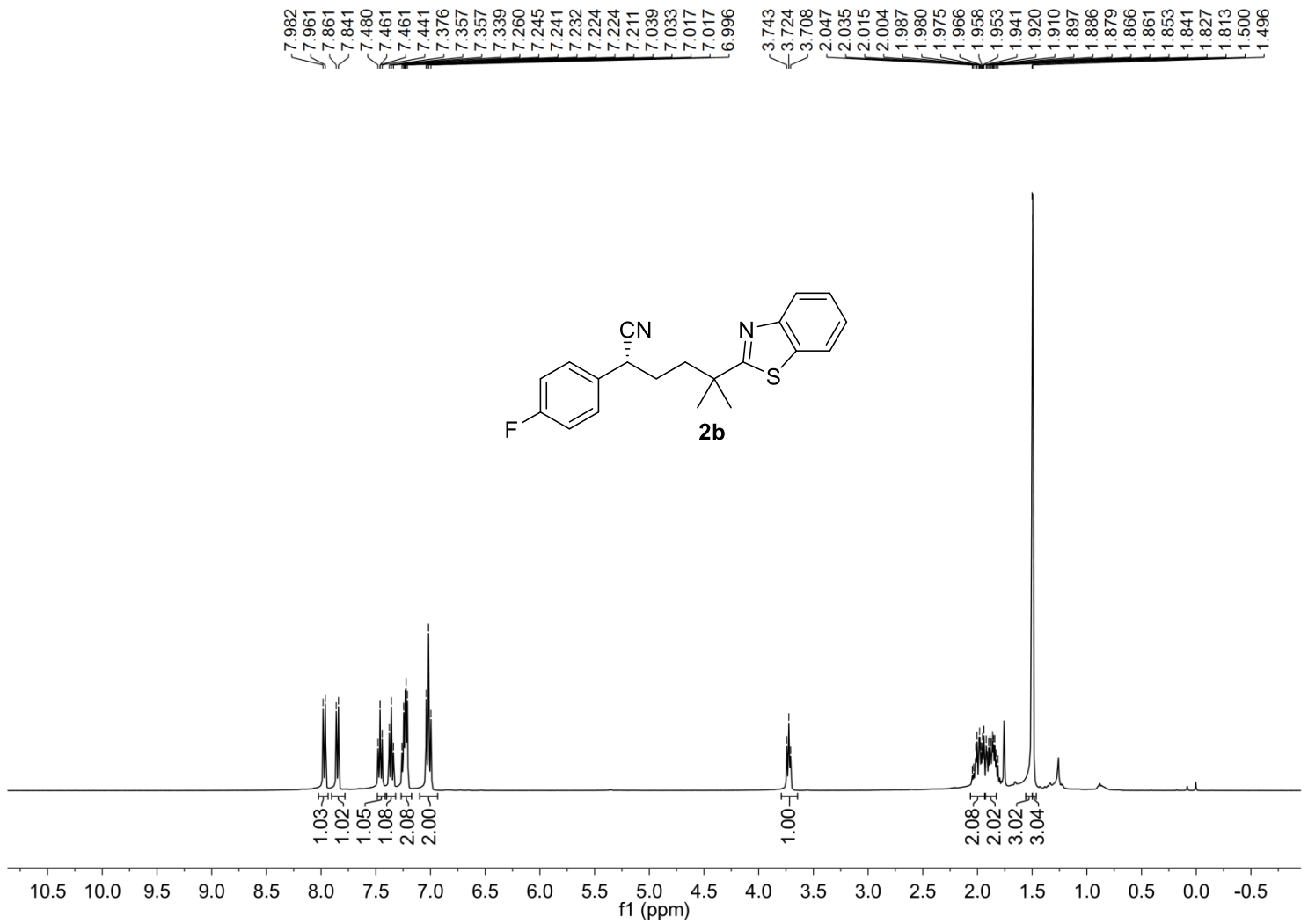
CN
N
S
2a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.339
7.260
7.245
7.241
7.232
7.224
7.224
7.211
7.039
7.033
7.017
7.017
6.996
3.743
3.724
3.708
2.047
2.035
2.015
2.004
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1.980
1.975
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1.953
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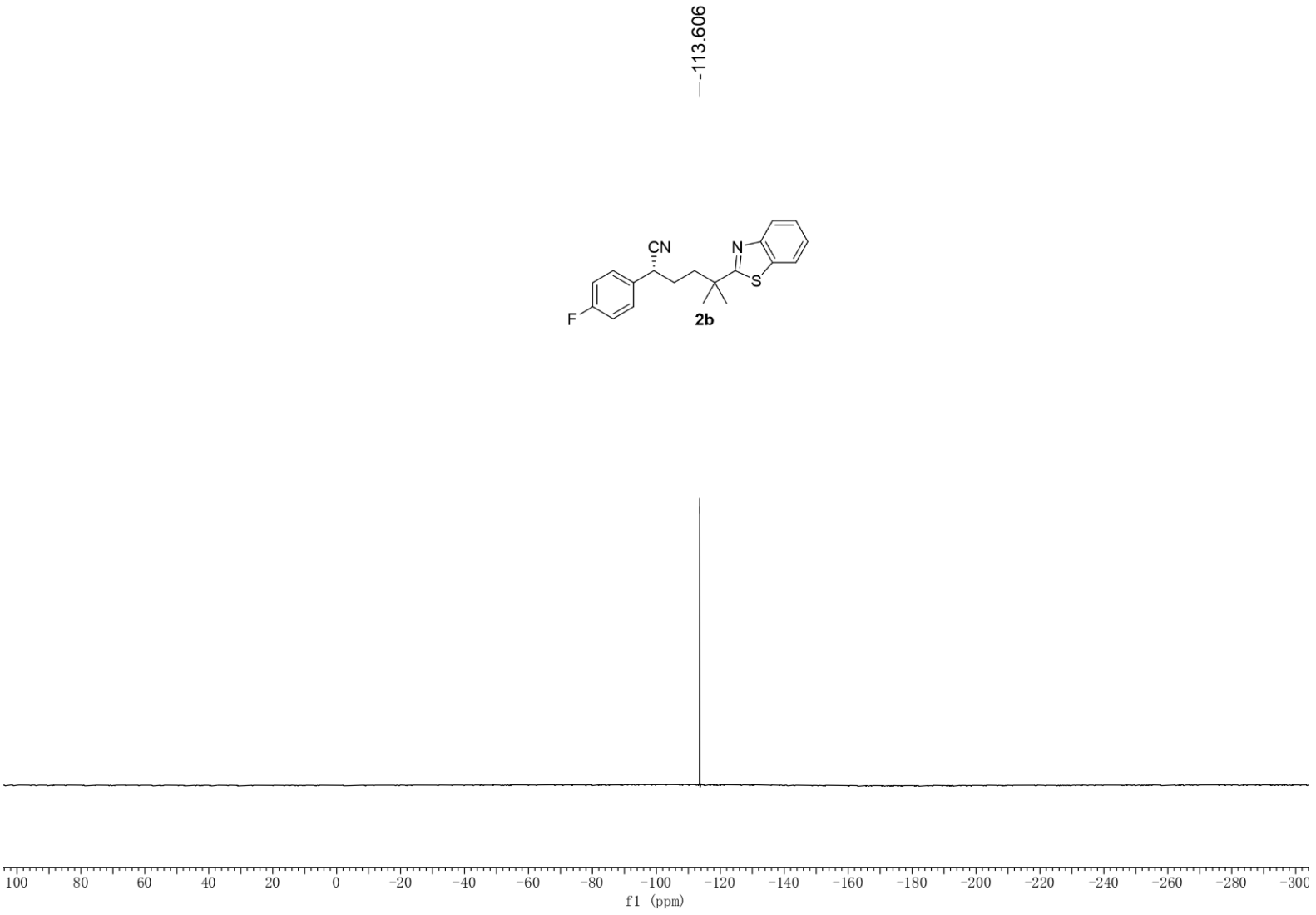
1.866
1.861
1.853
1.841
1.827
1.813
1.500
1.496
CN
N
S
F
2b
1.03
1.02
1.05
1.08
2.08
2.00
1.00
2.08
2.02
3.02
3.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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S
F
2b
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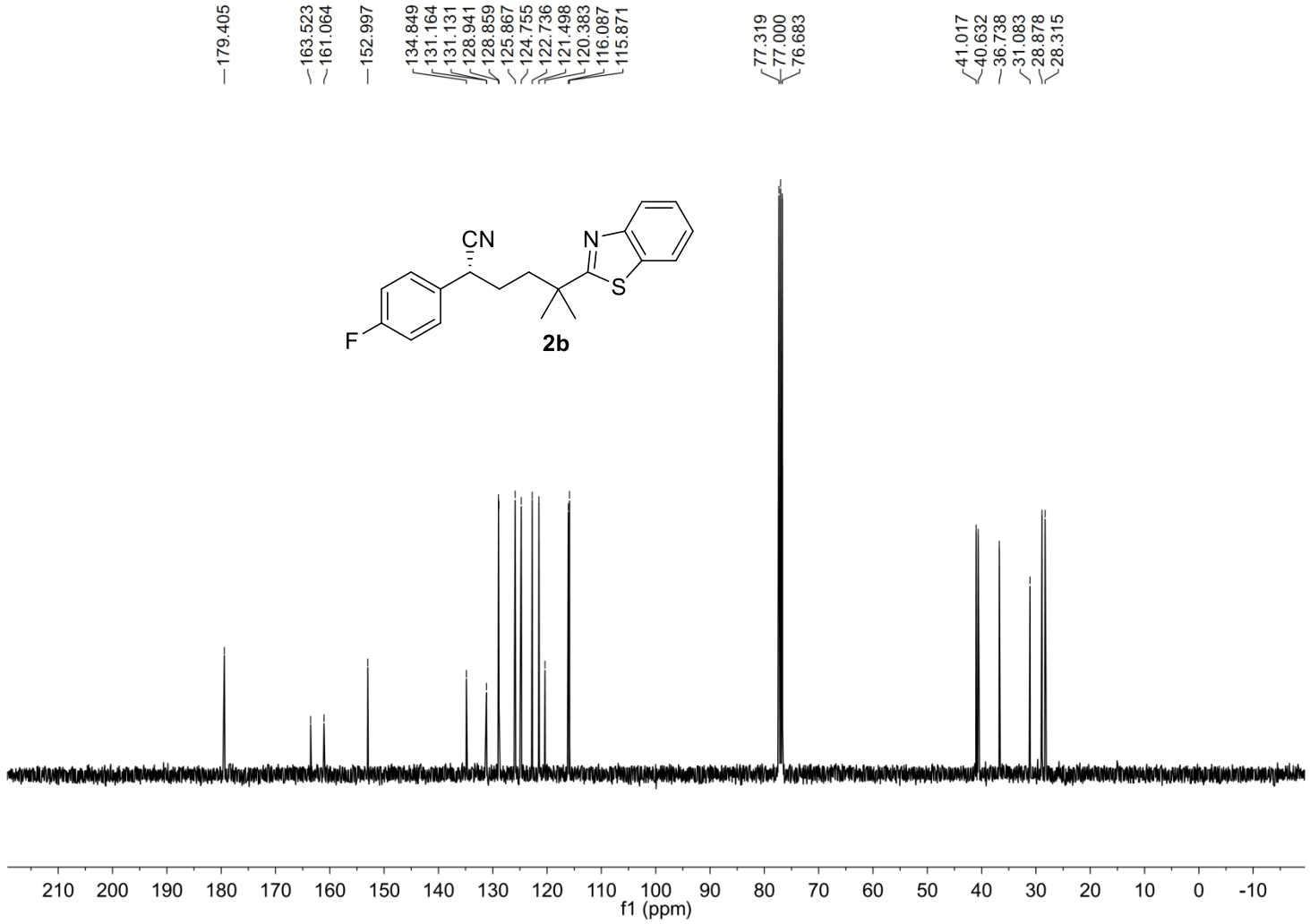
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
-260
-280
-300
f1 (ppm)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128.859
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121.498
120.383
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115.871
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77.000
76.683
41.017
40.632
36.738
31.083
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CN
N
S
F
2b
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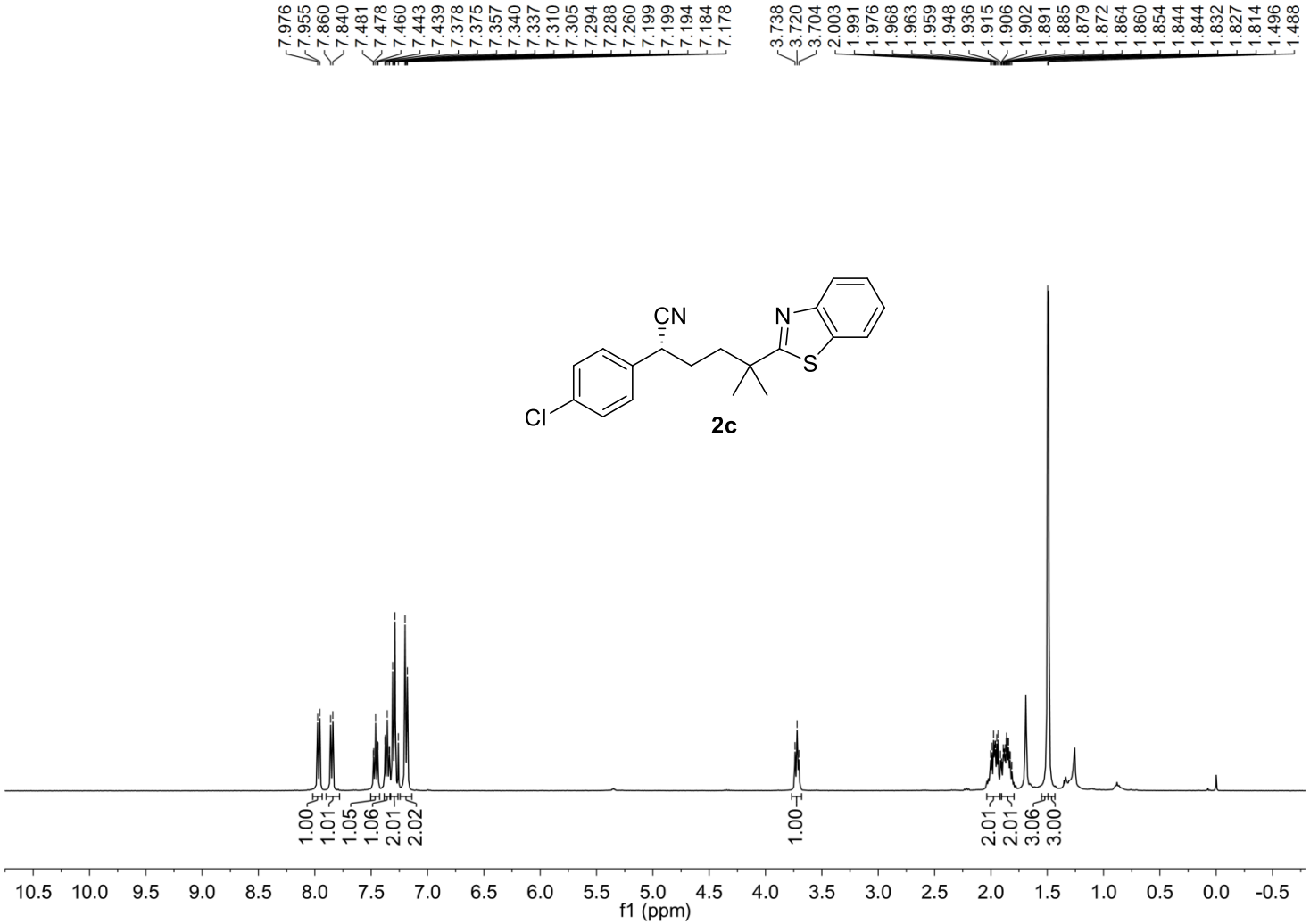
f1 (ppm)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7.340
7.337
7.310
7.305
7.294
7.288
7.260
7.199
7.199
7.194
7.184
7.178
3.738
3.720
3.704
2.003
1.991
1.976
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1.963
1.959
1.948
1.936
1.915
1.906
1.902
1.891
1.885
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1.860
1.854
1.844
1.844
1.832
1.827
1.814
1.496
1.488
CN
N
S
Cl
2c
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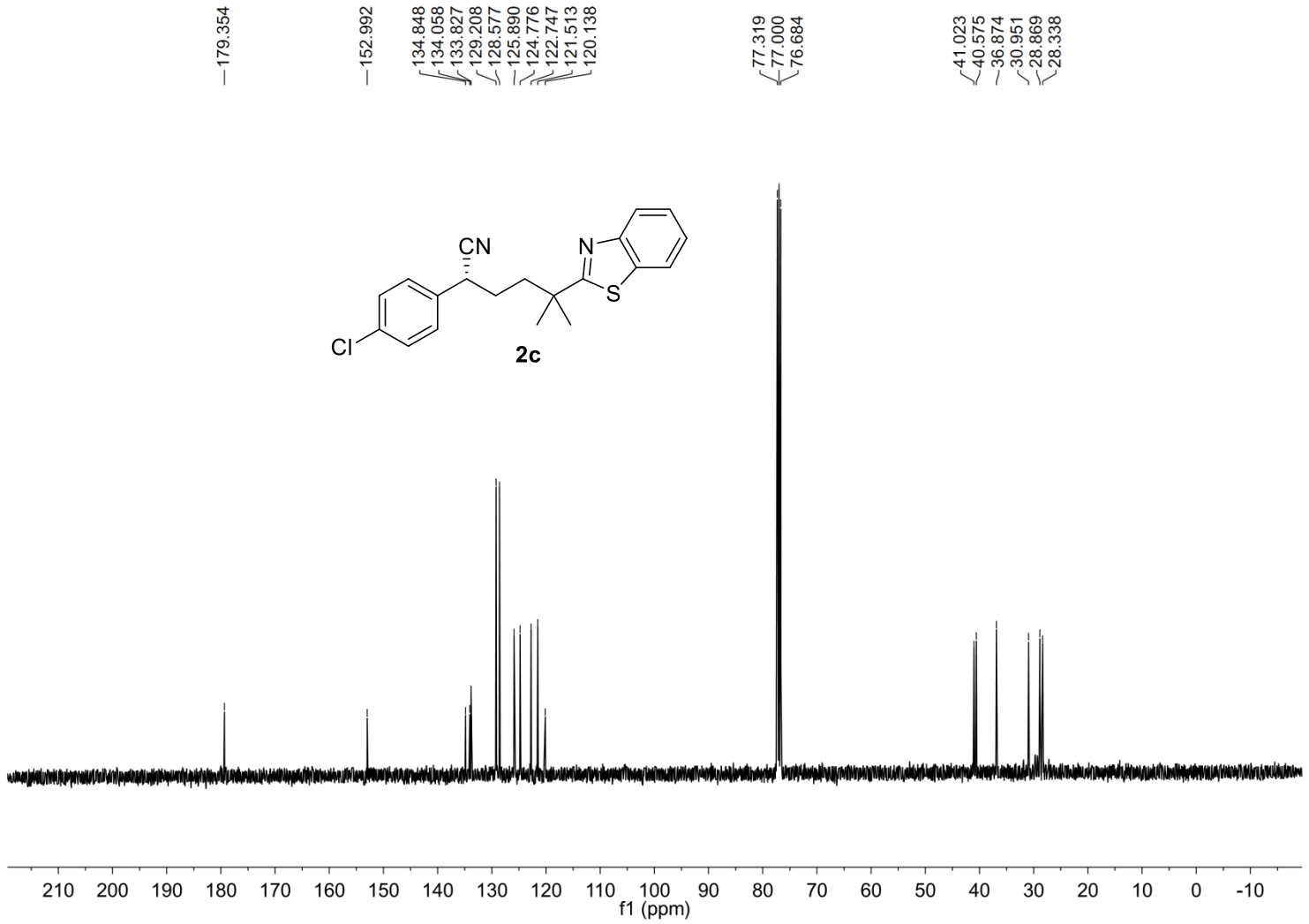
1.01
1.05
1.06
2.01
2.02
1.00
2.01
2.01
3.06
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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77.000
76.684
41.023
40.575
36.874
30.951
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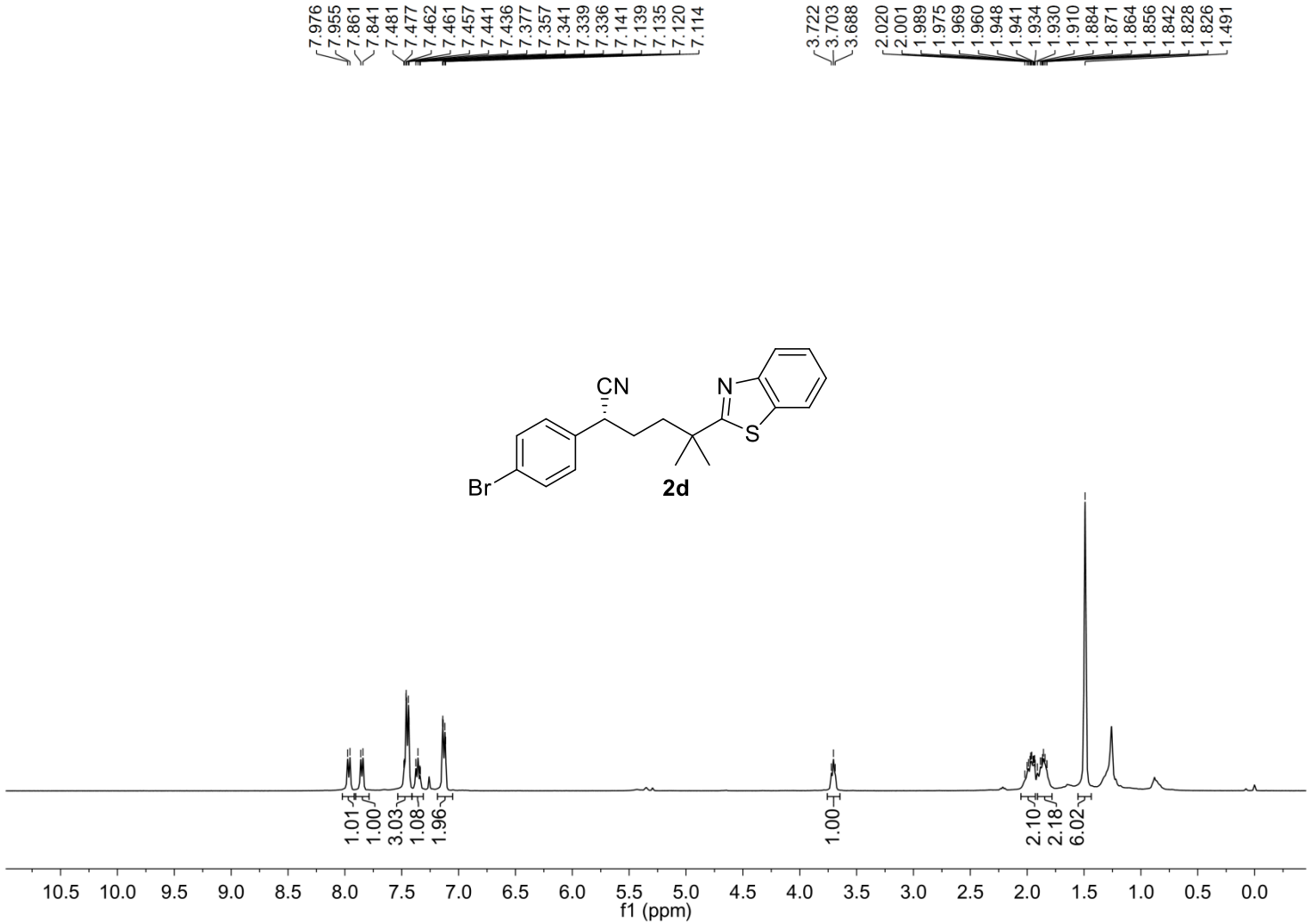
CN
N
S
Cl
2c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.339
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7.139
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1.941
1.934
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1.884
1.871
1.864
1.856
1.842
1.828
1.826
1.491
CN
N
S
Br
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1.00
3.03
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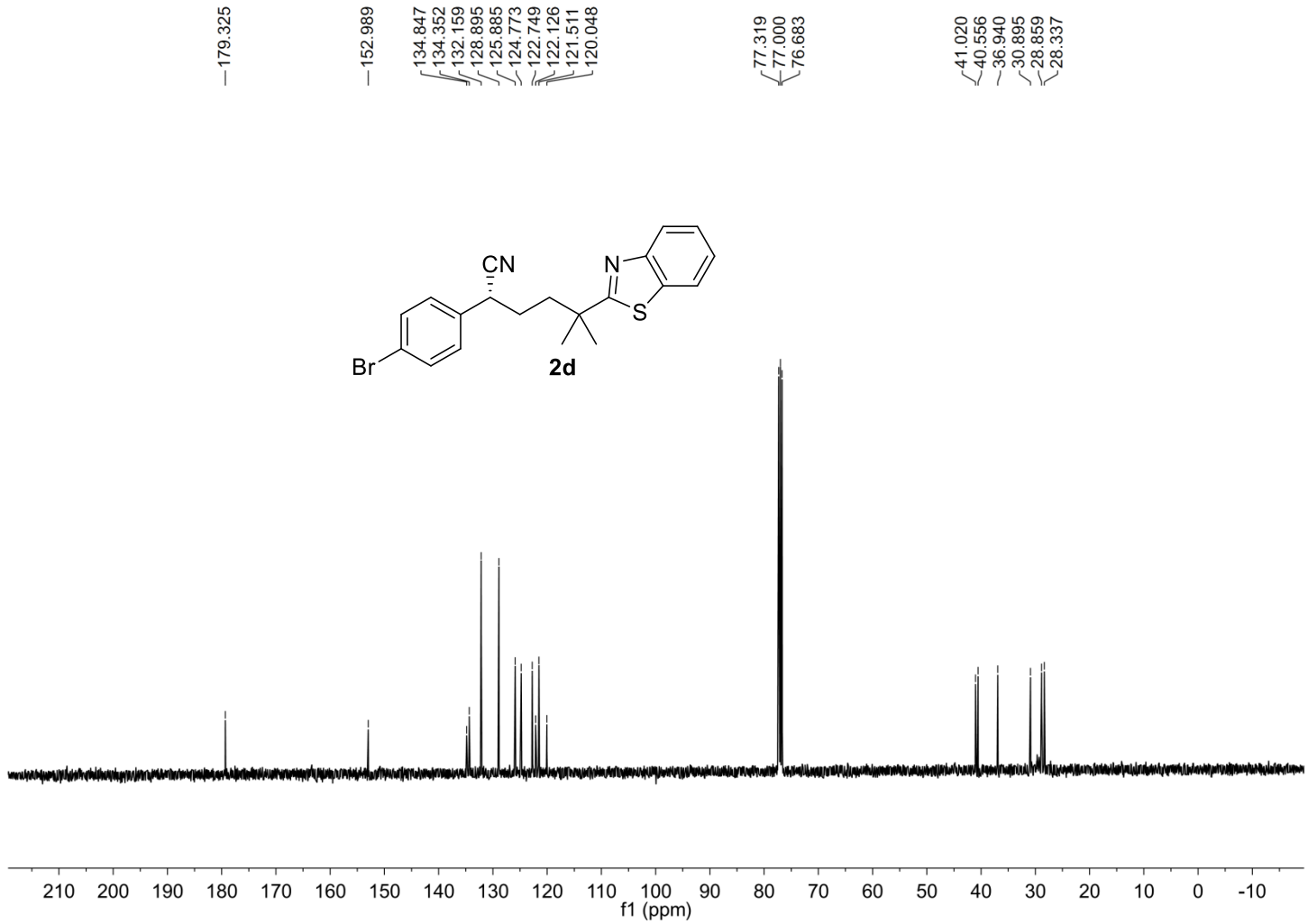
1.96
1.00
2.10
2.18
6.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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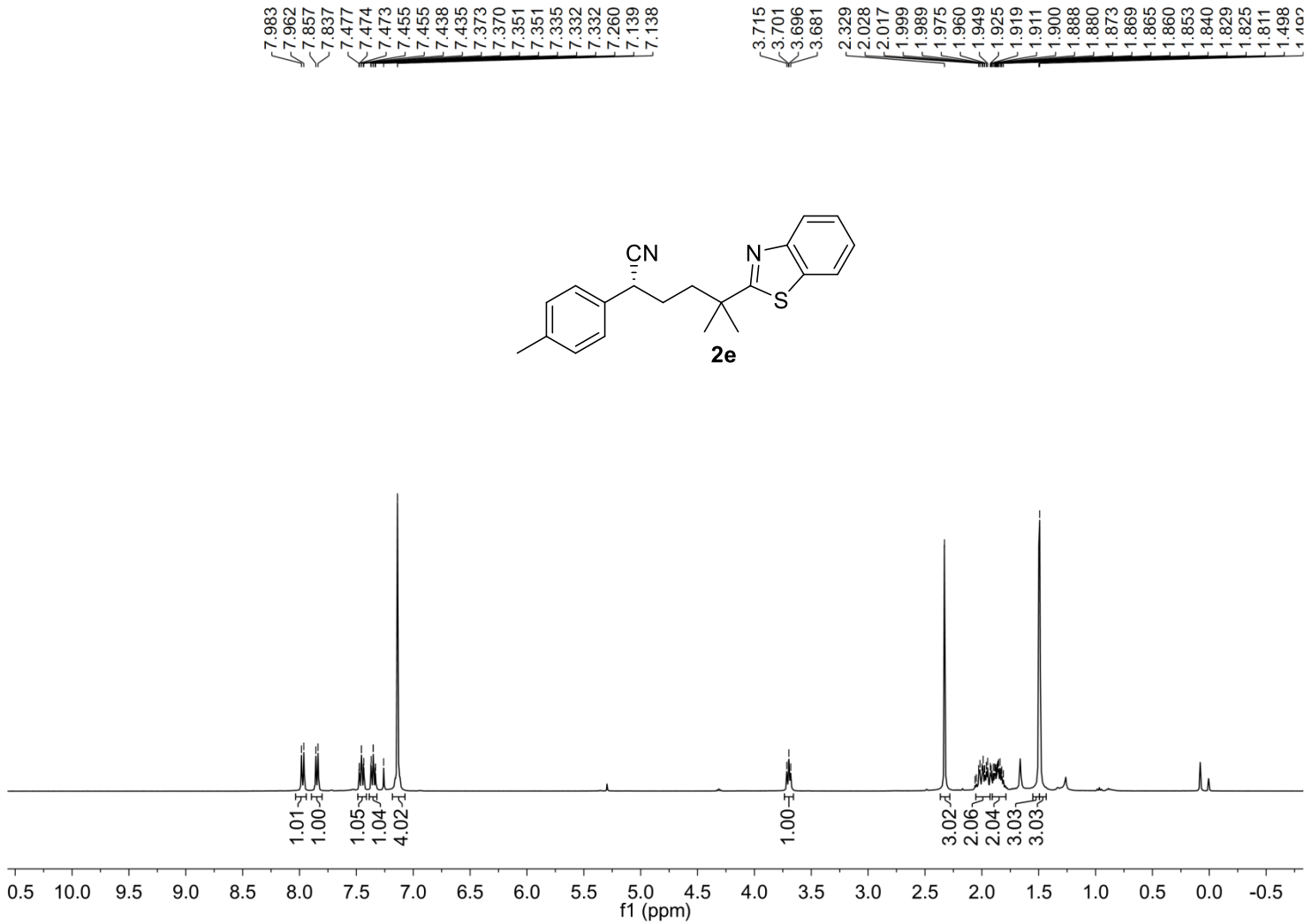
122.126
121.511
120.048
77.319
77.000
76.683
41.020
40.556
36.940
30.895
28.859
28.337
CN
N
S
Br
2d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.370
7.351
7.351
7.335
7.332
7.332
7.260
7.139
7.138
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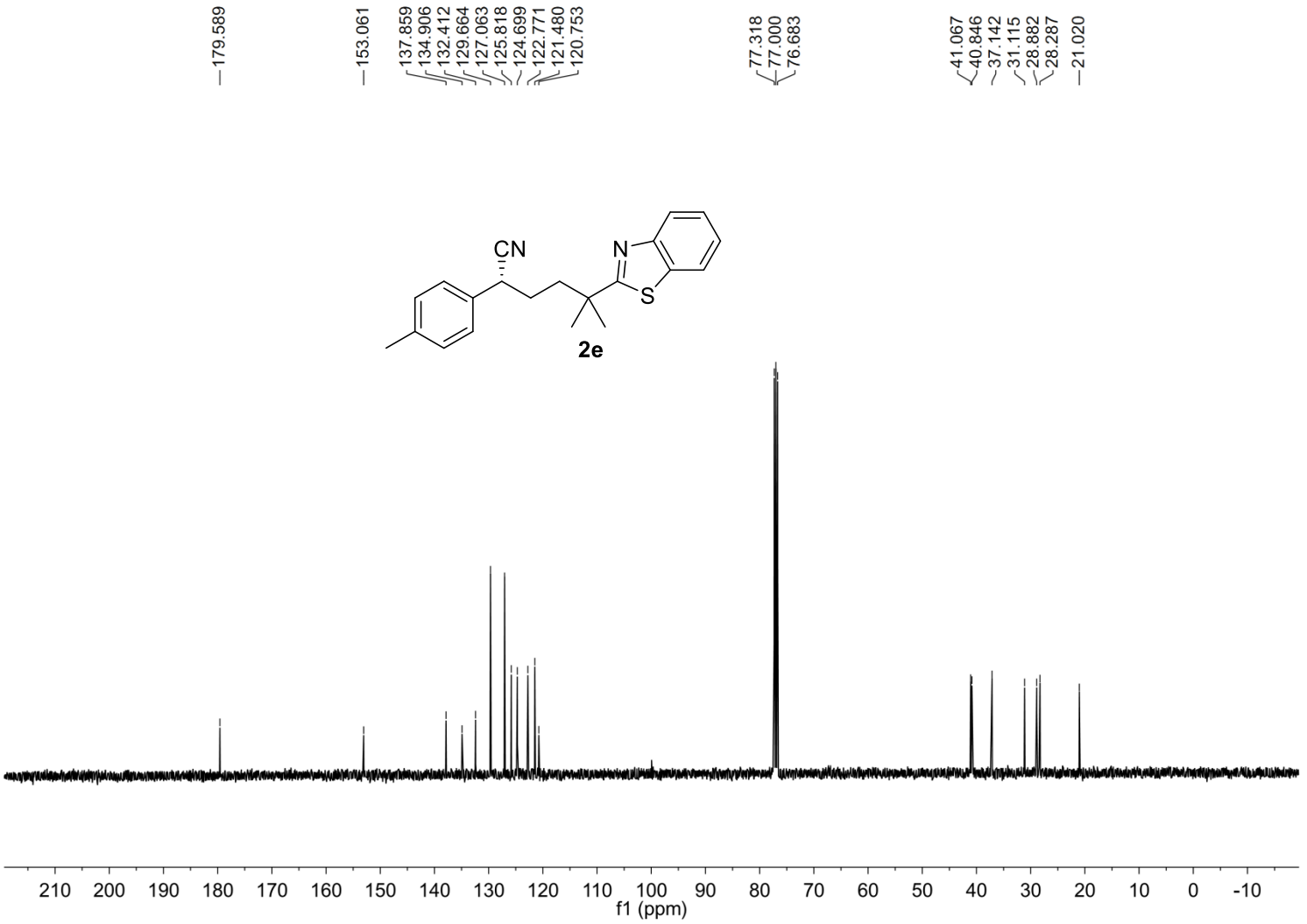
CN
N
S
2e
1.01
1.00
1.05
1.04
4.02
1.00
3.02
2.06
2.04
3.03
3.03
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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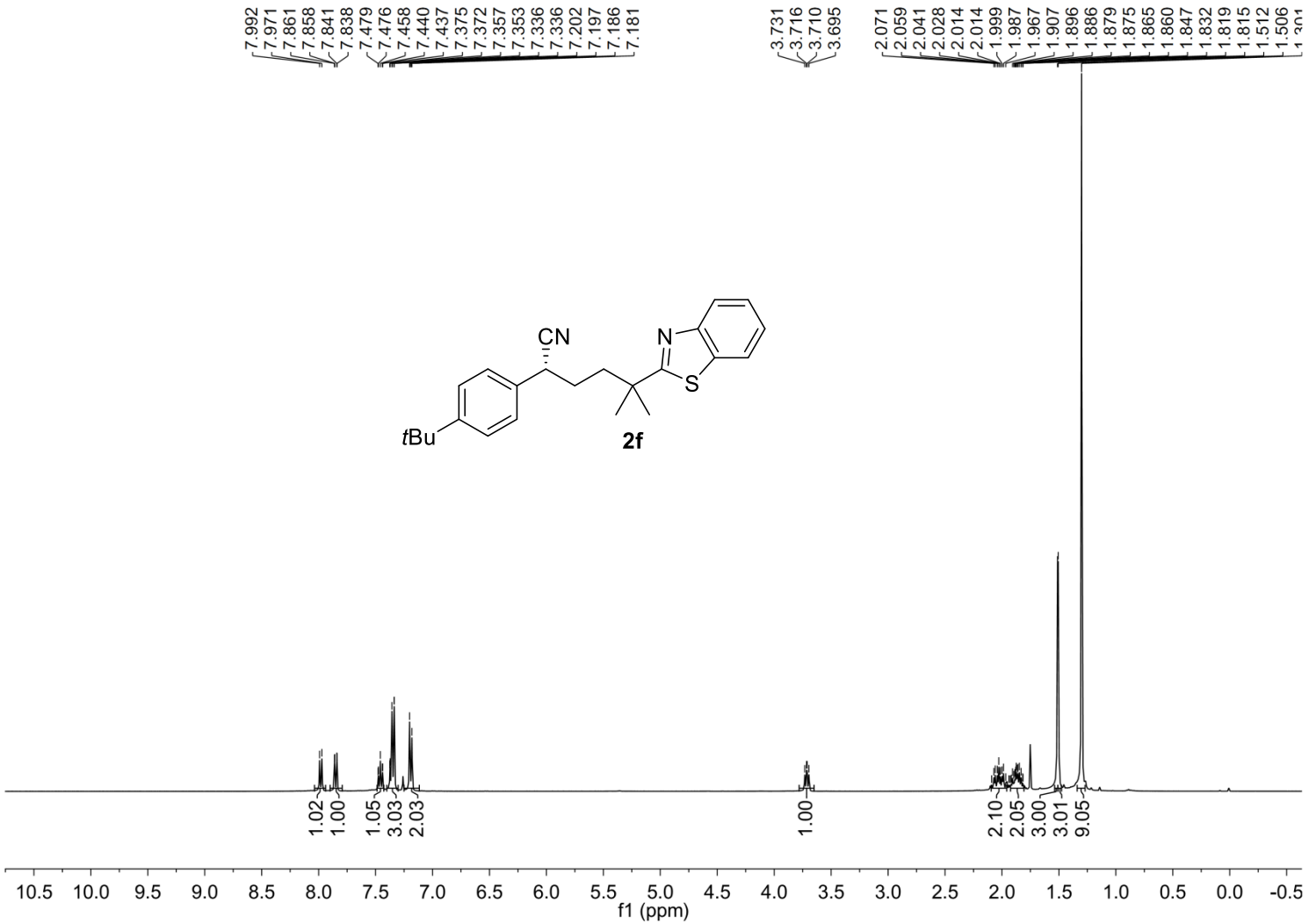
120.753
77.318
77.000
76.683
41.067
40.846
37.142
31.115
28.882
28.287
21.020
CN
N
S
2e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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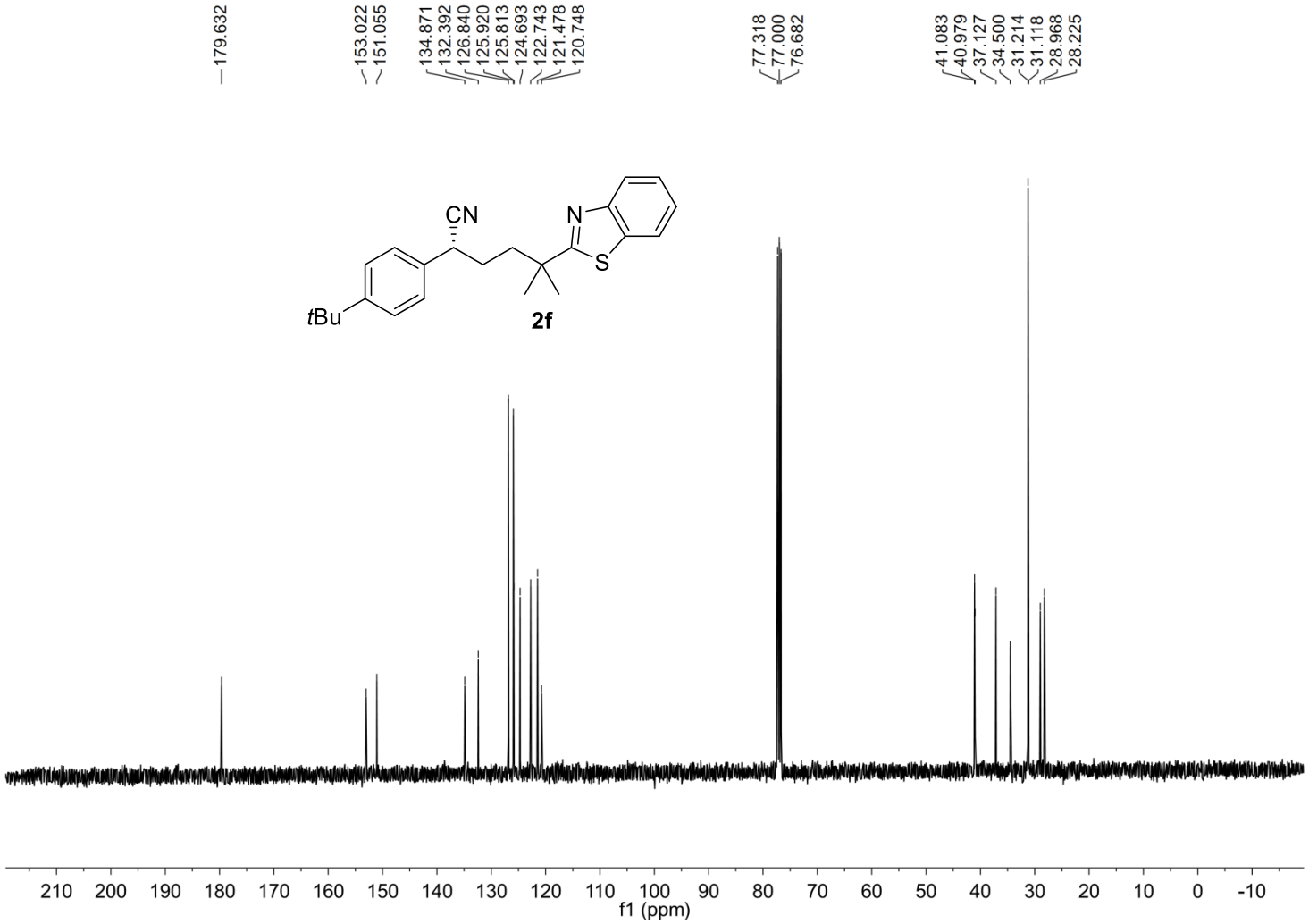
7.375
7.372
7.357
7.353
7.336
7.336
7.202
7.197
7.186
7.181
3.731
3.716
3.710
3.695
2.071
2.059
2.041
2.028
2.014
2.014
1.999
1.987
1.967
1.907
1.896
1.886
1.879
1.875
1.865
1.860
1.847
1.832
1.819
1.815
1.512
1.506
CN
N
S
tBu
2f
1.02
1.00
1.05
3.03
2.03
1.00
2.10
2.05
3.00
3.01
9.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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77.000
76.682
41.083
40.979
37.127
34.500
