Supporting Information

Enantioselective Synthesis of Arylglycine Derivatives by Direct C–H Oxidative Cross-coupling

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Contents:

General

All reactions involving air- or moisture-sensitive reagents were carried out under an argon atmosphere. All solvents were distilled under Ar before use. All chemicals were purchased from Aldrich and J&K Chemical and used without further purification. Thin-layer chromatography (TLC) was performed using 60 mesh silica gel plates visualized with short-wavelength UV light (254 nm). Silica gel 60 (230 - 400 mesh) was used for column chromatography. ^{1}H and ^{13}C NMR spectra were recorded using $CDCl_3$ solvent on a Bruker 400 MHz spectrometer at 298 K. The chemical shift is given indimensionless δ values and is frequency referenced relative to TMS in ^{1}H and ^{13}C NMR spectroscopy. Mass data were measured with a Thermo Scientific DSQ II mass spectrometer. Enantiomeric excess is determined by HPLC analysis (waters 600-2996). IR spectra were recorded on an FT-IR spectrometer and only major peaks are reported in cm^{-1}.

Experimental Section

1. Synthesis of Ethyl *N*-Aryl Glycine Esters 1a[1]

To the solution of ethyl bromoacetate (20.0 mmol) in anhydrous ethanol (3.0 mL) was added substituted benzenamine (20.0 mmol) and anhydrous NaOAc (20.0 mmol). The reaction mixture was refluxed for 6-10 h under N_2. Then, the mixture was filtered, and the filtrate was cooled at ice bath to precipitate. The precipitation was recrystallized from ethanol-hexane, giving the desired ethyl N-aryl glycine ester **1a**.

2. Synthesis of $T^{+}BF4^{-}$[2]

In a 250 mL round bottom flask, an aqueous solution of HBF_4 (48% aqueous solution, 10.9 mL, 83.2 mmol) was added to the heterogeneous solution of 1 (11.367g, 72.8 mmol) in purified water (31.15 mL). The reaction mixture was stirred at room temperature for 30 min to give a yellow orange mixture. In ice bath, an aqueous solution of NaOCl (5% aqueous solution, 48.5mL, 35.7 mmol) was added to the solution for 2 h. The mixture is filtered with grass filter and the yellow solid was washed with cooled water (4 ^{o}C, 4 × 20 mL) and dichloromethane (3 × 30 mL). After

1 J. Xie and Z-Z. Huang, *Angew. Chem. Int. Ed.* **2010**, *49*, 10181.
2 Y. Yonekuta, K. Oyaizu and H. Nishide, *Chem. Lett.* **2007**, *36*, 866.

dried under high vacuum at room temperature overnight, the product is obtained as a bright yellow solid.

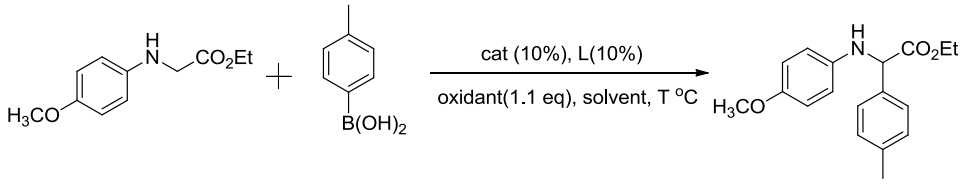
3. Synthesis of 3a and 3b[3]

2-Bromoacetyl bromide (2.4 g, 1.2 mmol) in CH_2Cl_2 (10 mL) was added dropwise to a mixture of $MeNH_2$ (1.0 g, 30 wt% in H_2O, 1.0 mmol) and K_2CO_3 (1.66 g, 1.2 mmol) in CH_2Cl_2/H_2O (30 mL/10 mL) at 0 ℃. The mixture was then allowed to warm up to room temperature and stirred for 6 h. Then, the organic layer was separated and the aqueous layer was extracted with CH_2Cl_2 (3*5 mL). The organic layers were combined and dried over Na_2SO_4, and CH2Cl2 was removed in vacuo. Subsequently, EtOH (5 mL), *p*-anisidine (1.23 g, 1 mmol), and NaOAc (0.84 g, 1 mmol) were added to the residue. The resulting mixture was refluxed for 6 h and was filtered. The solvent of the filtrate was removed in vacuo. Recrystallization (CH_2Cl_2/hexanes) gave the pure product 2-(4-methoxyphenylamino)-*N*-methylacetamide (**3a**).

$SOCl_2$ (3.6 g, 30 mmol) was added slowly to EtOH (30mL) at 0 ℃. After stirring at this temperature for 10 min, glycine (0.75 g, 10 mmol) was added to the solution. Then, the reaction was stirred at 70 ℃ for 3 h. EtOH was removed in vacuo. The resulting solid was then mixed with CH_2Cl_2 (30 mL) and NEt_3 (2.2 g, 22 mmol). The reaction mixture was cooled to -78 ℃, and $BrCH_2COBr$ (2.0 g, 10 mmol) was added dropwise to the solution at this temperature. The solution was allowed to warm up to room temperature and the stirring was continued for 6 h. After that, the solution was washed with H_2O (10 mL). The organic layer was dried over Na_2SO_4, and CH_2Cl_2 was removed in vacuo to afford $BrCH_2CONHCH_2CO_2Et$ (1.8 g, 81%). NaOAc (0.50 g, 6 mmol), *p*-anisole (0.74 g, 6 mmol), and $BrCH_2CONHCH_2CO_2Et$ (1.1 g, 5 mmol) were successively added to EtOH (4 mL). The reaction tube was heated at 80 ℃ for 6 h. EtOH was removed in vacuo and the residue was dissolved in CH_2Cl_2 (20 mL) and washed with H_2O (5 mL). The organic layer was dried over Na_2SO_4, and CH_2Cl_2 was removed in vacuo. Flash column chromatography on silica gel by using ethyl acetate/hexanes (1:1) furnished the final product *N*-(*N*-*p*-methoxyphenylglycyl)-glycine ethyl ester (**4a**).

3 L. Zhao, O. Basl é and C-J. Li, *Proc. Natl. Acad. Sci. USA*, **2009**, *106*, 4107.

4. Optimization of Reaction Conditions

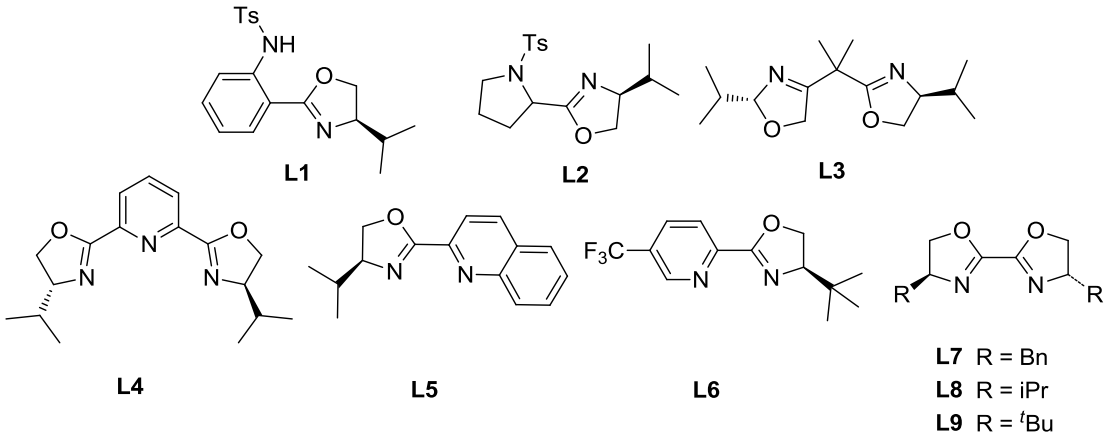


1a **2a**

Entry	Cat/L	Oxidant	Solvent	Temp	Yield [a,b](2a)	Ee [c](%)
1	$Pd(OAc)_2$/bpy	BQ	CH_3NO_2	60	24%	--
2	$Pd(OAc)_2$/bpy	TBHP	CH_3NO_2	60	trace	--
3	$Pd(OAc)_2$/bpy	$K_2S_2O_8$	CH_3NO_2	60	10%	--
4	$Pd(OAc)_2$/bpy	$(NH_4)_2S_2O_8$	CH_3NO_2	60	19%	--
5	$Pd(OAc)_2$/bpy	Selectflour	CH_3NO_2	60	17%	--
6	$Pd(OAc)_2$/bpy	$PhI(OAc)_2$	CH_3NO_2	60	NR	--
7	$Pd(OAc)_2$/bpy	IBX	CH_3NO_2	60	trace	--
8	$Pd(OAc)_2$/bpy	$T^+BF_4^-$	CH_3NO_2	60	32%	--
9	$Pd(OAc)_2$/bpy	$T^+BF_4^-$	$PhCH_3$	60	9%	--
10	$Pd(OAc)_2$/bpy	$T^+BF_4^-$	CH_3CN	60	11%	--
11	$Pd(OAc)_2$/bpy	$T^+BF_4^-$	THF	60	32%	--
12	$Pd(OAc)_2$/bpy	$T^+BF_4^-$	DME	60	46%	--
13	$Pd(OAc)_2$/bpy	$T^+BF_4^-$	DMF	60	61%	--
14	$Pd(OAc)_2$/bpy	$T^+BF_4^-$	DCE	60	70%	--
15	$Pd(OAc)_2$/bpy	$T^+BF_4^-$	DCM	60	34%	--
16	$Pd(OAc)_2$/bpy	$T^+BF_4^-$	DCE	30	32 %	--
17	$Pd(OAc)_2$/bpy	$T^+BF_4^-$	DCE	40	45 %	--
18	$Pd(OAc)_2$/bpy	$T^+BF_4^-$	DCE	50	61 %	--
19	$Pd(OAc)_2$/bpy	$T^+BF_4^-$	DCE	70	52 %	--
20	-/bpy	$T^+BF_4^-$	DCE	60	trace	--
21	$Pd(OAc)_2$/-	$T^+BF_4^-$	DCE	60	NR	--
22	-/-	$T^+BF_4^-$	DCE	60	NR	--
23	$Pd(OAc)_2$/L1	T^+BF_4	DCE	60	33%	0
24	$Pd(OAc)_2$/L2	T^+BF_4	DCE	60	31%	0
25	$Pd(OAc)_2$/L3	T^+BF_4	DCE	60	12%	26%
26	$Pd(OAc)_2$/L4	T^+BF_4	DCE	60	30%	6%
27	$Pd(OAc)_2$/L5	T^+BF_4	DCE	60	58%	51%

28	$Pd(OAc)_2$/L6	T^+BF_4	DCE	60	64%	31%
29	$Pd(OAc)_2$/L7	T^+BF_4	DCE	60	64%	89%
30	**$Pd(OAc)_2$/L8**	**T^+BF_4**	**DCE**	**60**	**69%**	**90%**
31	$Pd(OAc)_2$/L9	T^+BF_4	DCE	60	43%	62%
32	$Pd(OAc)_2$/L8	T^+BF_4	CH_3CN	60	trace	--
33	$Pd(OAc)_2$/L8	T^+BF_4	THF	60	57%	75%
34	$Pd(OAc)_2$/L8	T^+BF_4	DME	60	61%	86%
35	$Pd(OAc)_2$/L8	T^+BF_4	DMF	60	40%	77%
36	$Pd(OAc)_2$/L8	T^+BF_4	CH_3NO_2	60	16%	92%
37	$Pd(OAc)_2$/L8	T^+BF_4	DCM	60	58%	92%
38	$PdCl_2$/L8	T^+BF_4	DCE	60	trace	--
39	$Pd(TFA)_2$/L8	T^+BF_4	DCE	60	42%	84%
40	$Pd(PPh_3)_2Cl_2$/L8	T^+BF_4	DCE	60	trace	--
41	$Pd(CH_3CN)_2Cl_2$/L8	T^+BF_4	DCE	60	trace	--
42	$Pd(PhCN)_2Cl_2$/L8	T^+BF_4	DCE	60	trace	--
43	$Pd_2(dba)_3$/L8	T^+BF_4	DCE	60	ND	--
44	$Pd(OAc)_2$/L8	T^+BF_4	DCE	50	58%	92%
45	$Pd(OAc)_2$/L8	T^+BF_4	DCE	70	50%	89%

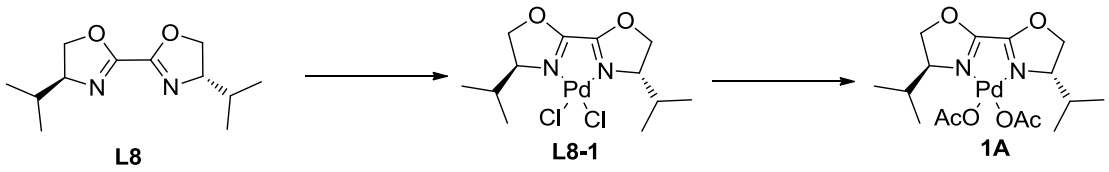
[a] Reaction conditions: 1a (0.3 mmol), 4-Tolylboronic acid (0.36 mmol, 1.2 equiv), $Pd(OAc)_2$ (0.03 mmol, 0.1 equiv), bpy (0.03 mmol, 0.1 equiv), Oxidant (0.33 mmol, 1.1 equiv), solvent (2.5 mL) under Ar, 16 h. [b] Isolated yield by column chromatography. [c] Enantiomeric excess of the major isomer was indicated, which was analyzed by chiral HPLC. bpy = 2,2'-bipyridine; $T^+BF_4^-$= 2,2,6,6-tetramethylpiperidine-1-oxoammonium tetra-fluoroborate.



In an initial study, we chose para-methoxyphenyl-(PMP)-protected glycine ester **1a** and para-methyphenyl boric acid as model substrates to identify suitable reaction conditions. We first selected achiral 2,2-bipyridine as ligand and 10 mol % $Pd(OAc)_2$

as catalyst to screen different oxidants(entries 1–7), To our delight, this reaction works with BQ as oxidant and affords the desired product **2a** in 24% yield (entries 1). Encouraged by this result, we further optimized the reaction conditions. First, we introduced these oxidant(BQ, $K_2S_2O_8$, $(NH_4)_2S_2O_8$, Selectflour). As a result, the yield of **2a** in low yield (entries 2-7). Subsequently, we evaluated a variety of oxidant for their potential in this transformation in the presence of 10 mol % $Pd(OAc)_2$ in CH_3NO_2 at 60 ℃. Results indicate that $T^+BF_4^-$ is the best choice; the product of **2a** improves to 32% yield (entry 8). We further investigated the different of solvent. To our delight the desired product of racemic **2a** was obtained in 70% yield by using the DCE as the solvent at 60 ℃.