31.214
31.118
28.968
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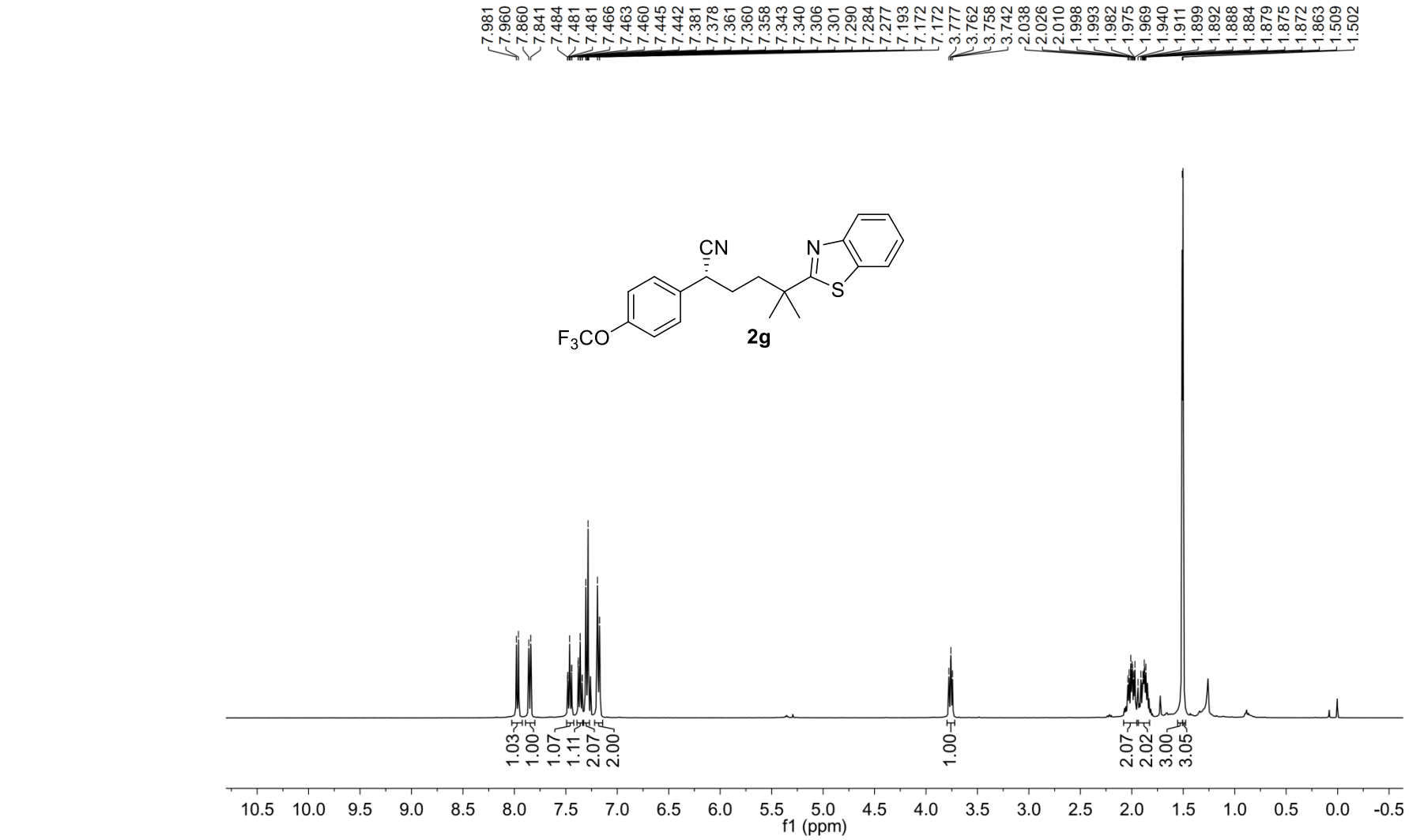
CN
N
S
tBu
2f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.442
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7.378
7.361
7.360
7.358
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7.284
7.277
7.193
7.172
7.172
3.777
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3.758
3.742
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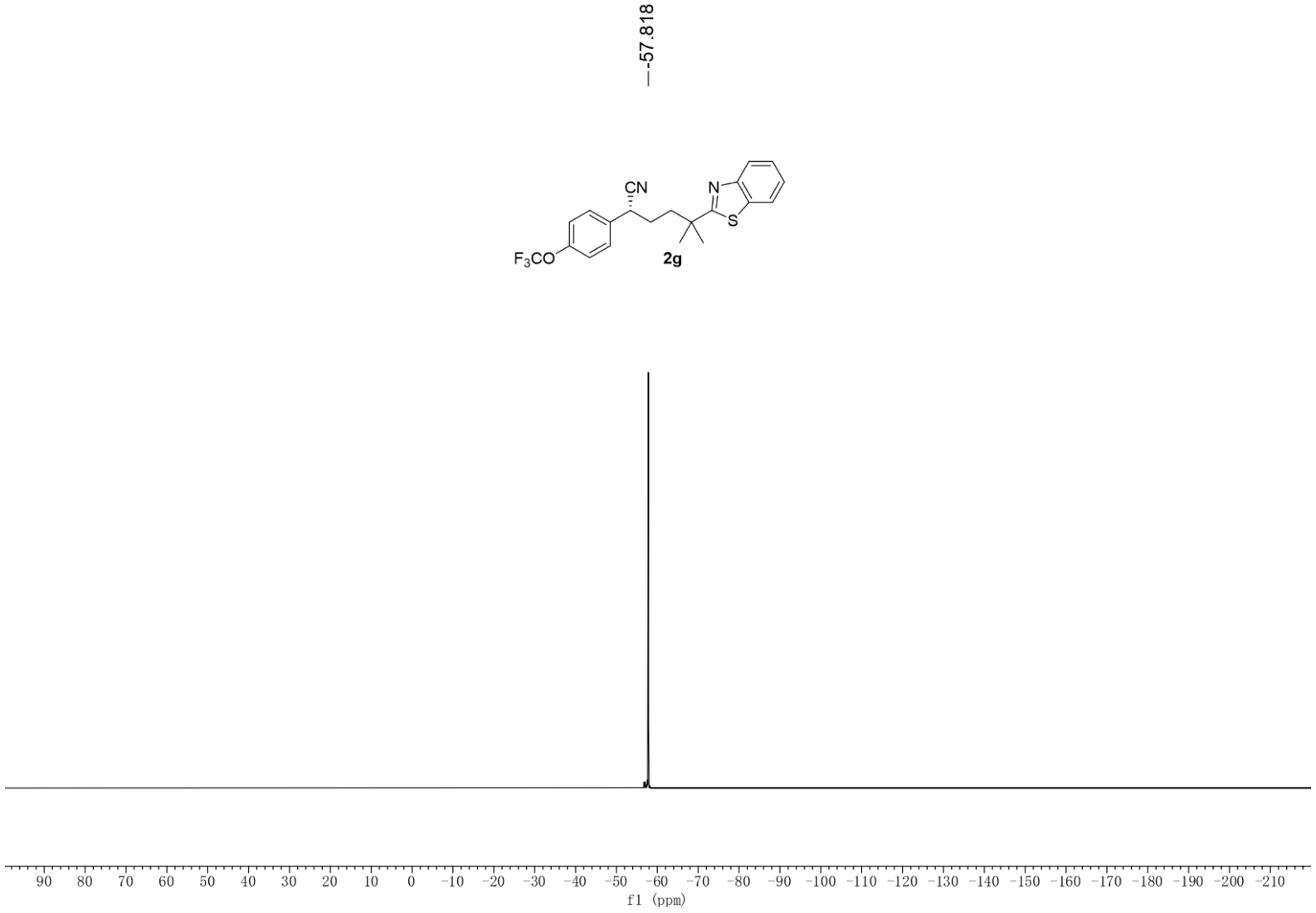
2.026
2.010
1.998
1.993
1.982
1.975
1.969
1.940
1.911
1.899
1.892
1.888
1.884
1.879
1.875
1.872
1.863
1.509
1.502
CN
N
S
F3CO
2g
1.03
1.00
1.07
1.11
2.07
2.00
1.00
2.07
2.02
3.00
3.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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N
S
F3CO
2g
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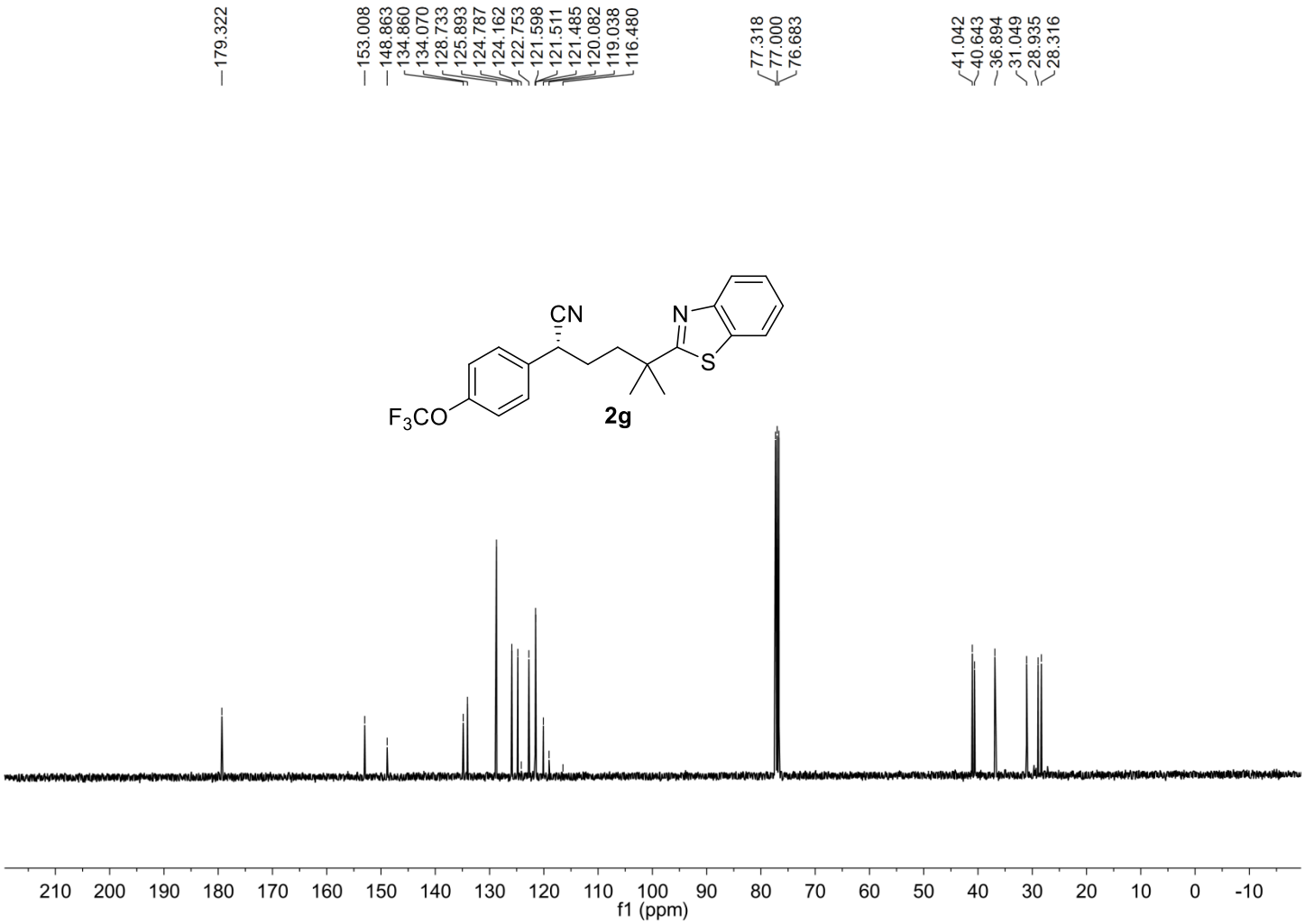
f1 (ppm)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121.485
120.082
119.038
116.480
77.318
77.000
76.683
41.042
40.643
36.894
31.049
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N
S
F3CO
2g
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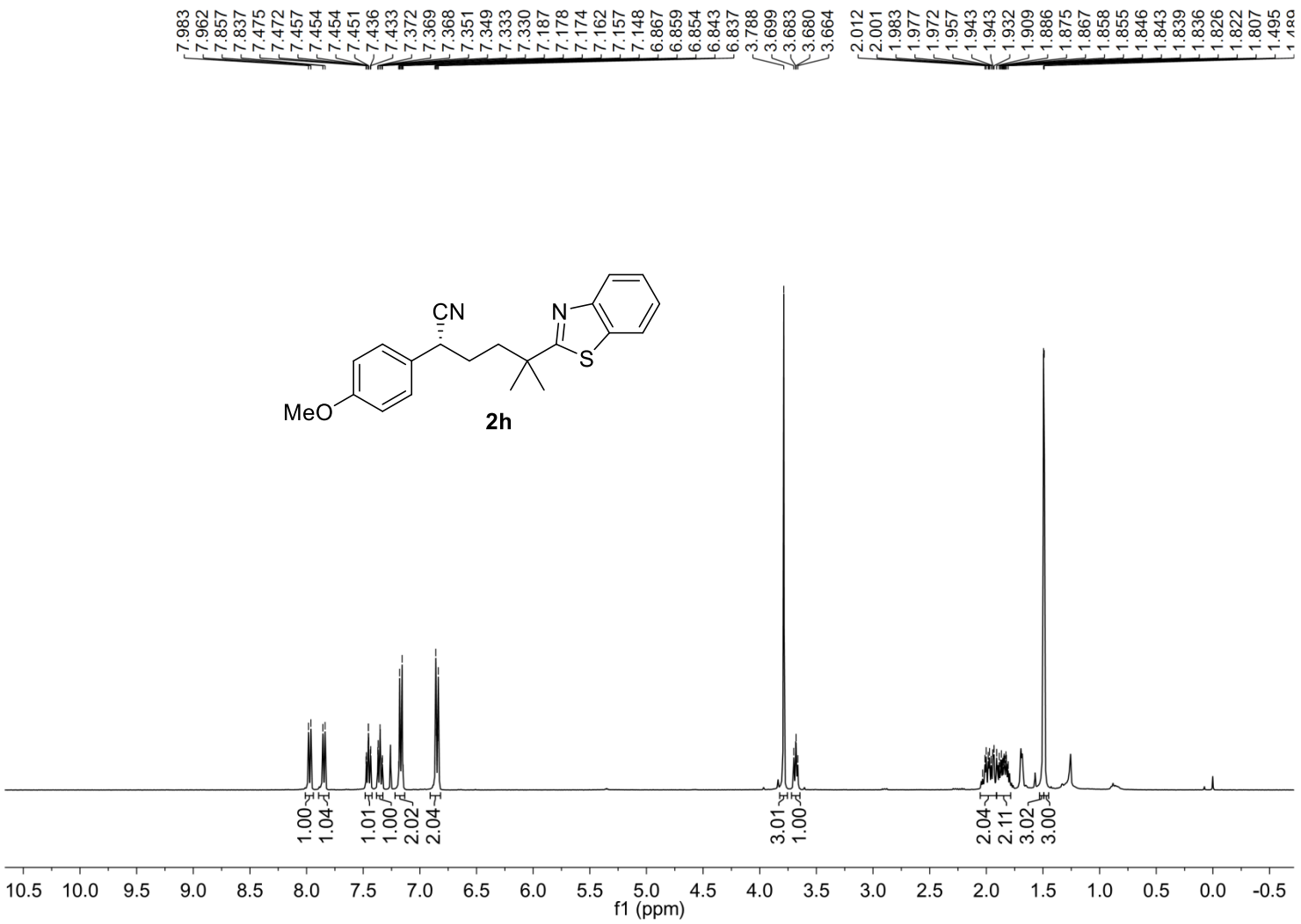
f1 (ppm)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7.454
7.454
7.451
7.436
7.433
7.372
7.369
7.368
7.351
7.349
7.333
7.330
7.187
7.178
7.174
7.162
7.157
7.148
6.867
6.859
6.854
6.843
6.837
3.788
3.699
3.683
3.680
3.664
2.012
2.001
1.983
1.977
1.972
1.957
1.943
1.943
1.932
1.909
1.886
1.875
1.867
1.858
1.855
1.846
1.843
1.839
1.836
1.826
1.822
1.807
1.495
CN
N
S
MeO
2h
1.00
1.04
1.01
1.00
2.02
2.04
3.01
1.00
2.04
2.11
3.02
3.00
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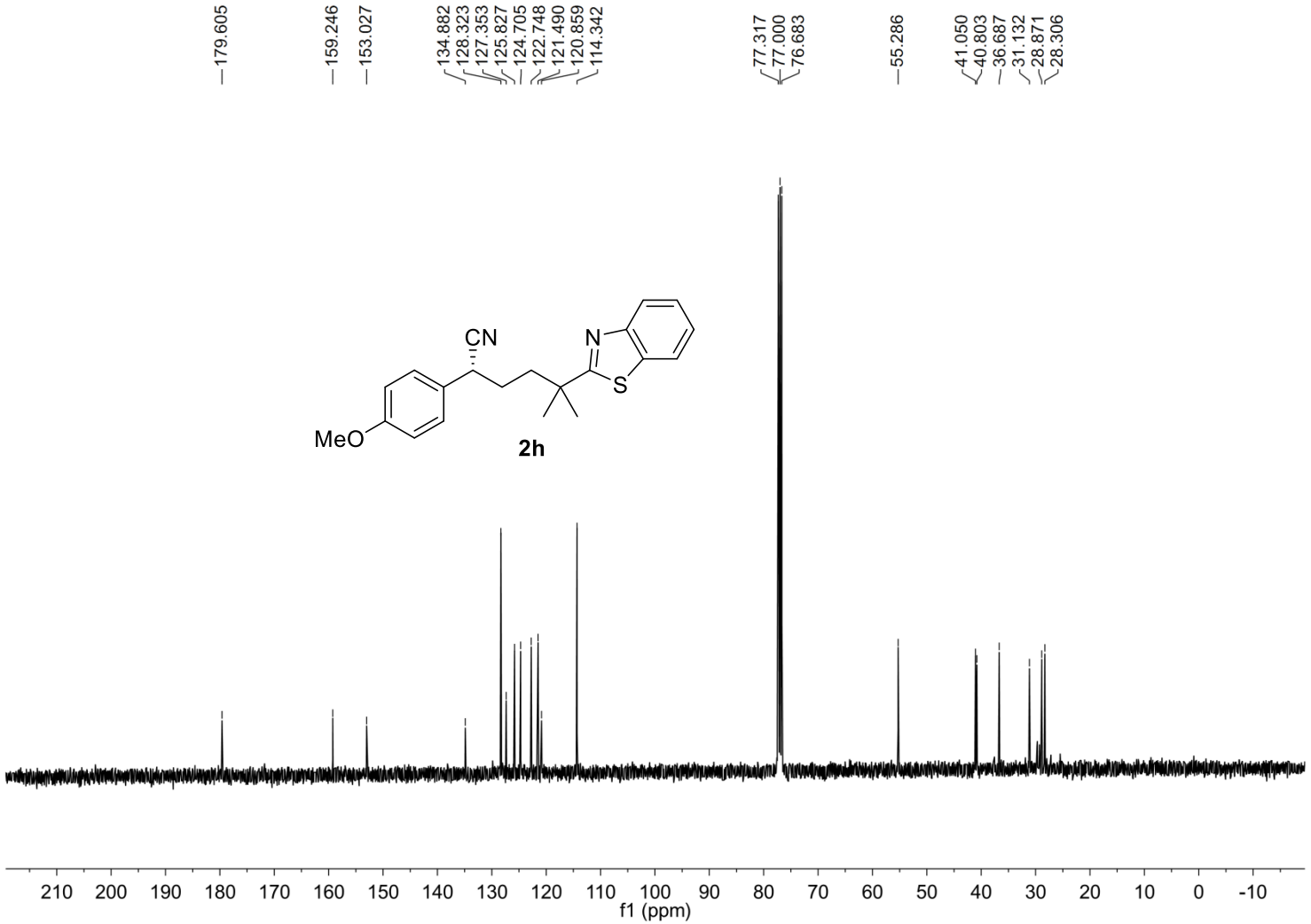
f1 (ppm)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127.353
125.827
124.705
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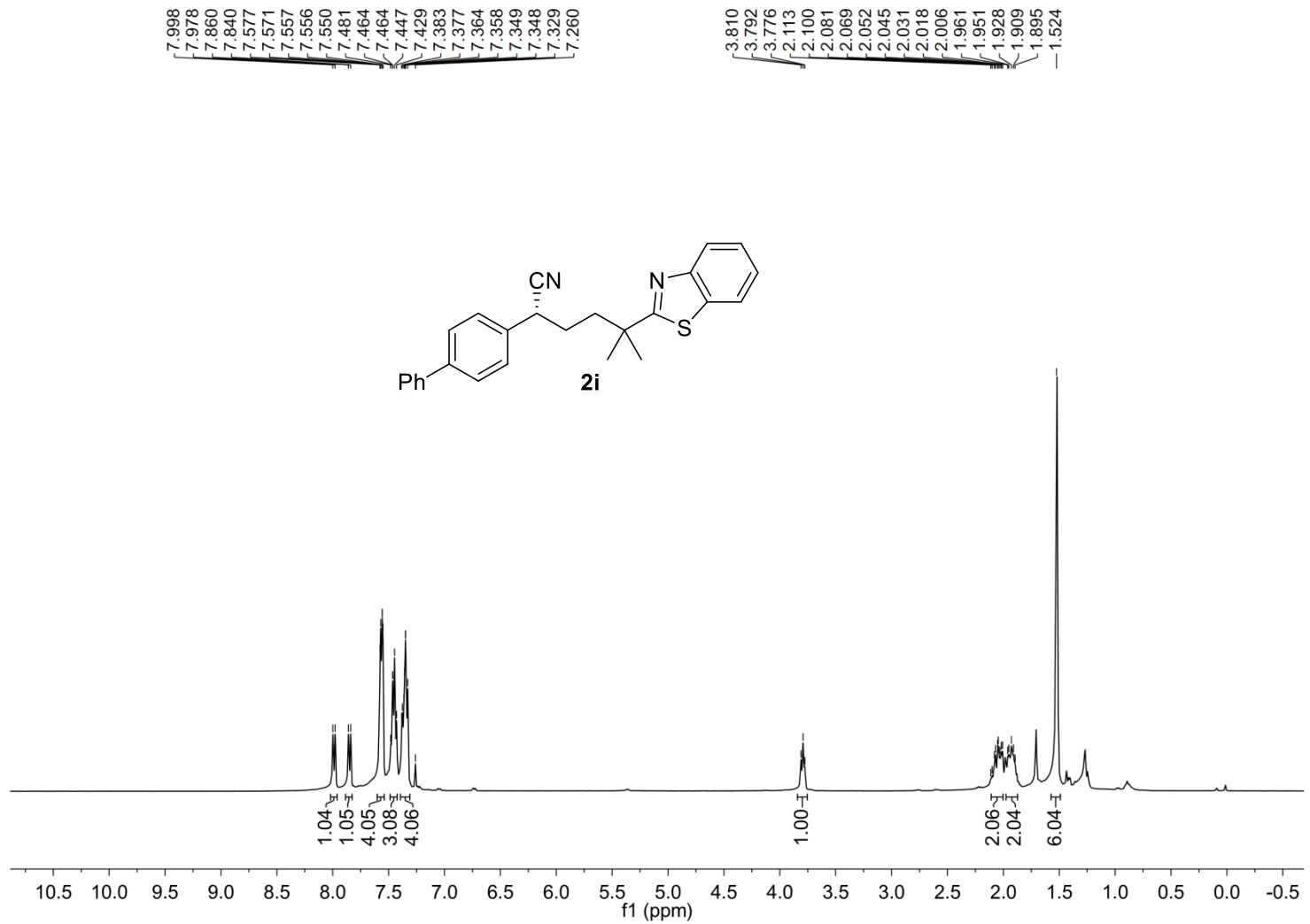
120.859
114.342
77.317
77.000
76.683
55.286
41.050
40.803
36.687
31.132
28.871
28.306
CN
N
S
MeO
2h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.556
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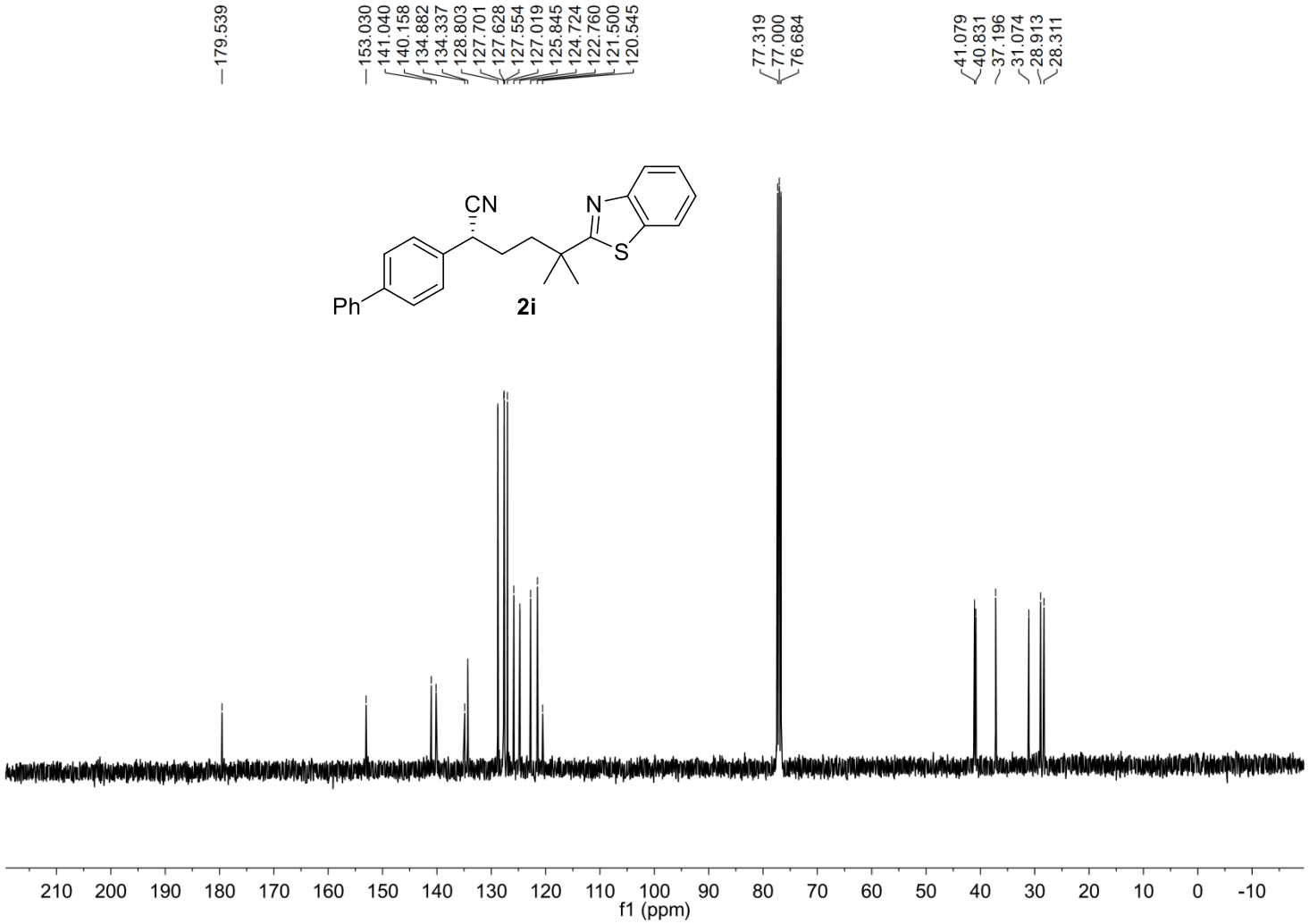
7.464
7.447
7.429
7.383
7.377
7.364
7.358
7.349
7.348
7.329
7.260
3.810
3.792
3.776
2.113
2.100
2.081
2.069
2.052
2.045
2.031
2.018
2.006
1.961
1.951
1.928
1.909
1.895
1.524
CN
N
S
Ph
2i
1.04
1.05
4.05
3.08
4.06
1.00
2.06
2.04
6.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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127.701
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127.554
127.019
125.845
124.724
122.760
121.500
120.545
77.319
77.000
76.684
41.079
40.831
37.196
31.074
28.913
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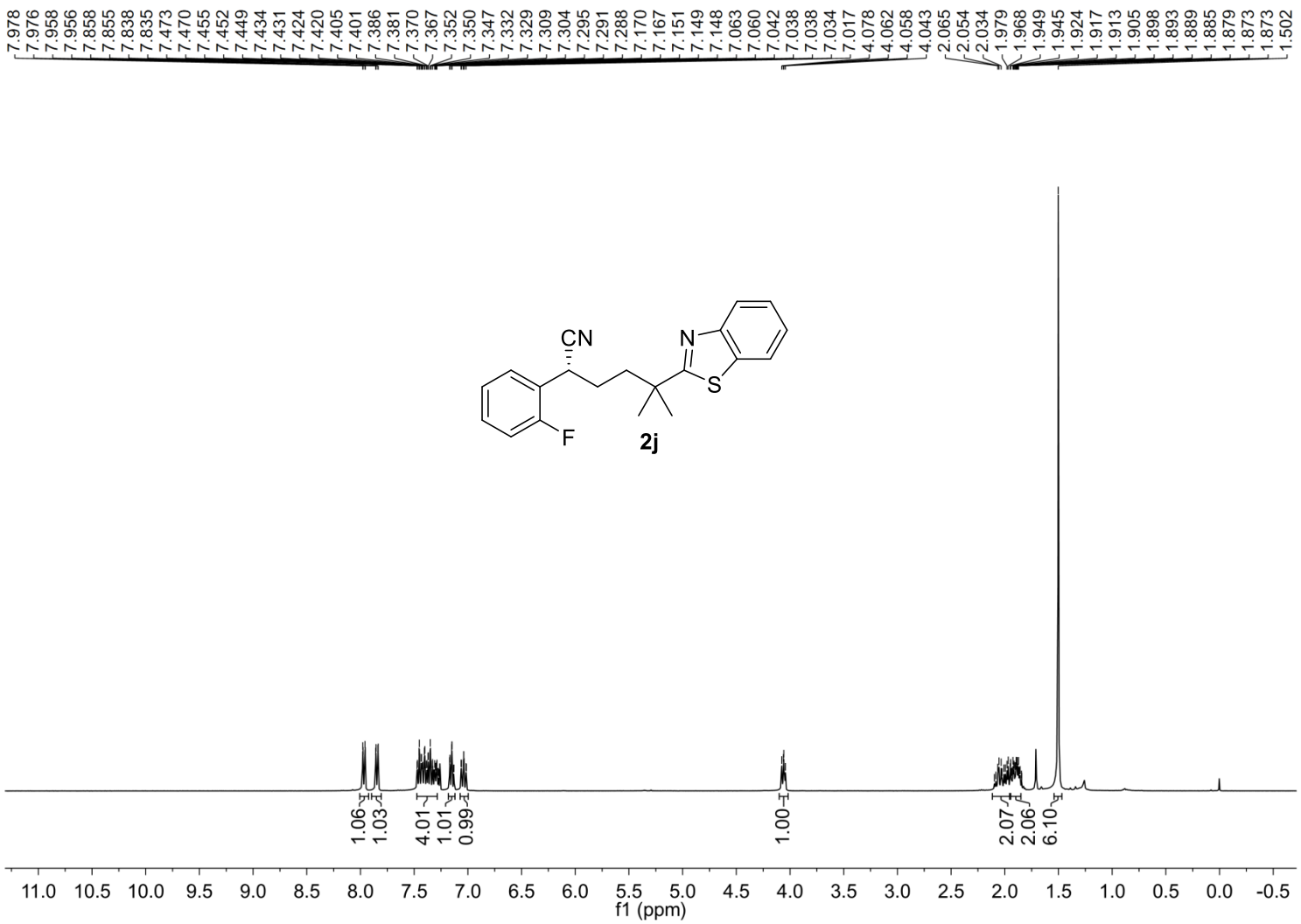
CN
N
S
Ph
2i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.449
7.434
7.431
7.424
7.420
7.405
7.401
7.386
7.381
7.370
7.367
7.352
7.350
7.347
7.332
7.329
7.309
7.304
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7.288
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7.167
7.151
7.149
7.148
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7.060
7.042
7.038
7.038
7.034
7.017
4.078
4.062
4.058
4.043
2.065
2.054
2.034
1.979
1.968
1.949
1.945
1.924
1.917
1.913
1.905
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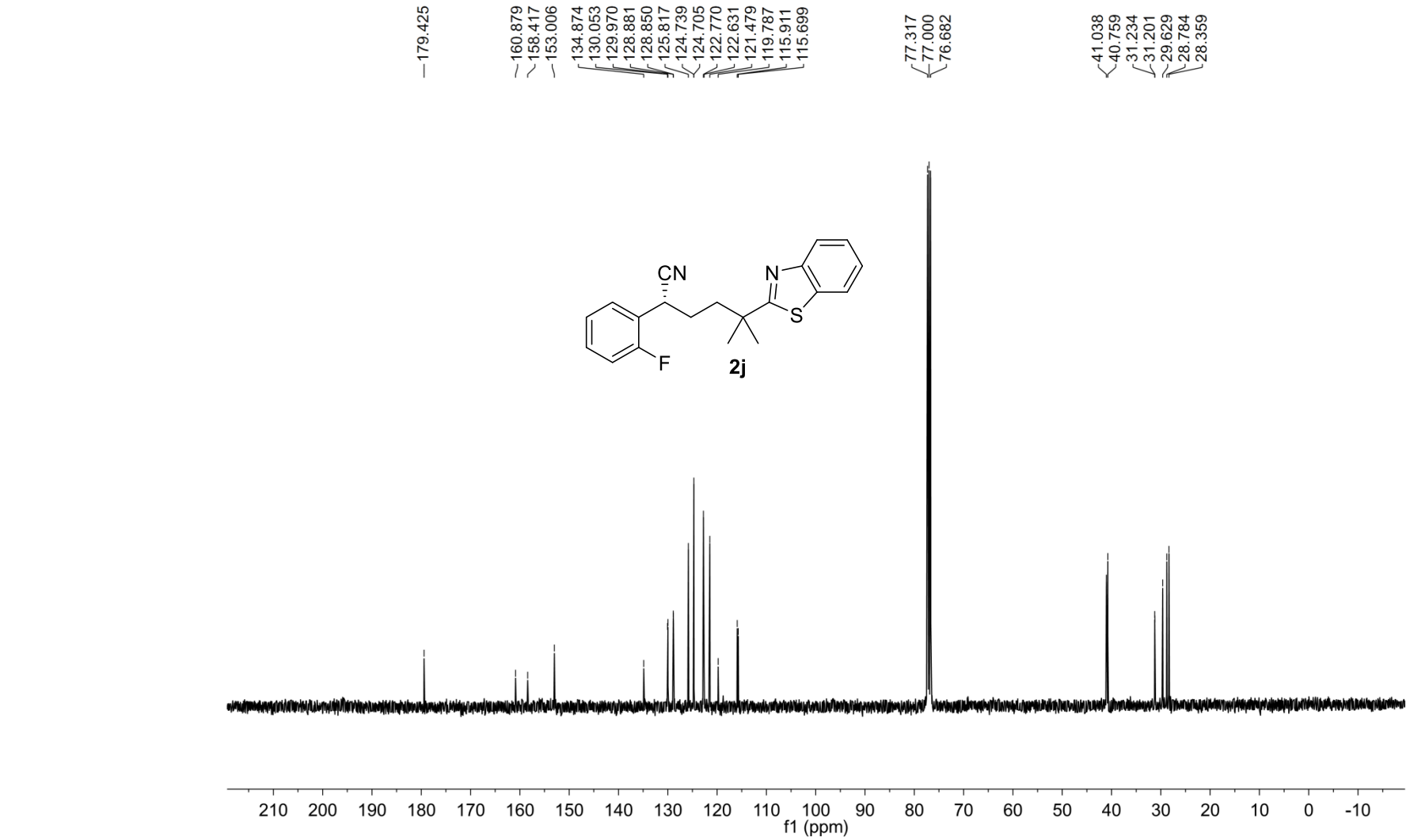
1.885
1.879
1.873
1.873
1.502
CN
N
S
F
2j
1.06
1.03
4.01
1.01
0.99
1.00
2.07
2.06
6.10
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


-118.170
CN
N
S
F
2j
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
-260
-280
-300
f1 (ppm)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121.479
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115.911
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77.317
77.000
76.682
41.038
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31.201
29.629
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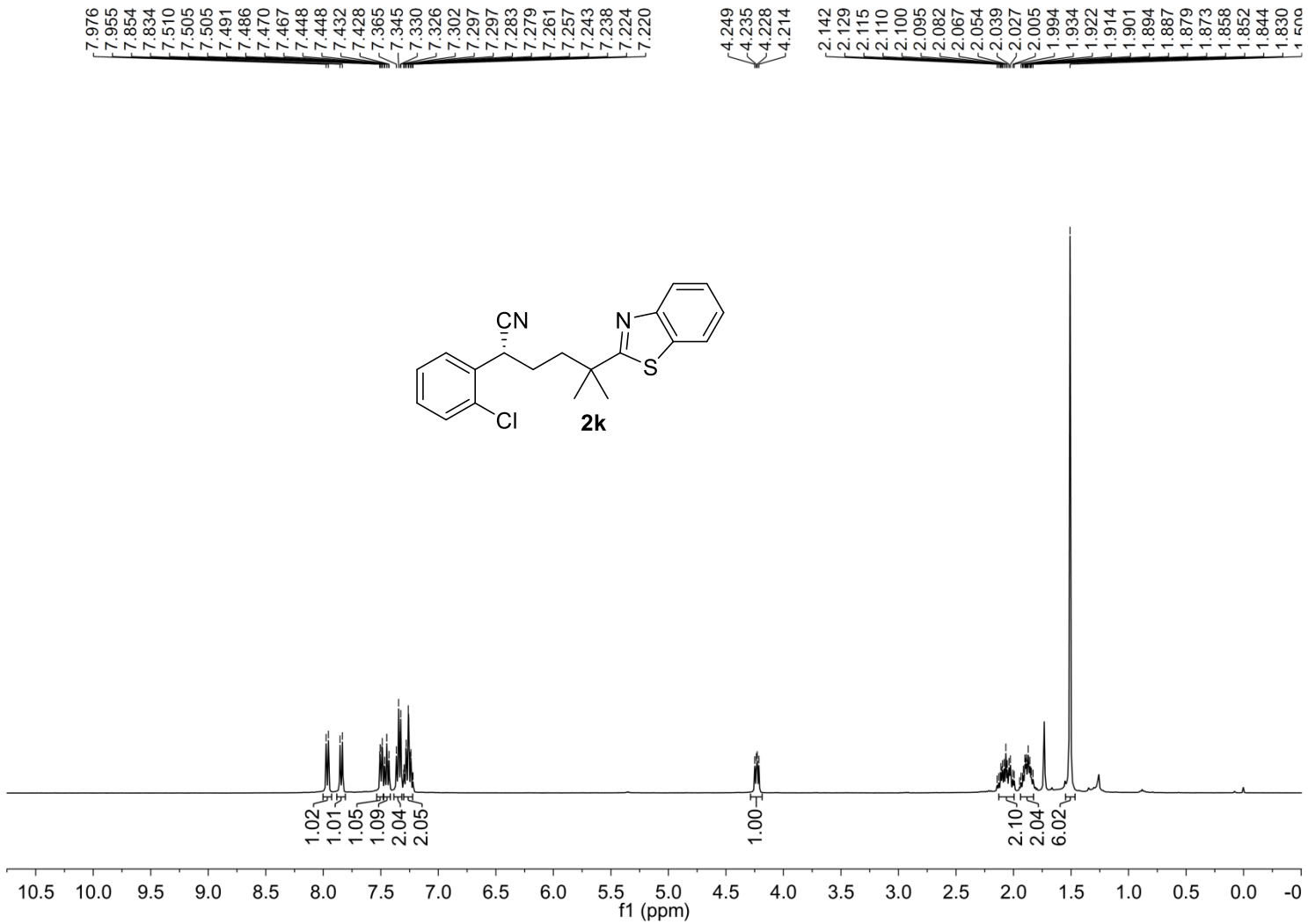
CN
N
S
F
2j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.467
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7.448
7.432
7.428
7.365
7.345
7.330
7.326
7.302
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7.297
7.283
7.279
7.261
7.257
7.243
7.238
7.224
7.220
4.249
4.235
4.228
4.214
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2.115
2.110
2.100
2.095
2.082
2.067
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1.914
1.901
1.894
1.887
1.879
1.873
1.858
1.852
1.844
1.830
CN
N
S
Cl
2k
1.02
1.01
1.05
1.09
2.04
2.05
1.00
2.10
2.04
6.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
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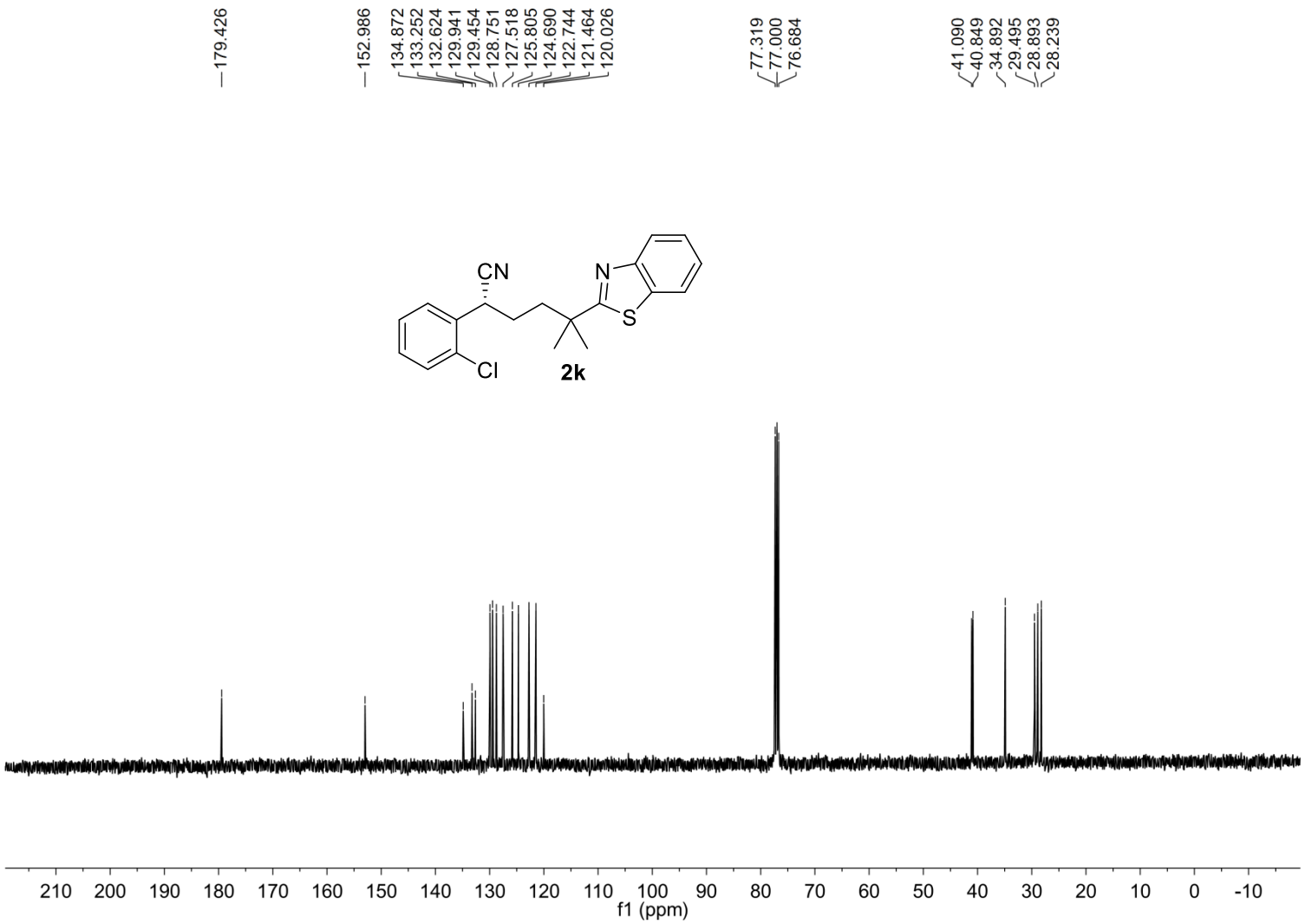
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120.026
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77.000
76.684
41.090
40.849
34.892
29.495
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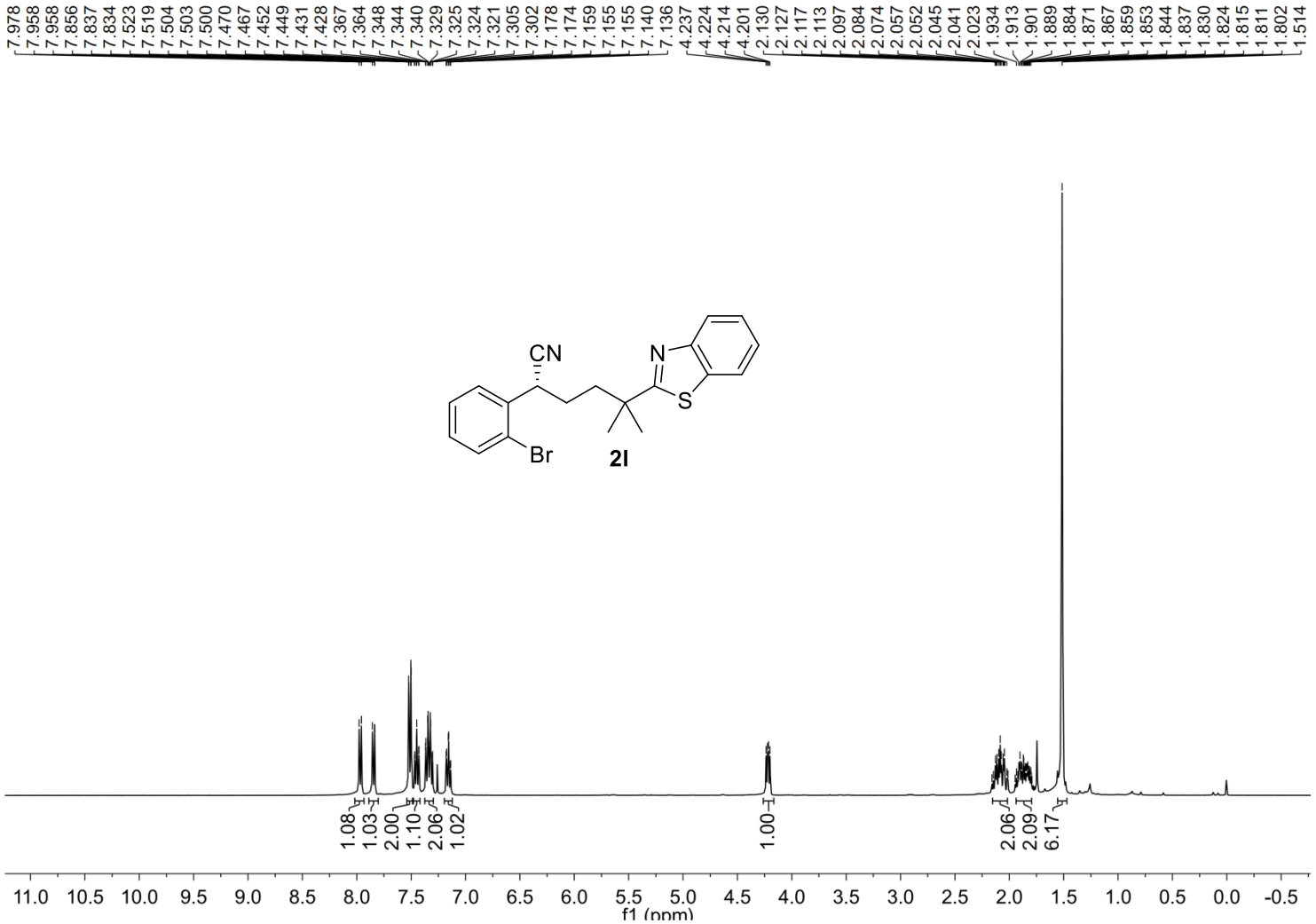
CN
N
S
Cl
2k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.519
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7.503
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7.470
7.467
7.452
7.449
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7.428
7.367
7.364
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7.344
7.340
7.329
7.325
7.324
7.321
7.305
7.302
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7.174
7.159
7.155
7.155
7.140
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4.214
4.201
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2.127
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2.113
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2.084
2.074
2.057
2.052
2.045
2.041
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1.853
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1.837
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1.824
1.815
1.811
1.802
1.514
CN
N
S
Br
2l
1.08
1.03
2.00
1.10
2.06
1.02
1.00
2.06
2.09
6.17
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.0
2.5
2.0
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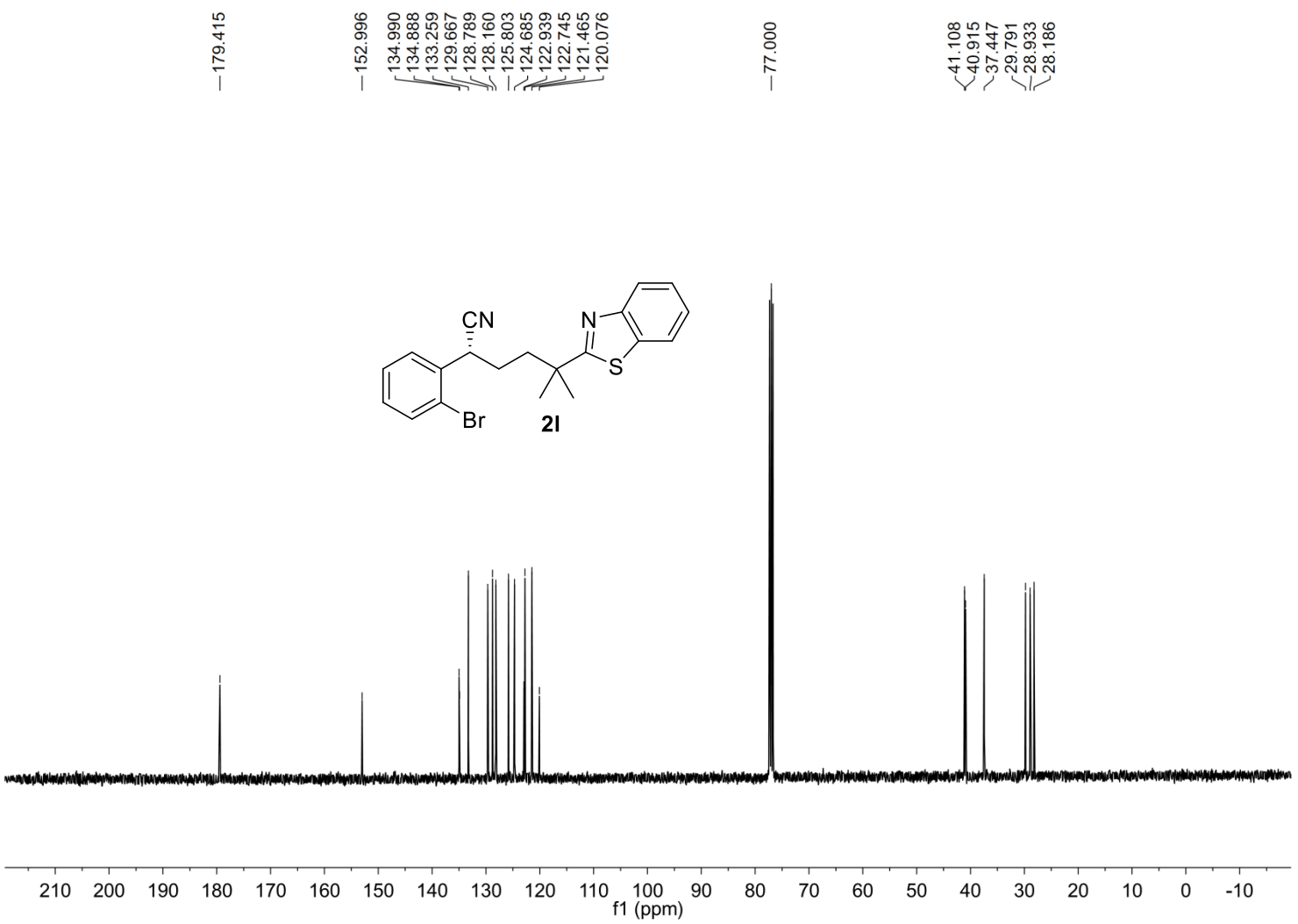
0.0
-0.5
f1 (ppm)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120.076
77.000
41.108
40.915
37.447
29.791
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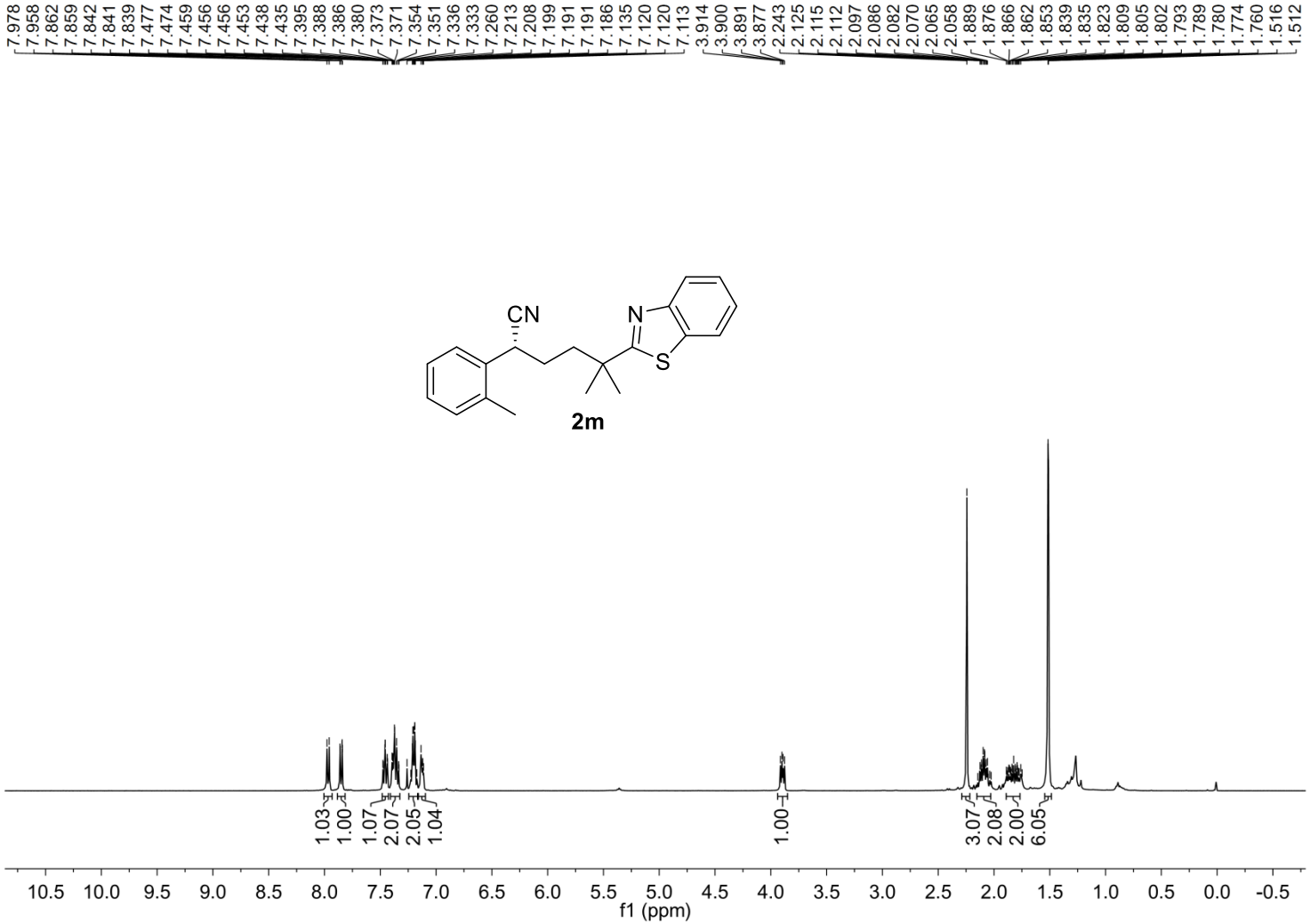
CN
N
S
Br
2l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.351
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7.333
7.260
7.213
7.208
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7.191
7.186
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7.120
7.113
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3.900
3.891
3.877
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2.115
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1.760
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1.512
CN
N
S
2m
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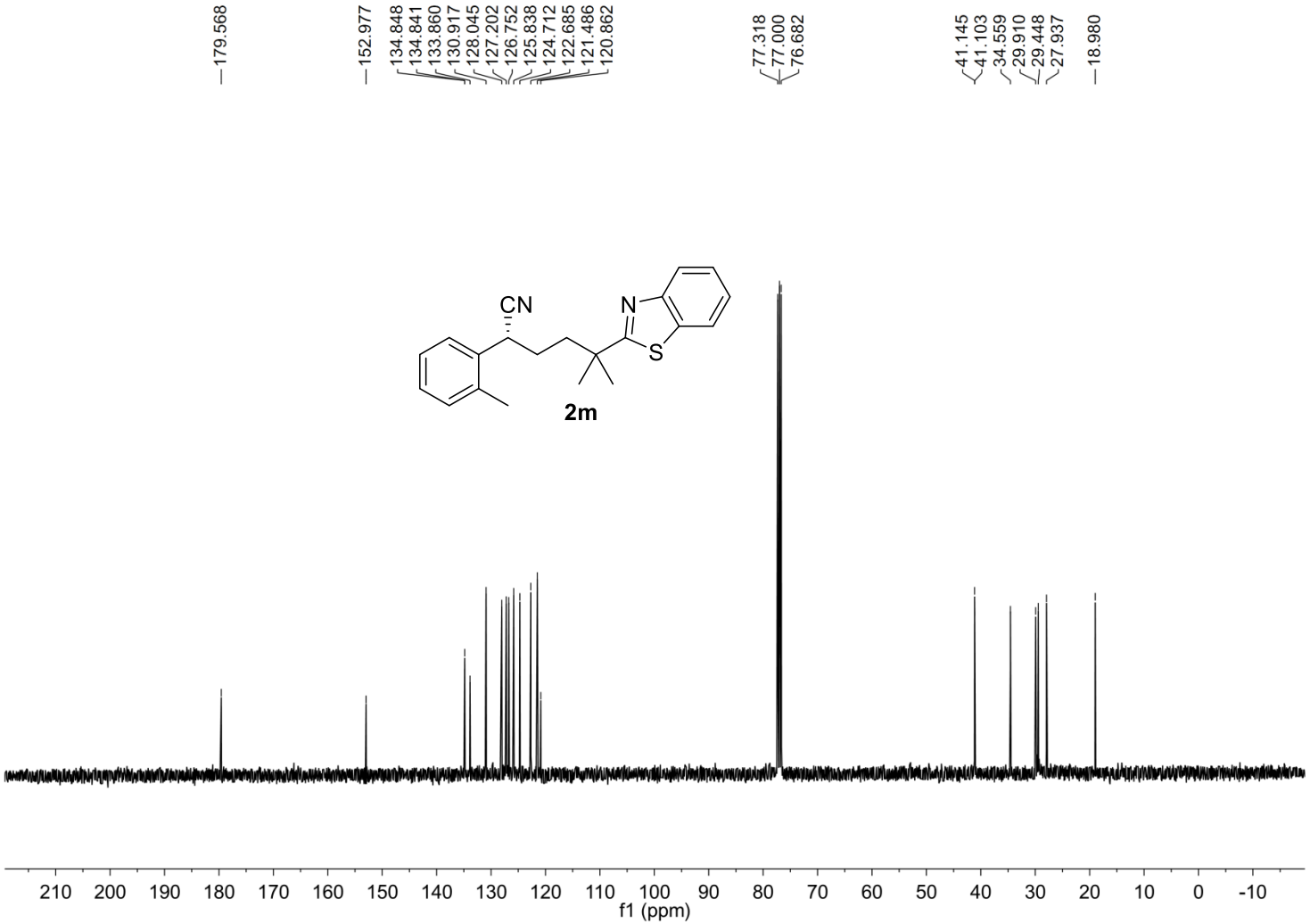
1.00
1.07
2.07
2.05
1.04
1.00
3.07
2.08
2.00
6.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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120.862
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77.000
76.682
41.145
41.103
34.559
29.910
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27.937
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CN
N
S
2m
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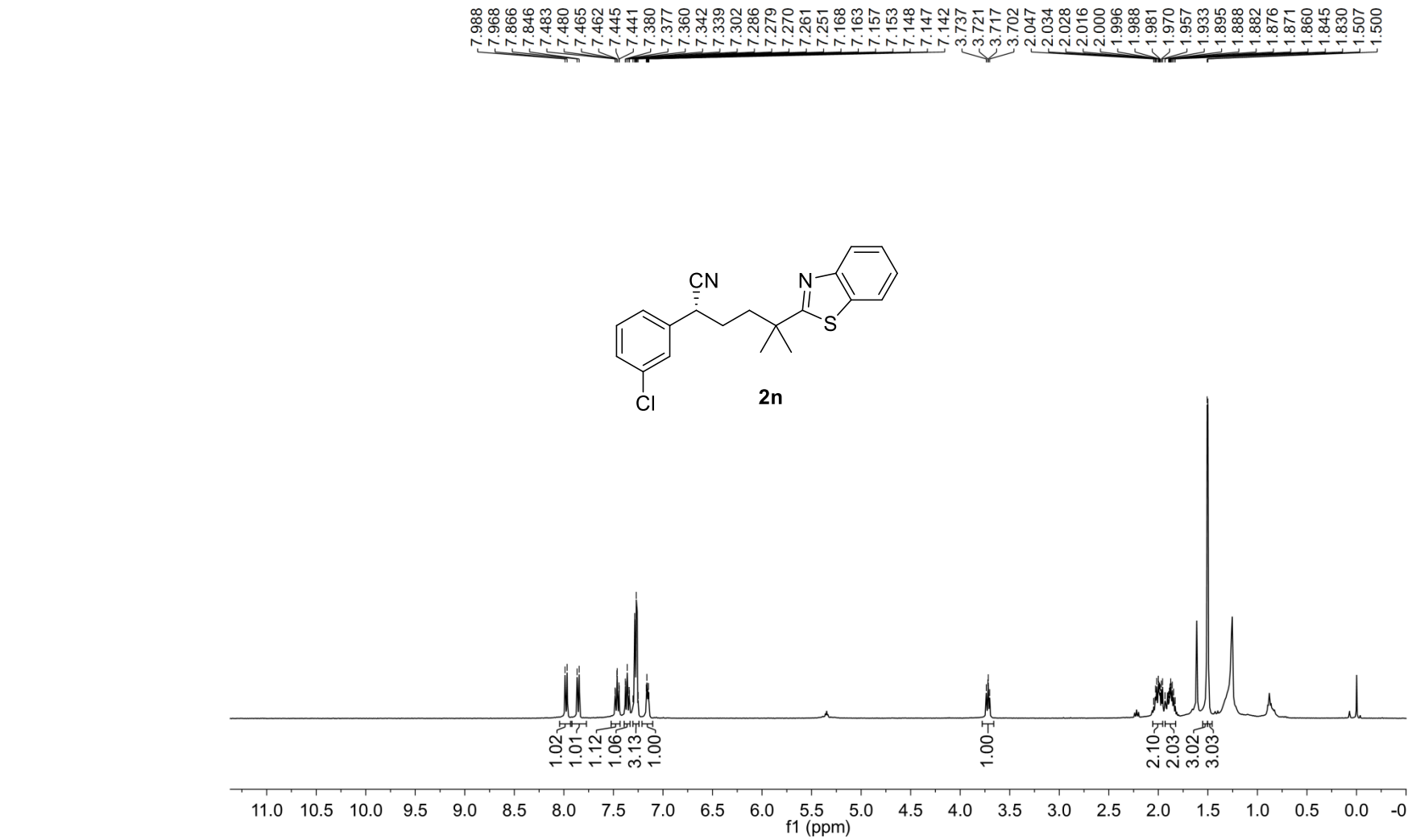
f1 (ppm)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7.339
7.302
7.286
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7.270
7.261
7.251
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7.163
7.157
7.153
7.148
7.147
7.142
3.737
3.721
3.717
3.702
2.047
2.034
2.028
2.016
2.000
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1.876