5. Synthesis of compound 1A[4]



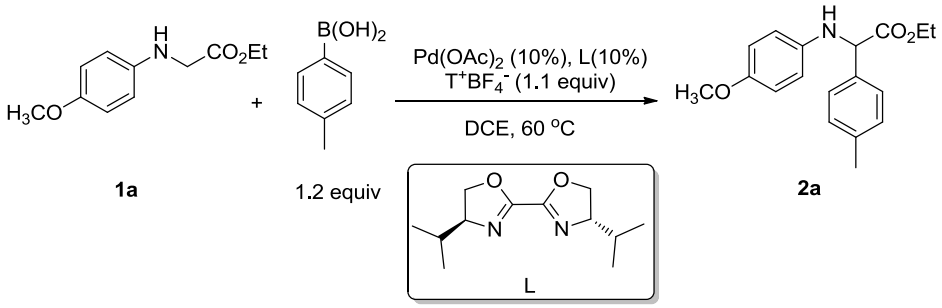
The mixture solution of (*S*, *S*)-isopropyl bisoxazoline compound **L8** (110 mg, 0.49 mmol) and $PdCl_2(CH_3CN)_2$ (127 mg, 0.49 mmol) in dichloromethane (4 mL) was stirred for 5 hours with exclusion of light at room temperature. The mixture was filtered through a celite pad and the solution was concentrated to ca. 1 mL in vacuo. The crude substrate was precipitated with hexane (2 mL). The resulting solid was filtered and washed with diethyl ether to give product **L8-1** as an orange solid. And then AgOAc (110 mg, 0.66 mmol) was added to a dichloromethane (4 mL) solution containing **L8-1** (132 mg, 0.33 mmol) in a aluminum foiled 10 mL vial. The vial was capped and the mixture was left to stir at room temperature for 35 min. The yellow solution was filtered through Celite and dried in vacuo to afford yellow/orange powder **1A.**

1A(0.03 mmol, 0.1 equiv), *N*-aryl α-imino ester (0.3 mmol, 1.0 equiv), arylboronic acid (0.36 mmol, 1.2 equiv) and 2,2,6,6-tetramethylpiperidine-1-oxoammonium tetra-fluoroborate ($T^+BF_4^-$) was added to an oven-dried 10 mL screw-capped vial and purged with Ar three times. Then, DCE (2.50 mL) was added *via* syringe. and heated to

4 (a) A. G. D. Crisci, K. Chung, A. G. Oliver, D. Solis-Ibarra and R. M. Waymouth, *Organometallics* **2013**, *32*, 2257. (b) K. S Yoo, C. P. Park, C. H. Yoon, S. Sakaguchi, J. O. Neill and K. W. Jung, *Org. Lett*, **2007**, *9*, 3933.

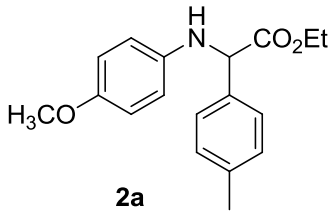
60 ℃ in an oil bath until the starting material has disappeared (monitored by TLC). And then the solvent was removed in vacuo and residue was purified on a silica gel column using EA/PE as eluent to afford the desired product **2a** (50% and 81% ee).

6. General procedure for the Pd-catalyzed synthesis of 2a-2z, 3b and 4b



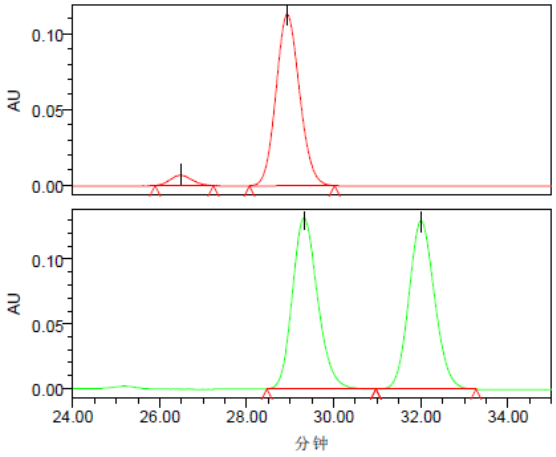
An oven-dried 10 mL screw-capped vial containing $Pd(OAc)_2$ (0.03 mmol, 0.1 equiv), (S, S)-isopropyl bisoxazoline L (0.03 mmol, 0.1 equiv) evacuated and purged with Ar three times. Then, DCE (2.50 mL) was added *via* syringe. The reaction mixture was stirred at room temperature for 1 h. Then, *N*-aryl *α*-imino ester (0.3 mmol, 1.0 equiv), arylboronic acid (0.36 mmol, 1.2 equiv) and 2,2,6,6-tetramethylpiperidine-1-oxoammonium tetra-fluoroborate ($T^+BF_4^-$) was added to the solution and heated to 60 ℃ in an oil bath until the starting material has disappeared (monitored by TLC). And then the solvent was removed in vacuo and residue was purified on a silica gel column using EA/PE as eluent to afford the desired product **2a**. The ee value of the product was determined by chiral HPLC analysis and compared with the racemate.

7. Analytical Data of Products



Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, J = 8.0 Hz, 2H), 7.14 (d, J = 7.9 Hz, 2H), 6.70 (d, J = 7.9 Hz, 2H), 6.53 (d, J = 6.1 Hz, 2H), 4.96 (s, 1H), 4.61 (s, 1H), 4.26 – 4.15 (m, 1H), 4.15 – 4.03 (m, 1H), 3.68 (s, 3H), 2.31 (s, 3H), 1.19 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.14, 152.37, 140.29, 137.83, 134.83, 129.41, 127.05, 114.77, 114.68, 61.53, 61.37, 55.59, 21.05, 13.99. IR ν_{max} (cm^{-1}) 3398, 2985,

2930, 1736, 1512, 1240, 1174, 1033, 820, 792, 762. MS (EI), m/z: 299[M]$^{+}$, 226, 211, 182, 167, 134, 107, 91, 77, 64, 50. Enantiomeric excess is 90% determined by HPLC analysis: Chiralcel AD-H (hexane/iPrOH = 98/2, flow rate = 1.0 mL/min, 242.1 nm), $t_{\text{r-minor}}$ 26.485 min, $t_{\text{r-major}}$ 28.930 min. $[\alpha]_D^{20}$ = 80 (c = 0.2, $CHCl_3$).



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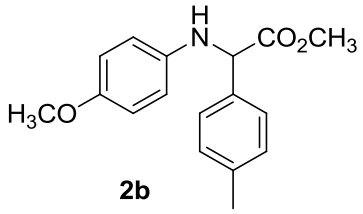
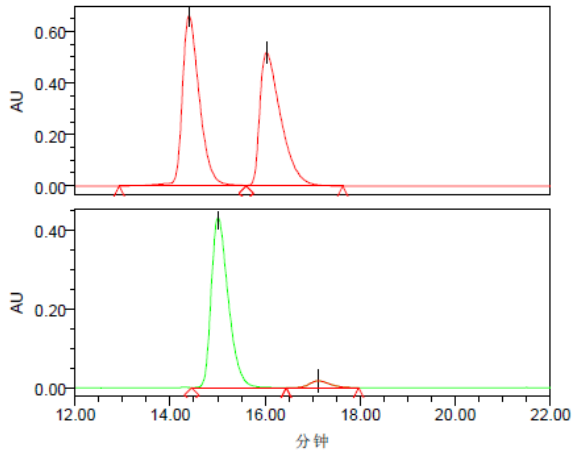


2b

Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, J = 7.8 Hz, 2H), 7.15 (d, J = 7.8 Hz, 2H), 6.71 (d, J = 8.9 Hz, 2H), 6.52 (d, J = 8.9 Hz, 2H), 4.98 (s, 1H), 4.62 (s, 1H), 3.69 (d, J = 3.9 Hz, 6H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.63, 152.42, 140.21, 137.96, 134.72, 129.47, 127.08, 114.78, 114.68, 61.31, 55.60, 52.55, 21.05. IR ν_{max} (cm^{-1}) 3399, 2952, 2927, 1739, 1513, 1311, 1239, 1175, 1037, 819, 737. MS (EI), m/z: 285[M]$^{+}$, 226, 211, 182, 167, 134, 122, 107, 91, 77, 65, 50. Enantiomeric excess is 91% determined by HPLC analysis: Chiralcel OD-H (hexane/iPrOH = 98/2, flow rate = 1.0 mL/min, 241.0 nm), $t_{\text{r-minor}}$ 17.123 min, $t_{\text{r-major}}$ 15.011 min. $[\alpha]_D^{20}$ = 125 (c = 0.2, $CHCl_3$).



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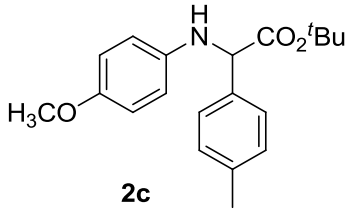
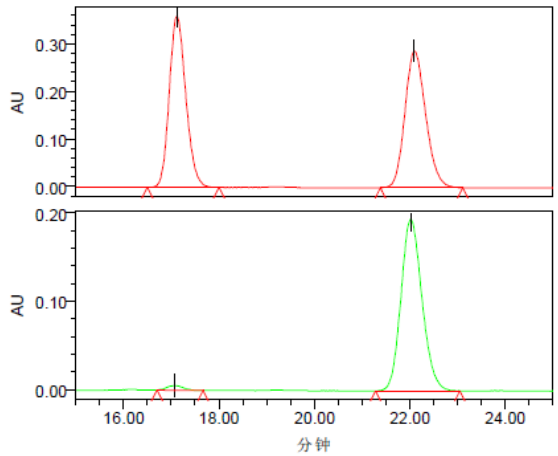


2c

Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (d, J = 8.0 Hz, 2H), 7.13 (d, J = 8.0 Hz, 2H), 6.70 (d, J = 8.9 Hz, 2H), 6.51 (d, J = 8.9 Hz, 2H), 4.86 (s, 1H), 4.60 (s, 1H), 3.69 (s, 3H), 2.32 (s, 3H), 1.37 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.28, 152.24, 140.54, 137.52, 135.31, 129.29, 126.98, 114.79, 114.62, 82.00, 61.85, 55.69, 27.83, 21.10. IR ν_{max} (cm^{-1}) 3400, 2978, 2928, 1727, 1513, 1239, 1153, 1038, 819, 791. MS (EI), m/z: 327[M]$^{+}$, 271, 226, 210, 182, 167, 134, 107, 92 77, 57, 50. Enantiomeric excess is 96% determined by HPLC analysis: Chiralcel AD-H (hexane/iPrOH = 98/2, flow rate = 1.0 mL/min, 242.1 nm), t $_{r\text{-minor}}$ 17.063 min, t $_{r\text{-major}}$ 22.023 min. $[\alpha]_D^{20}$ = 65 (c = 0.2, $CHCl_3$).



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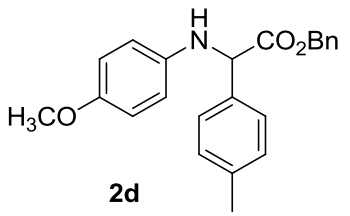
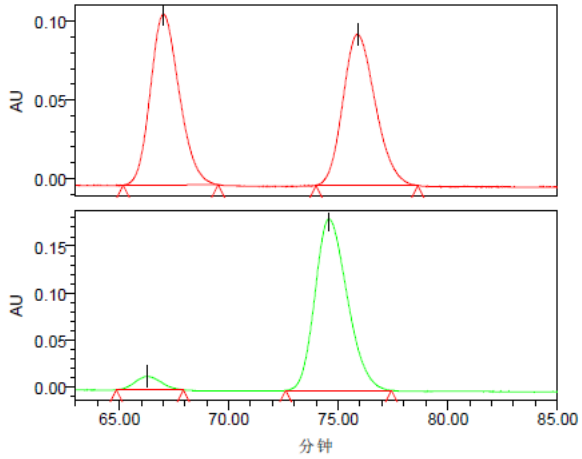


2d

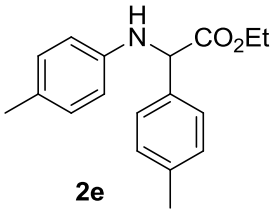
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, J = 8.0 Hz, 2H), 7.32 – 7.24 (m, 3H), 7.20 – 7.10 (m, 4H), 6.69 (d, J = 8.9 Hz, 2H), 6.51 (d, J = 8.9 Hz, 2H), 5.12 (dd, J = 48.3, 12.4 Hz, 2H), 5.03 (s, 1H), 4.62 (s, 1H), 3.68 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.97, 152.35, 140.11, 137.90, 135.27, 134.50, 129.39, 128.36, 128.11, 127.77, 127.06, 114.71, 114.66, 67.02, 61.36, 55.54, 21.02. IR ν_{max} (cm^{-1}) 3401, 2928, 2832, 1736, 1513, 1238, 1173, 1037, 909, 819, 733, 698. MS (EI), m/z: 361$[M]^+$, 270, 226, 210, 182, 167, 134, 107, 92 77, 57, 50. Enantiomeric excess is 88% determined by HPLC analysis: Chiralcel AD-H (hexane/iPrOH = 98/2, flow rate = 1.0 mL/min, 241.0 nm), t $_{r\text{-minor}}$ 66.308 min, t $_{r\text{-major}}$ 74.591 min. $[\alpha]_D^{20}$ = 70 (c = 0.2, $CHCl_3$).



样品名称： wxh-37-r, wxh-37-s
采集日期： 2014-5-27 10:34:13, 2014-5-27

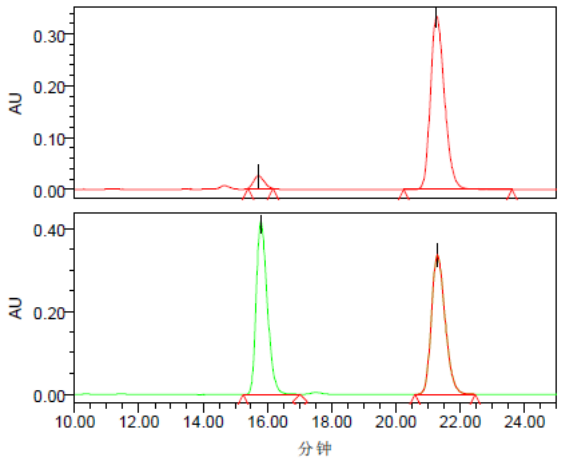
处理通道: **PDA 241.0** 纳米

	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 241.0 纳米	66.308	1191398	5.96	14238
2	PDA 241.0 纳米	67.018	9983467	50.14	108568
3	PDA 241.0 纳米	74.591	18784857	94.04	183090
4	PDA 241.0 纳米	75.902	9927730	49.86	96042



2e

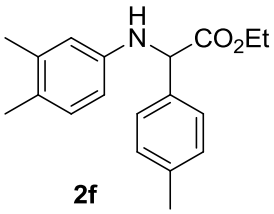
Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, J = 8.0 Hz, 2H), 7.14 (d, J = 7.9 Hz, 2H), 6.92 (d, J = 8.2 Hz, 2H), 6.48 (d, J = 8.4 Hz, 2H), 5.00 (d, J = 5.2 Hz, 1H), 4.77 (s, 1H), 4.29 – 4.04 (m, 2H), 2.32 (s, 3H), 2.19 (s, 3H), 1.21 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.09, 143.76, 137.86, 134.79, 129.67, 129.45, 127.11, 127.06, 113.48, 61.62, 60.76, 21.11, 20.36, 14.04. IR ν_{max} (cm^{-1}) 3404, 2923, 2862, 1735, 1521, 1250, 1178, 1137, 1022, 806, 738. MS (EI), m/z: 283$[M]^+$, 210, 208, 194, 118, 105, 91, 77, 65, 50. Enantiomeric excess is 90% determined by HPLC analysis: Chiralcel OD-H (hexane/iPrOH = 99/1, flow rate = 0.5 mL/min, 244.5 nm), t $_{r\text{-minor}}$ 15.726 min, t $_{r\text{-major}}$ 21.272 min. $[\alpha]_D^{20}$ = 120 (c = 0.2, $CHCl_3$).



样品名称: wxh-2-r-3, wxh-2-s-3
采集日期: 2014-4-20 22:16:44, 2014-4-20

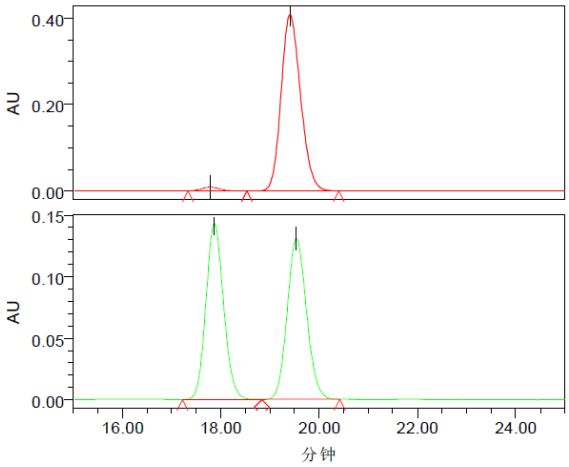
处理通道: **PDA 244.5** 纳米

	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 244.5 纳米	15.726	539274	5.02	24242
2	PDA 244.5 纳米	15.803	10005670	50.11	418329
3	PDA 244.5 纳米	21.272	10196043	94.98	334180
4	PDA 244.5 纳米	21.297	9962501	49.89	336102



2f

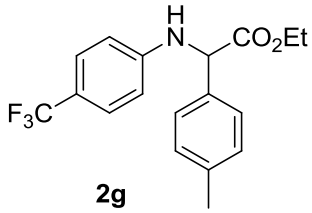
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, J = 8.0 Hz, 2H), 7.14 (d, J = 7.9 Hz, 2H), 6.86 (d, J = 8.1 Hz, 1H), 6.43 (s, 1H), 6.30 (d, J = 10.4 Hz, 1H), 4.99 (s, 1H), 4.70 (s, 1H), 4.30 – 4.04 (m, 2H), 2.32 (s, 3H), 2.14 (s, 3H), 2.10 (s, 3H), 1.21 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.19, 144.22, 137.81, 137.24, 134.90, 130.19, 129.44, 127.05, 125.96, 115.31, 110.61, 61.56, 60.74, 21.11, 19.98, 18.66, 14.04. IR ν_{max} (cm^{-1}) 3407, 2980, 2921, 1735, 1618, 1511, 1289, 1022, 803, 737. MS (EI), m/z: 297$[M]^+$, 224, 132, 105, 91, 77, 65. Enantiomeric excess is 96% determined by HPLC analysis: Chiralcel AD-H (hexane/iPrOH = 98/2, flow rate = 1.0 mL/min, 244.5 nm), $t_{\text{r-minor}}$ 17.781 min, $t_{\text{r-major}}$ 19.408 min. $[\alpha]_D^{20}$ = 20 (c = 0.2, $CHCl_3$).



样品名称: wxh-3-r, wxh-3-s
采集日期: 2014-4-19 21:47:35, 2014-4-19

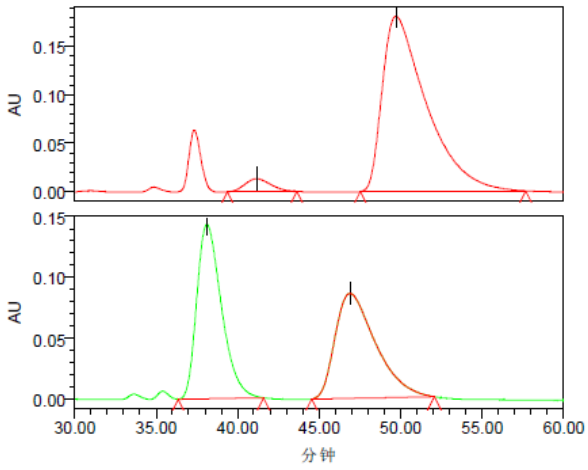
处理通道: **PDA 244.5** 纳米

	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 244.5 纳米	17.781	226210	1.98	9062
2	PDA 244.5 纳米	17.868	3583823	50.00	143286
3	PDA 244.5 纳米	19.408	11208695	98.02	408532
4	PDA 244.5 纳米	19.538	3584375	50.00	130959



2g

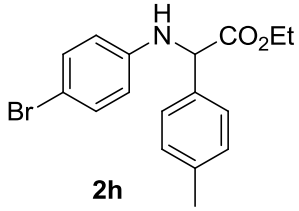
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.30 (m, 4H), 7.16 (d, J = 7.9 Hz, 2H), 6.55 (d, J = 8.5 Hz, 2H), 5.31 (d, J = 5.6 Hz, 1H), 5.04 (d, J = 5.8 Hz, 1H), 4.28 – 4.07 (m, 2H), 2.33 (s, 3H), 1.22 (t, J = 7.1 Hz, 3H). 13C NMR (101 MHz, CDCl3) δ 171.39, 148.34, 138.31, 133.82, 130.89, 129.65, 126.97, 126.55 (q, J.C-F = 3.7 Hz), 124.81 (d, J C-F = 270.5 Hz), 112.57, 62.04, 59.92, 21.13, 14.01. IR νmax (cm^{-1}) 3402, 2983, 2926, 1735, 1618, 1321, 1136, 1111, 826, 790. MS (EI), m/z: 337[M]+, 318, 264, 172, 145, 118, 91, 77, 65, 50. Enantiomeric excess is 92% determined by HPLC analysis: Chiralcel AD-H (hexane/iPrOH = 98/2, flow rate = 1.0 mL/min, 253.9 nm), $t_{r\text{-minor}}$ 41.180 min, $t_{r\text{-major}}$ 49.723 min. $[\alpha]_D^{20}$ = 95 (c = 0.2, CHCl3).



样品名称: wxh-4-r-6, wxh-4-s-6
采集日期: 2014-4-22 15:24:10, 2014-4-22

处理通道: **PDA 253.9** 纳米

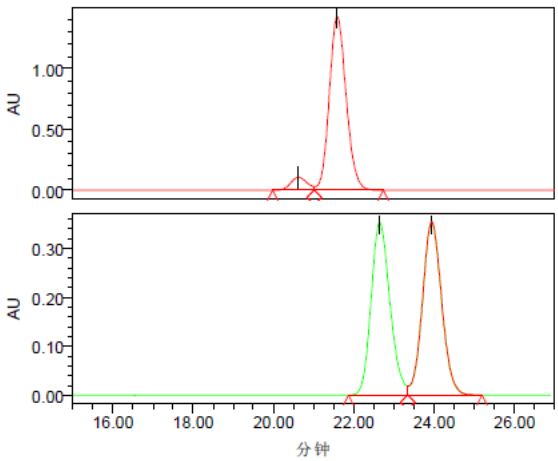
	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 253.9 纳米	38.118	15131497	50.37	143310
2	PDA 253.9 纳米	41.180	1471390	4.12	13256
3	PDA 253.9 纳米	46.918	14911754	49.63	86338
4	PDA 253.9 纳米	49.723	34243507	95.88	181102



2h

Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (d, *J* = 8.1 Hz, 2H), 7.16 (td, *J* = 9.2, 4.5 Hz, 4H), 6.41 (d, *J* = 8.7 Hz, 2H), 5.04 – 4.93 (m, 2H), 4.28 – 4.17 (m, 1H), 4.17 – 4.05 (m, 1H), 2.31 (s, 3H), 1.19 (d, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.55, 144.90, 138.06, 134.08, 131.82, 129.51, 126.96, 114.91, 109.56, 61.78, 60.28, 21.05, 13.96. IR ν_{max} (cm^{-1}) 3404, 2928, 2922, 1724, 1595, 1498, m1315, 1255, 1176, 1021, 842, 813, 739. MS (EI), m/z: 347$[M]^+$, 274, 182, 155, 118, 103, 91, 76, 65, 50. Enantiomeric excess is 88% determined by HPLC analysis: Chiralcel AD-H

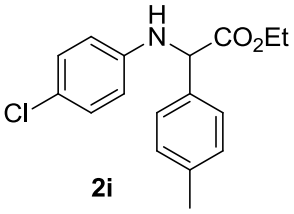
(hexane/iPrOH = 98/2, flow rate = 1.0 mL/min, 250.4 nm), $t_{\text{r-minor}}$ 20.623 min, $t_{\text{r-major}}$ 21.588 min. $[\alpha]_D^{20}$ = 55 (c = 0.2, $CHCl_3$).



样品名称： wxh-7-r, wxh-743-15
采集日期： 2014-4-18 20:21:47, 2014-5-27

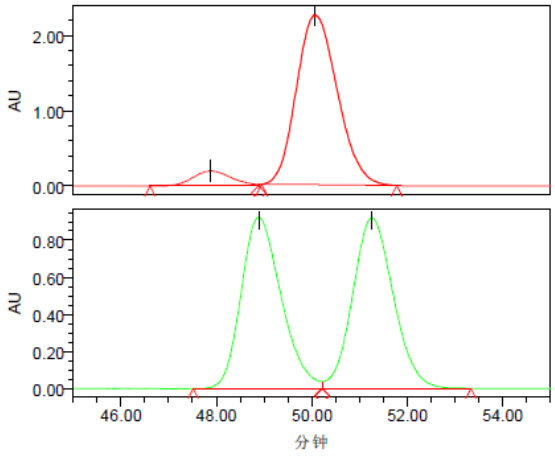
处理通道: **PDA 250.4** 纳米

	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 250.4 纳米	20.623	2978877	6.66	105459
2	PDA 250.4 纳米	21.588	41720758	93.34	1425220
3	PDA 250.4 纳米	22.648	11519551	49.40	352257
4	PDA 250.4 纳米	23.943	11798910	50.60	353503



2i

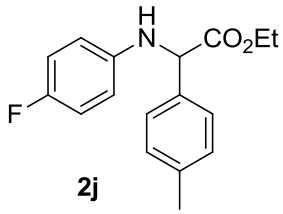
Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (d, J = 8.0 Hz, 2H), 7.07 (d, J = 7.9 Hz, 2H), 6.97 (d, J = 8.7 Hz, 2H), 6.38 (d, J = 8.7 Hz, 2H), 4.89 (s, 2H), 4.23 – 3.96 (m, 2H), 2.25 (s, 3H), 1.13 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.65, 144.51, 138.11, 134.16, 129.54, 129.00, 126.99, 122.53, 114.44, 77.32, 60.42, 21.10, 14.00. IR ν_{max} (cm^{-1}) 3404, 2981, 2925, 1734, 1601, 1501, 1314, 1254, 1176, 1021, 816, 739. MS (EI), m/z: 303$[M]^+$, 230, 195, 138, 111, 91, 77, 65, 50. Enantiomeric excess is 85% determined by HPLC analysis: Chiralcel AD-H (hexane/iPrOH = 99/1, flow rate = 0.5 mL/min, 251.6 nm), $t_{\text{r-minor}}$ 47.883 min, $t_{\text{r-major}}$ 50.079 min. $[\alpha]_D^{20}$ = 85 (c = 0.2, $CHCl_3$).



样品名称： wxh-6-r-1, wxh-6-s-1
采集日期： 2014-4-20 13:29:46, 2014-4-20

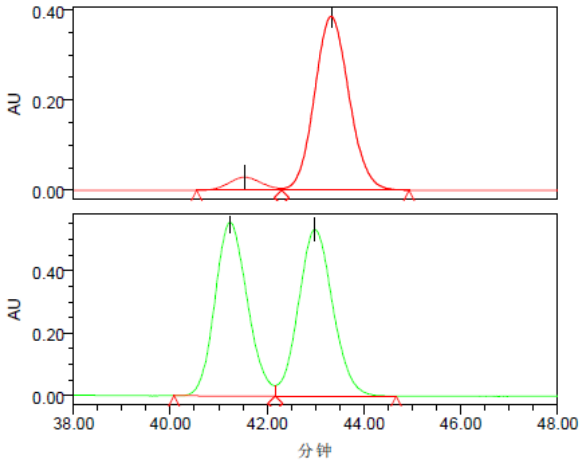
处理通道: **PDA 251.6** 纳米

	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 251.6 纳米	47.883	11251477	7.71	199830
2	PDA 251.6 纳米	48.888	53726139	49.66	922556
3	PDA 251.6 纳米	50.079	134684326	92.29	2254404
4	PDA 251.6 纳米	51.258	54467122	50.34	918300



2j

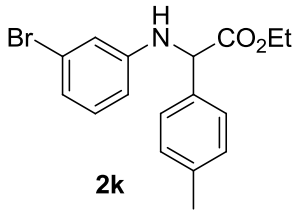
Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, J = 8.0 Hz, 2H), 7.15 (d, J = 7.9 Hz, 2H), 6.81 (t, J = 8.7 Hz, 2H), 6.48 (dd, J = 9.0, 4.4 Hz, 2H), 4.96 (d, J = 4.9 Hz, 1H), 4.82 (s, 1H), 4.28 – 4.05 (m, 2H), 2.32 (s, 3H), 1.20 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.93, 156.06 (d, J = 235.6 Hz), 142.45, 138.09, 134.50, 129.57, 127.09, 115.67 (d, J = 22.4 Hz), 114.27 (d, J = 7.4 Hz), 77.38, 77.06, 76.74, 61.78, 61.06, 21.15, 14.06. IR ν_{max} (cm^{-1}) 3402, 2982, 2925, 1734, 1512, 1313, 1203, 1022, 820. MS (EI), m/z: 287$[M]^+$, 214, 198, 122, 95, 75, 65, 50. Enantiomeric excess is 87% determined by HPLC analysis: Chiralcel AD-H (hexane/iPrOH = 99/1, flow rate = 0.5 mL/min, 235.1 nm), $t_{\text{r-minor}}$ 41.533 min, $t_{\text{r-major}}$ 43.324 min. $[\alpha]_D^{20}$ = 80 (c = 0.2, $CHCl_3$).