1.871
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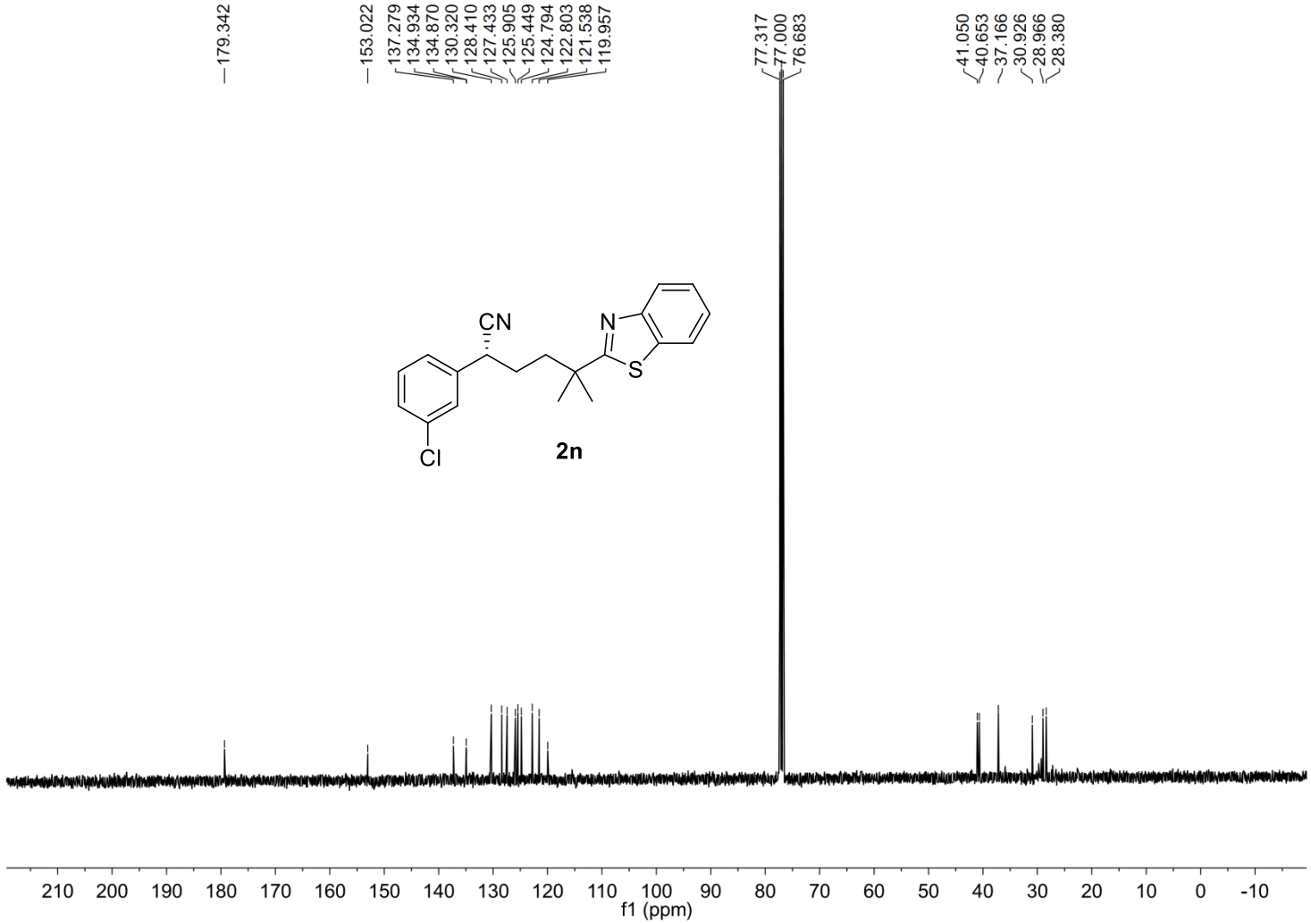
1.830
1.507
1.500
CN
N
S
Cl
2n
1.02
1.01
1.12
1.06
3.13
1.00
1.00
2.10
2.03
3.02
3.03
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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77.317
77.000
76.683
41.050
40.653
37.166
30.926
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CN
N
S
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2n
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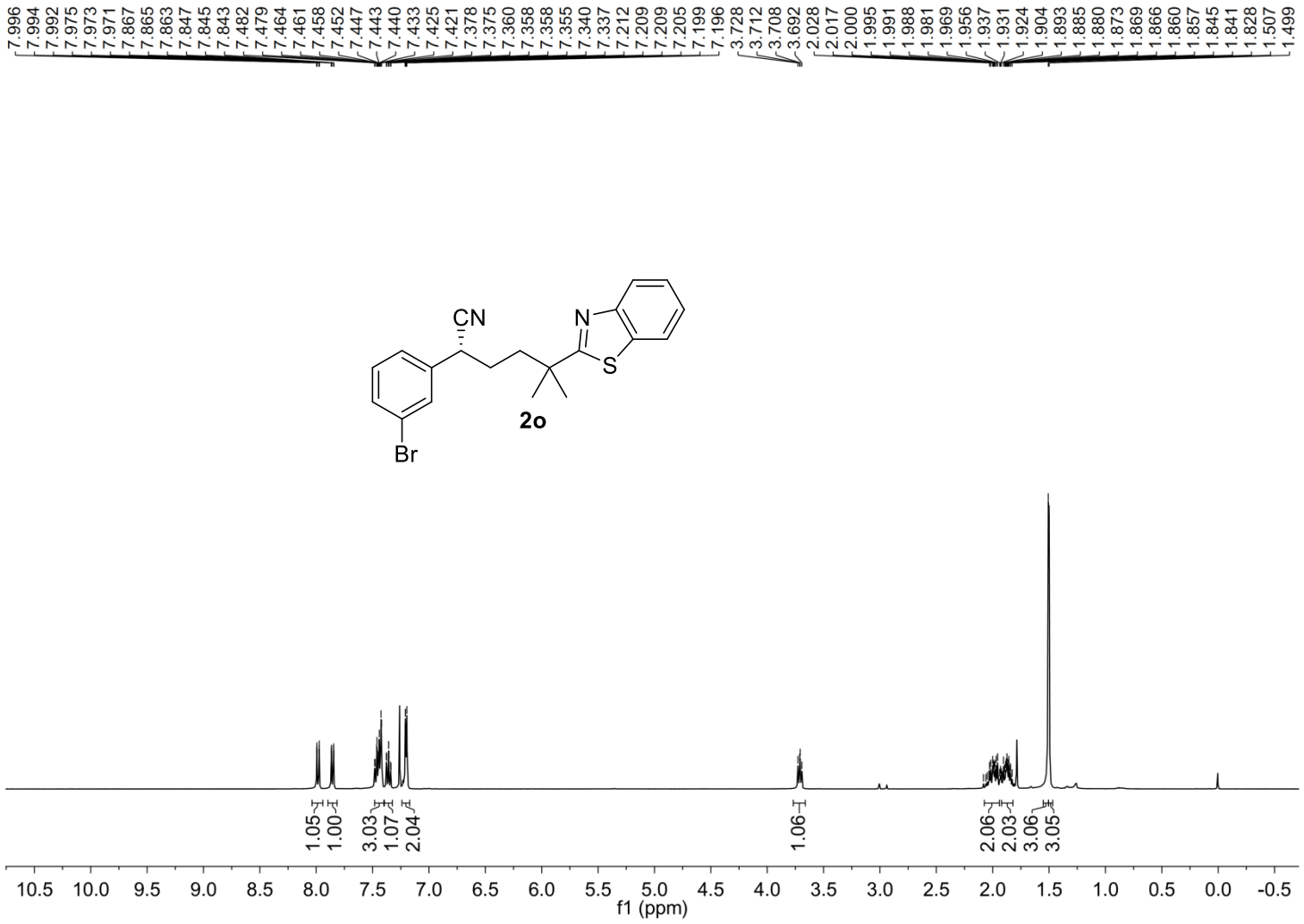
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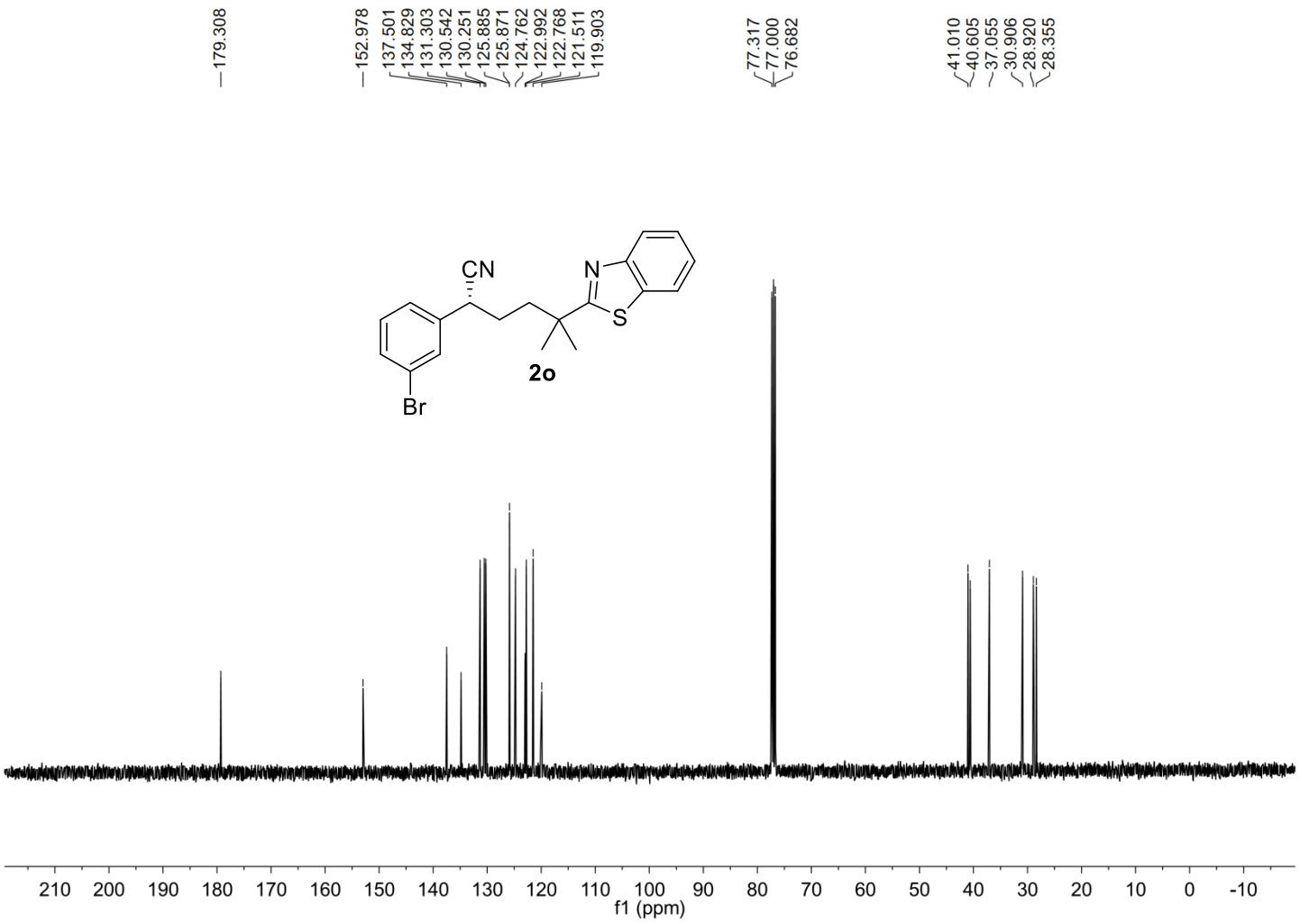
7.479
7.464
7.461
7.458
7.452
7.447
7.443
7.440
7.433
7.425
7.421
7.378
7.375
7.360
7.358
7.358
7.355
7.340
7.337
7.212
7.209
7.209
7.205
7.199
7.196
3.728
3.712
3.708
3.692
2.028
2.017
2.000
1.995
1.991
1.988
1.981
1.969
1.956
1.937
1.931
1.924
1.904
1.893
1.885
1.880
1.873
1.869
1.866
1.860
1.857
1.845
1.841
1.828
1.507
1.499
CN
N
S
Br
2o
1.05
1.00
3.03
1.07
2.04
1.06
2.06
2.03
3.06
3.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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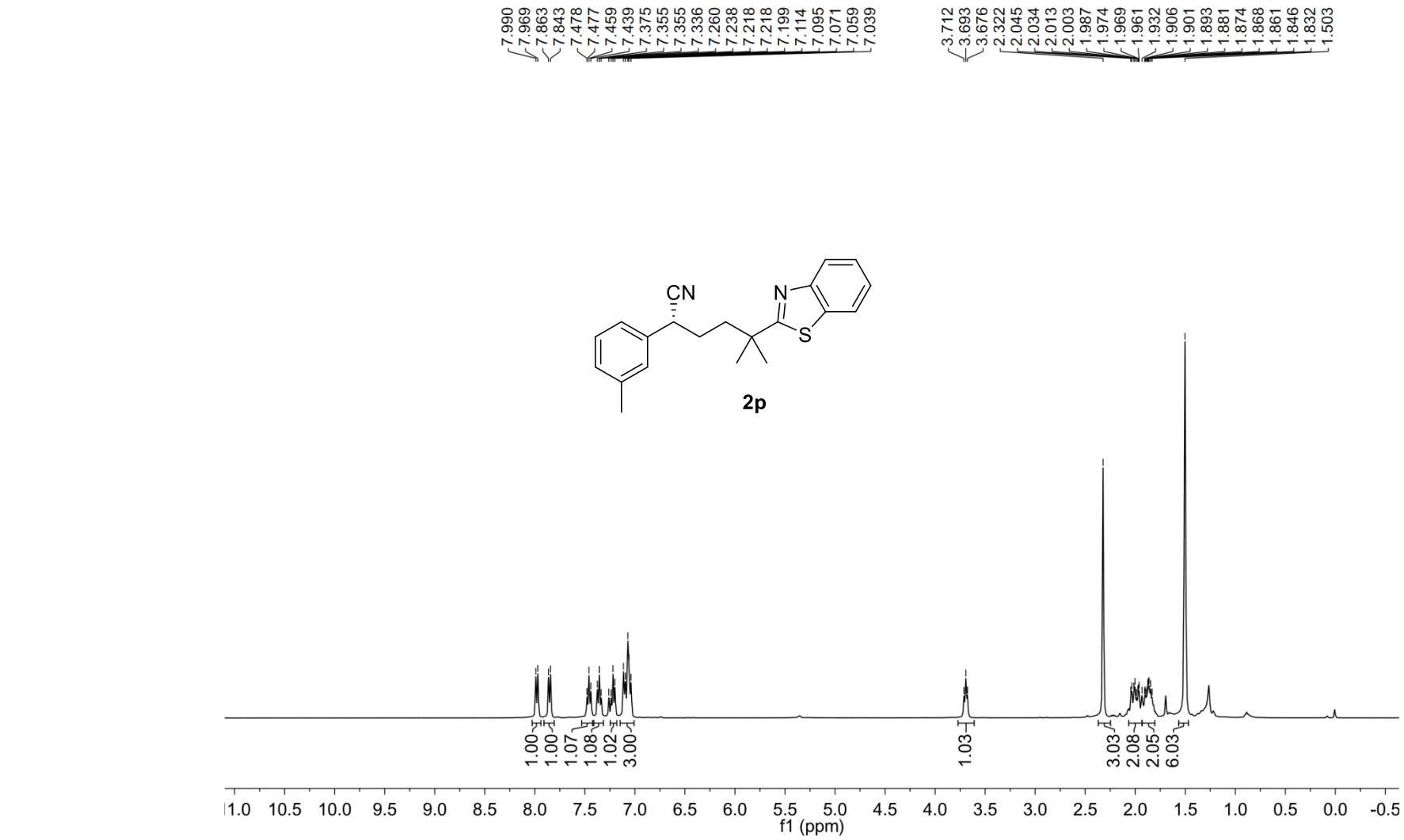
121.511
119.903
77.317
77.000
76.682
41.010
40.605
37.055
30.906
28.920
28.355
CN
N
S
Br
2o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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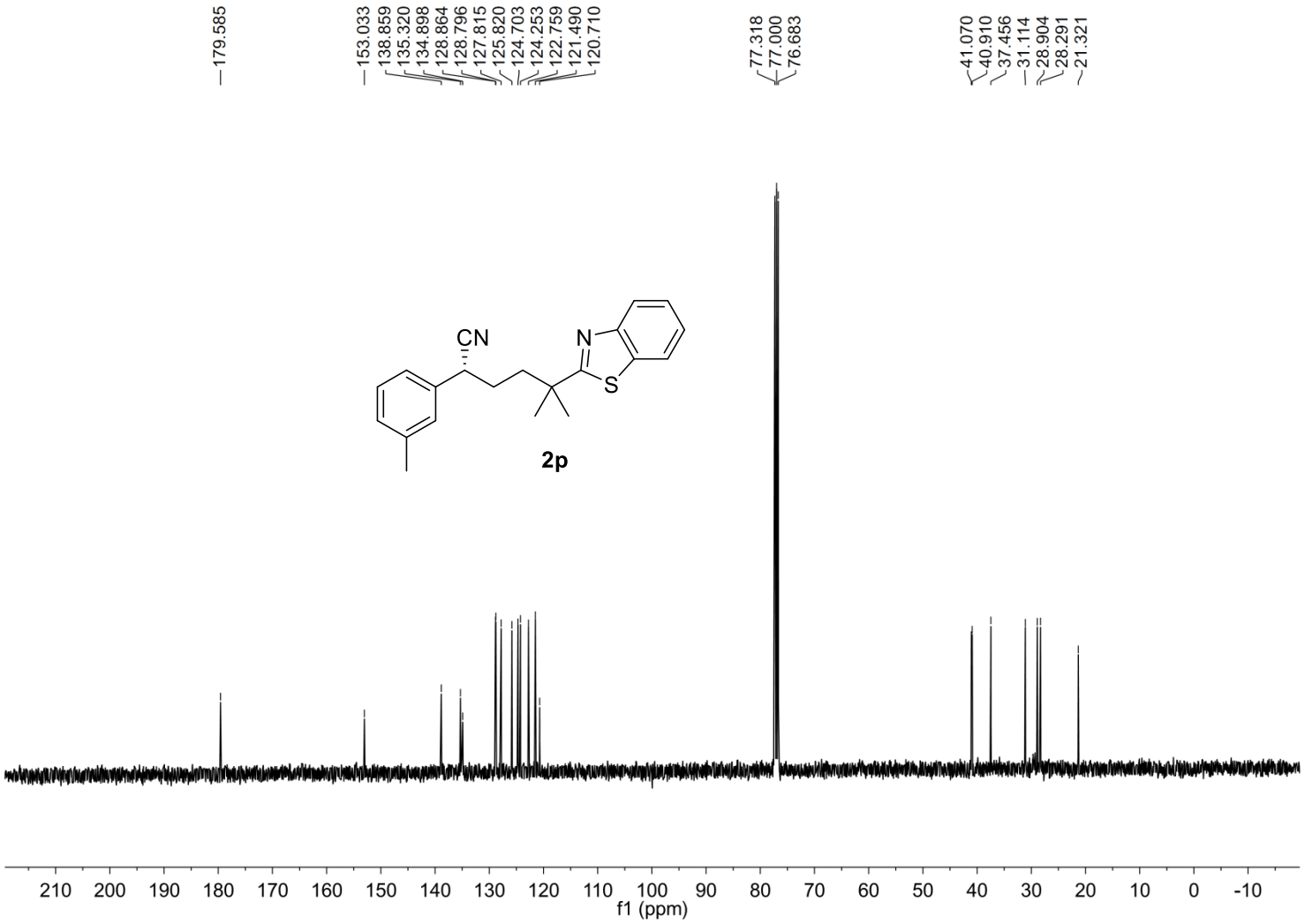
7.355
7.336
7.260
7.238
7.218
7.218
7.199
7.114
7.095
7.071
7.059
7.039
3.712
3.693
3.676
2.322
2.045
2.034
2.013
2.003
1.987
1.974
1.969
1.961
1.932
1.906
1.901
1.893
1.881
1.874
1.868
1.861
1.846
1.832
1.503
CN
N
S
2p
1.00
1.00
1.07
1.08
1.02
3.00
1.03
3.03
2.08
2.05
6.03
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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77.000
76.683
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40.910
37.456
31.114
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CN
N
S
2p
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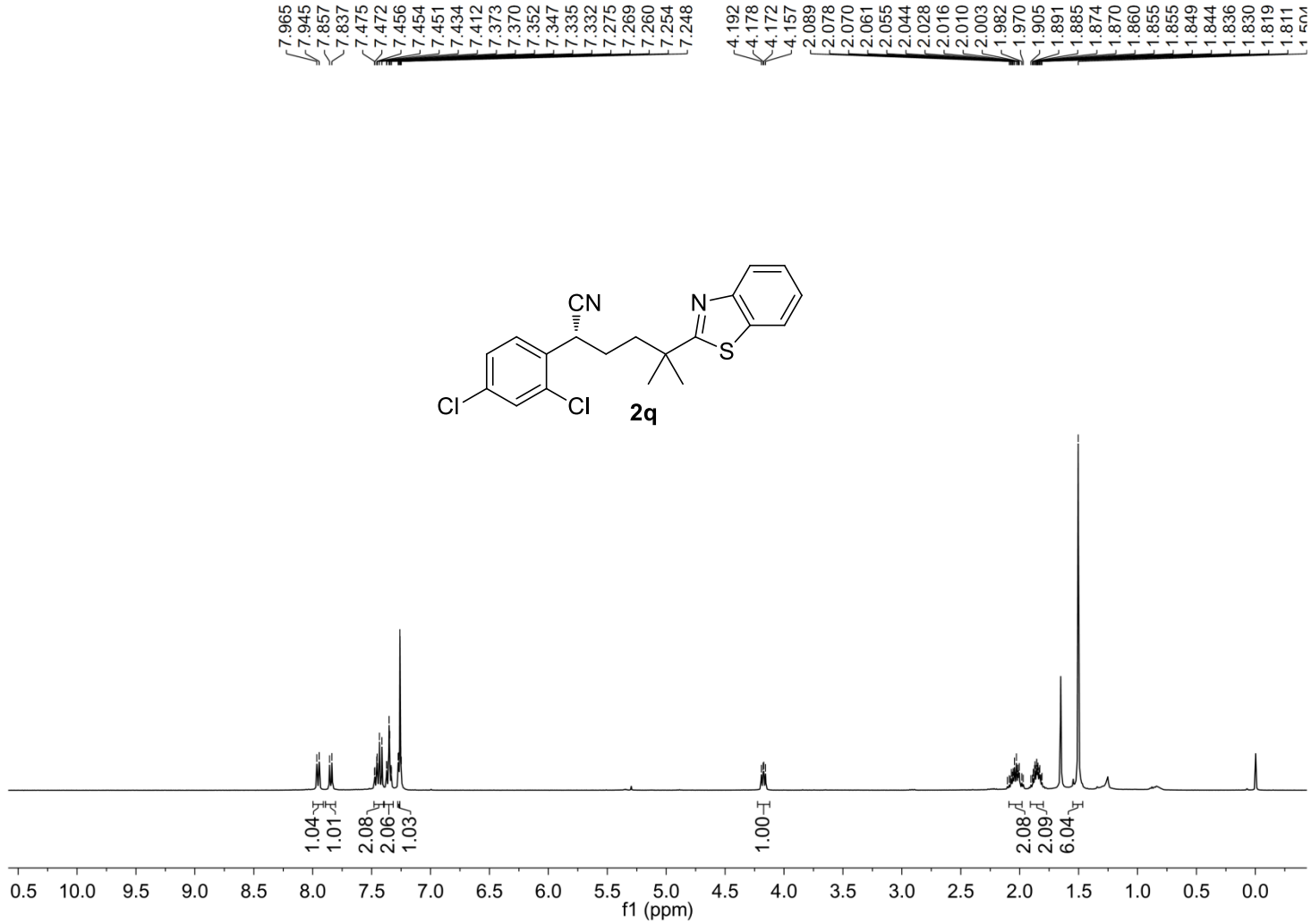
f1 (ppm)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7.451
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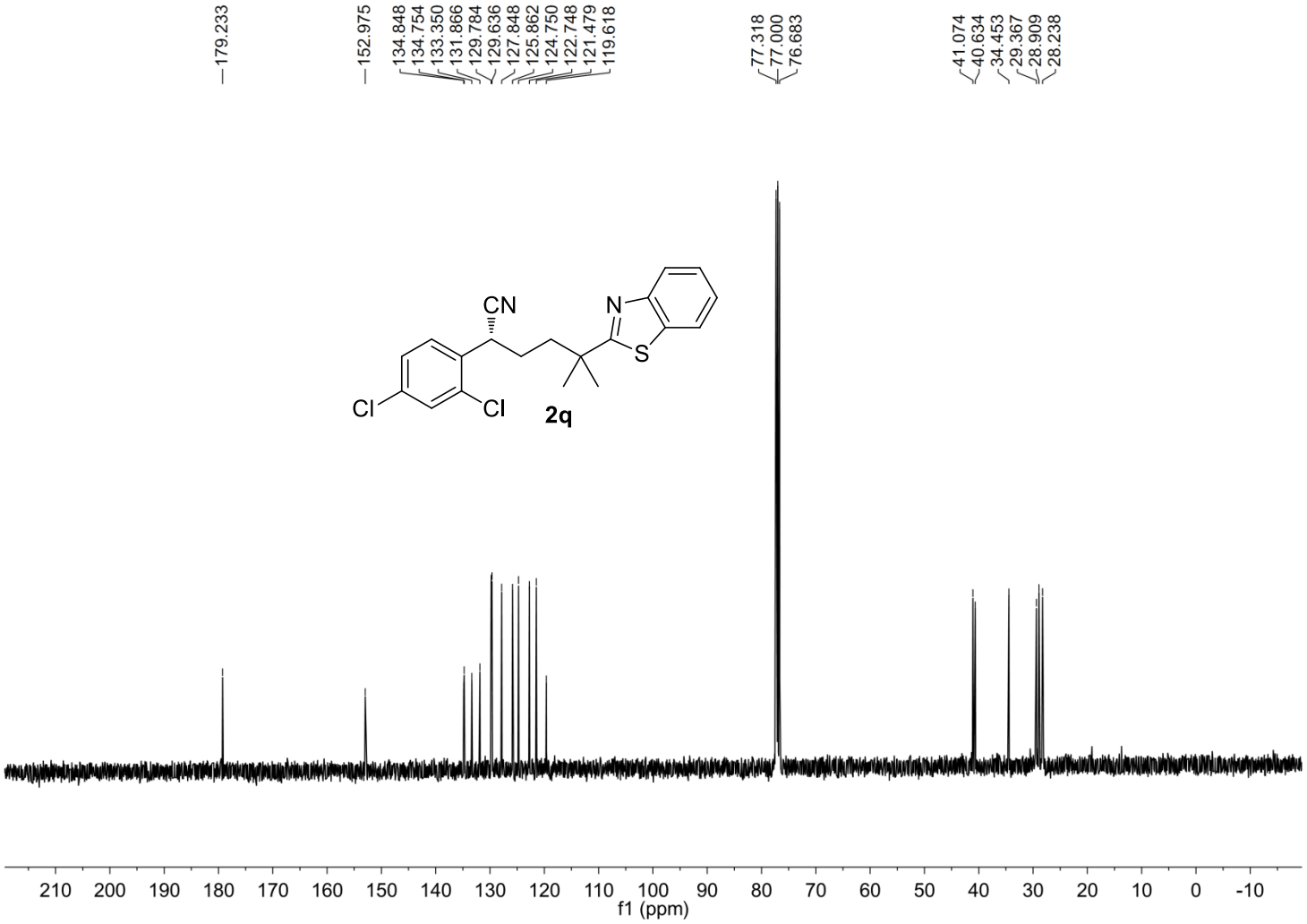
7.373
7.370
7.352
7.347
7.335
7.332
7.275
7.269
7.260
7.254
7.248
4.192
4.178
4.172
4.157
2.089
2.078
2.070
2.061
2.055
2.044
2.028
2.016
2.010
2.003
1.982
1.970
1.905
1.891
1.885
1.874
1.870
1.860
1.855
1.855
1.849
1.844
1.836
1.830
1.819
1.811
CN
N
S
Cl
Cl
2q
1.04
1.01
2.08
2.06
1.03
1.00
2.08
2.09
6.04
0.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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133.350
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127.848
125.862
124.750
122.748
121.479
119.618
77.318
77.000
76.683
41.074
40.634
34.453
29.367
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28.238
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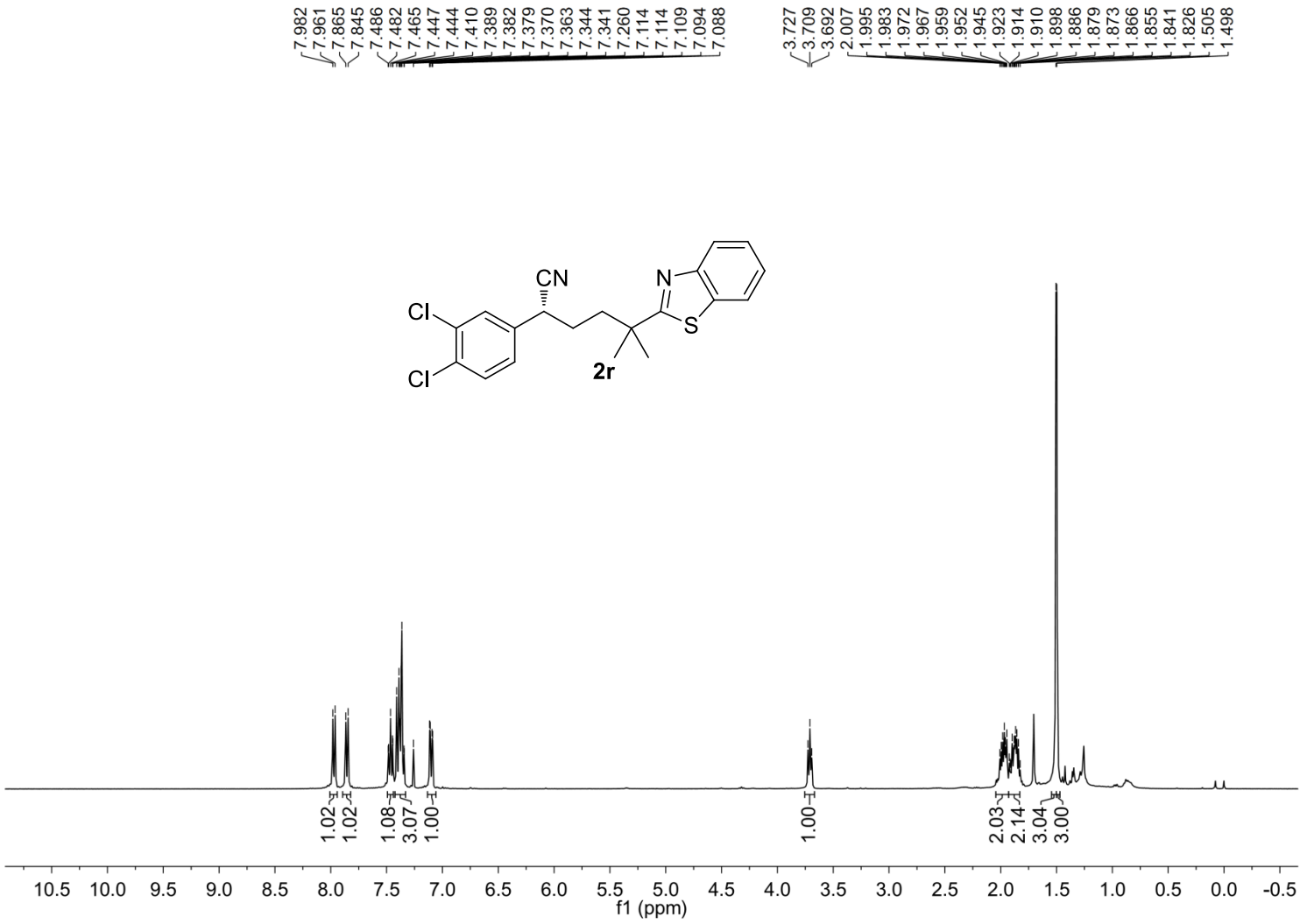
N
S
Cl
Cl
2q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.444
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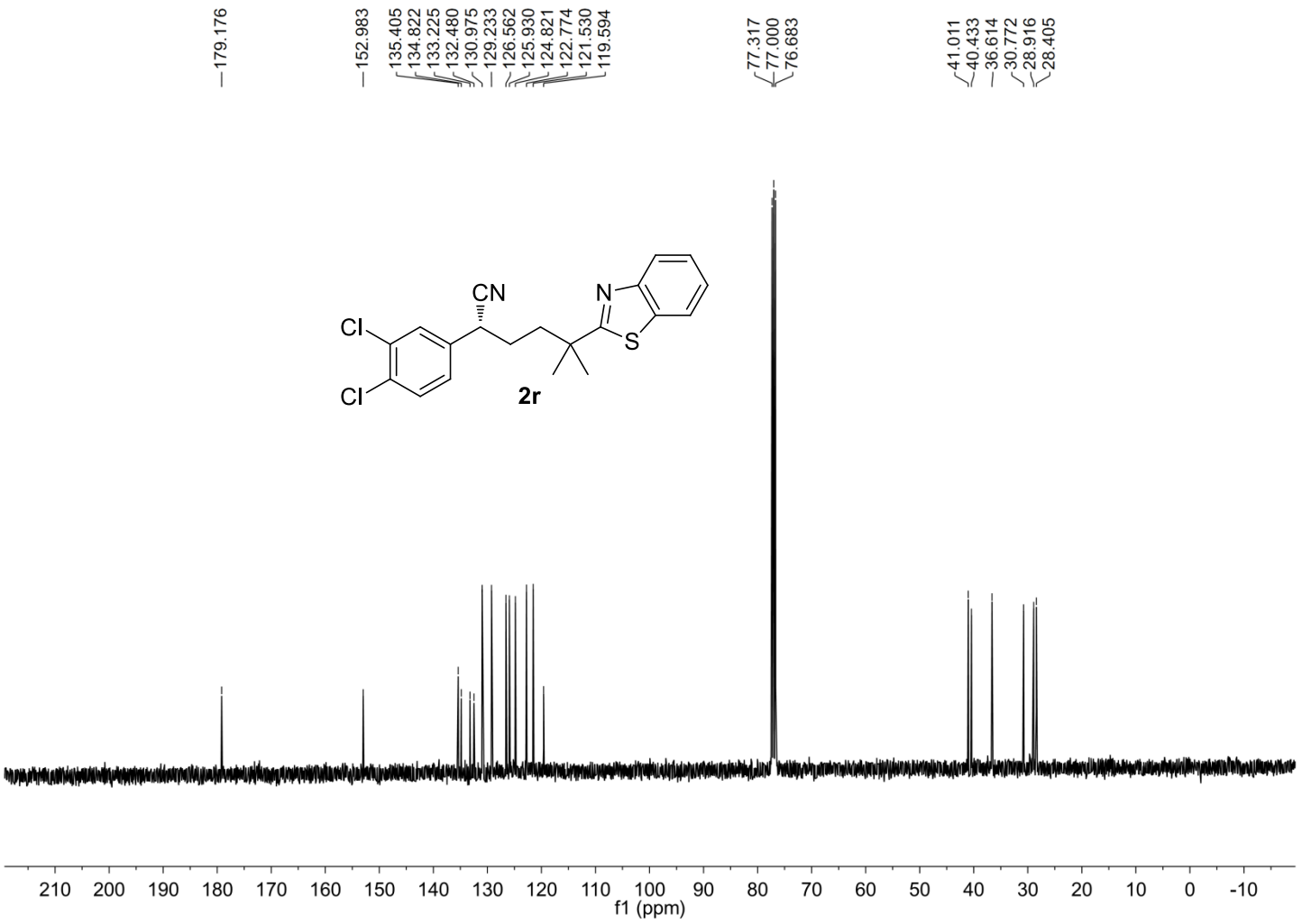
7.382
7.379
7.370
7.363
7.344
7.341
7.260
7.114
7.114
7.109
7.094
7.088
3.727
3.709
3.692
2.007
1.995
1.983
1.972
1.967
1.959
1.952
1.945
1.923
1.914
1.910
1.898
1.886
1.879
1.873
1.866
1.855
1.841
1.826
1.505
1.498
CN
N
S
Cl
Cl
2r
1.02
1.02
1.08
3.07
1.00
1.00
2.03
2.14
3.04
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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129.233
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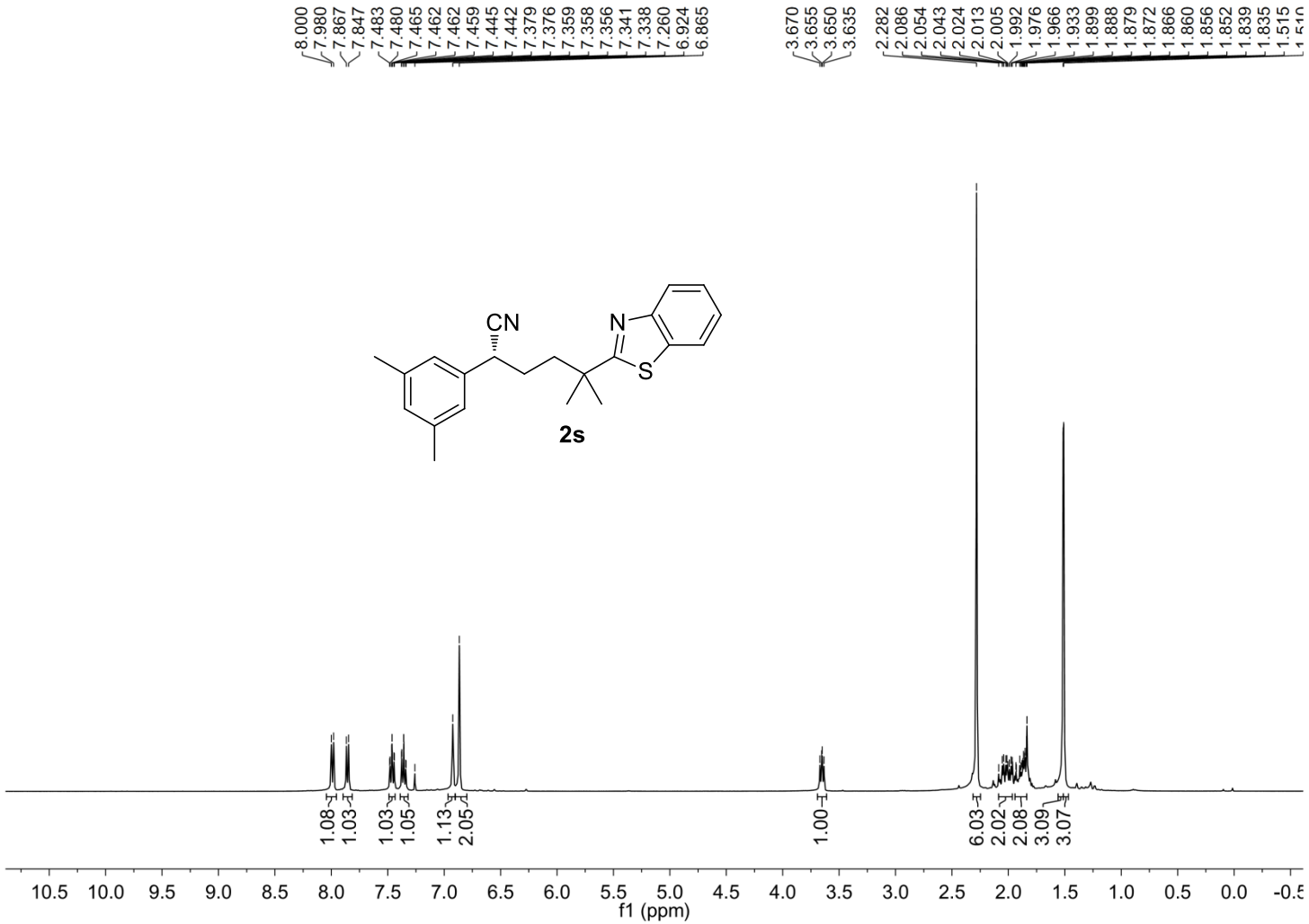
122.774
121.530
119.594
77.317
77.000
76.683
41.011
40.433
36.614
30.772
28.916
28.405
CN
N
S
Cl
Cl
2r
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.462
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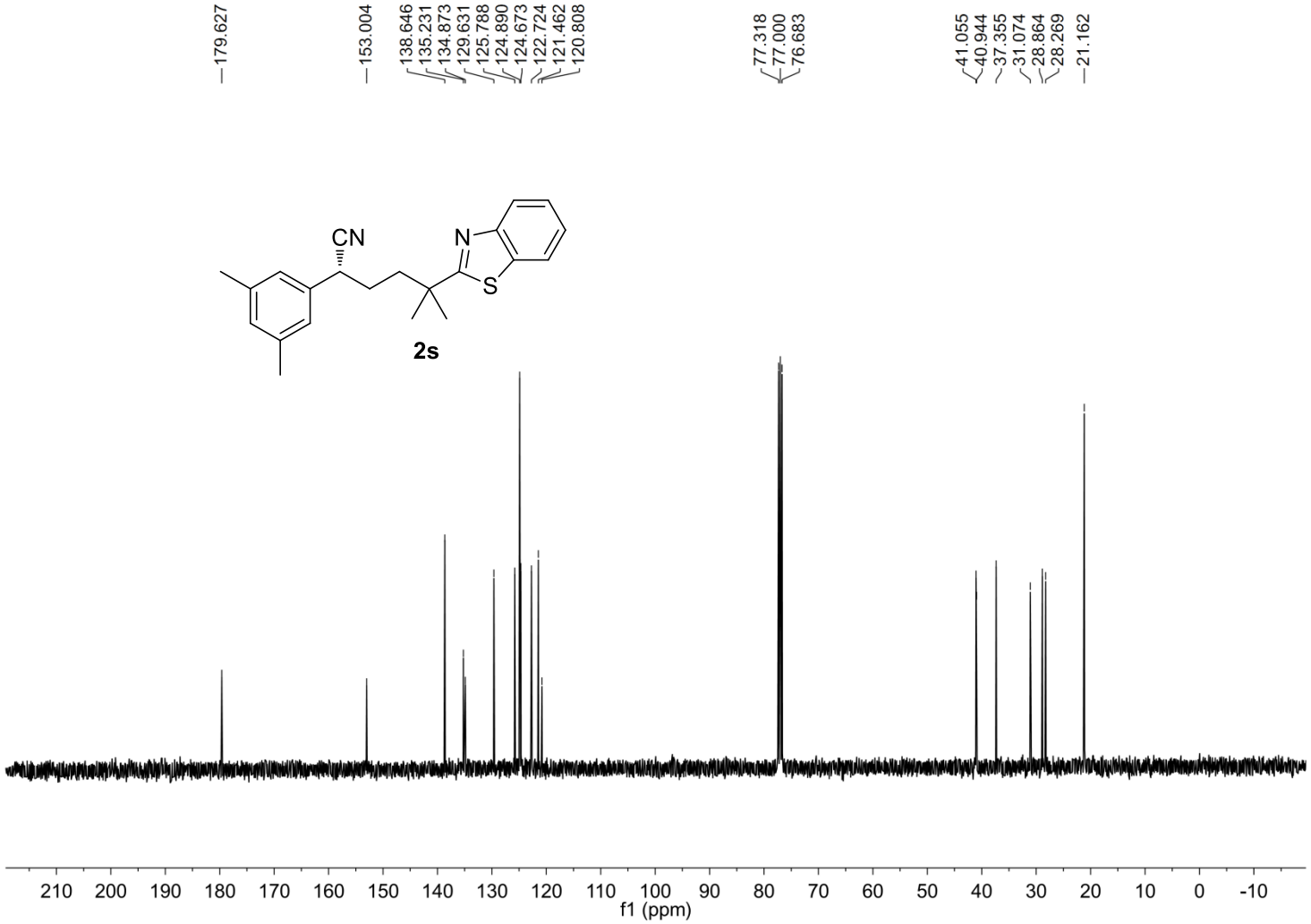
7.442
7.379
7.376