样品名称: wxh-5-r-1, wxh-5-s-1
采集日期: 2014-4-20 11:48:44, 2014-4-20

处理通道: **PDA 235.1** 纳米

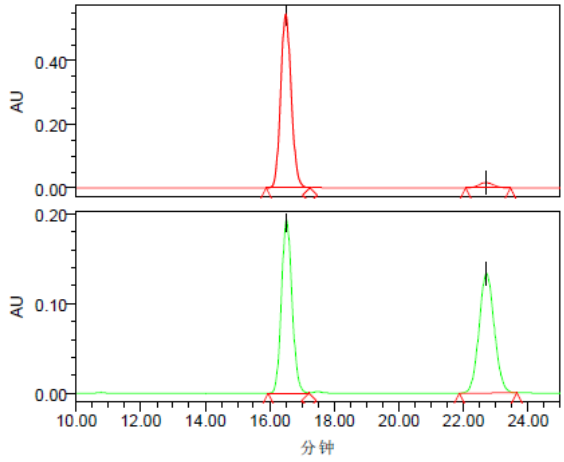
	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 235.1 纳米	41.239	25896636	49.60	556047
2	PDA 235.1 纳米	41.533	1354230	6.60	28561
3	PDA 235.1 纳米	42.988	26313496	50.40	532859
4	PDA 235.1 纳米	43.324	19160085	93.40	386169



2k

White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (d, J = 8.1 Hz, 1H), 7.15 (d, J = 7.9 Hz, 1H), 6.93 (t, J = 8.0 Hz, 1H), 6.78 (d, J = 8.7 Hz, 1H), 6.70 (s, 1H), 6.44 (d, J = 8.2 Hz, 1H), 5.04 (d, J = 5.9 Hz, 1H), 4.98 (d, J = 6.0 Hz, 1H), 4.30 – 4.04 (m, 1H), 2.32 (s, 1H), 1.19 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.54, 147.22, 138.14, 134.01, 130.41, 129.56, 126.95, 123.06, 120.68, 116.05, 111.87, 61.87, 60.08, 21.09, 13.99. IR ν_{max} (cm^{-1}) 3403, 2924, 2858, 1724, 1637, 1597, 1184, 804, 739. MS (EI), m/z: 347$[M]^+$,

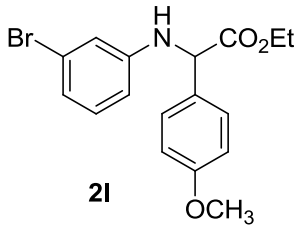
274, 182, 155, 103, 91, 77, 65, 50. Enantiomeric excess is 92% determined by HPLC analysis: Chiralcel AD-H (hexane/iPrOH = 98/2, flow rate = 1.0 mL/min, 246.9 nm), $t_{\text{r-minor}}$ 22.705 min, $t_{\text{r-major}}$ 16.497 min. $[\alpha]_D^{20}$ = 80 (c = 0.2, $CHCl_3$).



样品名称: wxh-8-r, wxh-8-s
采集日期: 2014-4-18 21:20:58, 2014-4-18

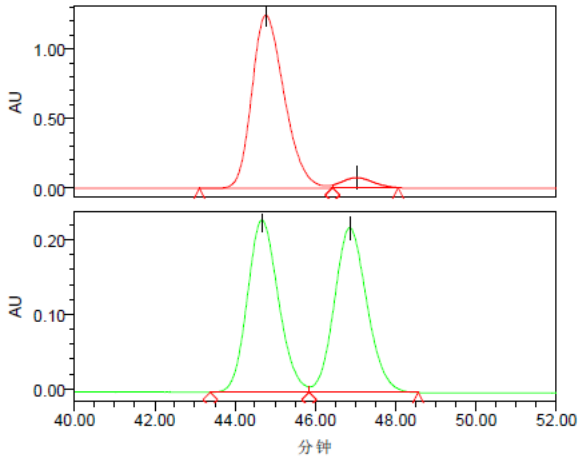
处理通道: **PDA 246.9** 纳米

	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 246.9 纳米	16.497	12431143	96.01	545113
2	PDA 246.9 纳米	16.522	4400237	50.08	193174
3	PDA 246.9 纳米	22.705	517118	3.99	16501
4	PDA 246.9 纳米	22.719	4385357	49.92	133237



2l

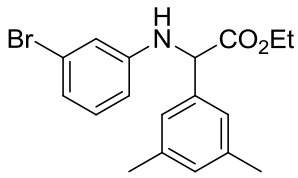
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, J = 8.6 Hz, 2H), 6.94 (t, J = 8.0 Hz, 1H), 6.87 (d, J = 8.6 Hz, 2H), 6.79 (d, J = 8.0 Hz, 1H), 6.70 (d, J = 1.6 Hz, 1H), 6.44 (d, J = 8.1 Hz, 1H), 4.99 (dd, J = 25.8, 5.1 Hz, 2H), 4.31 – 4.04 (m, 2H), 3.78 (s, 3H), 1.21 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.61, 159.54, 147.18, 130.41, 128.92, 128.21, 123.06, 120.68, 116.04, 114.23, 111.90, 77.32, 77.00, 76.68, 61.85, 59.72, 55.21, 14.01. IR ν_{max} (cm^{-1}) 3398, 2977, 2927, 1732, 1596, 1499, 1246, 1178, 1035,765, 738. MS (EI), m/z: 363$[M]^+$, 292, 277, 211, 184, 155, 120, 107, 91, 77, 65, 50. Enantiomeric excess is 90% determined by HPLC analysis: Chiralcel AD-H (hexane/iPrOH = 98/2, flow rate = 0.6 mL/min, 242.1 nm), $t_{\text{r-minor}}$ 47.031 min, $t_{\text{r-major}}$ 44.771 min. $[\alpha]_D^{20}$ = 100 (c = 0.2, $CHCl_3$).



样品名称： wxh-28-r-2, wxh-28-s
采集日期： 2014-5-13 15:47:11, 2014-5-13

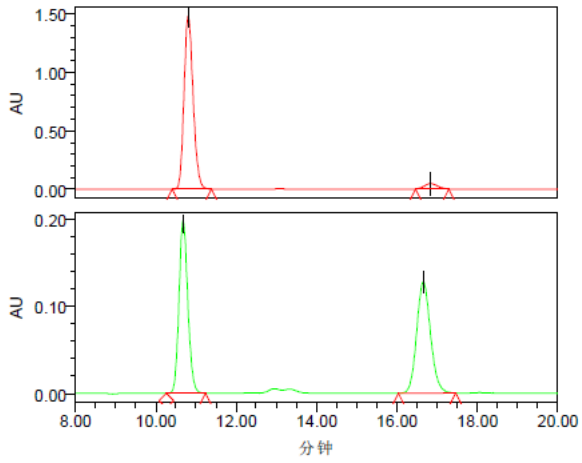
处理通道: **PDA 242.1** 纳米

	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 242.1 纳米	44.672	12447410	49.90	231001
2	PDA 242.1 纳米	44.771	69513111	94.82	1239417
3	PDA 242.1 纳米	46.859	12498888	50.10	220593
4	PDA 242.1 纳米	47.031	3794847	5.18	71864



2m

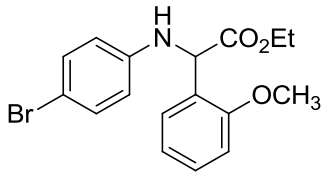
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.06 (s, 2H), 7.01 – 6.92 (m, 2H), 6.80 (d, J = 7.9 Hz, 1H), 6.72 (d, J = 1.9 Hz, 1H), 6.45 (d, J = 8.1 Hz, 1H), 4.98 – 4.88 (m, 2H), 4.33 – 4.06 (m, 2H), 2.30 (s, 6H), 1.22 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.67, 147.43, 138.47, 136.94, 130.47, 130.15, 124.86, 123.11, 120.77, 116.11, 111.87, 61.84, 60.51, 21.31, 14.04. IR ν_{max} (cm^{-1}) 3396, 2980, 2919, 1734, 1596, 1498, 1480, 1196, 1160, 1025, 853, 763, 681. MS (EI), m/z: 361[M]$^{+}$, 288, 209, 184, 155, 117, 103, 91, 76, 65, 50. Enantiomeric excess is 92% determined by HPLC analysis: Chiralcel AD-H (hexane/iPrOH = 98/2, flow rate = 1.0 mL/min, 246.9 nm), $t_{r\text{-minor}}$ 16.842 min, $t_{r\text{-major}}$ 10.807 min. $[\alpha]_D^{20}$ = 80 (c = 0.2, $CHCl_3$).



样品名称： wxh-33-r, wxh-33-s
采集日期： 2014-5-12 21:36:36, 2014-5-12

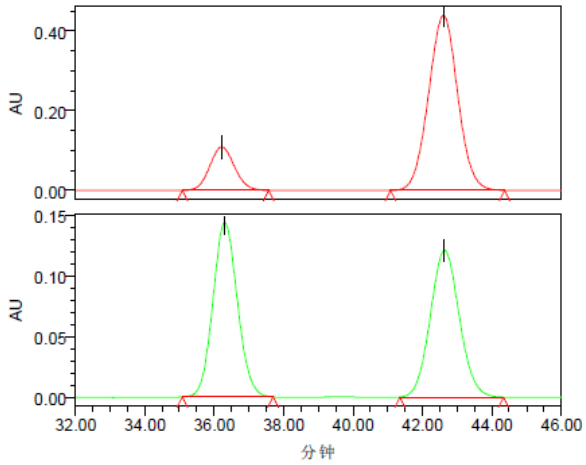
处理通道: **PDA 246.9** 纳米

	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 246.9 纳米	10.681	3026025	49.77	197529
2	PDA 246.9 纳米	10.807	23239489	95.80	1482148
3	PDA 246.9 纳米	16.659	3053978	50.23	127486
4	PDA 246.9 纳米	16.842	1018191	4.20	44829



2n

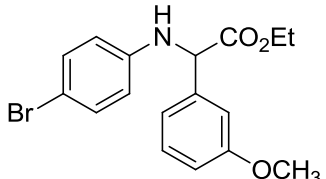
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.22 (m, 2H), 7.18 (d, J = 12.0 Hz, 2H), 6.90 (d, J = 7.9 Hz, 2H), 6.48 (d, J = 8.9 Hz, 2H), 5.44 (d, J = 7.3 Hz, 1H), 4.93 (d, J = 7.1 Hz, 1H), 4.25 – 4.03 (m, 2H), 3.88 (s, 3H), 1.17 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.91, 157.10, 145.31, 131.78, 129.44, 127.92, 125.94, 120.97, 114.98, 111.13, 109.52, 61.52, 55.69, 54.65, 13.99. IR ν_{max} (cm^{-1}) 3403, 2980, 2937, 1734, 1596, 1496, 1247, 1026, 814, 755, 737. MS (EI), m/z: 363[M]$^{+}$, 292, 211, 184, 157, 121, 103, 91, 76, 65, 50. Enantiomeric excess is 66% determined by HPLC analysis: Chiralcel AD-H (hexane/iPrOH = 98/2, flow rate = 1.0 mL/min, 251.6 nm), $t_{r\text{-minor}}$ 36.214 min, $t_{r\text{-major}}$ 42.605 min. $[\alpha]_D^{20}$ = 65 (c = 0.2, $CHCl_3$).



样品名称： wxh-11-r, wxh-11-s
采集日期： 2014-4-18 18:44:47, 2014-4-18

处理通道: **PDA 251.6** 纳米

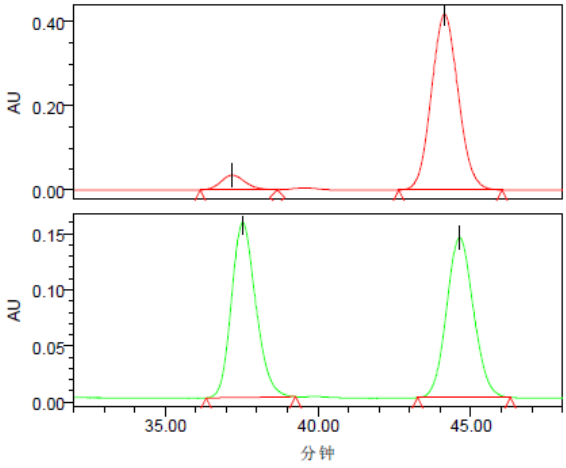
	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 251.6 纳米	36.214	5364682	17.26	108389
2	PDA 251.6 纳米	36.304	7064026	50.05	143731
3	PDA 251.6 纳米	42.605	25721246	82.74	438301
4	PDA 251.6 纳米	42.637	7050328	49.95	121058



2o

White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (t, J = 7.9 Hz, 1H), 7.17 (d, J = 8.9 Hz, 2H), 7.05 (d, J = 7.7 Hz, 1H), 7.02 – 6.98 (m, 1H), 6.83 (dd, J = 8.0, 2.2 Hz, 1H), 6.42 (d, J = 8.9 Hz, 2H), 5.02 (s, 1H), 4.97 (s, 1H), 4.31 – 4.05 (m, 2H), 3.77 (s, 3H), 1.21 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.28, 159.93, 144.83, 138.72, 131.85, 129.81, 119.42, 114.92, 113.65, 112.69, 109.66, 61.92, 60.54, 55.17, 13.98. IR ν_{max} (cm^{-1}) 3402, 2981, 2937, 1733, 1596, 1495, 1311, 1199, 1046, 814, 738. MS (EI), m/z: 363[M]$^{+}$, 292, 211, 184, 157, 103, 91, 76, 65, 50. Enantiomeric excess is 86%

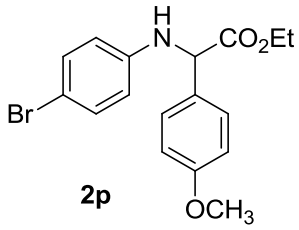
determined by HPLC analysis: Chiralcel AD-H (hexane/iPrOH = 98/2, flow rate = 1.0 mL/min, 250.4 nm), $t_{\text{r-minor}}$ 37.183 min, $t_{\text{r-major}}$ 44.138 min. $[\alpha]_D^{20}$ = 45 (c = 0.2, $CHCl_3$).