7.359
7.358
7.356
7.341
7.338
7.260
6.924
6.865
3.670
3.655
3.650
3.635
2.282
2.086
2.054
2.043
2.024
2.013
2.005
1.992
1.976
1.966
1.933
1.899
1.888
1.879
1.872
1.866
1.860
1.856
1.852
1.839
1.835
1.515
CN
N
S
2s
1.08
1.03
1.03
1.05
1.13
2.05
1.00
6.03
2.02
2.08
3.09
3.07
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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77.000
76.683
41.055
40.944
37.355
31.074
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CN
N
S
2s
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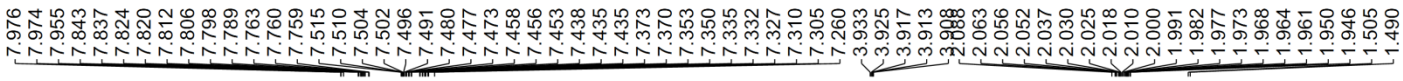
f1 (ppm)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7.798
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7.763
7.760
7.759
7.515
7.510
7.504
7.502
7.496
7.491
7.480
7.477
7.473
7.458
7.456
7.453
7.438
7.435
7.435
7.373
7.370
7.353
7.350
7.335
7.332
7.327
7.310
7.305
7.260
3.933
3.925
3.917
3.913
2.063
2.056
2.052
2.037
2.030
2.025
2.018
2.010
2.000
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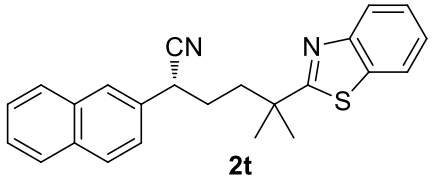
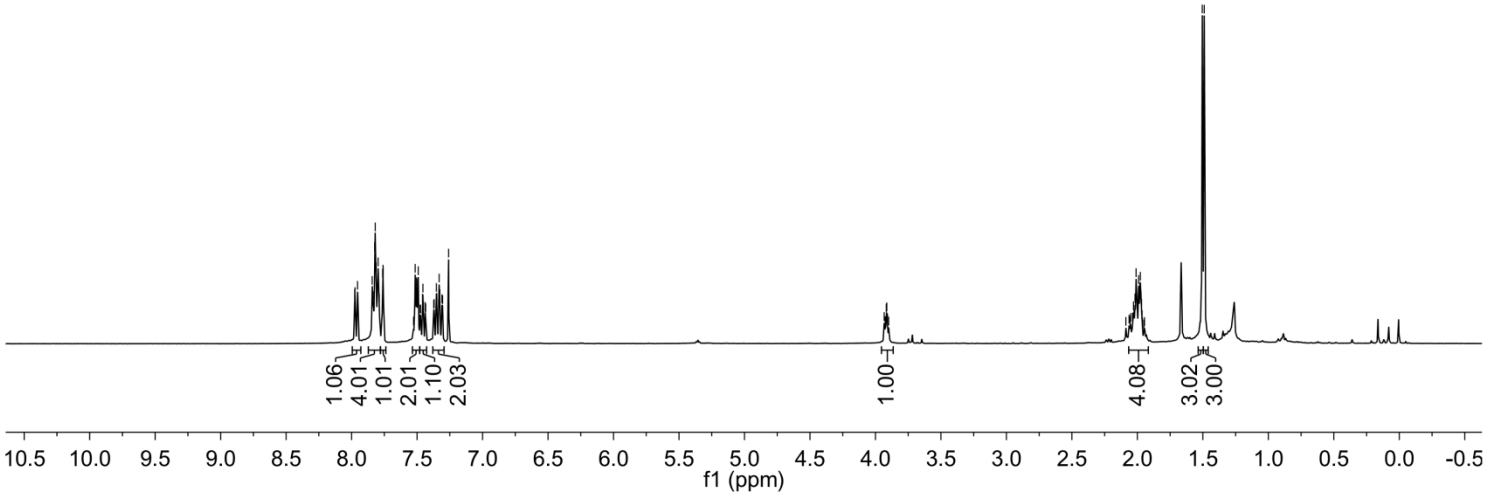

CN
N
S

2t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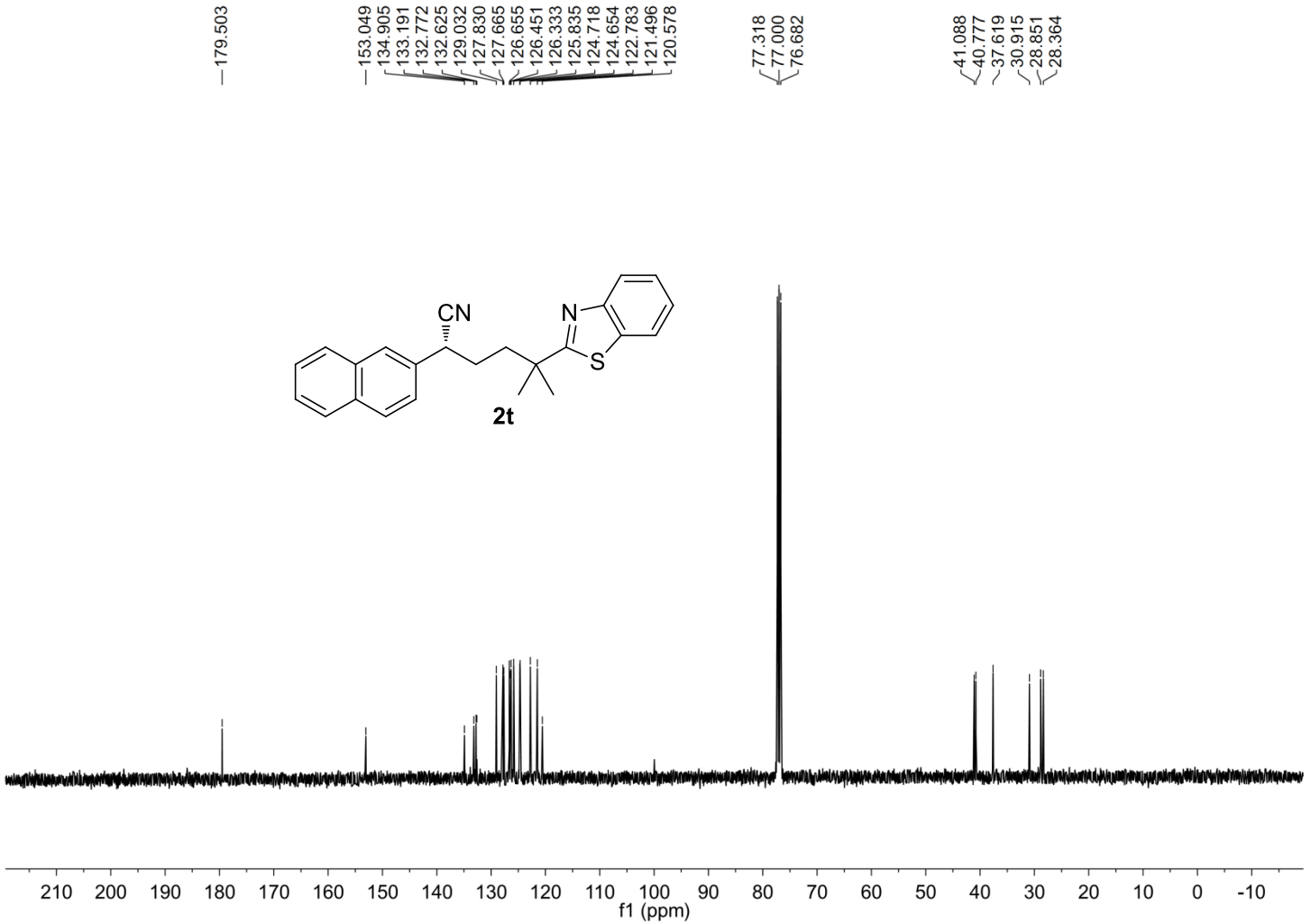
1.01
2.01
1.10
2.03
1.00
4.08
3.02
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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126.333
125.835
124.718
124.654
122.783
121.496
120.578
77.318
77.000
76.682
41.088
40.777
37.619
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CN
N
S
2t
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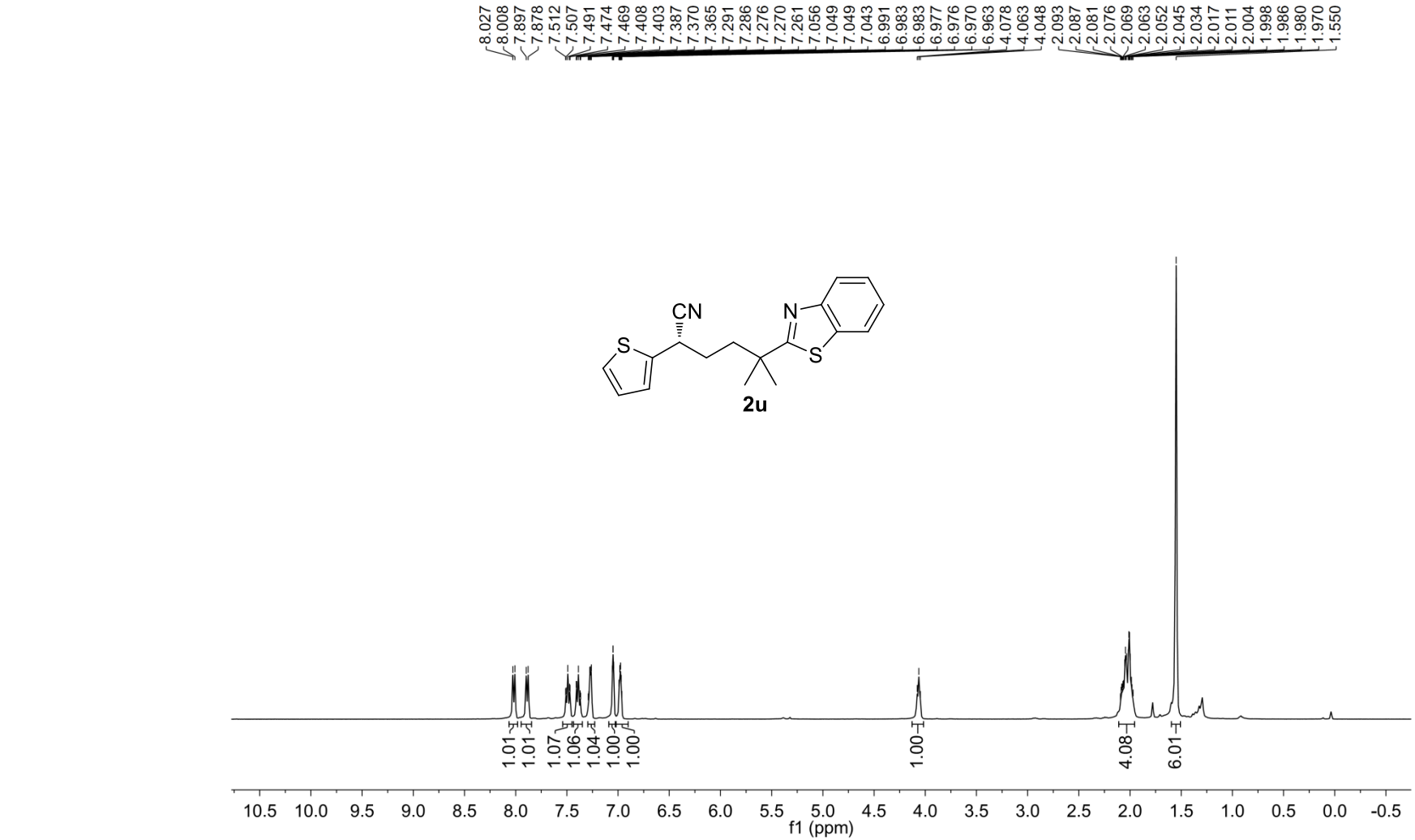
f1 (ppm)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7.049
7.043
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4.063
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2.087
2.081
2.076
2.069
2.063
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2.034
2.017
2.011
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1.550
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S
S
2u
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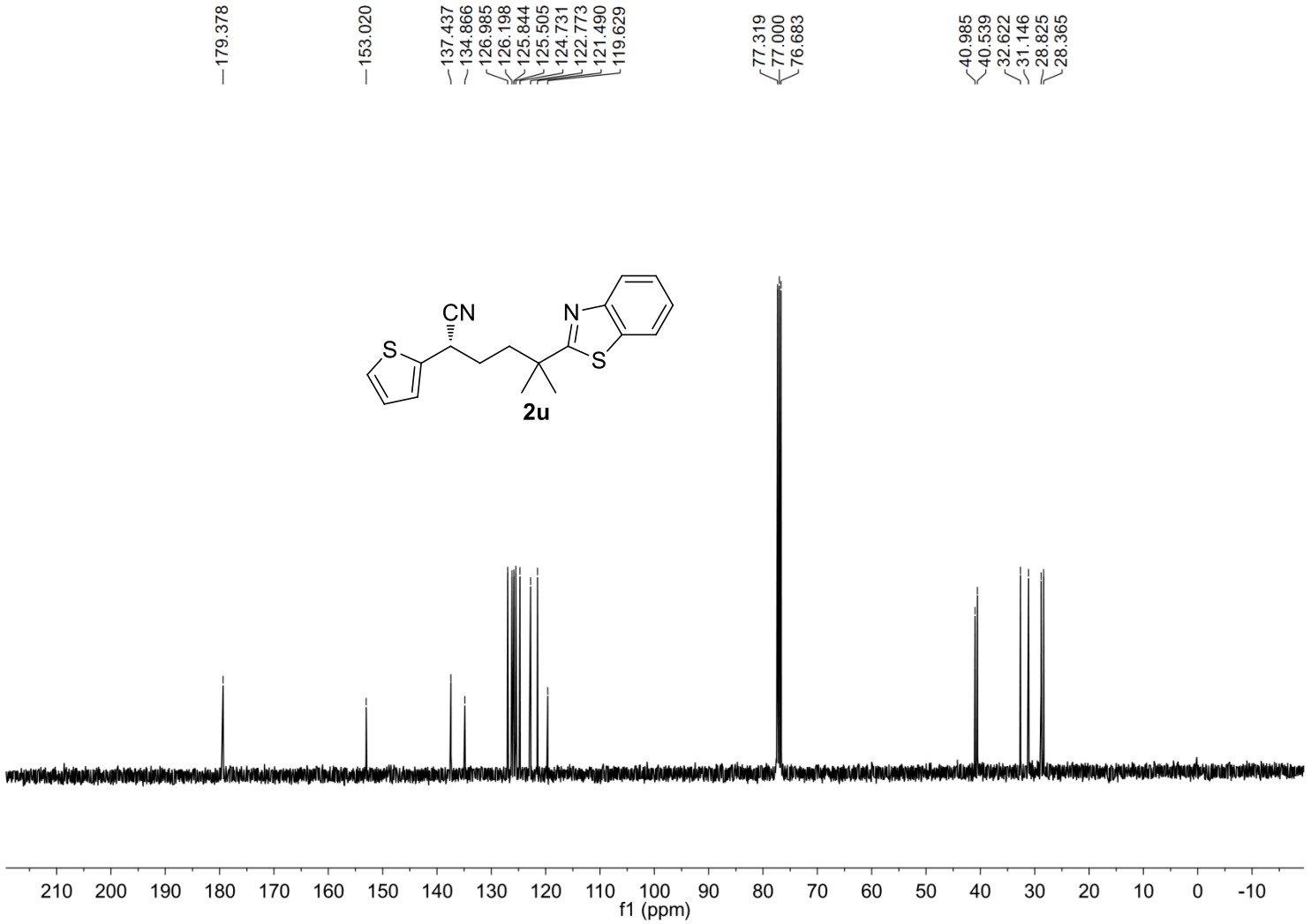
1.01
1.07
1.06
1.04
1.00
1.00
1.00
4.08
6.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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40.539
32.622
31.146
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CN
N
S
S
2u
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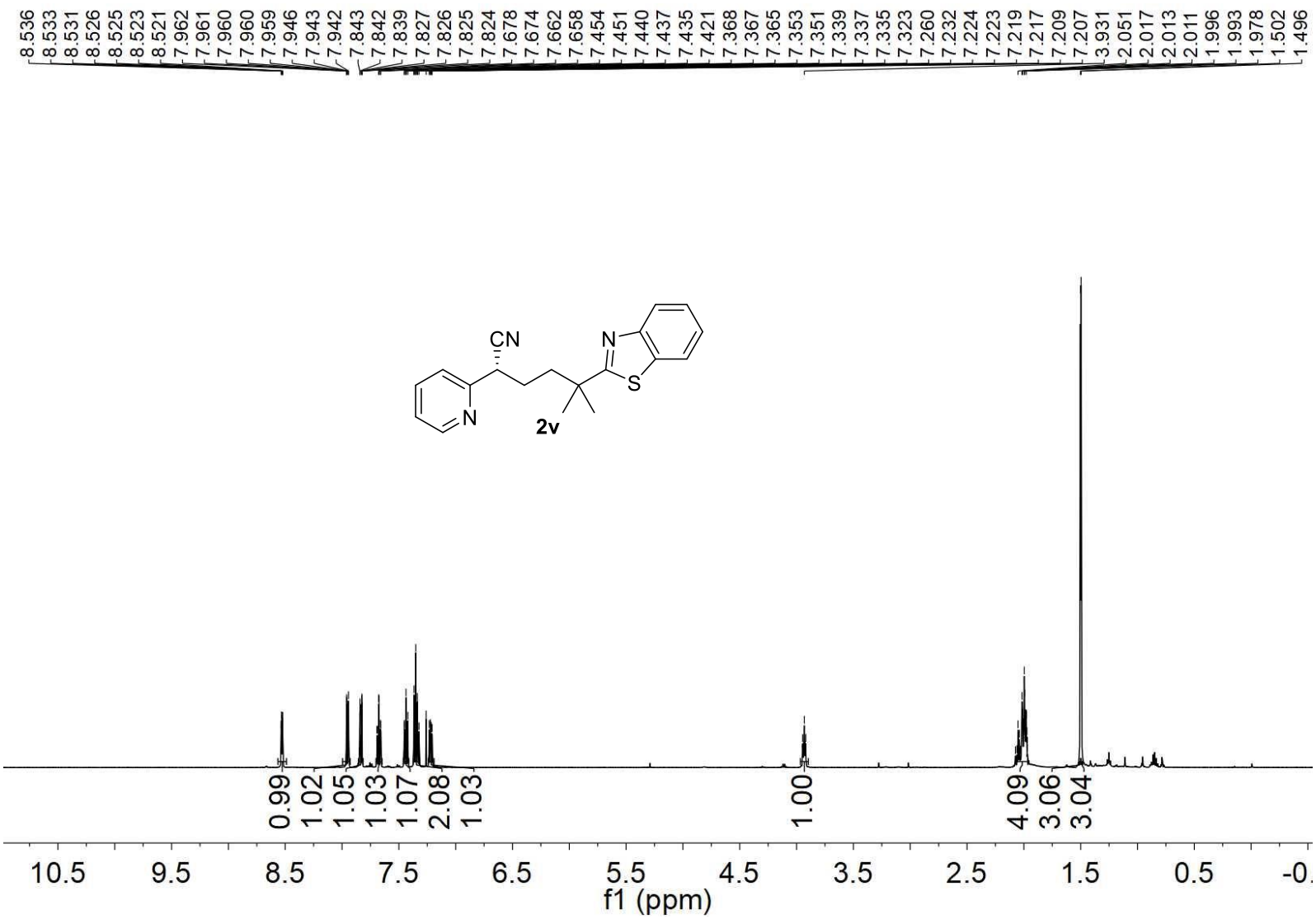
f1 (ppm)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S
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2v
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1.03
1.07
2.08
1.03
1.00
4.09
3.06
3.04
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6.5
5.5
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3.5
2.5
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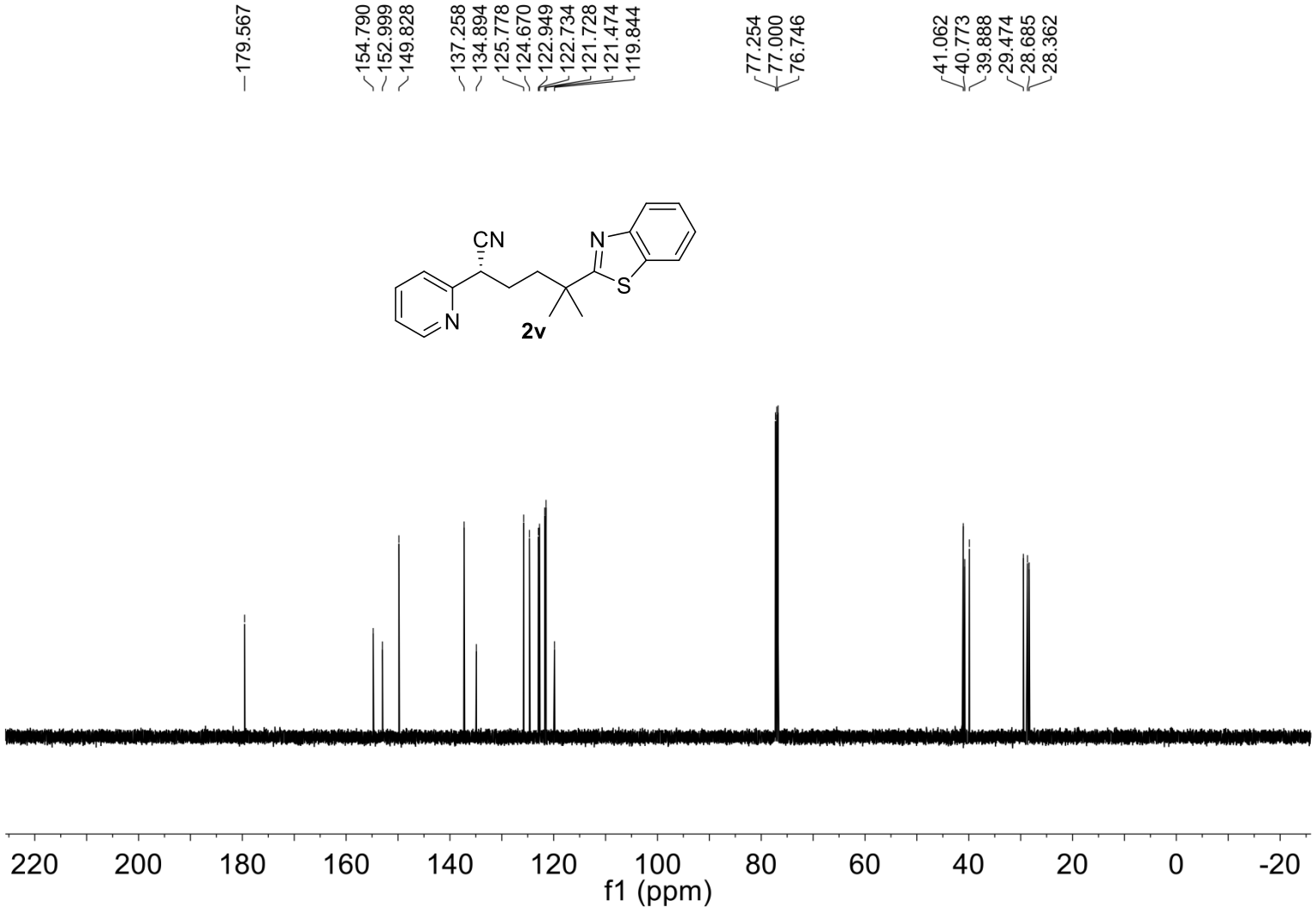
f1 (ppm)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122.734
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77.254
77.000
76.746
41.062
40.773
39.888
29.474
28.685
28.362
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N
S
N
2v
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200
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140
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80
60
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20
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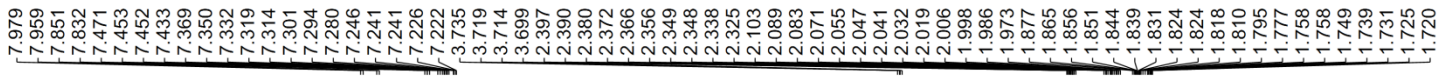
-20
f1 (ppm)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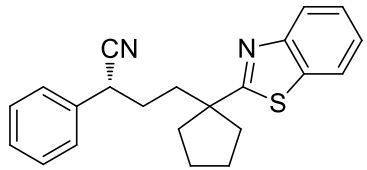
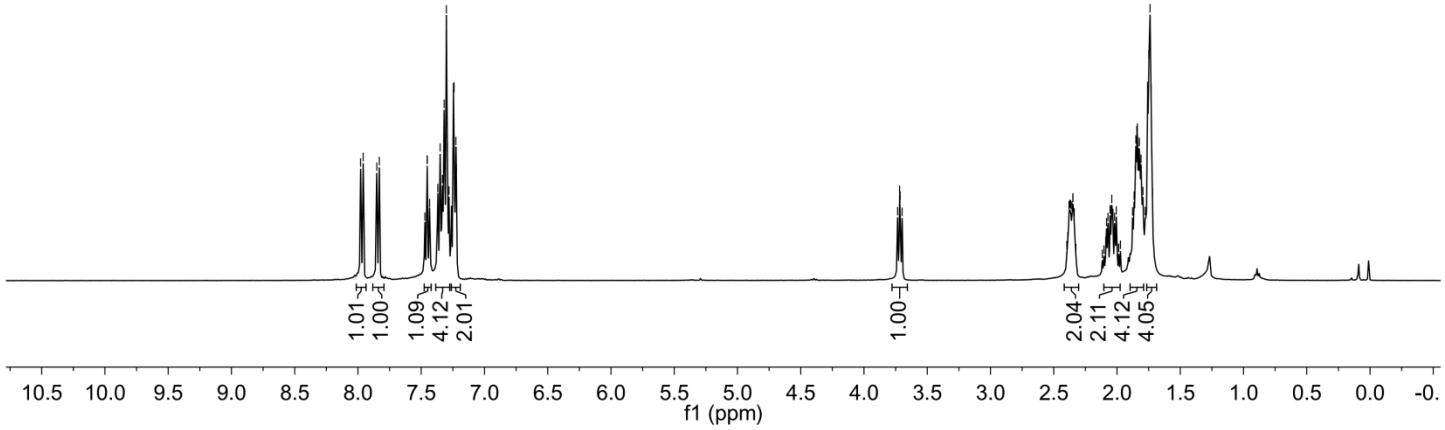
1.720


CN
N
S

2w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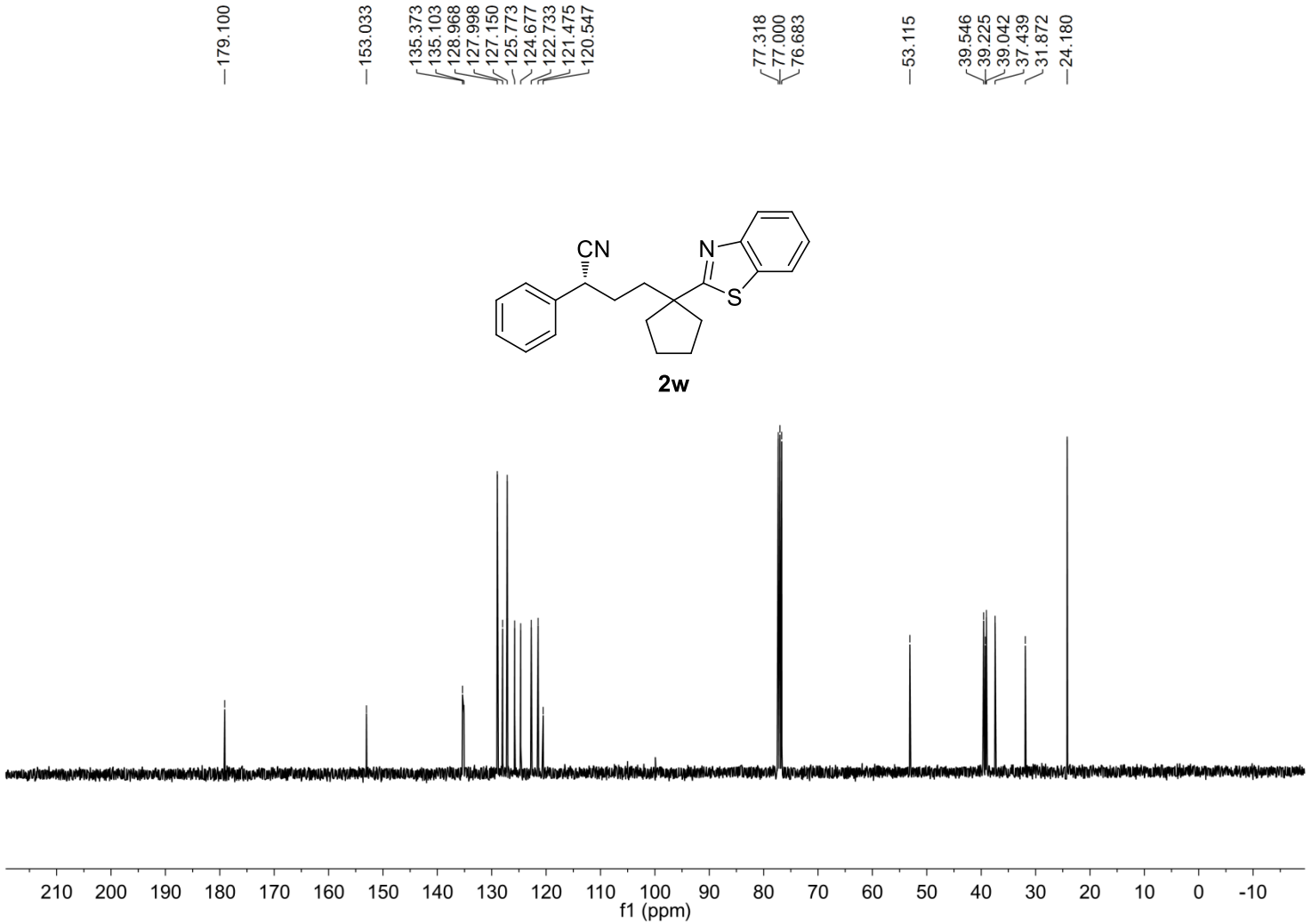
1.00
2.04
2.11
4.12
4.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)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125.773
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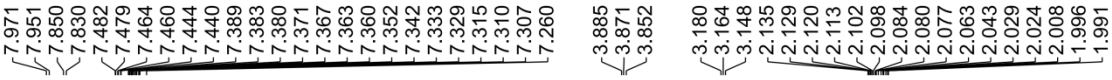