样品名称： wxh-10-r, wxh-10-s
采集日期： 2014-4-18 17:01:18, 2014-4-18

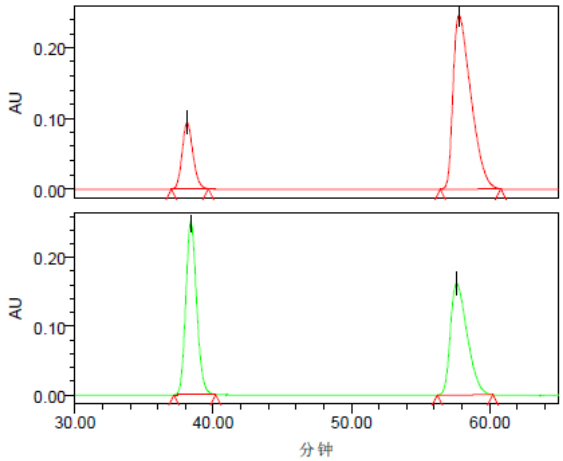
处理通道: **PDA 250.4** 纳米

	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 250.4 纳米	37.183	1926094	7.02	34729
2	PDA 250.4 纳米	37.527	8650516	49.62	156267
3	PDA 250.4 纳米	44.138	25521096	92.98	417587
4	PDA 250.4 纳米	44.631	8782516	50.38	142934



2p

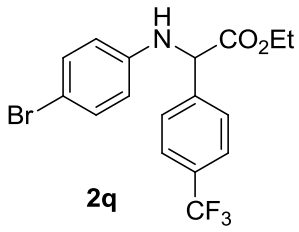
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, J = 6.7 Hz, 2H), 7.17 (d, J = 8.9 Hz, 2H), 6.86 (d, J = 8.8 Hz, 2H), 6.41 (d, J = 8.9 Hz, 2H), 4.95 (t, J = 7.0 Hz, 2H), 4.28 – 4.05 (m, 2H), 3.76 (s, 3H), 1.20 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.64, 159.55, 144.91, 131.83, 129.01, 128.21, 114.94, 114.21, 109.57, 61.77, 59.95, 55.18, 13.98. IR ν_{max} (cm^{-1}) 3402, 2981, 2934, 1733, 1596, 1499, 1176, 1030, 814, 737. MS (EI), m/z: 363[M]$^+$, 292, 211, 184, 157, 103, 91, 76, 65, 50. Enantiomeric excess is 62% determined by HPLC analysis: Chiralcel AD-H (hexane/iPrOH = 98/2, flow rate = 1.0 mL/min, 246.9 nm), $t_{\text{r-minor}}$ 38.130 min, $t_{\text{r-major}}$ 57.788 min. $[\alpha]_D^{20}$ = 95 (c = 0.2, $CHCl_3$).



样品名称： wxh-9, wxh-9'
采集日期： 2014-4-17 17:57:38, 2014-4-17

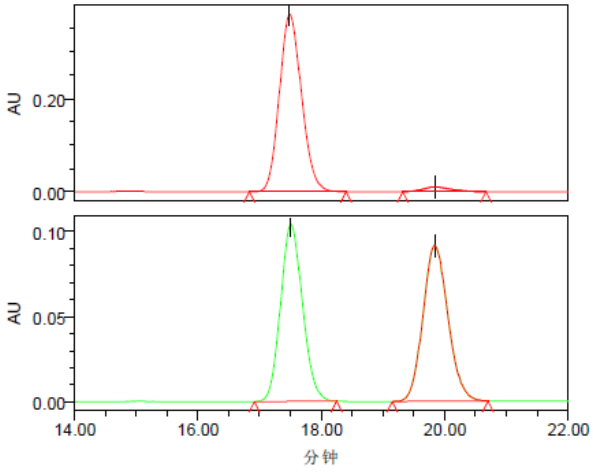
处理通道: **PDA 246.9** 纳米

	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 246.9 纳米	38.130	5086638	18.78	93496
2	PDA 246.9 纳米	38.394	13690853	49.98	252382
3	PDA 246.9 纳米	57.623	13703984	50.02	162257
4	PDA 246.9 纳米	57.788	22004184	81.22	245392



2q

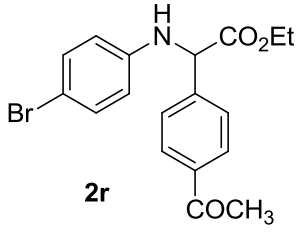
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (q, J = 8.6 Hz, 1H), 7.61 (s, 3H), 7.20 (d, J = 6.9 Hz, 2H), 6.39 (d, J = 8.8 Hz, 2H), 5.11 (s, 1H), 5.07 (s, 1H), 4.34 – 4.04 (m, 2H), 1.22 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.56, 144.36, 141.32, 132.04, 130.63 (q, $J_{C\text{-}F}$ = 32.5 Hz), 127.62, 126.71 (q, $J_{C\text{-}F}$ = 183.8 Hz), 125.85 (q, $J_{C\text{-}F}$ = 3.7 Hz), 114.96, 110.13, 62.40, 60.26, 13.98. IR ν_{max} (cm^{-1}) 3405, 2983, 2928, 1737, 1596, 1498, 1324, 1068, 1018, 8314, 739. MS (EI), m/z: 401$[M]^+$, 330, 248, 182, 157, 145, 127, 104, 76, 63, 50. Enantiomeric excess is 94% determined by HPLC analysis: Chiralcel AD-H (hexane/iPrOH = 98/2, flow rate = 1.0 mL/min, 248.0 nm), $t_{\text{r-minor}}$ 19.847 min, $t_{\text{r-major}}$ 17.488 min. $[\alpha]_D^{20}$ = 75 (c = 0.2, $CHCl_3$).



样品名称: wxh-15-r, wxh-15-s
采集日期: 2014-4-19 14:53:06, 2014-4-19

处理通道: **PDA 248.0** 纳米

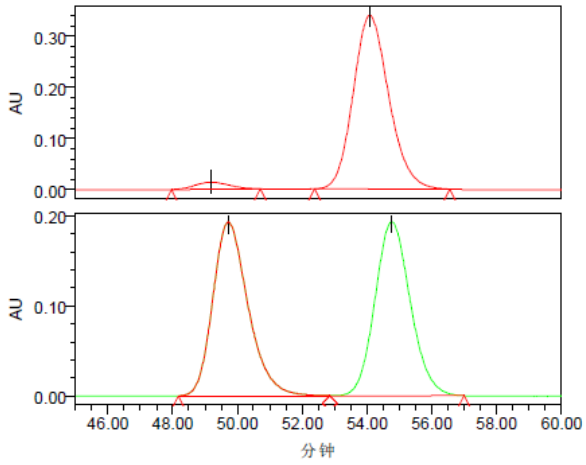
	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 248.0 纳米	17.488	9521486	96.83	380500
2	PDA 248.0 纳米	17.507	2580168	49.93	104028
3	PDA 248.0 纳米	19.839	2587556	50.07	91439
4	PDA 248.0 纳米	19.847	311384	3.17	9771



2r

Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, J = 8.2 Hz, 2H), 7.58 (d, J = 8.3 Hz, 2H), 7.18 (d, J = 8.7 Hz, 2H), 6.39 (d, J = 8.8 Hz, 2H), 5.09 (d, J = 18.4 Hz, 2H), 4.35 – 3.97 (m, 2H), 2.59 (s, 3H), 1.21 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.47, 170.61, 144.45, 142.52, 137.15, 132.00, 128.89, 127.38, 115.00, 110.06, 62.33, 60.44, 26.62, 13.97. IR ν_{max} (cm^{-1}) 3396, 2982, 2926, 1736, 1684, 1595, 1497, 1265, 1177, 1018, 814, 737. MS (EI), m/z: 375$[M]^+$, 306, 225, 182, 155, 135, 103, 93, 76, 65, 50. Enantiomeric excess is 93% determined by HPLC analysis: Chiralcel

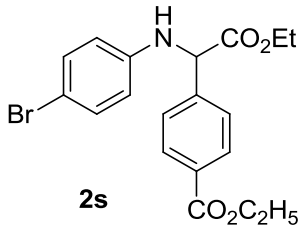
AD-H (hexane/iPrOH = 98/2, flow rate = 1.0 mL/min, 250.4 nm), $t_{\text{r-minor}}$ 49.189 min, $t_{\text{r-major}}$ 54.089 min. $[\alpha]_D^{20}$ = 85 (c = 0.2, $CHCl_3$).



样品名称: wxh-31-r_1, wxh-31-s
采集日期: 2014-5-13 19:48:00, 2014-5-13

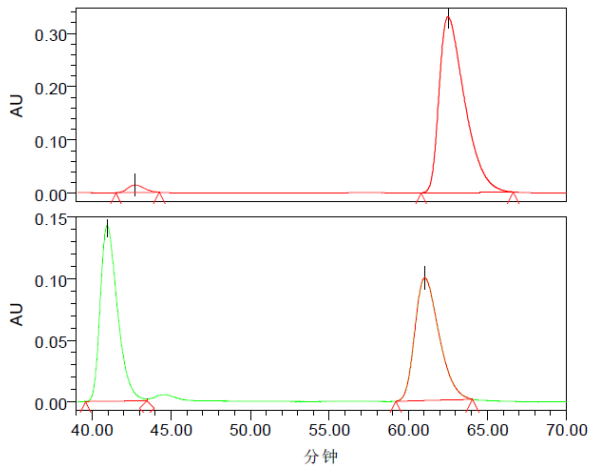
处理通道: **PDA 250.4** 纳米

	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 250.4 纳米	49.189	1000994	3.70	13756
2	PDA 250.4 纳米	49.722	14626548	49.91	193049
3	PDA 250.4 纳米	54.089	26069557	96.30	339764
4	PDA 250.4 纳米	54.766	14680386	50.09	193284



2s

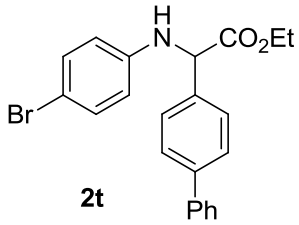
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, J = 8.4 Hz, 2H), 7.55 (d, J = 8.3 Hz, 2H), 7.18 (d, J = 8.8 Hz, 2H), 6.39 (d, J = 8.8 Hz, 2H), 5.08 (dd, J = 22.4, 5.5 Hz, 2H), 4.44 – 4.31 (m, 2H), 4.30 – 4.08 (m, 2H), 1.38 (t, J = 7.1 Hz, 3H), 1.21 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.70, 166.11, 144.47, 142.19, 131.97, 130.61, 130.09, 127.13, 114.98, 109.99, 62.28, 61.04, 60.45, 14.30, 13.96. IR ν_{max} (cm^{-1}) 3395, 1978, 1924, 1735, 1718, 1595, 1498, 1277, 1107, 814, 745. MS (EI), m/z: 405$[M]^+$, 334, 304, 259, 224, 180, 152, 104, 89, 76, 63, 50. Enantiomeric excess is 94% determined by HPLC analysis: Chiralcel AD-H (hexane/iPrOH = 98/2, flow rate = 1.0 mL/min, 246.9 nm), $t_{\text{r-minor}}$ 42.703 min, $t_{\text{r-major}}$ 62.512 min. $[\alpha]_D^{20}$ = 90 (c = 0.2, $CHCl_3$).



样品名称: wxh-13-r-2, wxh-13-s-2
采集日期: 2014-4-21 9:40:04, 2014-4-21

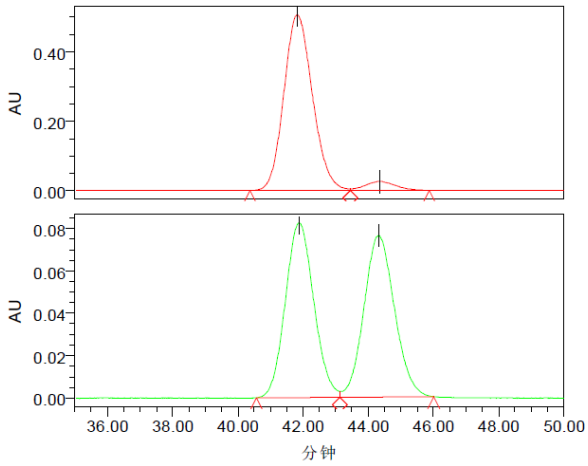
处理通道: **PDA 246.9** 纳米

	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 246.9 纳米	40.950	10847843	50.45	142836
2	PDA 246.9 纳米	42.703	1037101	2.72	14440
3	PDA 246.9 纳米	61.036	10652262	49.55	99832
4	PDA 246.9 纳米	62.512	37161740	97.28	331231



2t

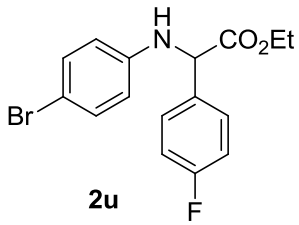
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (q, J = 8.4 Hz, 6H), 7.40 (t, J = 7.5 Hz, 2H), 7.32 (t, J = 7.3 Hz, 1H), 7.23 – 7.15 (m, 2H), 6.44 (d, J = 8.8 Hz, 2H), 5.05 (q, J = 5.7 Hz, 2H), 4.29 – 4.07 (m, 2H), 1.21 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.35, 144.83, 141.22, 140.37, 136.08, 131.91, 128.73, 127.54, 127.49, 127.42, 127.00, 114.98, 109.73, 77.32, 77.00, 76.68, 61.98, 60.32, 14.00. IR ν_{max} (cm^{-1}) 3405, 2982, 2927, 1735, 1596, 1497, 1315, 1264, 1177, 1022, 814, 737, 699. MS (EI), m/z: 409$[M]^+$, 336, 257, 184, 155, 127, 115, 103, 76, 63, 50. Enantiomeric excess is 90% determined by HPLC analysis: Chiralcel AD-H (hexane/iPrOH = 98/2, flow rate = 1.0 mL/min, 255.1 nm), $t_{r\text{-minor}}$ 44.349 min, $t_{r\text{-major}}$ 41.823 min. $[\alpha]_D^{20}$ = 135 (c = 0.2, $CHCl_3$).



样品名称: wxh-16-r, wxh-16-s
采集日期: 2014-4-19 15:47:24, 2014-4-19

处理通道: **PDA 255.1** 纳米

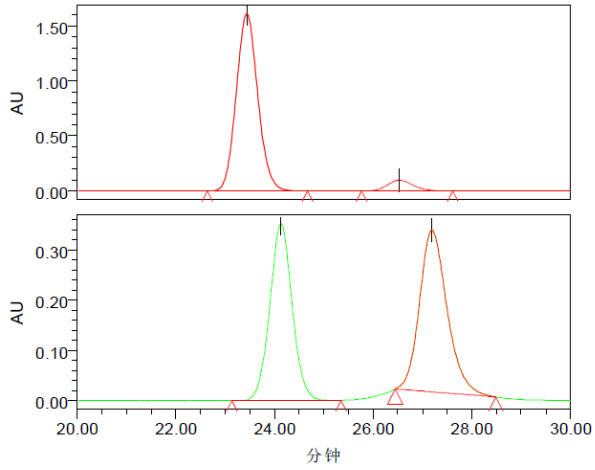
	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 255.1 纳米	41.823	30872620	94.89	506141
2	PDA 255.1 纳米	41.880	5014363	50.16	82617
3	PDA 255.1 纳米	44.319	4983079	49.84	76417
4	PDA 255.1 纳米	44.349	1663274	5.11	25326



2u

Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.43 (m, 2H), 7.22 (d, J = 6.8 Hz, 2H), 7.07 (t, J = 8.6 Hz, 2H), 6.43 (d, J = 8.9 Hz, 2H), 5.07 (s, 1H), 5.01 (s, 1H), 4.32 – 4.11 (m, 2H), 1.24 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.19, 162.63 (d, J = 247.2 Hz), 144.62, 132.89 (d, J = 3.2 Hz), 131.94, 128.75 (d, J = 8.3 Hz), 115.81 (d, J = 21.7 Hz), 115.64 (d, J = 21.6 Hz), 109.88, 62.07, 59.90, 13.98. IR ν_{max} (cm^{-1}) 3402, 2982, 2930, 1735, 1596, 1505, 1311, 1226, 1178, 1019, 811. MS (EI), m/z: 351$[M]^+$,

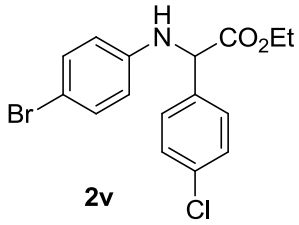
278, 198, 182, 155, 122, 107, 95, 76, 63, 50. Enantiomeric excess is 87% determined by HPLC analysis: Chiralcel AD-H (hexane/iPrOH = 98/2, flow rate = 1.0 mL/min, 249.2 nm), $t_{\text{r-minor}}$ 26.531 min, $t_{\text{r-major}}$ 23.438 min. $[\alpha]_D^{20}$ = 80 (c = 0.2, $CHCl_3$).