120.547
77.318
77.000
76.683
53.115
39.546
39.225
39.042
37.439
31.872
24.180
CN
N
S
2w
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.380
7.371
7.367
7.363
7.360
7.352
7.342
7.333
7.329
7.315
7.310
7.307
7.260
3.885
3.871
3.852
3.180
3.164
3.148
2.135
2.129
2.120
2.113
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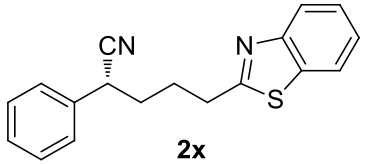
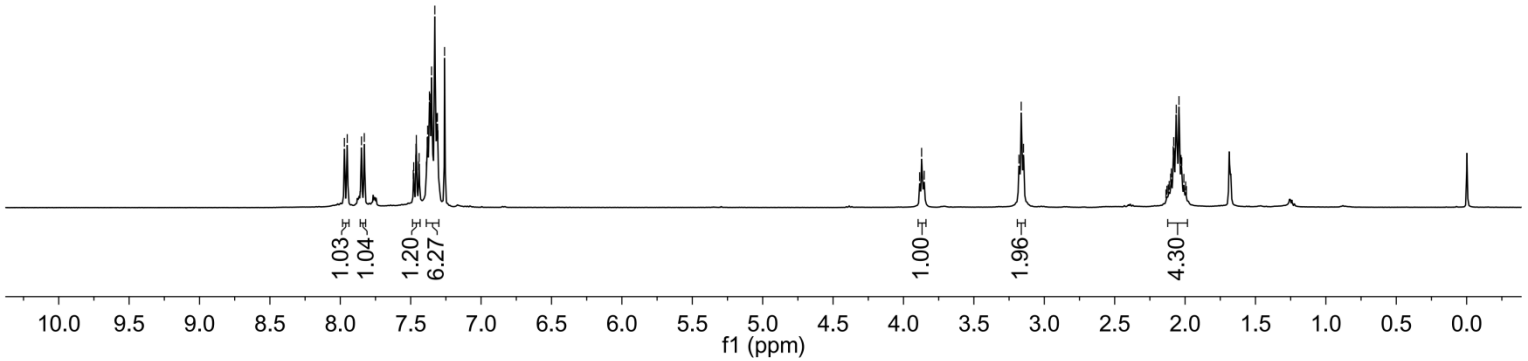
2.084
2.080
2.077
2.063
2.043
2.029
2.024
2.008
1.996
1.991


CN
N
S

2x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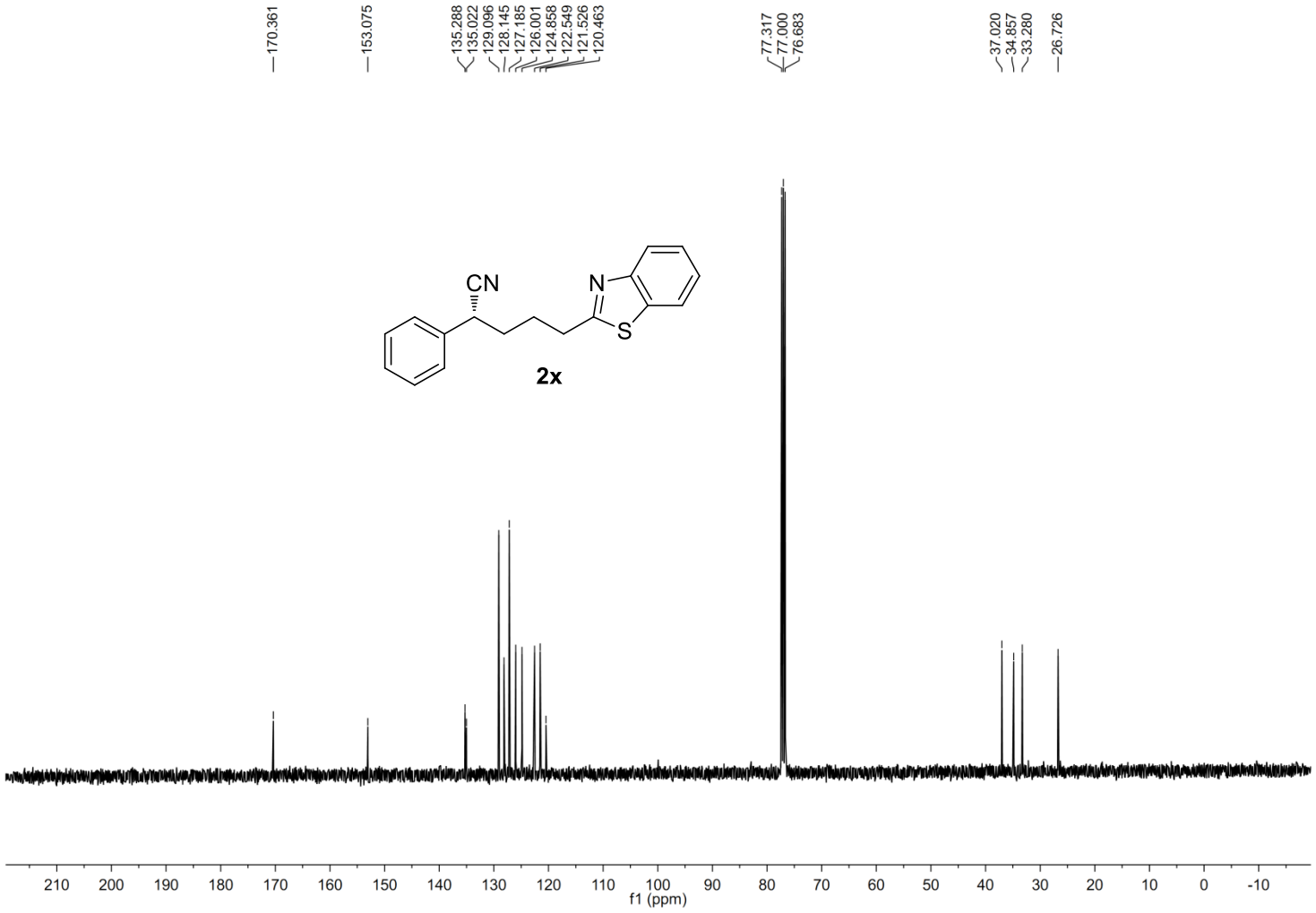
1.04
1.20
6.27
1.00
1.96
4.30
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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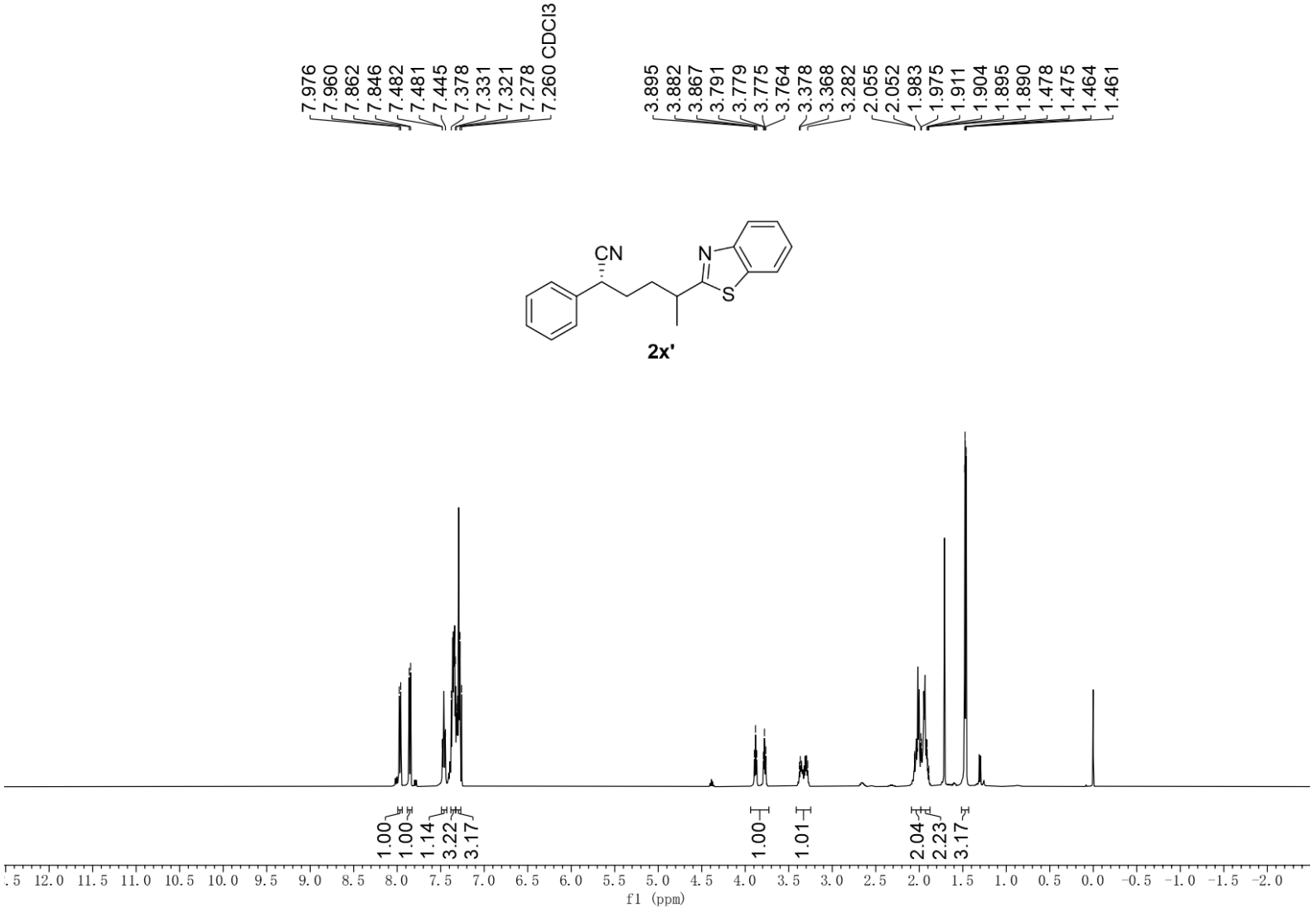
128.145
127.185
126.001
124.858
122.549
121.526
120.463
77.317
77.000
76.683
37.020
34.857
33.280
26.726
CN
N
S
2x
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.862
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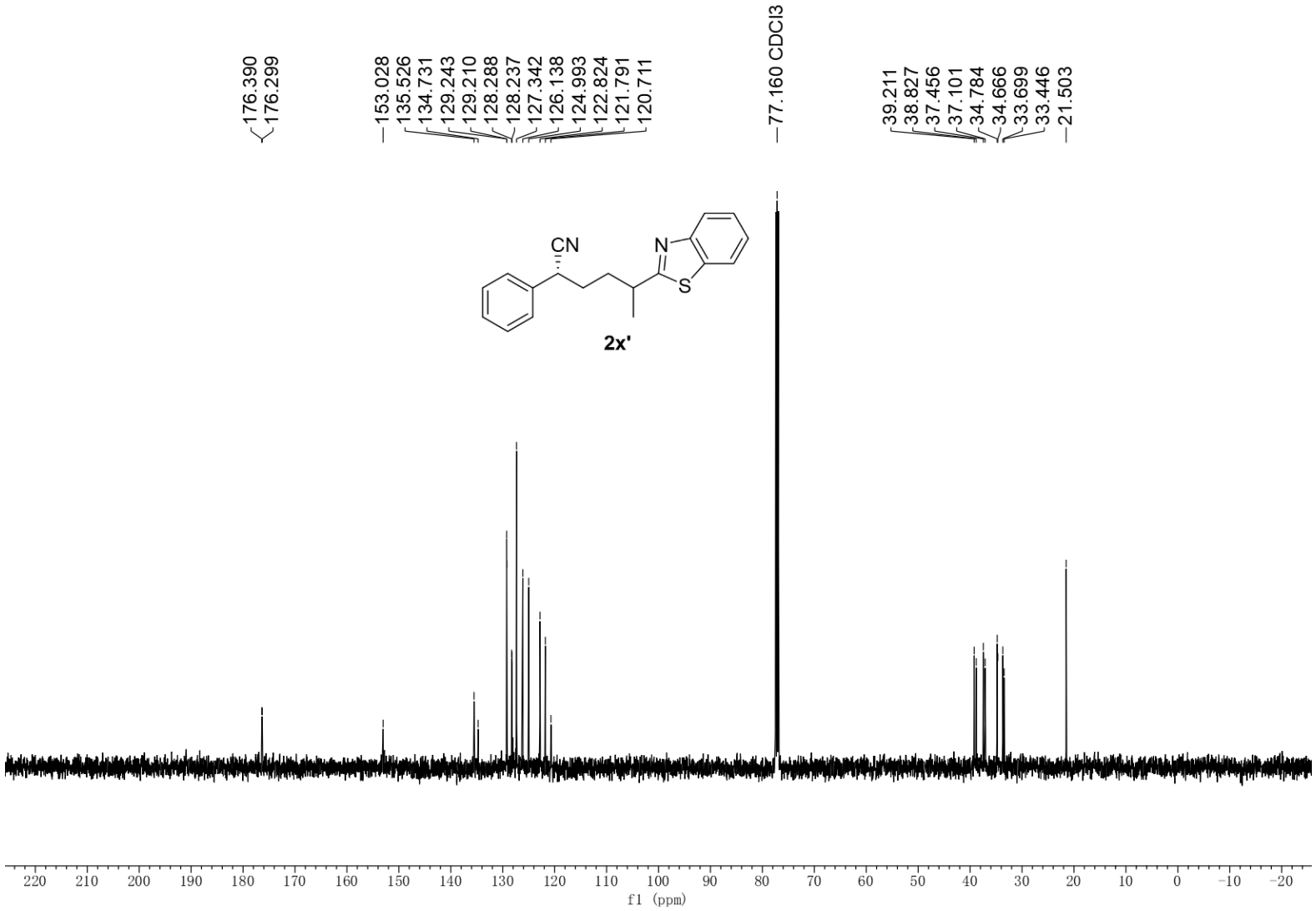
7.482
7.481
7.445
7.378
7.331
7.321
7.278
7.260 CDCl3
3.895
3.882
3.867
3.791
3.779
3.775
3.764
3.378
3.368
3.282
2.055
2.052
1.983
1.975
1.911
1.904
1.895
1.890
1.478
1.475
1.464
1.461
CN
N
S
2x'
1.00
1.00
1.14
3.22
3.17
1.00
1.01
2.04
2.23
3.17
f1 (ppm)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128.288
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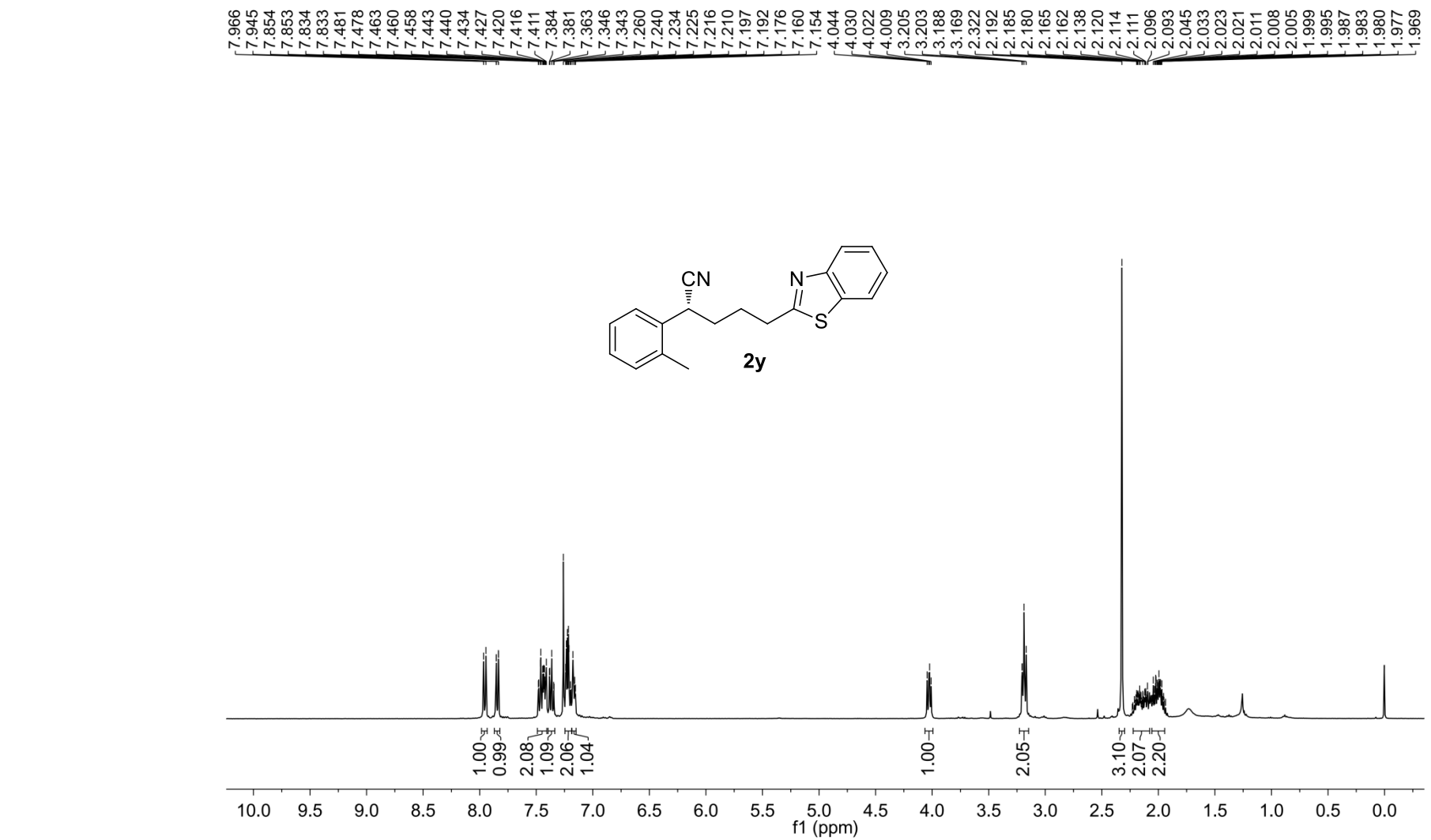
124.993
122.824
121.791
120.711
77.160 CDCl3
39.211
38.827
37.456
37.101
34.784
34.666
33.699
33.446
21.503
CN
N
S
2x'
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20
f1 (ppm)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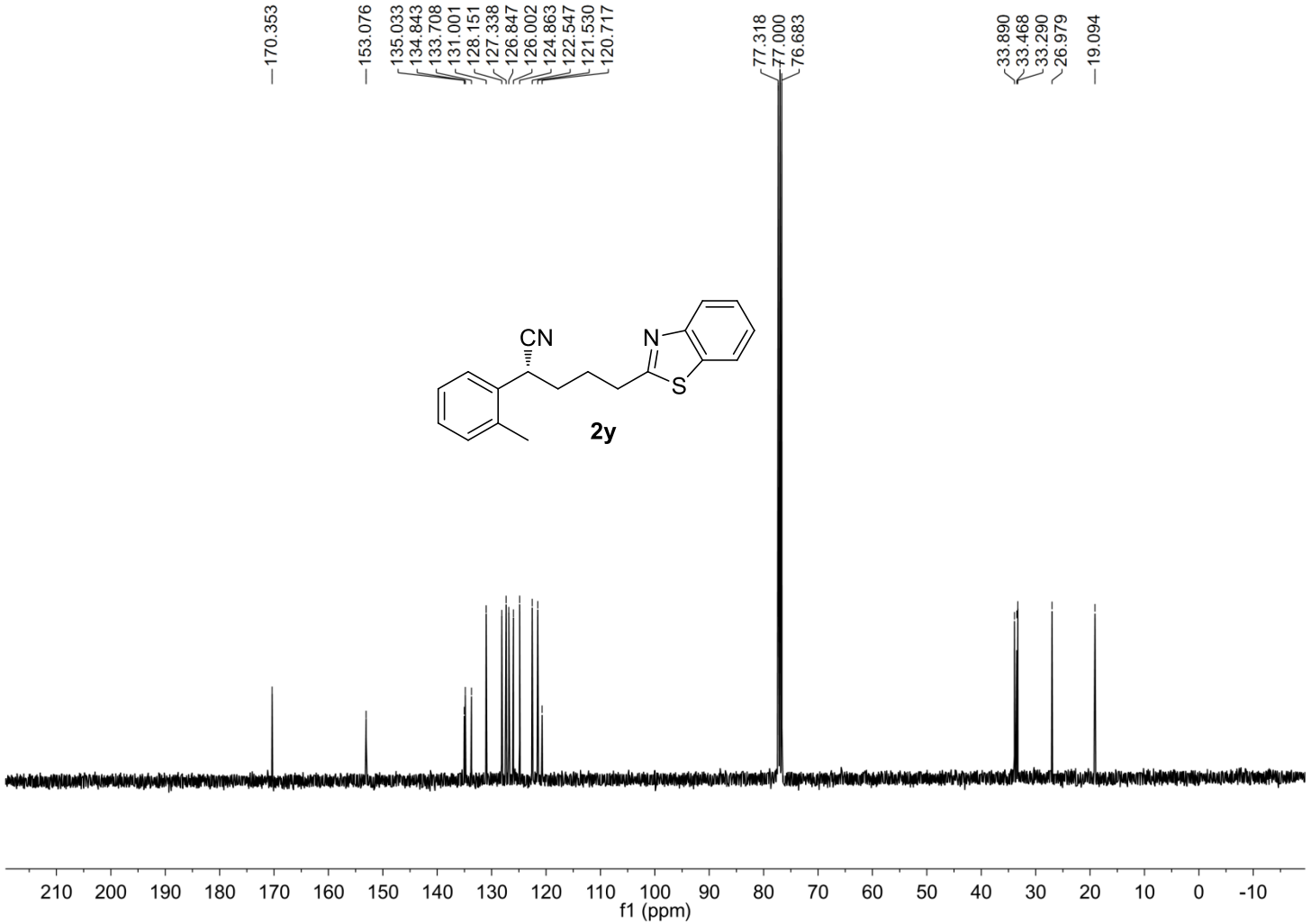
7.854
7.853
7.834
7.833
7.481
7.478
7.463
7.460
7.458
7.443
7.440
7.434
7.427
7.420
7.416
7.411
7.384
7.381
7.363
7.346
7.343
7.260
7.240
7.234
7.225
7.216
7.210
7.197
7.192
7.176
7.160
7.154
4.044
4.030
4.022
4.009
3.205
3.203
3.188
3.169
2.322
2.192
2.185
2.180
2.165
2.162
2.138
2.120
2.114
2.111
2.096
2.093
2.045
2.033
2.023
2.021
2.011
2.008
2.005
1.999
1.995
1.987
1.983
1.980
1.977
1.969
CN
N
S
2y
1.00
0.99
2.08
1.09
2.06
1.04
1.00
2.05
3.10
2.07
2.20
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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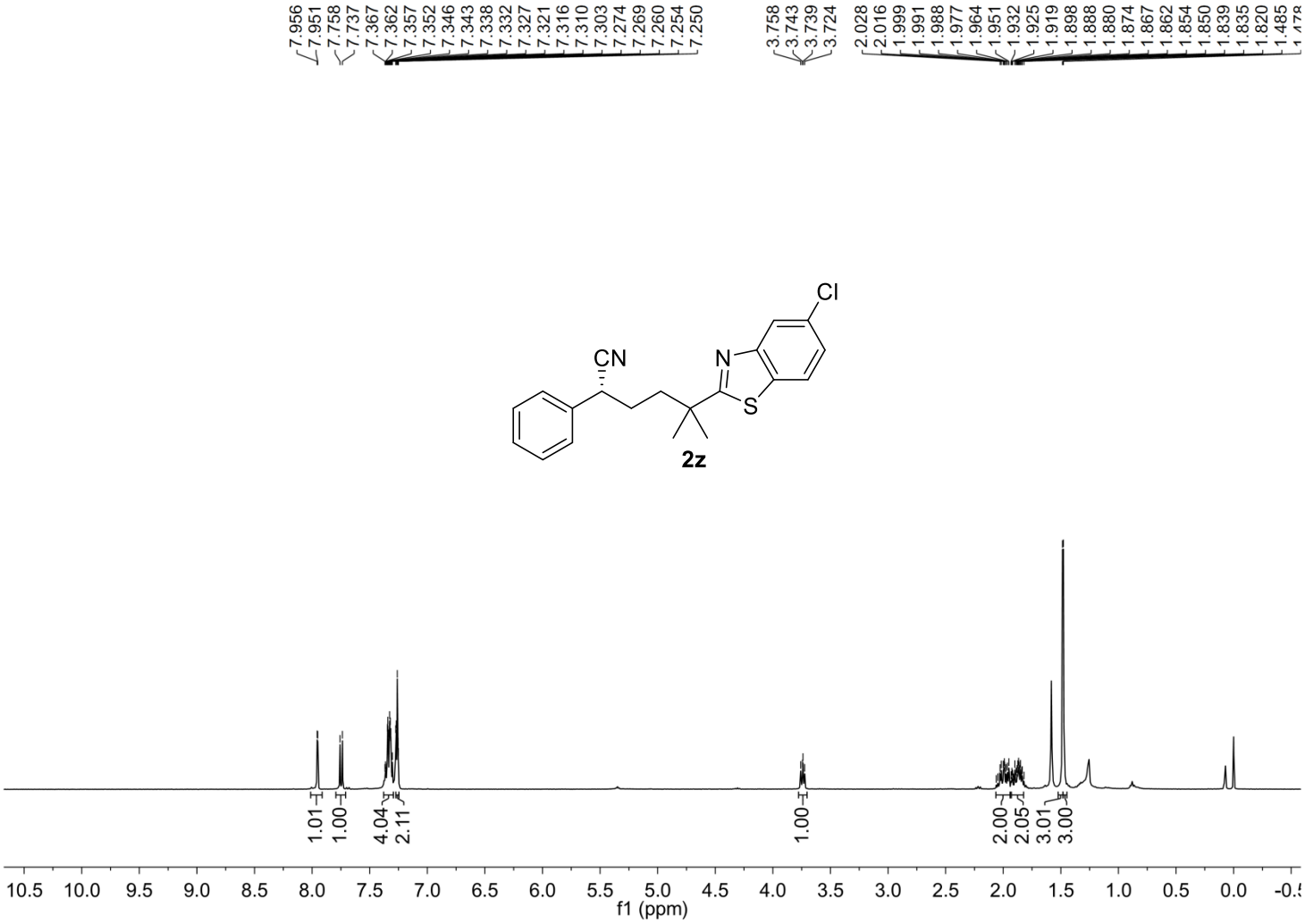
128.151
127.338
126.847
126.002
124.863
122.547
121.530
120.717
77.318
77.000
76.683
33.890
33.468
33.290
26.979
19.094
CN
N
S
2y
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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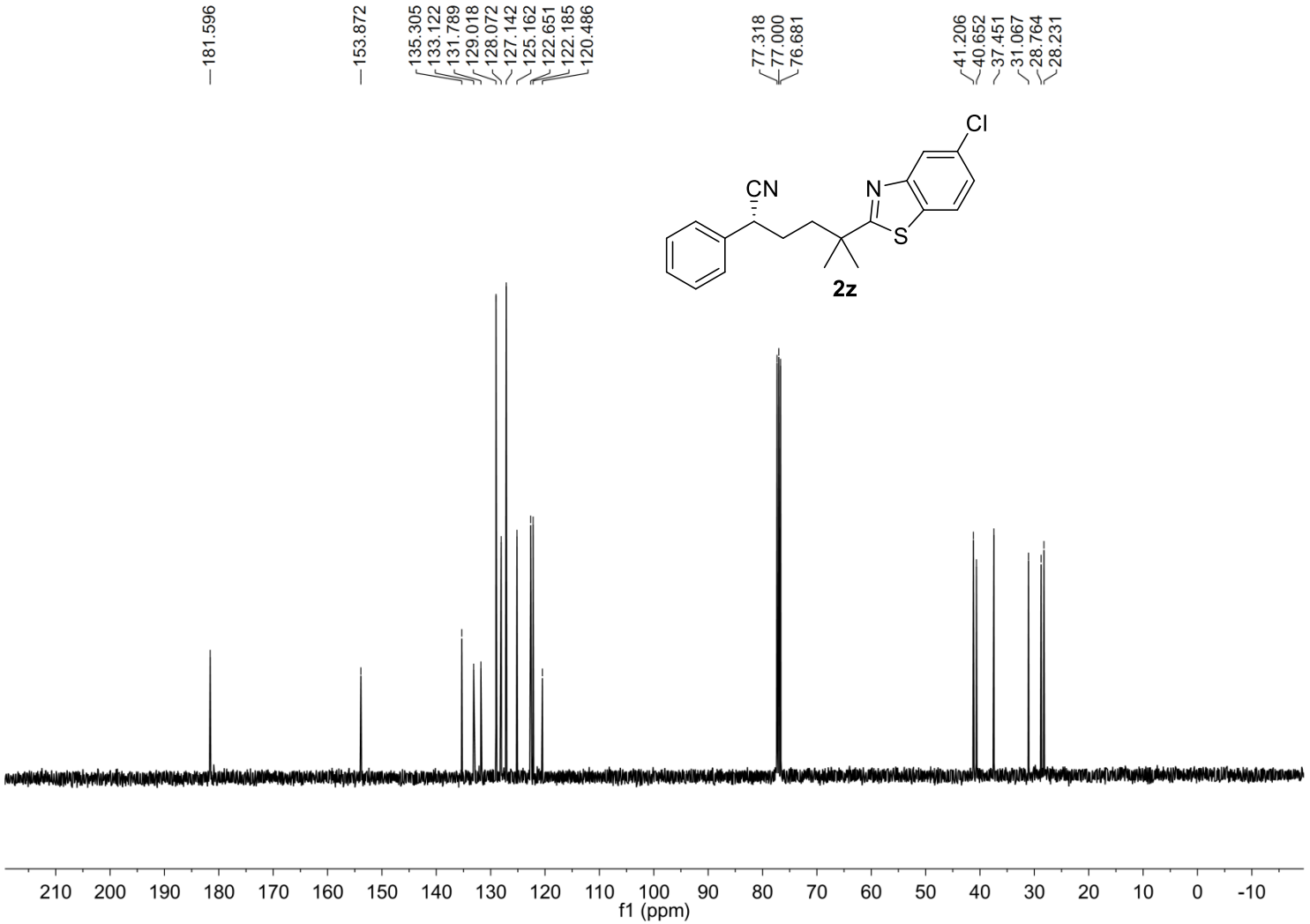
7.758
7.737
7.367
7.362
7.357
7.352
7.346
7.343
7.338
7.332
7.327
7.321
7.316
7.310
7.303
7.274
7.269
7.260
7.254
7.250
3.758
3.743
3.739
3.724
2.028
2.016
1.999
1.991
1.988
1.977
1.964
1.951
1.932
1.925
1.919
1.898
1.888
1.880
1.874
1.867
1.862
1.854
1.850
1.839
1.835
1.820
1.485
Cl
CN
N
S
2z
1.01
1.00
4.04
2.11
1.00
2.00
2.05
3.01
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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131.789
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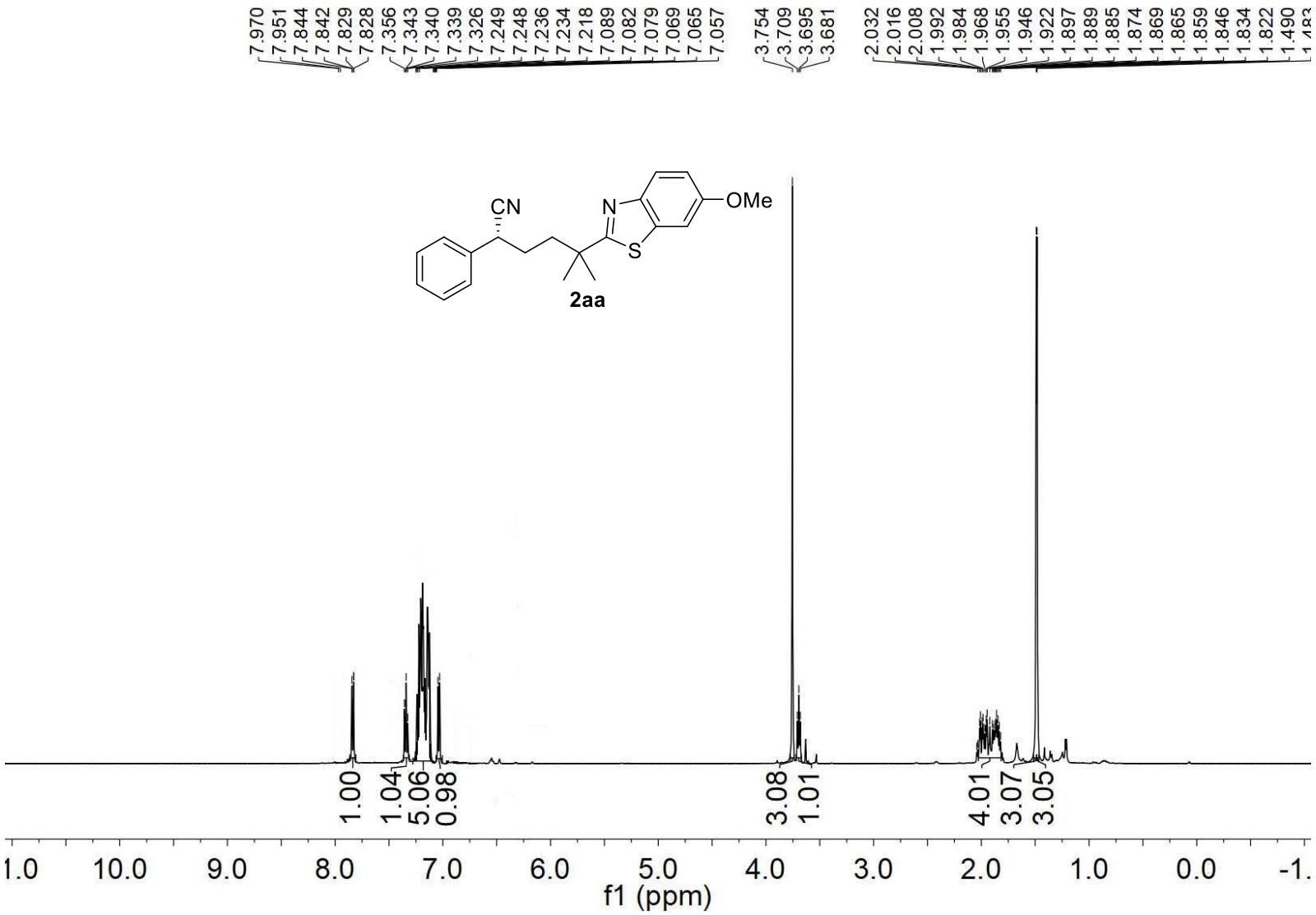
128.072
127.142
125.162
122.651
122.185
120.486
77.318
77.000
76.681
41.206
40.652
37.451
31.067
28.764
28.231
Cl
CN
N
S
2z
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.828
7.356
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7.340
7.339
7.326
7.249
7.248
7.236
7.234
7.218
7.089
7.082
7.079
7.069
7.065
7.057
3.754
3.709
3.695
3.681
2.032
2.016
2.008
1.992
1.984
1.968
1.955
1.946
1.922
1.897
1.889
1.885
1.874
1.869
1.865
1.859
1.846
1.834
1.822
1.490
CN
N
OMe
S
2aa
1.00
1.04
5.06
0.98
3.08
1.01
4.01
3.07
3.05
1.0
10.0
9.0
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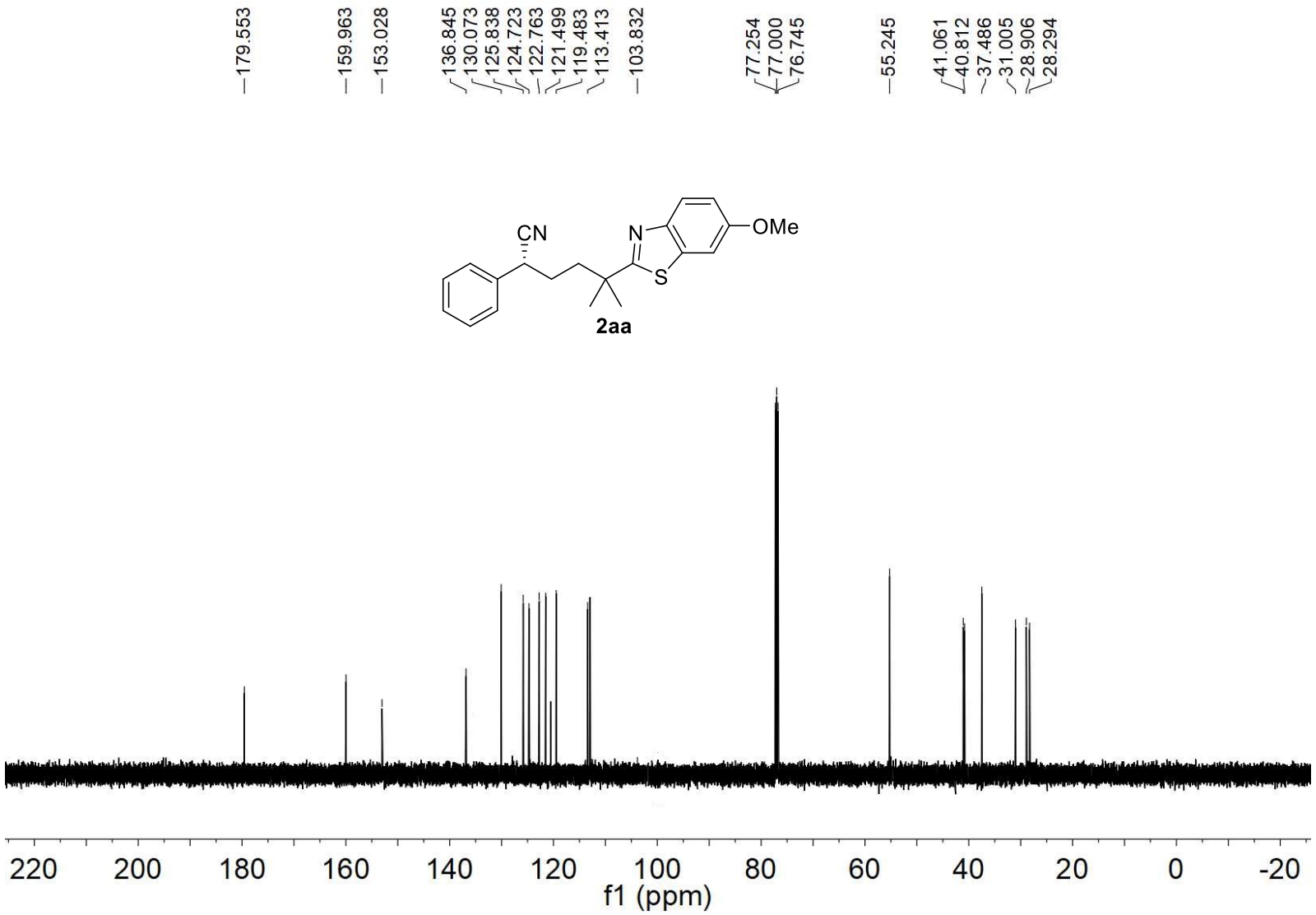
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.
f1 (ppm)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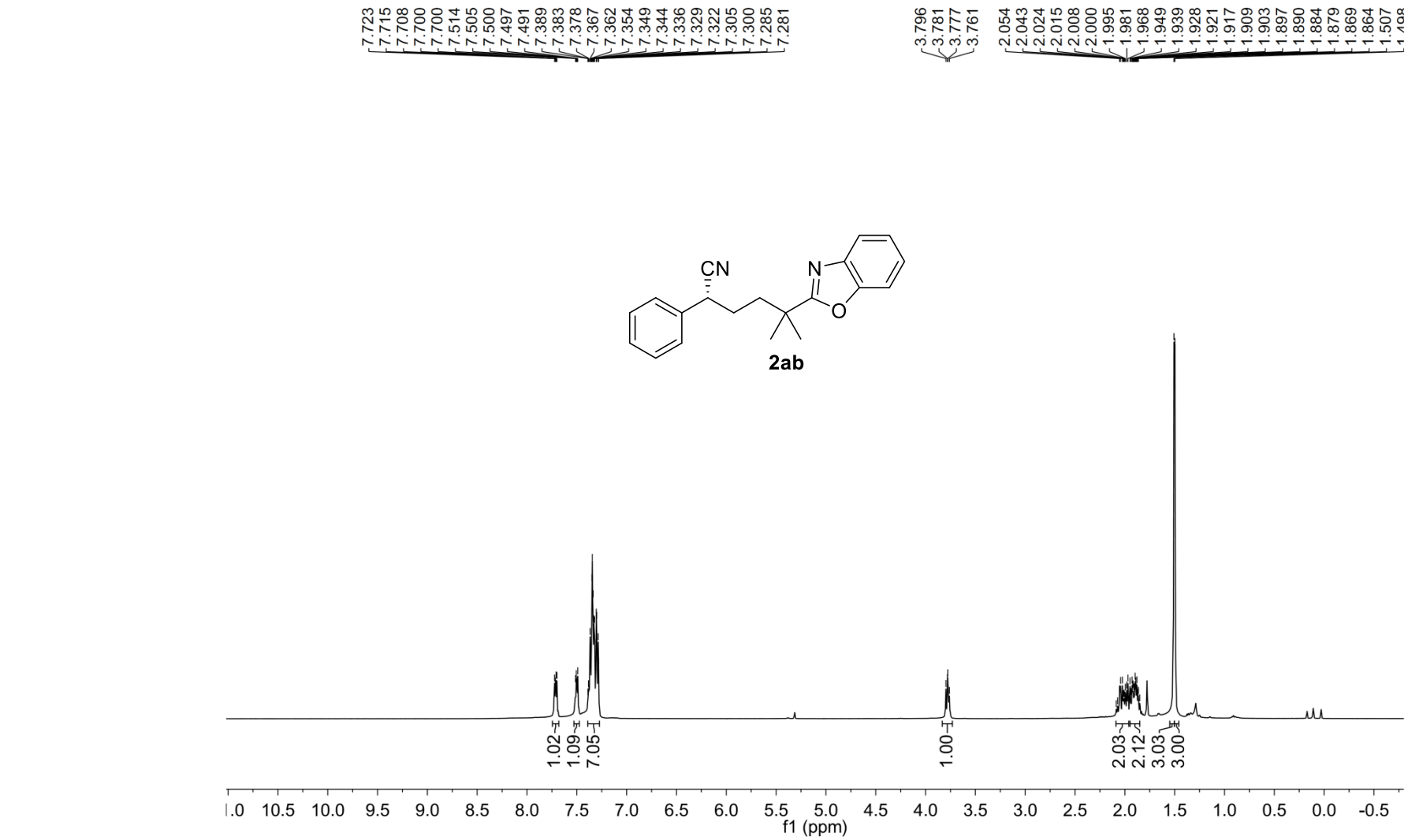
136.845
130.073
125.838
124.723
122.763
121.499
119.483
113.413
103.832
77.254
77.000
76.745
55.245
41.061
40.812
37.486
31.005
28.906
28.294
CN
N
OMe
S
2aa
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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7.500
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7.389
7.383
7.378
7.367
7.362
7.354
7.349
7.344
7.336
7.329
7.322
7.305
7.300
7.285
7.281
3.796
3.781
3.777
3.761
2.054
2.043
2.024
2.015
2.008
2.000
1.995
1.981
1.968
1.949
1.939
1.928
1.921
1.917
1.909
1.903
1.897
1.890
1.884
1.879
1.869
1.864
1.507
CN
N
O
2ab
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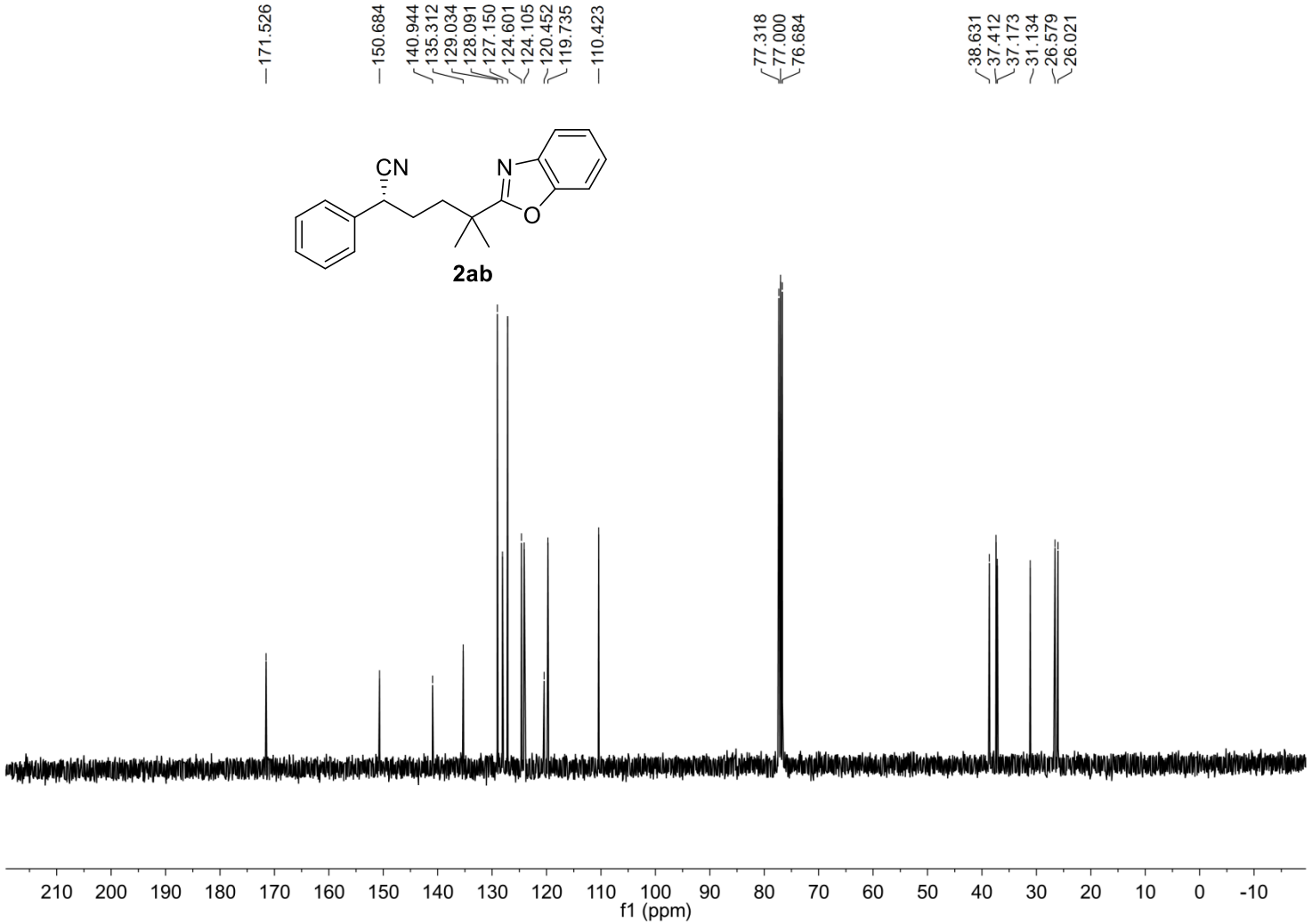
1.09
7.05
1.00
2.03
2.12
3.03
3.00
f1 (ppm)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127.150
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120.452
119.735
110.423
77.318
77.000
76.684
38.631
37.412
37.173
31.134
26.579
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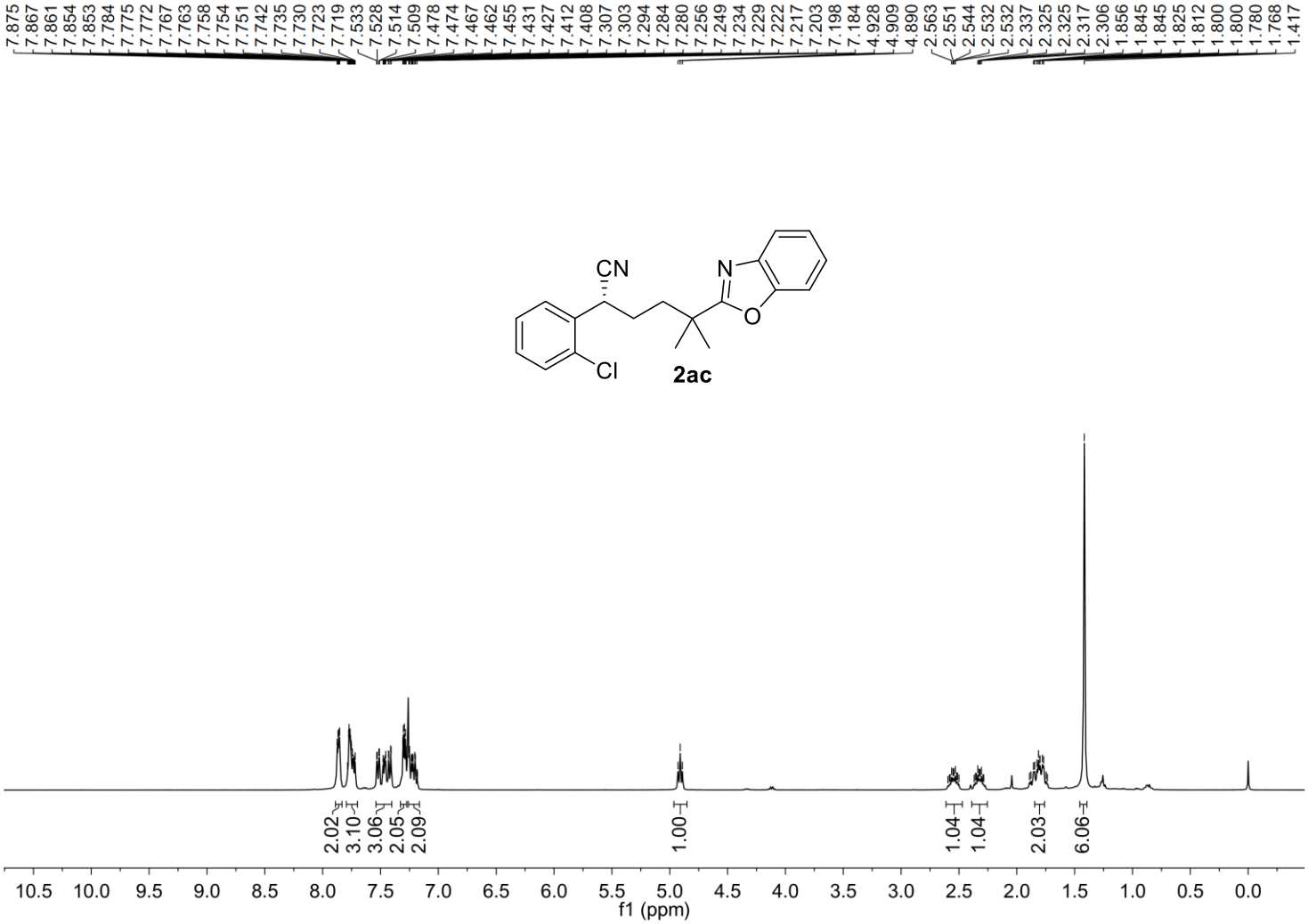
CN
N
O
2ab
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.751
7.742
7.735
7.730
7.723
7.719
7.533
7.528
7.514
7.509
7.478
7.474
7.467
7.462
7.455
7.431
7.427
7.412
7.408
7.307
7.303
7.294
7.284
7.280
7.256
7.249
7.234
7.229
7.222
7.217
7.203
7.198
7.184
4.928
4.909
4.890
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2.551
2.544
2.532
2.532
2.337
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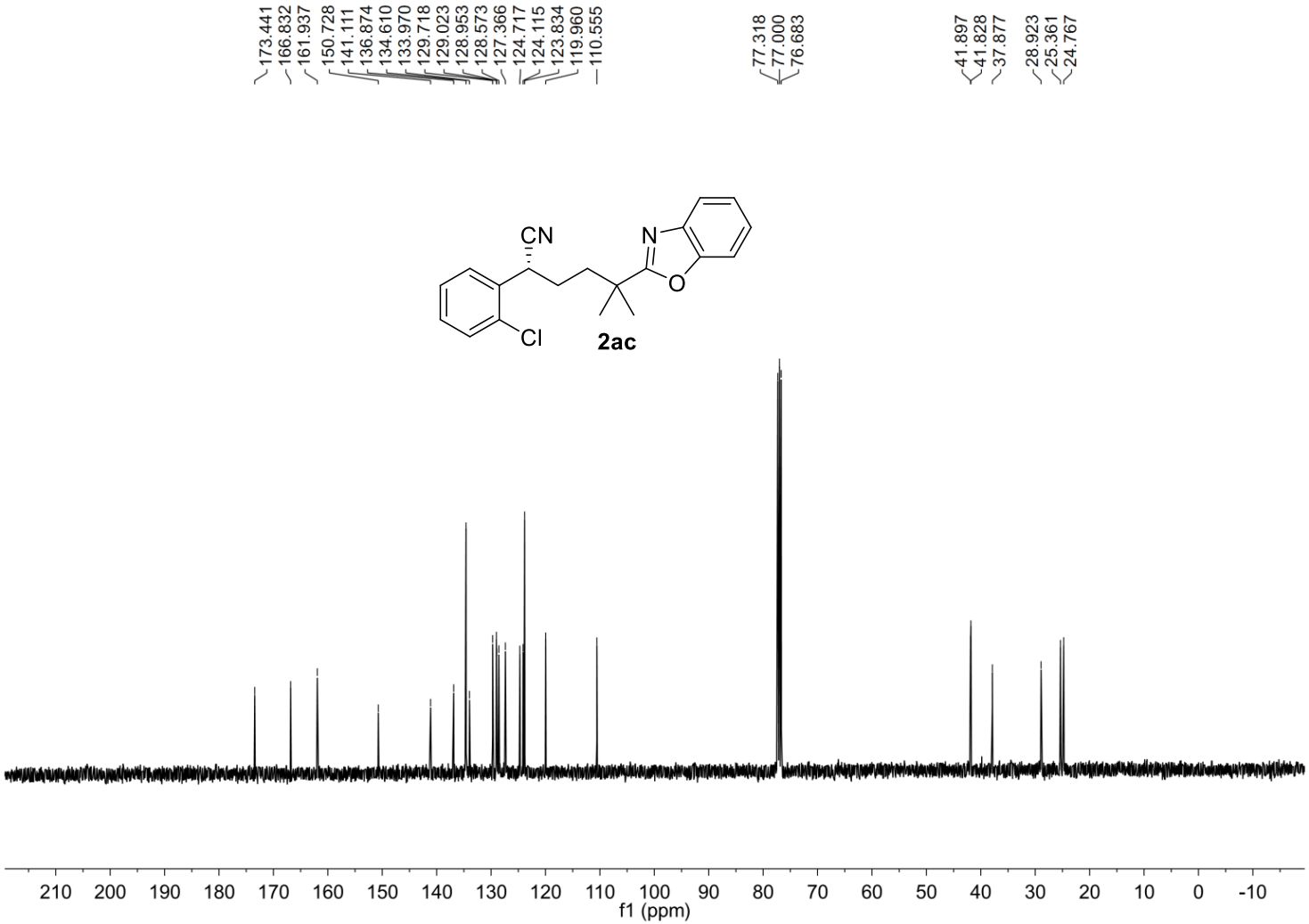
2.325
2.317
2.306
1.856
1.845
1.845
1.825
1.812
1.800
1.800
1.780
1.768
1.417
CN
N
O
Cl
2ac
2.02
3.10
3.06
2.05
2.09
1.00
1.04
1.04
2.03
6.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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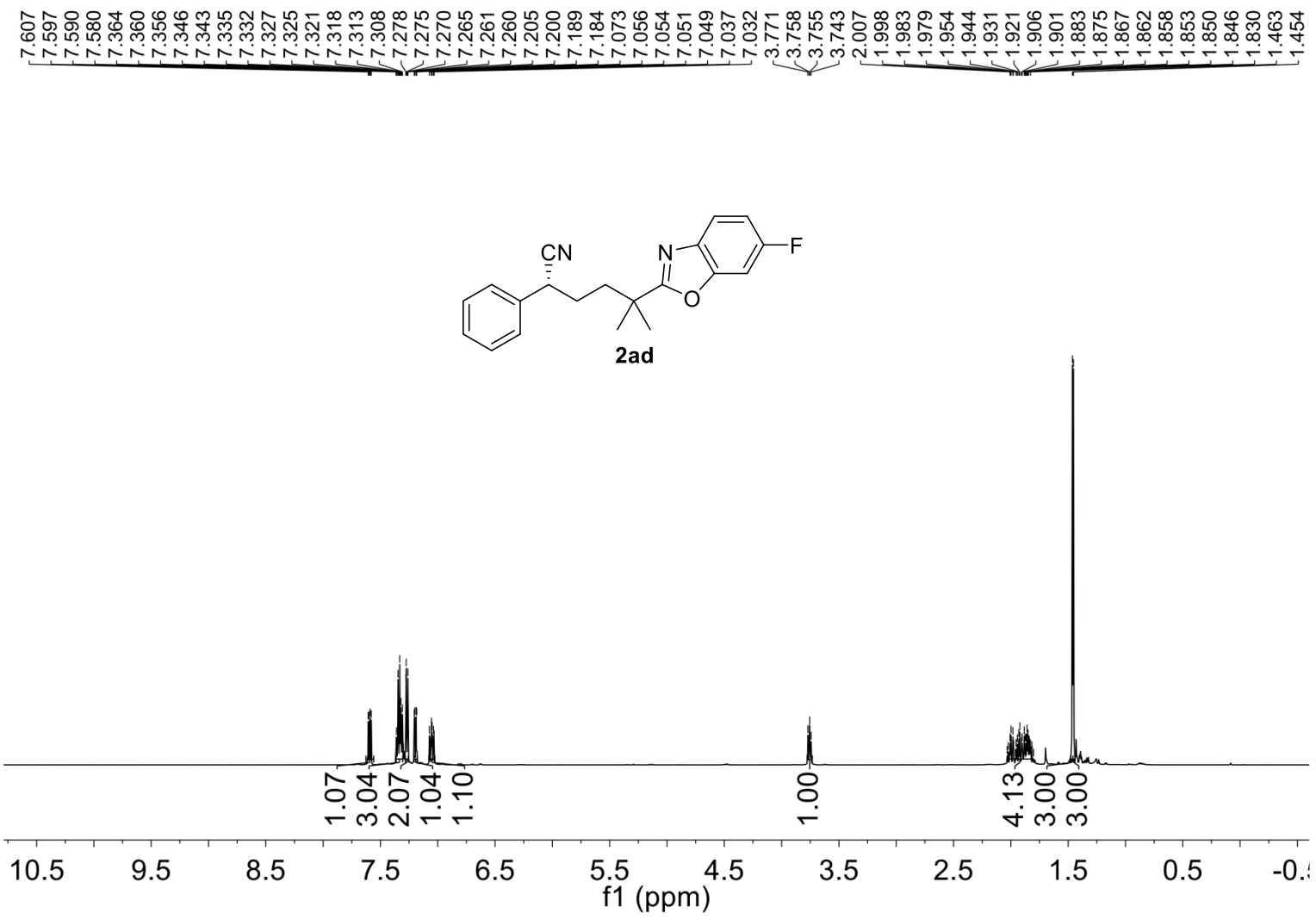
128.953
128.573
127.366
124.717
124.115
123.834
119.960
110.555
77.318
77.000
76.683
41.897
41.828
37.877
28.923
25.361
24.767
CN
N
O
Cl
2ac
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.332
7.327
7.325
7.321
7.318
7.313
7.308
7.278
7.275
7.270
7.265
7.261
7.260
7.205
7.200
7.189
7.184
7.073
7.056
7.054
7.051
7.049
7.037
7.032
3.771
3.758
3.755
3.743
2.007
1.998
1.983
1.979
1.954
1.944
1.931
1.921
1.906
1.901
1.883
1.875
1.867
1.862
1.858
1.853
1.850
1.846
1.830
1.463
1.454
CN
N
F
O
2ad
1.07
3.04
2.07
1.04
1.10
1.00
4.13
3.00
3.00
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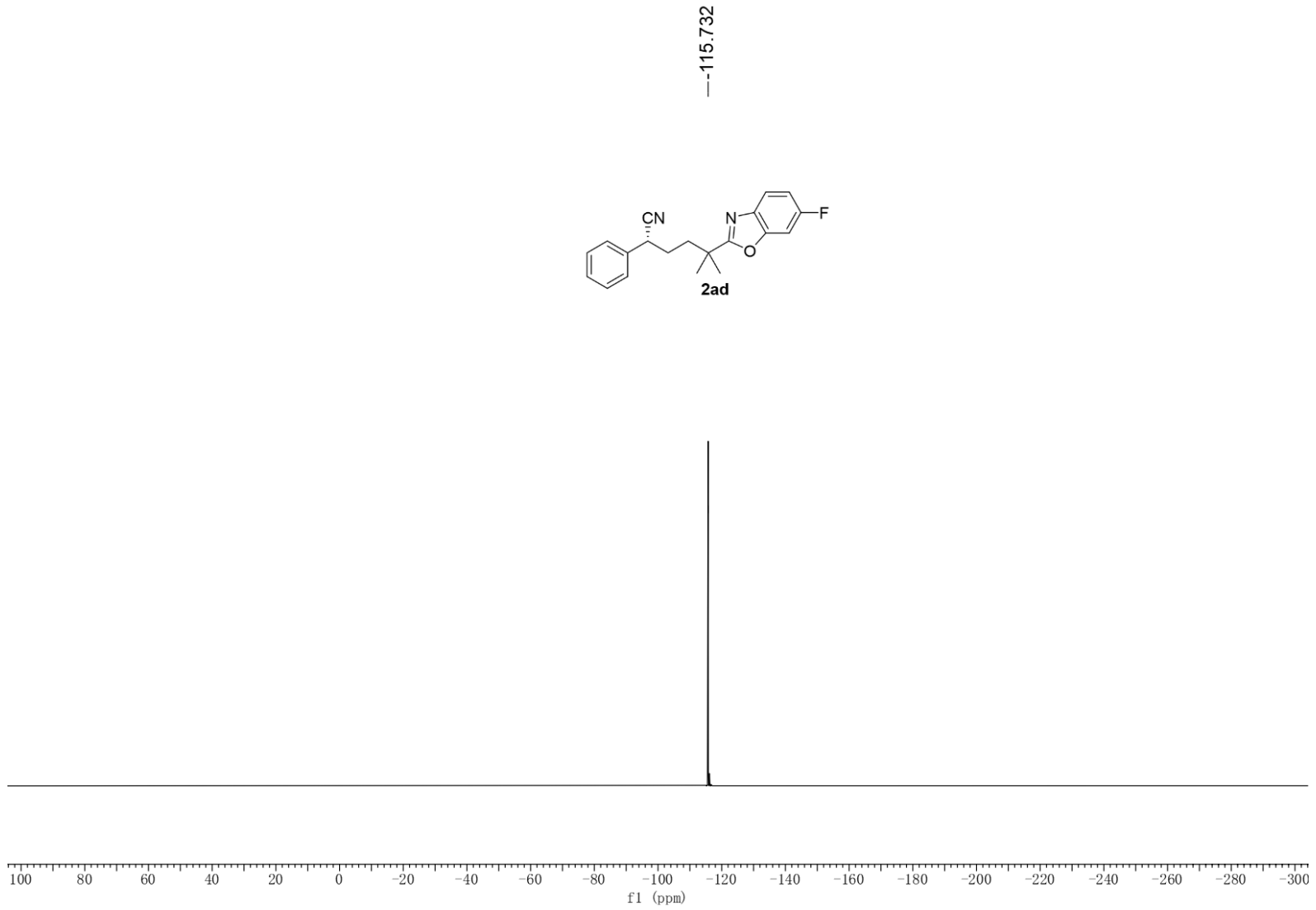
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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CN
N
F
O
2ad
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80
60
40
20
0
-20
-40
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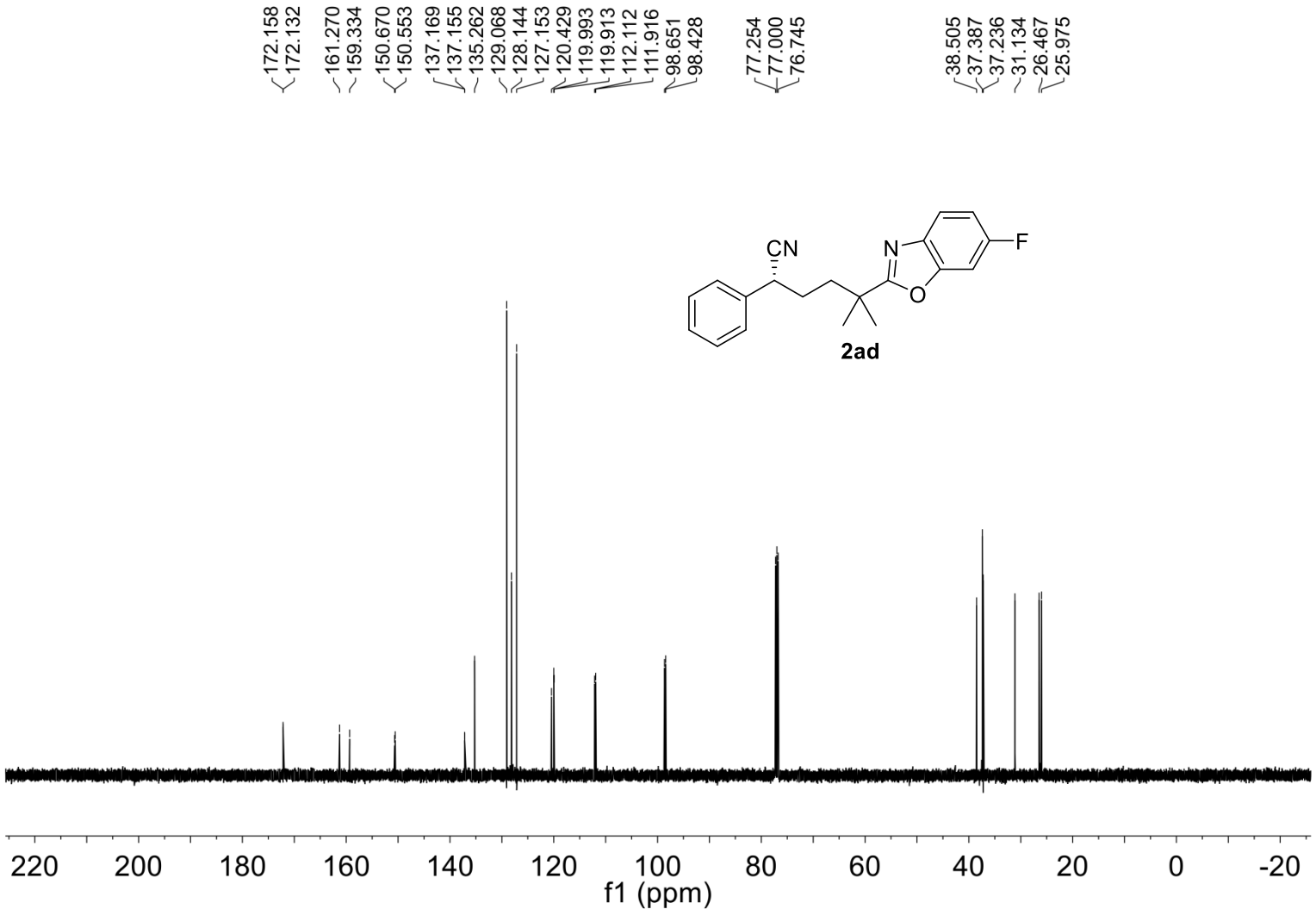
-100
-120
-140
-160
-180
-200
-220
-240
-260
-280
-300
f1 (ppm)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137.155
135.262
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128.144
127.153
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119.993
119.913
112.112
111.916
98.651
98.428
77.254
77.000
76.745
38.505
37.387
37.236
31.134
26.467
25.975
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220
200
180
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140
120
100
80
60
40
20
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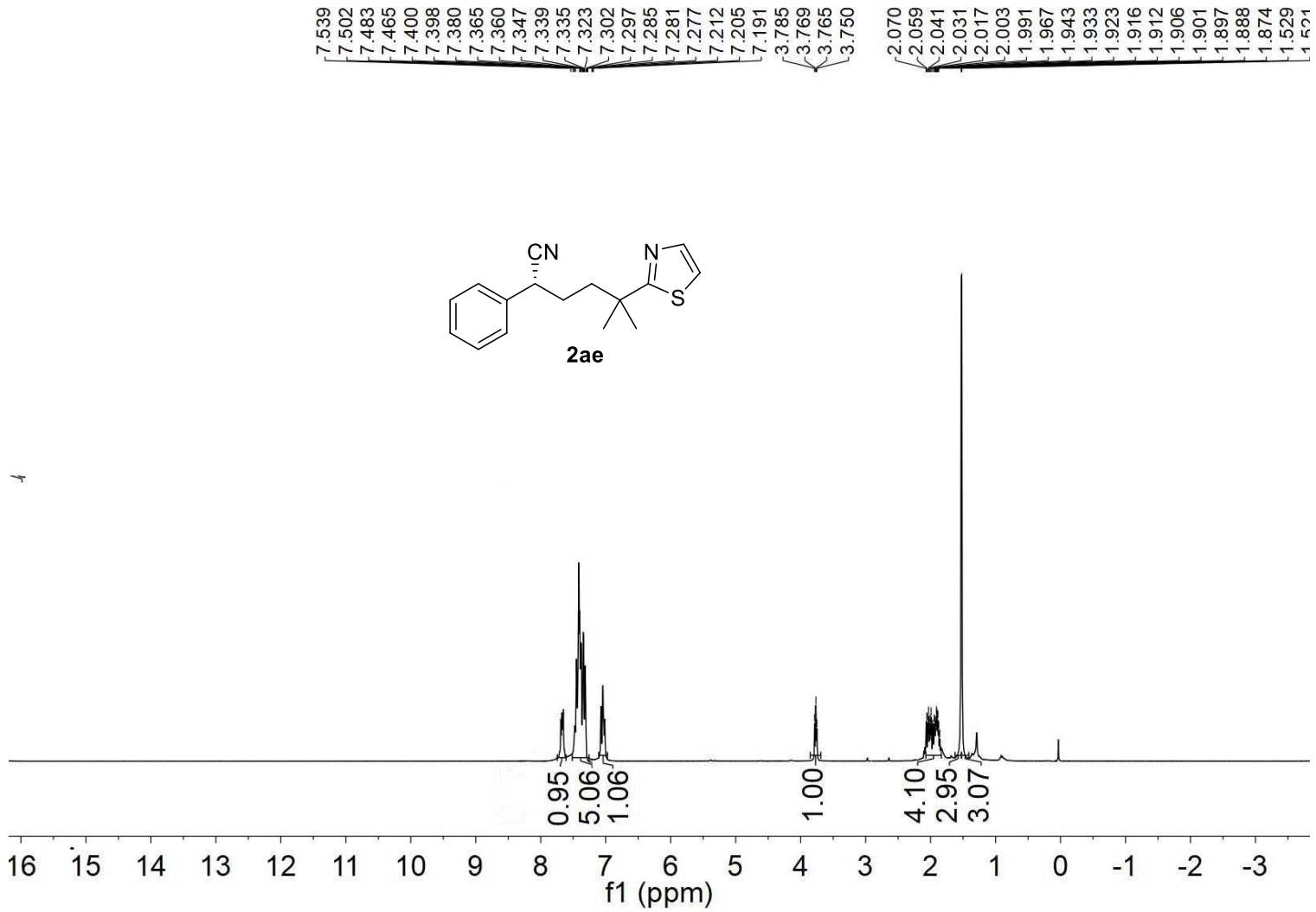
-20
f1 (ppm)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7.302
7.297
7.285
7.281
7.277
7.212
7.205
7.191
3.785
3.769
3.765
3.750
2.070
2.059
2.041
2.031
2.017
2.003
1.991
1.967
1.943
1.933
1.923
1.916
1.912
1.906
1.901
1.897
1.888
1.874
1.529
CN
N
S
2ae
0.95
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4.10
2.95
3.07
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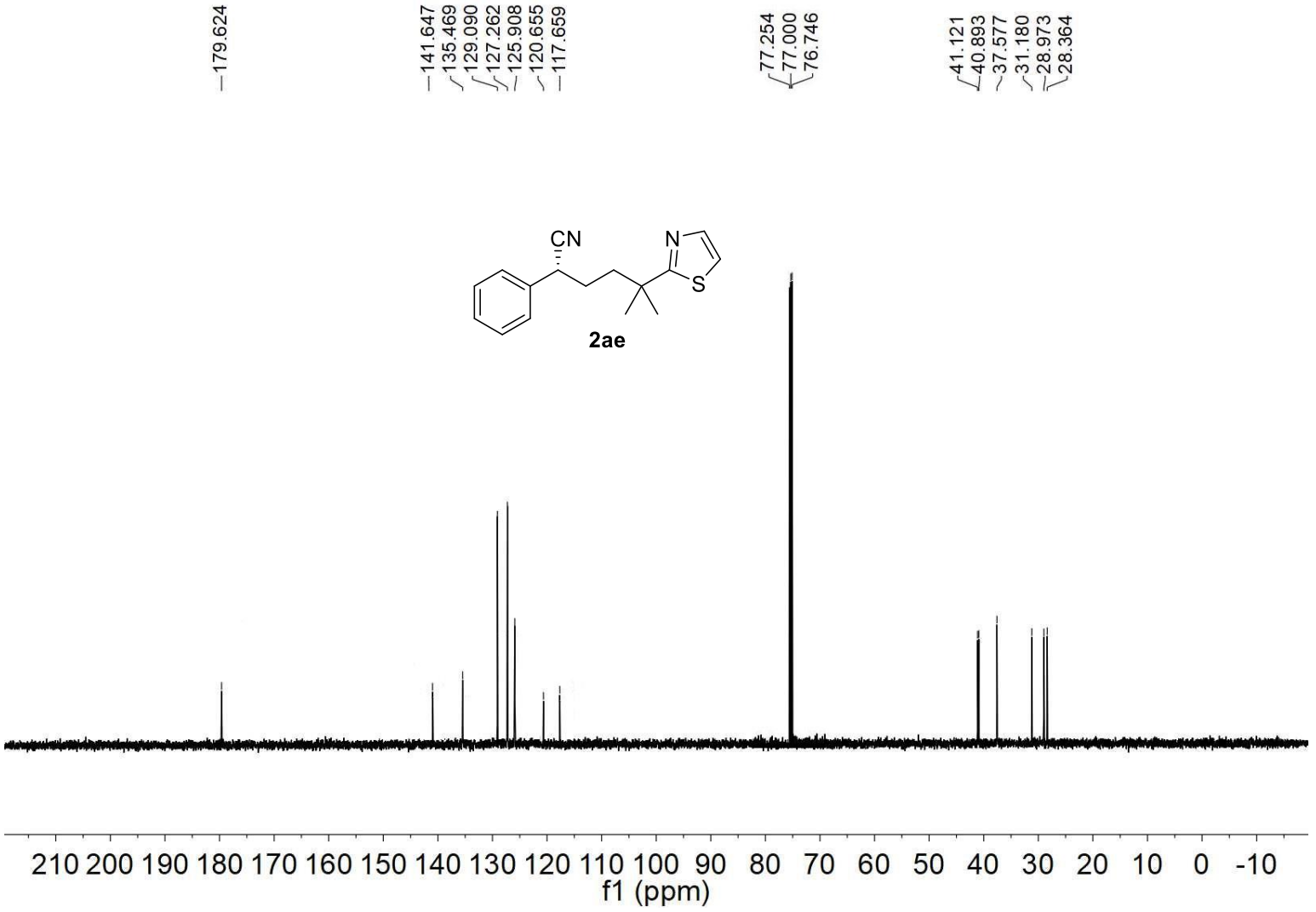
f1 (ppm)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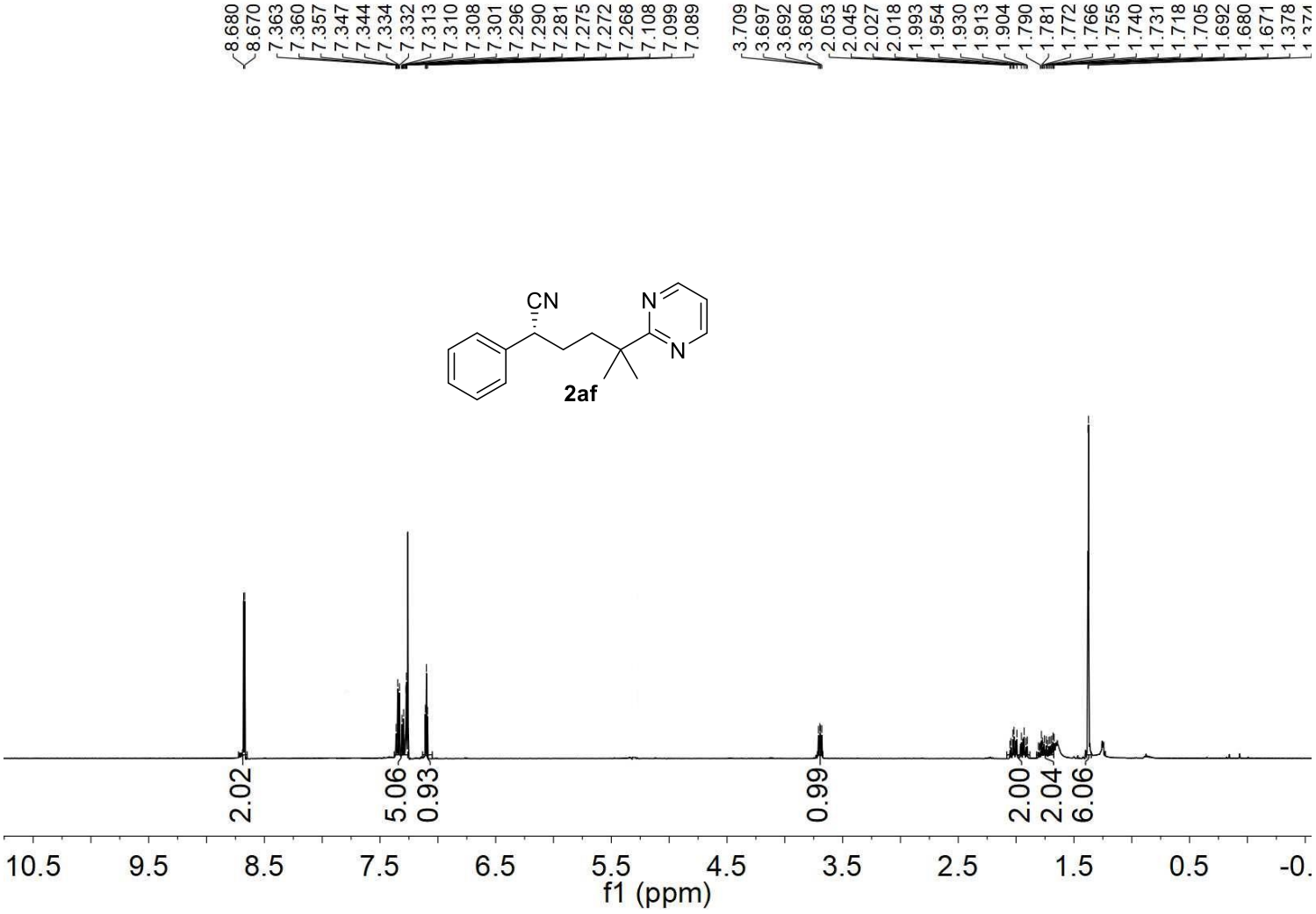
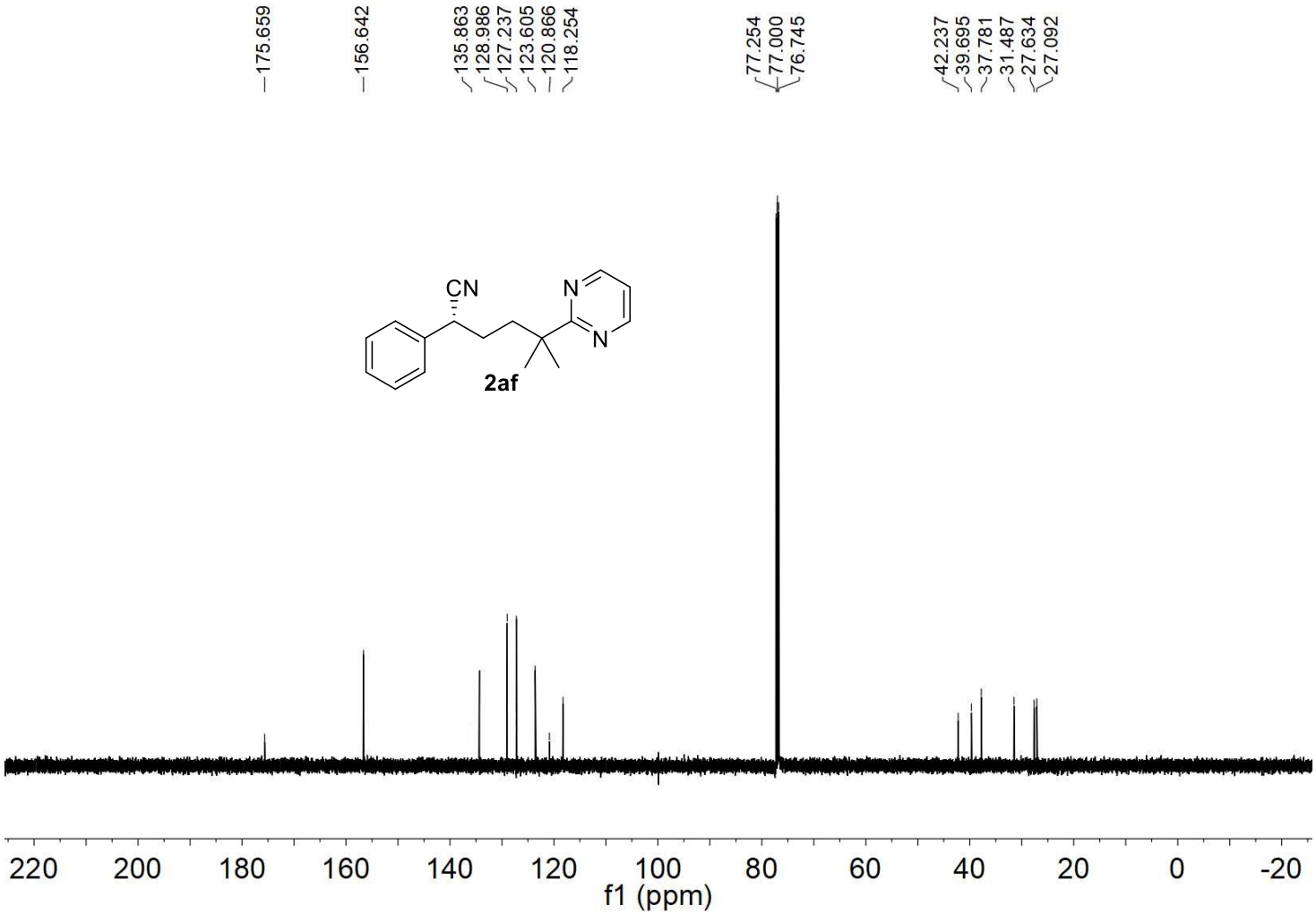
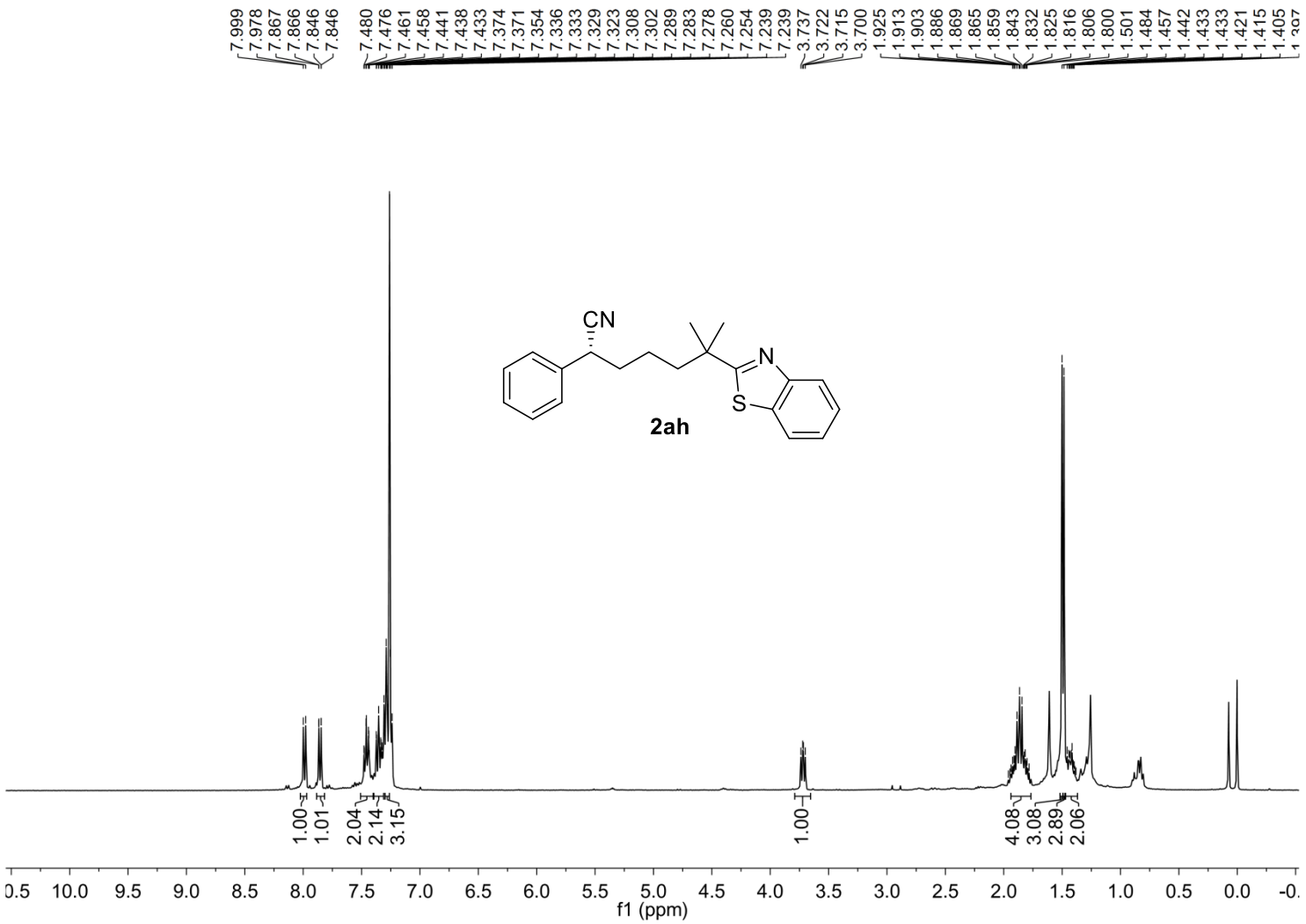