样品名称: wxh-29-r, wxh-29-s
采集日期: 2014-5-12 12:45:34, 2014-5-12

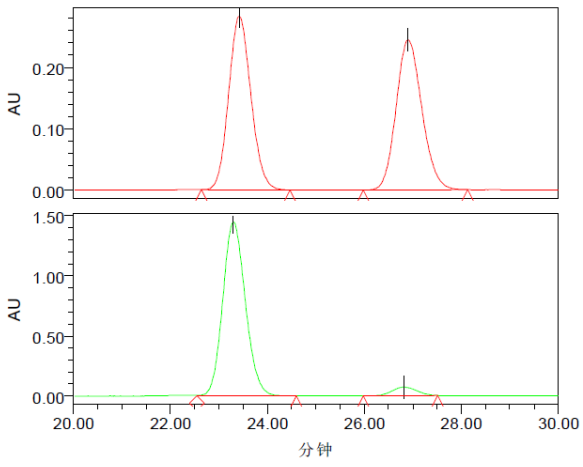
处理通道: **PDA 249.2** 纳米

	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 249.2 纳米	23.438	49082516	93.28	1610534
2	PDA 249.2 纳米	24.131	11112470	46.96	353360
3	PDA 249.2 纳米	26.531	3537954	6.72	97608
4	PDA 249.2 纳米	27.191	12551420	53.04	322825



2v

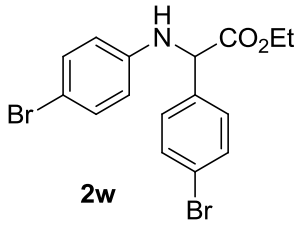
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, J = 8.5 Hz, 2H), 7.32 (d, J = 8.5 Hz, 2H), 7.19 (d, J = 8.8 Hz, 2H), 6.39 (d, J = 8.8 Hz, 2H), 5.05 (d, J = 5.3 Hz, 1H), 4.97 (d, J = 5.5 Hz, 1H), 4.31 – 4.06 (m, 2H), 1.22 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.94, 144.50, 135.73, 134.21, 131.97, 129.06, 128.45, 114.97, 109.95, 62.20, 59.97, 13.99. IR ν_{max} (cm^{-1}) 3402, 2981, 2928, 1735, 1596, 1495, 1311, 1251, 1177, 1015, 813, 738. MS (EI), m/z: 367[M]$^+$, 196, 260, 209, 184, 152, 138, 125, 105, 89, 76, 63, 50. Enantiomeric excess is 90% determined by HPLC analysis: Chiralcel AD-H (hexane/iPrOH = 98/2, flow rate = 1.0 mL/min, 248.0 nm), $t_{\text{r-minor}}$ 26.820 min, $t_{\text{r-major}}$ 23.299 min. $[\alpha]_D^{20}$ = 105 (c = 0.2, $CHCl_3$).



样品名称: wxh-14-r, wxh-14-s
采集日期: 2014-4-19 13:43:26, 2014-4-19

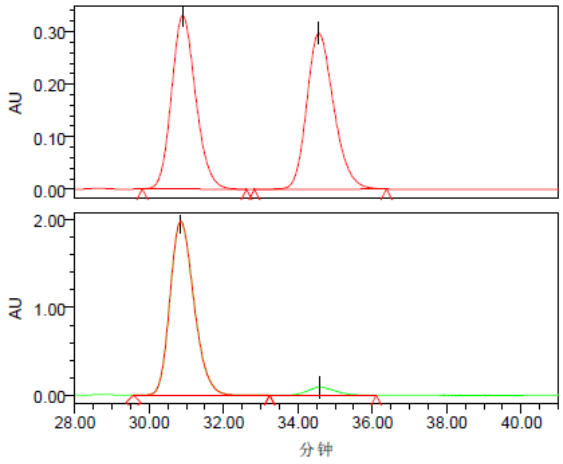
处理通道: **PDA 248.0** 纳米

	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 248.0 纳米	23.299	47021761	94.76	1447779
2	PDA 248.0 纳米	23.420	9067009	50.04	283038
3	PDA 248.0 纳米	26.820	2598254	5.24	72799
4	PDA 248.0 纳米	26.903	9051541	49.96	244971



2w

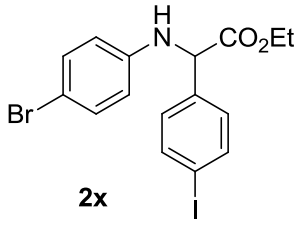
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, J = 8.5 Hz, 2H), 7.35 (d, J = 8.4 Hz, 2H), 7.18 (d, J = 8.8 Hz, 2H), 6.38 (d, J = 8.8 Hz, 2H), 5.05 (d, J = 5.2 Hz, 1H), 4.95 (d, J = 5.4 Hz, 1H), 4.30 – 4.07 (m, 2H), 1.21 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.84, 144.48, 136.28, 132.00, 131.96, 128.78, 122.35, 114.97, 109.96, 62.20, 60.03, 13.98. IR ν_{max} (cm^{-1}) 3401, 2981, 2930, 1735, 1596, 1498, 1311, 1177, 1073, 1011, 813. MS (EI), m/z: 411[M]$^{+}$, 340, 259, 182, 157, 103, 90, 76, 63, 50. Enantiomeric excess is 90% determined by HPLC analysis: Chiralcel AD-H (hexane/iPrOH = 98/2, flow rate = 1.0 mL/min, 248.0 nm), $t_{\text{r-minor}}$ 34.595 min, $t_{\text{r-major}}$ 30.853 min. $[\alpha]_D^{20}$ = 115 (c = 0.2, $CHCl_3$).



样品名称： wxh-22, wxh-22-s
采集日期： 2014-5-12 9:52:40, 2014-5-12

处理通道: **PDA 248.0** 纳米

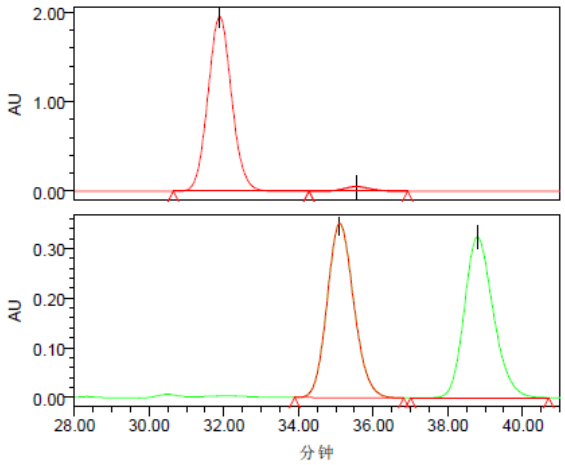
	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 248.0 纳米	30.853	88847703	94.99	1984521
2	PDA 248.0 纳米	30.904	14899505	49.95	330470
3	PDA 248.0 纳米	34.560	14927419	50.05	297041
4	PDA 248.0 纳米	34.595	4684018	5.01	91430



2x

Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, J = 8.4 Hz, 2H), 7.19 (dd, J = 13.4, 8.6 Hz, 4H), 6.37 (d, J = 8.8 Hz, 2H), 5.03 (s, 1H), 4.93 (s, 1H), 4.28 – 4.05 (m, 2H), 1.21 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.83, 144.48, 137.96, 137.01, 131.98, 129.02, 114.97, 109.98, 94.06, 62.22, 60.15, 14.00. IR ν_{max} (cm^{-1}) 3402, 2980, 2928, 1735, 1595, 1497, 1309, 1249, 1177, 1006, 812, 737. MS (EI), m/z: 459[M]$^{+}$, 386, 307, 259, 182, 152, 134, 103, 90, 76, 63, 50. Enantiomeric excess is 94% determined by HPLC analysis: Chiralcel AD-H (hexane/iPrOH = 98/2, flow rate = 1.0 mL/min, 243.3

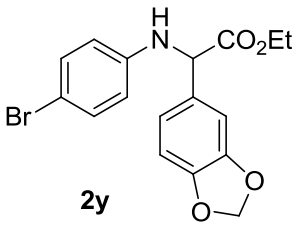
nm), $t_{r\text{-minor}}$ 35.549 min, $t_{r\text{-major}}$ 31.892 min. $[\alpha]_D^{20}$ = 110 (c = 0.2, $CHCl_3$).



样品名称： wxh-30-r, wxh-30-s
采集日期： 2014-5-12 11:18:17, 2014-5-12

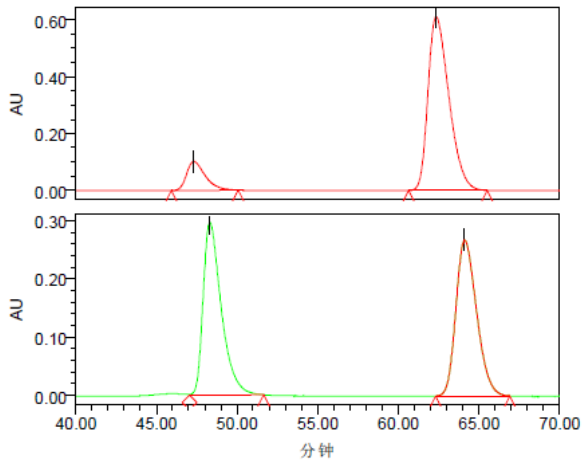
处理通道: **PDA 243.3** 纳米

	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 243.3 纳米	31.892	86192706	97.14	1950460
2	PDA 243.3 纳米	35.104	17439556	49.93	350627
3	PDA 243.3 纳米	35.549	2539977	2.86	50732
4	PDA 243.3 纳米	38.790	17486579	50.07	323486



2y

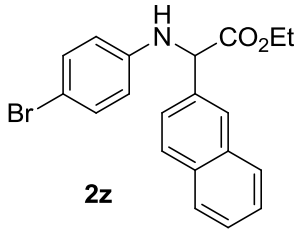
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 (d, J = 8.8 Hz, 2H), 6.94 (s, 2H), 6.76 (d, J = 8.0 Hz, 1H), 6.41 (d, J = 8.8 Hz, 2H), 5.93 (d, J = 2.4 Hz, 2H), 5.01 (d, J = 4.9 Hz, 1H), 4.89 (d, J = 5.3 Hz, 1H), 4.27 – 4.06 (m, 2H), 1.22 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.39, 148.09, 147.62, 144.70, 131.86, 130.93, 120.69, 114.93, 109.67, 108.44, 107.26, 101.20, 61.94, 60.19, 14.00. IR ν_{max} (cm^{-1}) 3402, 2981, 2899, 1733, 1595, 1500, 1489, 1318, 1244, 1039, 930, 813, 737. MS (EI), m/z: 377$[M]^+$, 306, 225, 182, 155, 135, 103, 93, 76, 65, 50. Enantiomeric excess is 74% determined by HPLC analysis: Chiralcel AD-H (hexane/iPrOH = 98/2, flow rate = 1.0 mL/min, 249.2 nm), $t_{r\text{-minor}}$ 47.331 min, $t_{r\text{-major}}$ 62.358 min. $[\alpha]_D^{20}$ = 80 (c = 0.2, $CHCl_3$).



样品名称： wxh-26-r, wxh-26-s
采集日期： 2014-5-12 16:20:43, 2014-5-12

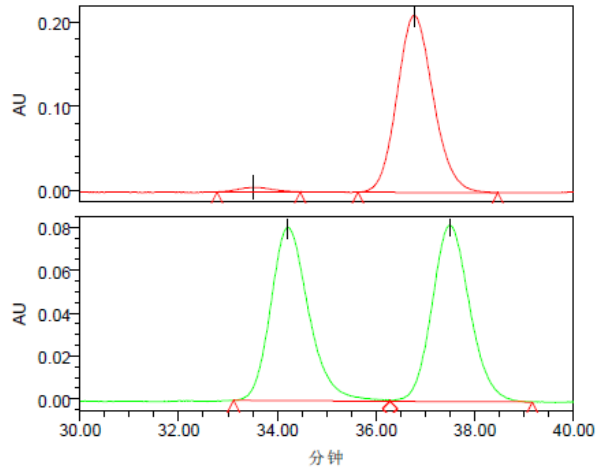
处理通道: **PDA 249.2** 纳米

	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 249.2 纳米	47.331	8107574	12.80	101664
2	PDA 249.2 纳米	48.327	23151790	49.25	295425
3	PDA 249.2 纳米	62.358	55229922	87.20	611116
4	PDA 249.2 纳米	64.130	23857419	50.75	266946



2z

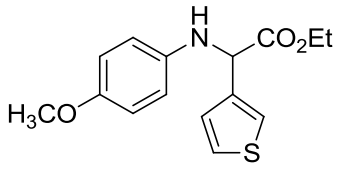
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (s, 1H), 7.81 (t, J = 8.0 Hz, 3H), 7.57 (d, J = 8.5 Hz, 1H), 7.51 – 7.42 (m, 2H), 7.16 (d, J = 8.8 Hz, 2H), 6.45 (d, J = 8.8 Hz, 2H), 5.15 (s, 2H), 4.30 – 4.03 (m, 2H), 1.18 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.37, 144.82, 134.59, 133.26, 133.21, 131.88, 128.74, 127.98, 127.65, 126.33, 126.32, 126.28, 124.70, 115.00, 109.72, 62.02, 60.74, 13.99. IR ν_{max} (cm^{-1}) 3396, 2985, 2930, 1730, 1596, 1498, 1265, 1166, 1022, 813, 738. MS (EI), m/z: 383[M]$^+$, 356, 310, 226, 182, 155, 127, 115, 103, 76, 63, 50. Enantiomeric excess is 95% determined by HPLC analysis: Chiralcel AD-H (hexane/iPrOH = 98/2, flow rate = 1.0 mL/min, 225.7 nm), $t_{r\text{-minor}}$ 33.524 min, $t_{r\text{-major}}$ 36.777 min. $[\alpha]_D^{20}$ = 135 (c = 0.2, $CHCl_3$).