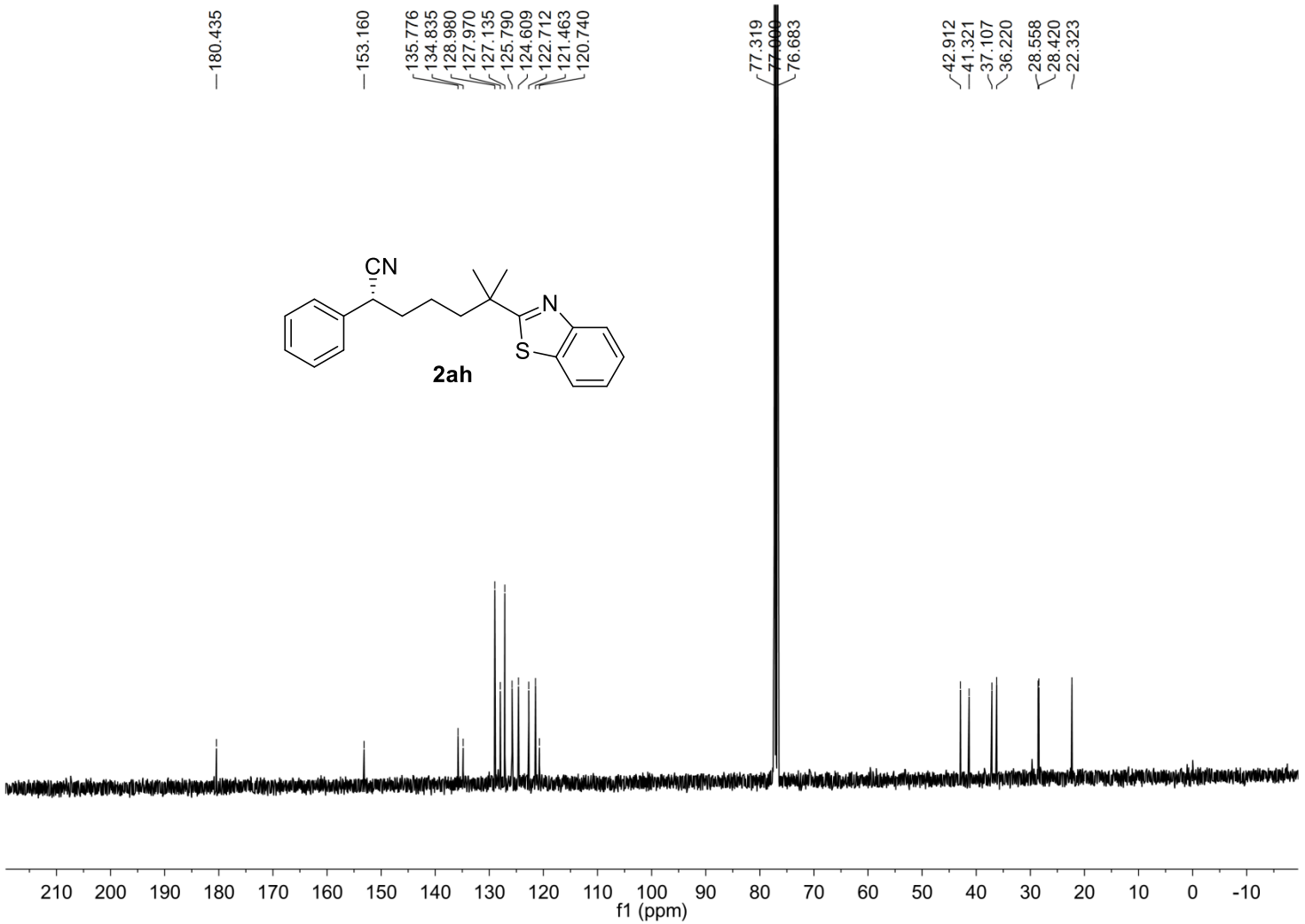
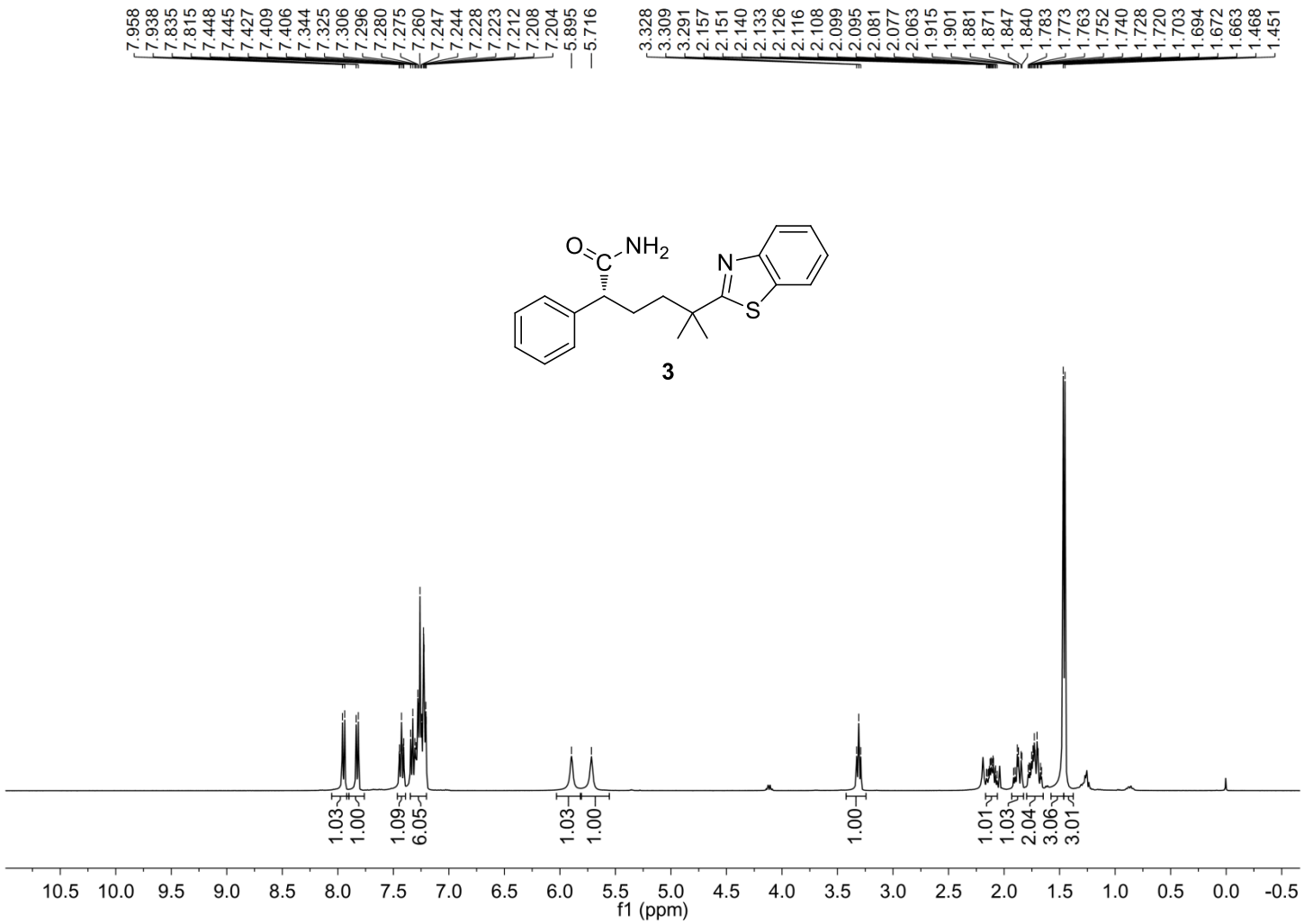
129.090
127.262
125.908
120.655
117.659
77.254
77.000
76.746
41.121
40.893
37.577
31.180
28.973
28.364
CN
N
S
2ae
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.680
8.670
7.363
7.360
7.357
7.347
7.344
7.334
7.332
7.313
7.310
7.308
7.301
7.296
7.290
7.281
7.275
7.272
7.268
7.108
7.099
7.089
3.709
3.697
3.692
3.680
2.053
2.045
2.027
2.018
1.993
1.954
1.930
1.913
1.904
1.790
1.781
1.772
1.766
1.755
1.740
1.731
1.718
1.705
1.692
1.680
1.671
CN
N
N
2af
2.02
5.06
0.93
0.99
2.00
2.04
6.06
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)


175.659
156.642
135.863
128.986
127.237
123.605
120.866
118.254
77.254
77.000
76.745
42.237
39.695
37.781
31.487
27.634
27.092
CN
N
N
2af
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)


7.999
7.978
7.867
7.866
7.846
7.846
7.480
7.476
7.461
7.458
7.441
7.438
7.433
7.374
7.371
7.354
7.336
7.333
7.329
7.323
7.308
7.302
7.289
7.283
7.278
7.260
7.254
7.239
7.239
3.737
3.722
3.715
3.700
1.925
1.913
1.903
1.886
1.869
1.865
1.859
1.843
1.832
1.825
1.816
1.806
1.800
1.501
1.484
1.457
1.442
1.433
1.433
1.421
1.415
1.405
CN
N
S
2ah
1.00
1.01
2.04
2.14
3.15
1.00
4.08
3.08
2.89
2.06
f1 (ppm)


180.435
153.160
135.776
134.835
128.980
127.970
127.135
125.790
124.609
122.712
121.463
120.740
77.319
77.000
76.683
42.912
41.321
37.107
36.220
28.558
28.420
22.323
CN
N
S
2ah
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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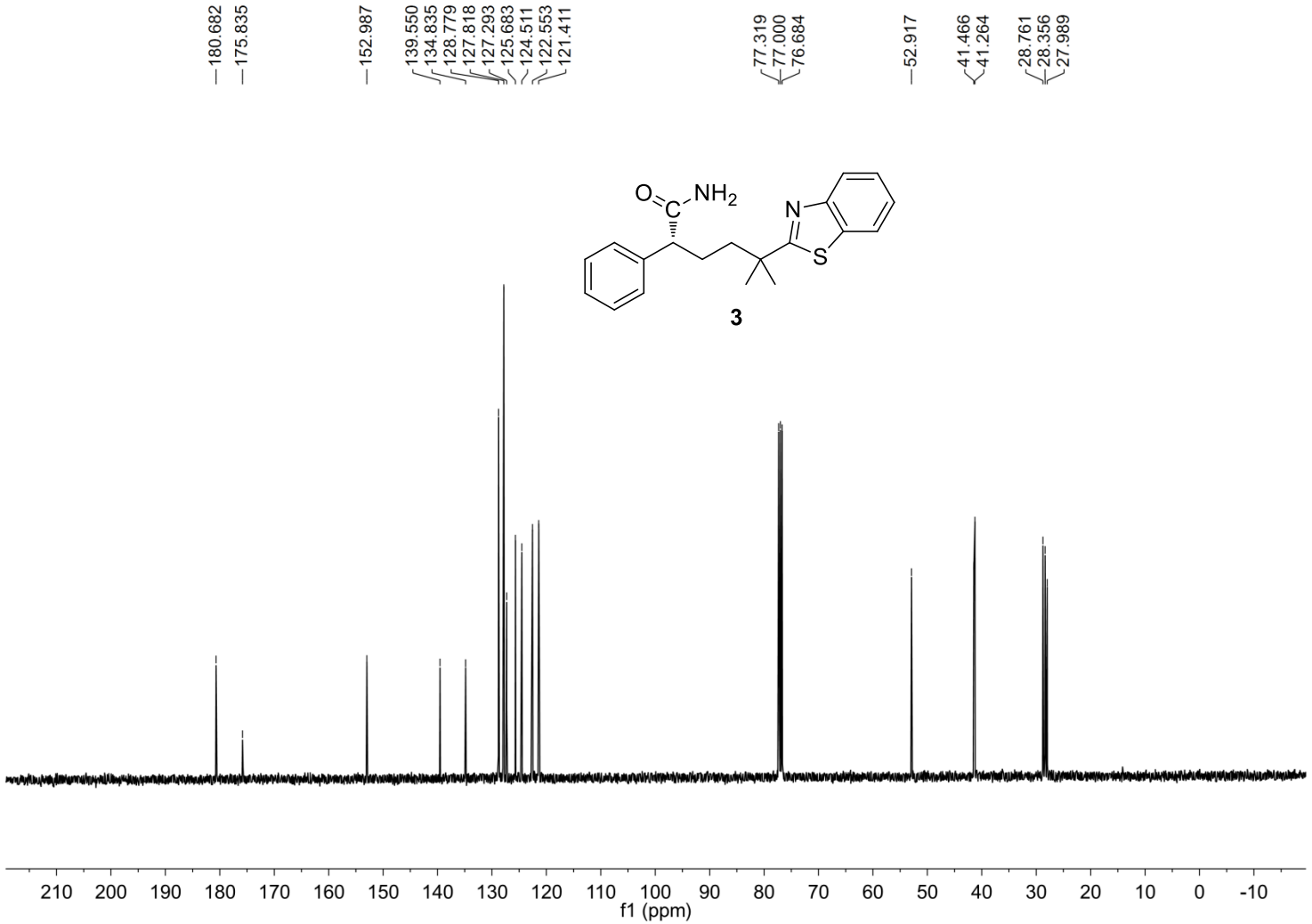
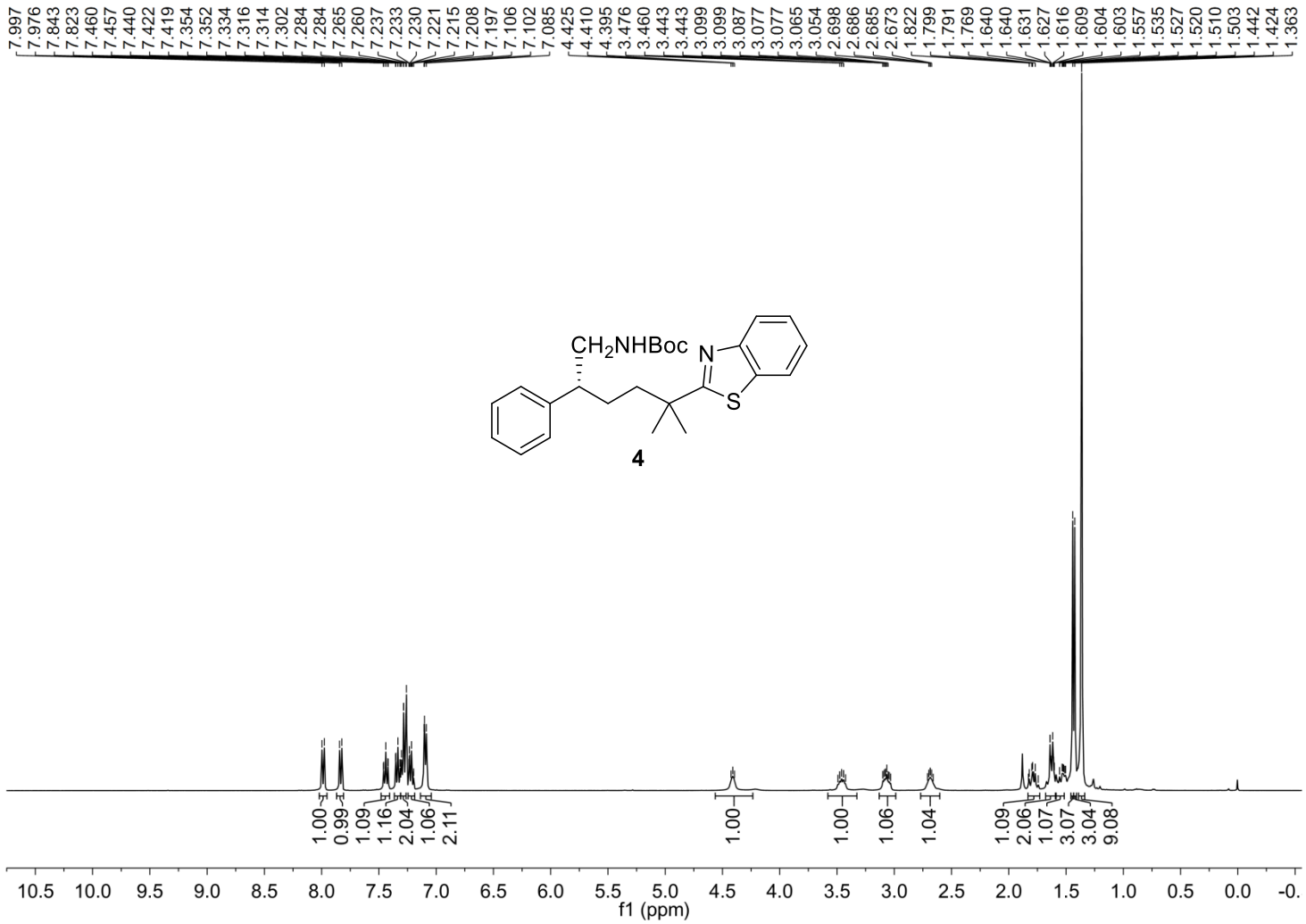
7.835
7.815
7.448
7.445
7.427
7.409
7.406
7.344
7.325
7.306
7.296
7.280
7.275
7.260
7.247
7.244
7.228
7.223
7.212
7.208
7.204
5.895
5.716
3.328
3.309
3.291
2.157
2.151
2.140
2.133
2.126
2.116
2.108
2.099
2.095
2.081
2.077
2.063
1.915
1.901
1.881
1.871
1.847
1.840
1.783
1.773
1.763
1.752
1.740
1.728
1.720
1.703
1.694
1.672
1.663
1.468
1.451
O
NH2
C
N
S
3
1.03
1.00
1.09
6.05
1.03
1.00
1.00
1.01
1.03
2.04
3.06
3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


180.682
175.835
152.987
139.550
134.835
128.779
127.818
127.293
125.683
124.511
122.553
121.411
77.319
77.000
76.684
52.917
41.466
41.264
28.761
28.356
27.989
O
C
NH2
N
S
3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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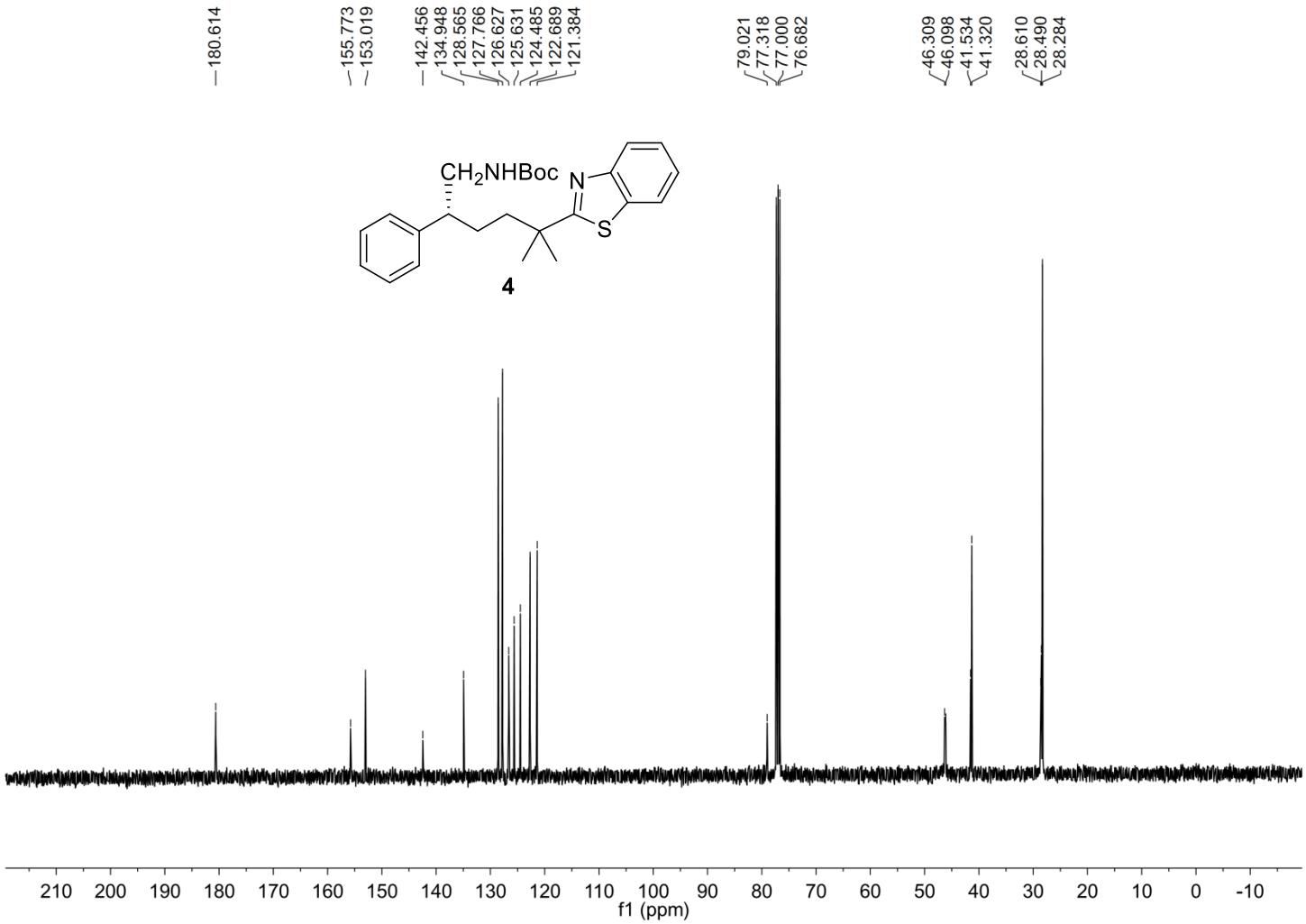
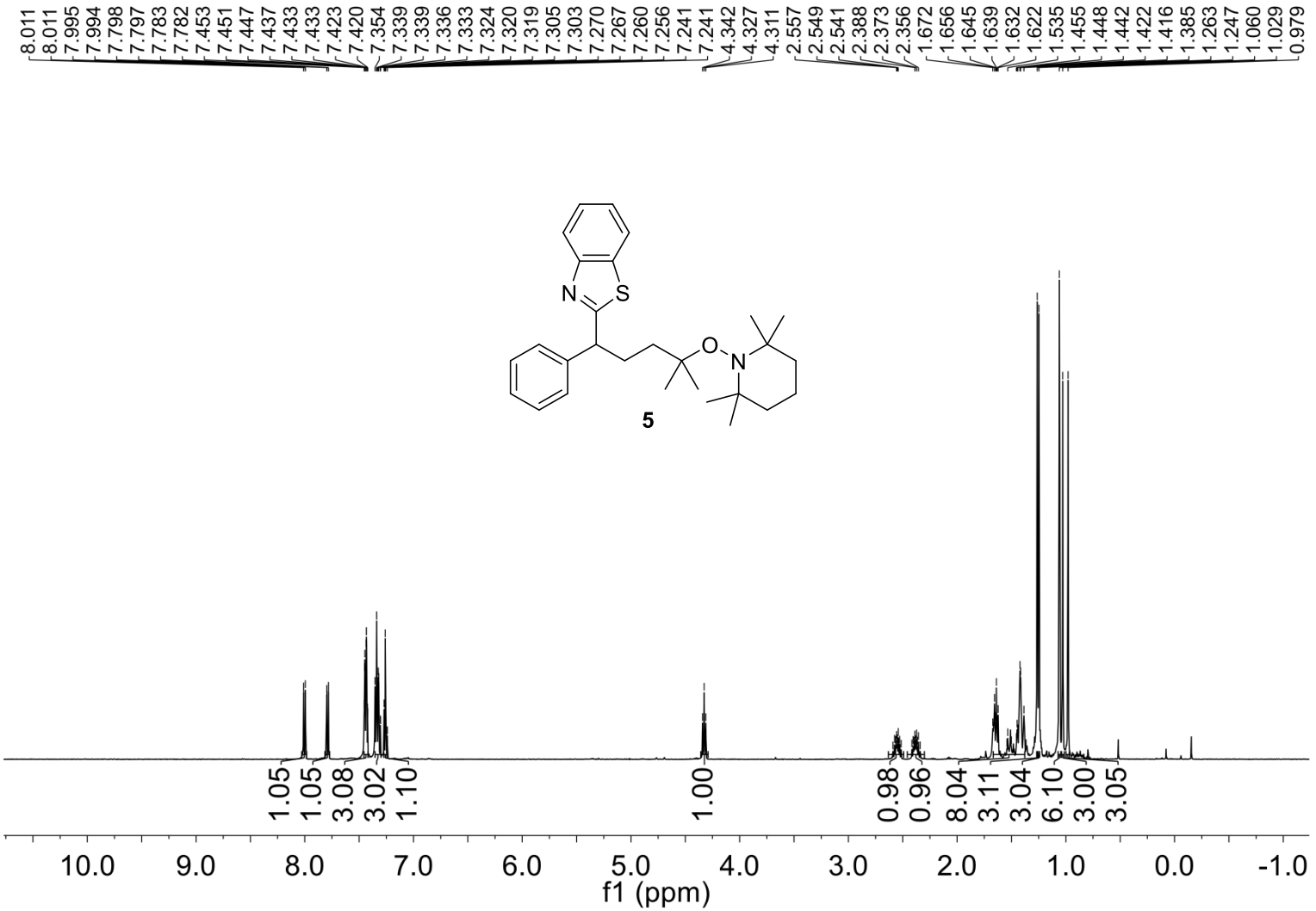
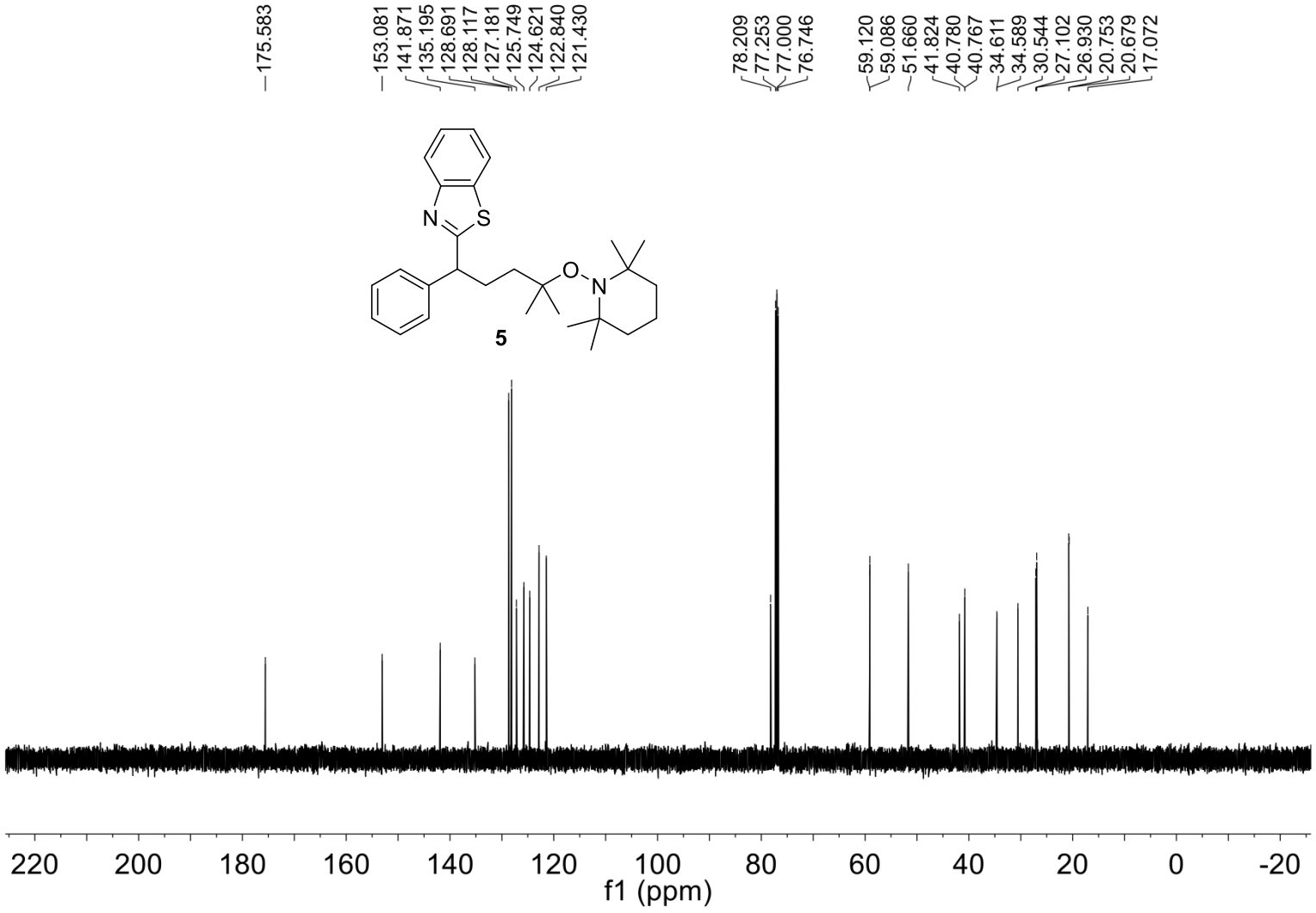
7.976
7.843
7.823
7.460
7.457
7.440
7.422
7.419
7.354
7.352
7.334
7.316
7.314
7.302
7.284
7.284
7.265
7.260
7.237
7.233
7.230
7.221
7.215
7.208
7.197
7.106
7.102
7.085
4.425
4.410
4.395
3.476
3.460
3.443
3.443
3.099
3.099
3.087
3.077
3.077
3.065
3.054
2.698
2.686
2.685
2.673
1.822
1.799
1.791
1.769
1.640
1.640
1.631
1.627
1.616
1.609
1.604
1.603
1.557
1.535
1.527
1.520
1.510
1.503
1.442
1.424
1.363
CH2NHBoc
N
S
4
1.00
0.99
1.09
1.16
2.04
1.06
2.11
1.00
1.00
1.06
1.04
1.09
2.06
1.07
3.07
3.04
9.08
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)


180.614
155.773
153.019
142.456
134.948
128.565
127.766
126.627
125.631
124.485
122.689
121.384
79.021
77.318
77.000
76.682
46.309
46.098
41.534
41.320
28.610
28.490
28.284
CH2NHBoc
N
S
4
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.011
8.011
7.995
7.994
7.798
7.797
7.783
7.782
7.453
7.451
7.447
7.437
7.433
7.433
7.423
7.420
7.354
7.339
7.339
7.336
7.333
7.324
7.320
7.319
7.305
7.303
7.270
7.267
7.260
7.256
7.241
7.241
4.342
4.327
4.311
2.557
2.549
2.541
2.388
2.373
2.356
1.672
1.656
1.645
1.639
1.632
1.622
1.535
1.455
1.448
1.442
1.422
1.416
1.385
1.263
1.247
1.060
1.029
0.979
N
S
O
N
5
1.05
1.05
3.08
3.02
1.10
1.00
0.98
0.96
8.04
3.11
3.04
6.10
3.00
3.05
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)


175.583
153.081
141.871
135.195
128.691
128.117
127.181
125.749
124.621
122.840
121.430
78.209
77.253
77.000
76.746
59.120
59.086
51.660
41.824
40.780
40.767
34.611
34.589
30.544
27.102
26.930
20.753
20.679
17.072
N
S
O
N
5
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)