样品名称： wxh-25-r, wxh-25-s
采集日期： 2014-5-12 14:43:01, 2014-5-12

处理通道: **PDA 225.7** 纳米

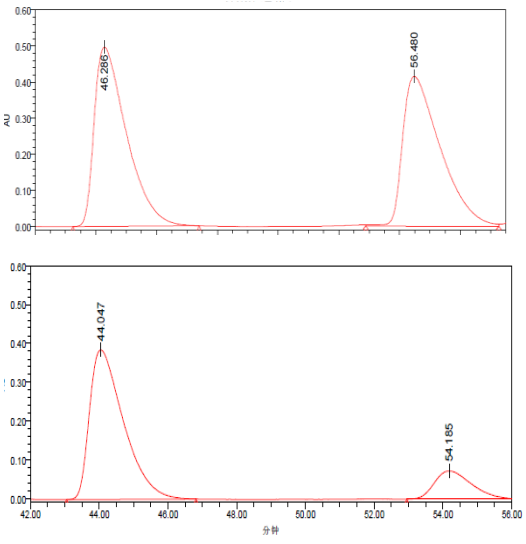
	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 225.7 纳米	33.524	257620	2.34	5270
2	PDA 225.7 纳米	34.215	4314999	49.71	80652
3	PDA 225.7 纳米	36.777	10738090	97.66	210115
4	PDA 225.7 纳米	37.500	4364938	50.29	82111



2aa

Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (dd, J = 10.2, 5.2 Hz, 2H), 7.16 (d, J = 5.0 Hz, 1H), 6.74 (d, J = 8.9 Hz, 2H), 6.58 (d, J = 8.9 Hz, 2H), 5.12 (s, 1H), 4.51 (s, 1H), 4.20 (qd, J = 10.8, 5.4 Hz, 2H), 3.71 (s, 3H), 1.23 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.74, 152.70, 140.33, 138.49, 126.47, 126.25, 122.74, 114.96, 114.83, 61.66, 58.04, 55.66, 14.07. IR ν_{max} (cm^{-1}) 3388, 2933, 2905, 1735, 1513, 1283, 1185, 1157, 1035, 820, 774. MS (EI), m/z: 291[M]$^+$, 218, 174, 134, 122, 107, 92, 77, 64, 50. Enantiomeric excess is 66% determined by HPLC analysis:

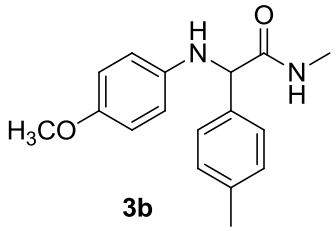
Chiralcel OD-H (hexane/iPrOH = 98/2, flow rate = 1.0 mL/min, 241.0 nm), t $_{r\text{-minor}}$ 54.185 min, t $_{r\text{-major}}$ 44.047 min. $[\alpha]_D^{20}$ = 40 (c = 0.2, $CHCl_3$).



样品名称： wxh-39-r-1, wxh-39-s-1
采集日期： 2014-5-28 9:53:47, 2014-5-28

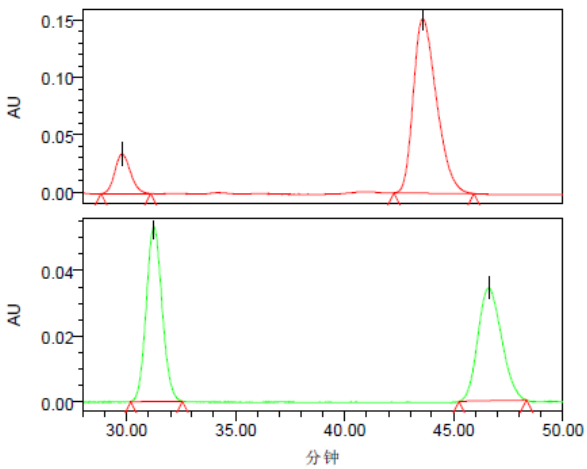
处理通道: **PDA 241.0** 纳米

	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 241.0 纳米	44.047	26529928	82.91	385844
2	PDA 241.0 纳米	46.286	36675346	50.61	496853
3	PDA 241.0 纳米	54.185	5467514	17.09	72841
4	PDA 241.0 纳米	56.480	35786551	49.39	415433



3b

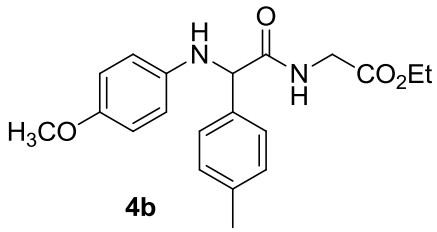
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (d, J = 8.0 Hz, 2H), 7.17 (d, J = 7.9 Hz, 2H), 6.85 (s, 1H), 6.76 (d, J = 8.9 Hz, 2H), 6.56 (d, J = 8.9 Hz, 2H), 4.63 (s, 1H), 4.43 (s, 1H), 3.72 (s, 3H), 2.80 (d, J = 4.9 Hz, 3H), 2.33 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.20, 153.01, 140.83, 138.21, 135.98, 129.73, 127.18, 114.86, 114.79, 64.55, 55.64, 26.22, 21.06. IR ν_{max} (cm^{-1}) 3321, 2928, 2833, 1656, 1512, 1241, 1178, 1036, 820, 773, 737. MS (EI), m/z: 284[M]$^+$, 226, 182, 168, 134, 119, 107, 77, 57, 51. Enantiomeric excess is 74% determined by HPLC analysis: Chiralcel AD-H (hexane/iPrOH = 90/10, flow rate = 1.0 mL/min, 242.1 nm), t $_{r\text{-minor}}$ 29.788 min, t $_{r\text{-major}}$ 43.583 min. $[\alpha]_D^{20}$ = 95 (c = 0.2, $CHCl_3$).



样品名称： wxh-21-r, wxh-21-s-2
采集日期： 2014-4-18 14:40:51, 2014-5-14

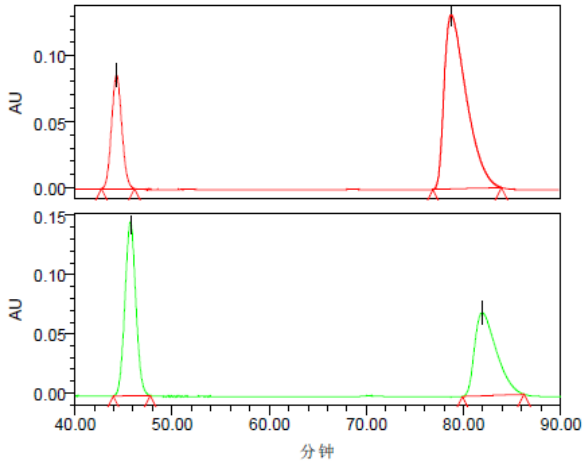
处理通道: **PDA 242.1** 纳米

	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 242.1 纳米	29.788	1718820	13.23	34423
2	PDA 242.1 纳米	31.248	2683646	50.89	53105
3	PDA 242.1 纳米	43.583	11271155	86.77	151742
4	PDA 242.1 纳米	46.607	2589292	49.11	34316



4b

Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.32 (m, 3H), 7.18 (d, J = 7.9 Hz, 2H), 6.77 (d, J = 8.8 Hz, 2H), 6.60 (d, J = 8.9 Hz, 2H), 4.68 (s, 1H), 4.21 – 4.08 (m, 4H), 3.96 – 3.86 (m, 1H), 3.73 (s, 3H), 2.33 (s, 3H), 1.24 (t, J = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.97, 169.49, 153.10, 140.70, 138.33, 135.64, 129.76, 127.31, 115.00, 114.75, 64.64, 61.38, 55.61, 41.18, 21.07, 14.02. IR ν_{max} (cm^{-1}) 3368, 2986, 2934, 1744, 1666, 1512, 1241, 1202, 1035, 821, 735. MS (EI), m/z: 356$[M]^+$, 226, 207, 168, 134, 119, 107, 91, 77, 56, 50. Enantiomeric excess is 54% determined by HPLC analysis: Chiralcel AD-H (hexane/iPrOH = 90/10, flow rate = 1.0 mL/min, 242.1 nm), $t_{r\text{-minor}}$ 44.281 min, $t_{r\text{-major}}$ 78.744 min. $[\alpha]_D^{20}$ = 60 (c = 0.2, $CHCl_3$).

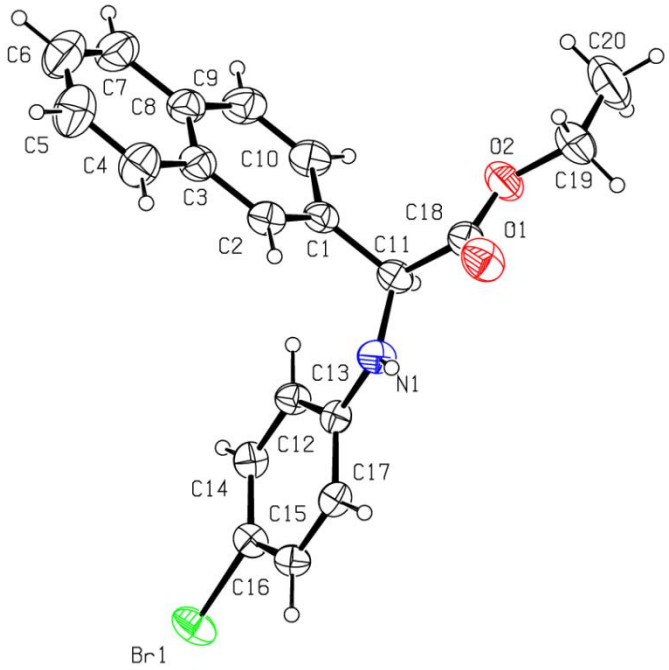


样品名称: wxh-20-race, wxh-20-s
采集日期: 2014-4-18 11:34:15, 2014-4-18

处理通道: **PDA 242.1** 纳米

	处理通道	保留时间 (分钟)	面积	% 面积	峰高
1	PDA 242.1 纳米	44.281	6331191	23.23	85869
2	PDA 242.1 纳米	45.713	11416965	51.16	146559
3	PDA 242.1 纳米	78.744	20926880	76.77	131441
4	PDA 242.1 纳米	81.946	10898313	48.84	69880

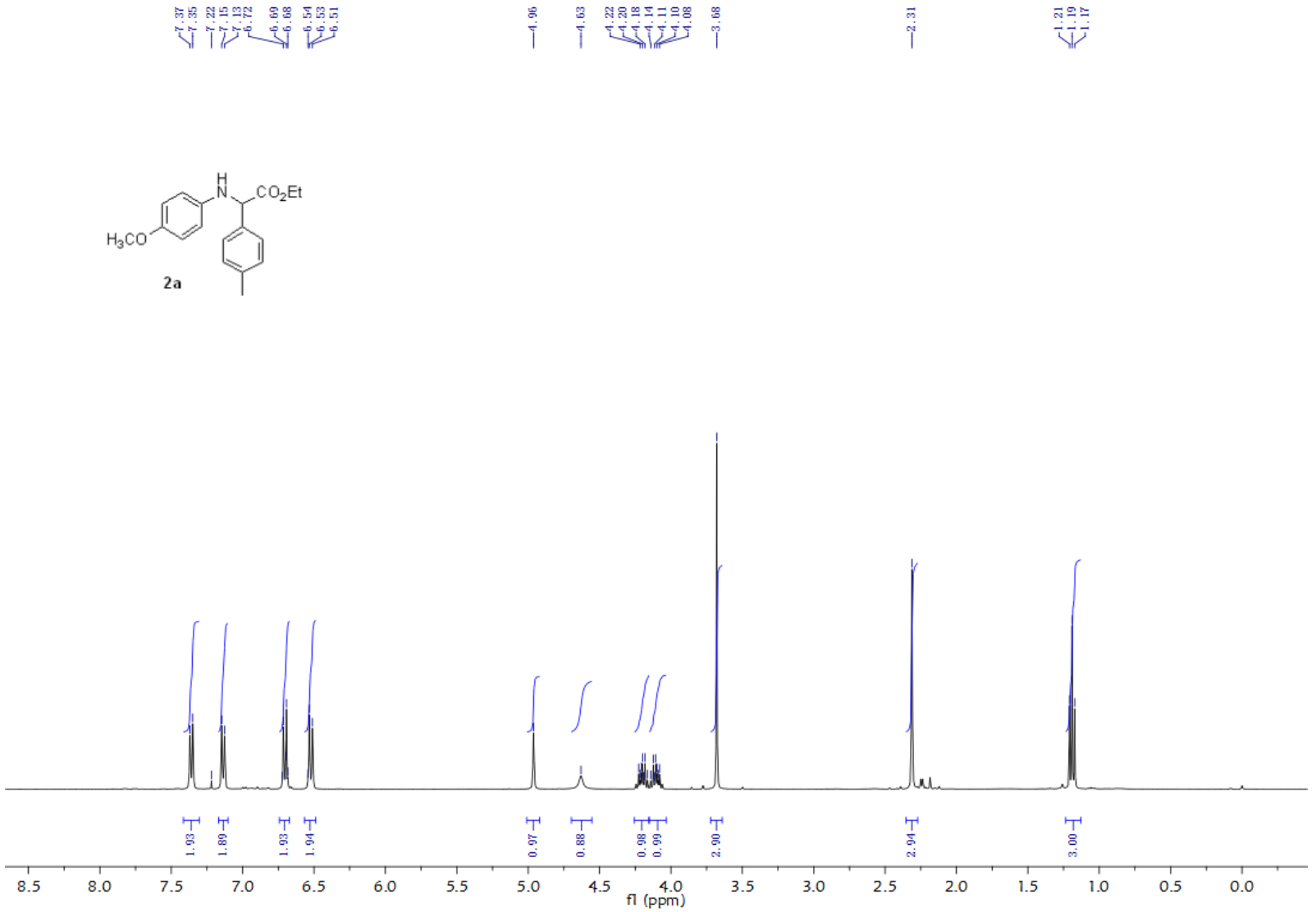
8. Crystal structure for 2z.



(*S*)-ethyl 2-((4-bromophenyl)amino)-2-(naphthalen-2-yl)acetate

(CCDC 1005709)

^{1}H and ^{13}C NMR spectra of Products


7.37
7.35
7.22
7.15
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6.72
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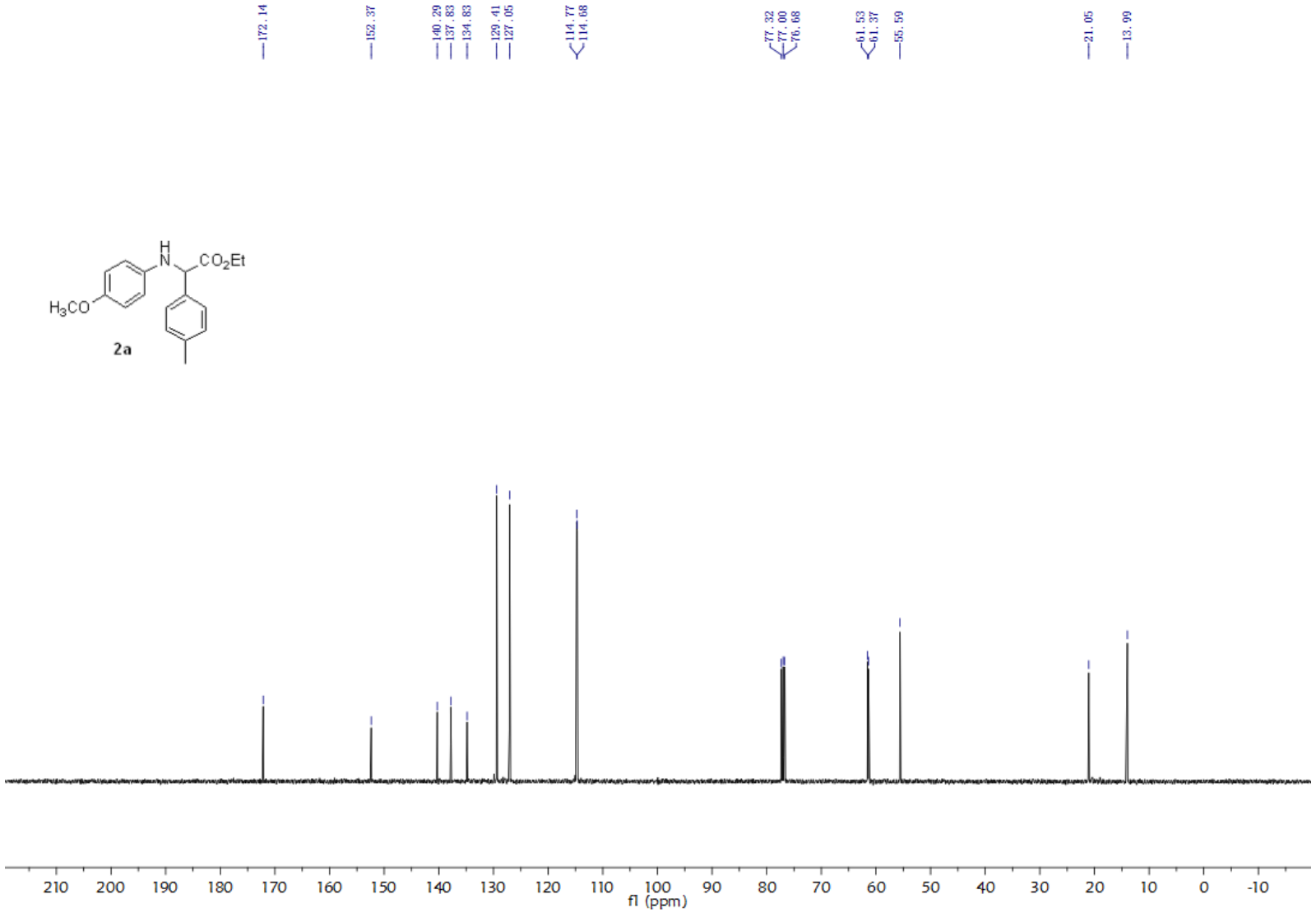
6.68
6.54
6.53
6.51
4.96
4.63
4.22
4.20
4.18
4.14
4.11
4.10
4.08
3.68
2.31
1.21
1.19
1.17
H
N
CO2Et
H3CO
2a
1.93
1.89
1.93
1.94
0.97
0.88
0.98
0.99
2.90
2.94
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


172.14
152.37
140.29
137.83
134.83
129.41
127.05
114.77
114.68
77.32
77.00
76.68
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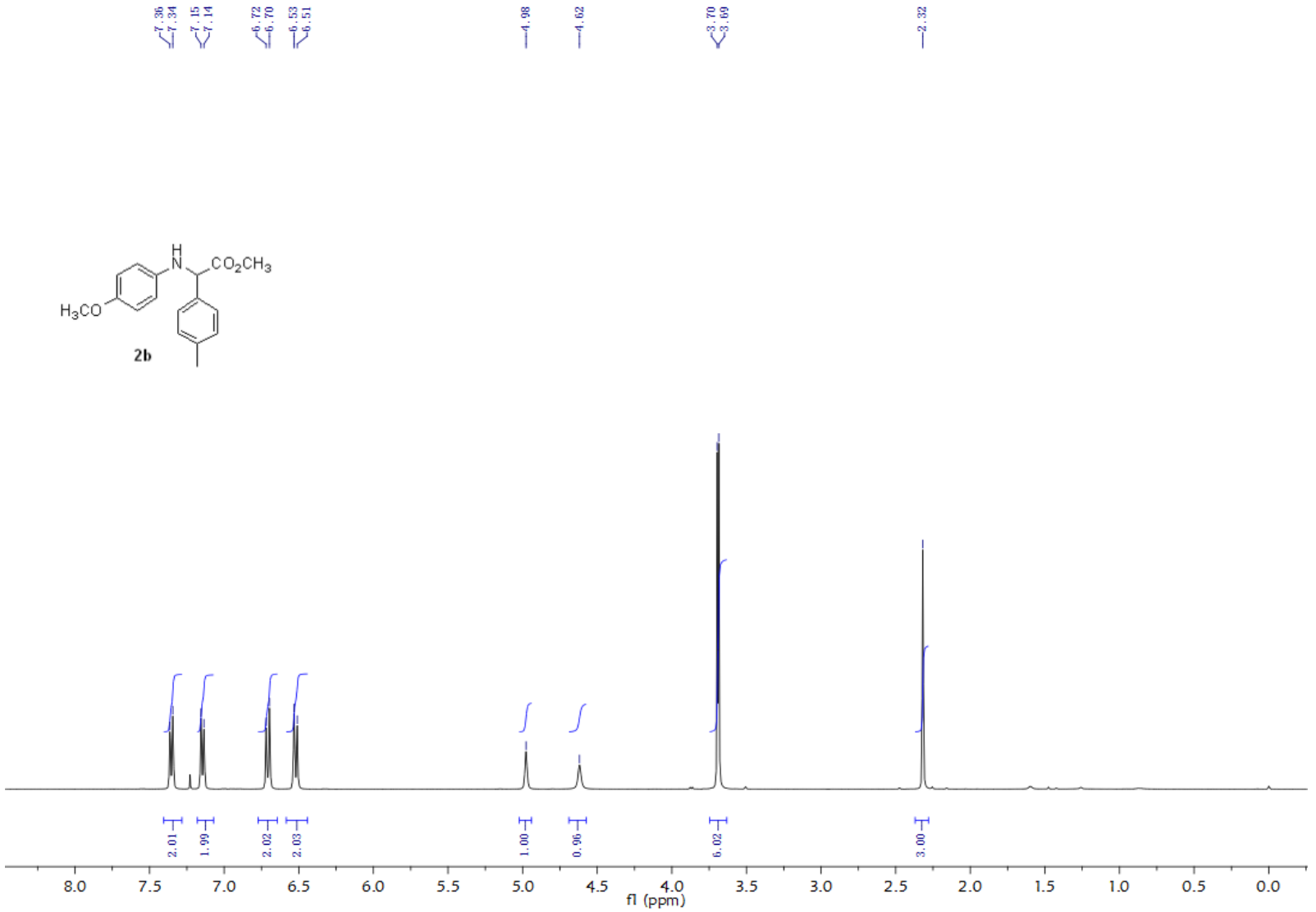
61.37
55.59
21.05
13.99
H
N
CO2Et
H3CO
2a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.14
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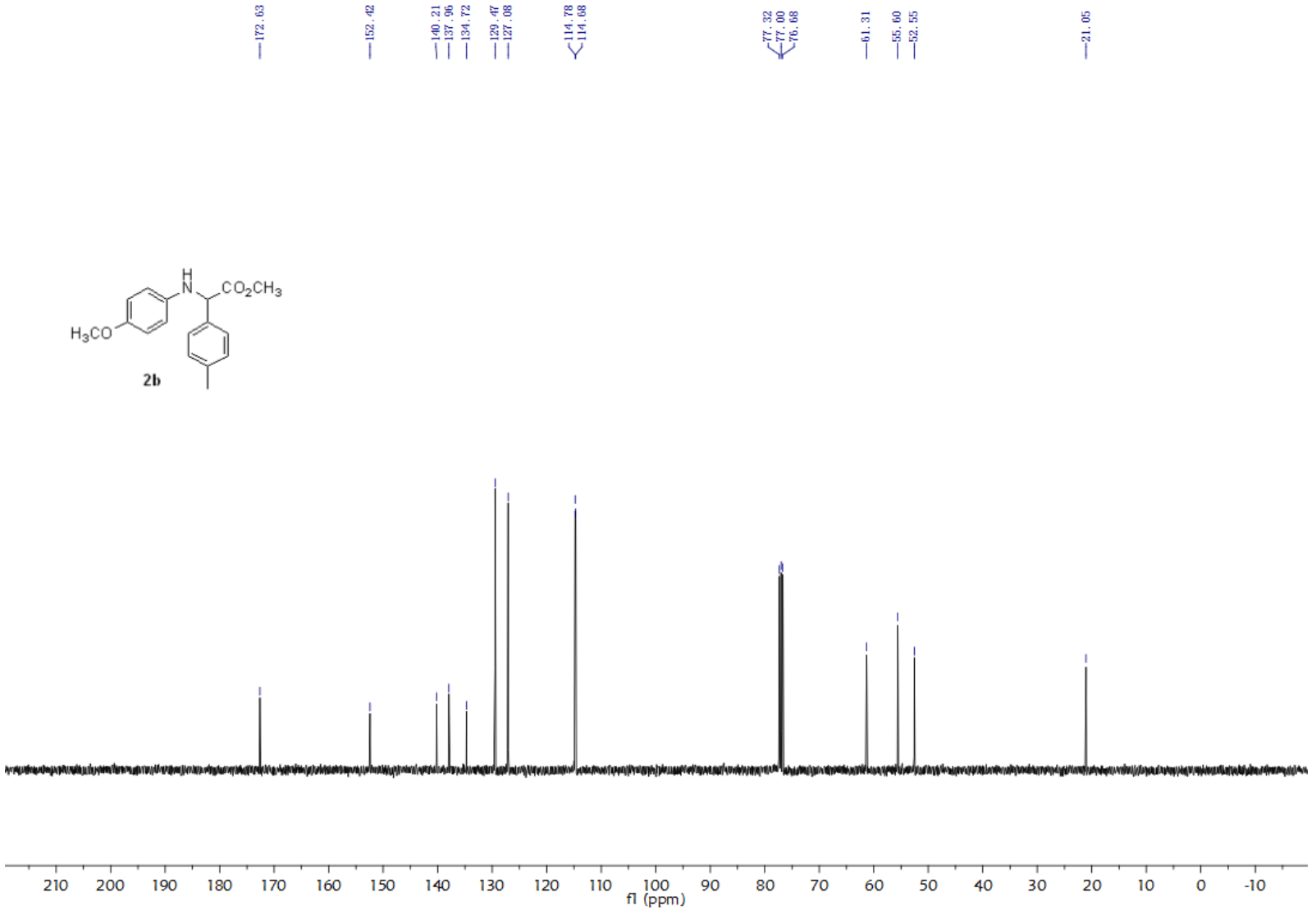
6.70
6.53
6.51
4.98
4.62
3.70
3.69
2.32
H
N
CO2CH3
H3CO
2b
2.01
1.99
2.02
2.03
1.00
0.96
6.02
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


172.63
152.42
140.21
137.96
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129.47
127.08
114.78
114.68
77.32
77.00
76.68
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55.60
52.55
21.05
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N
CO2CH3
H3CO
2b
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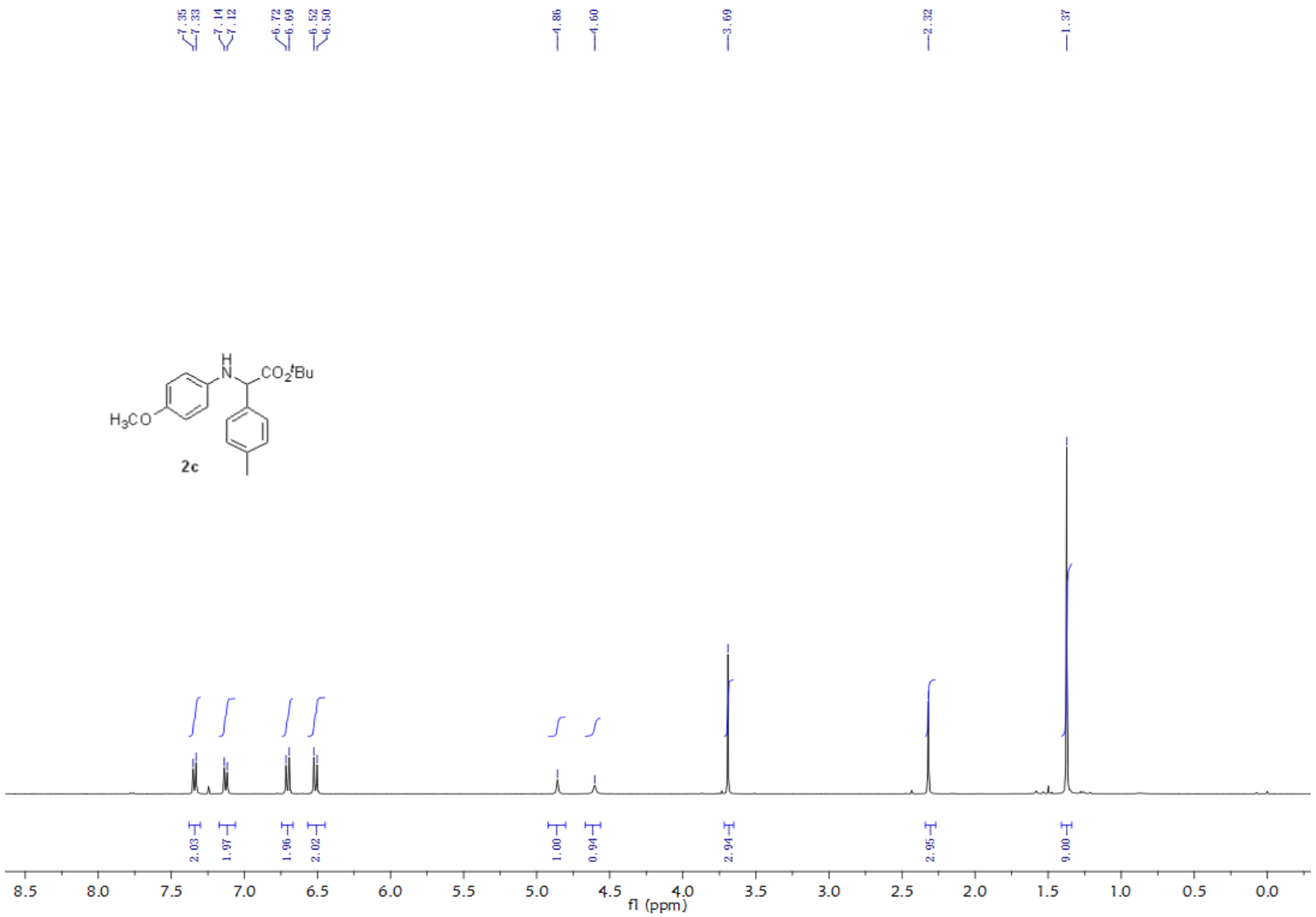
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.33
7.14
7.12
6.72
6.69
6.52
6.50
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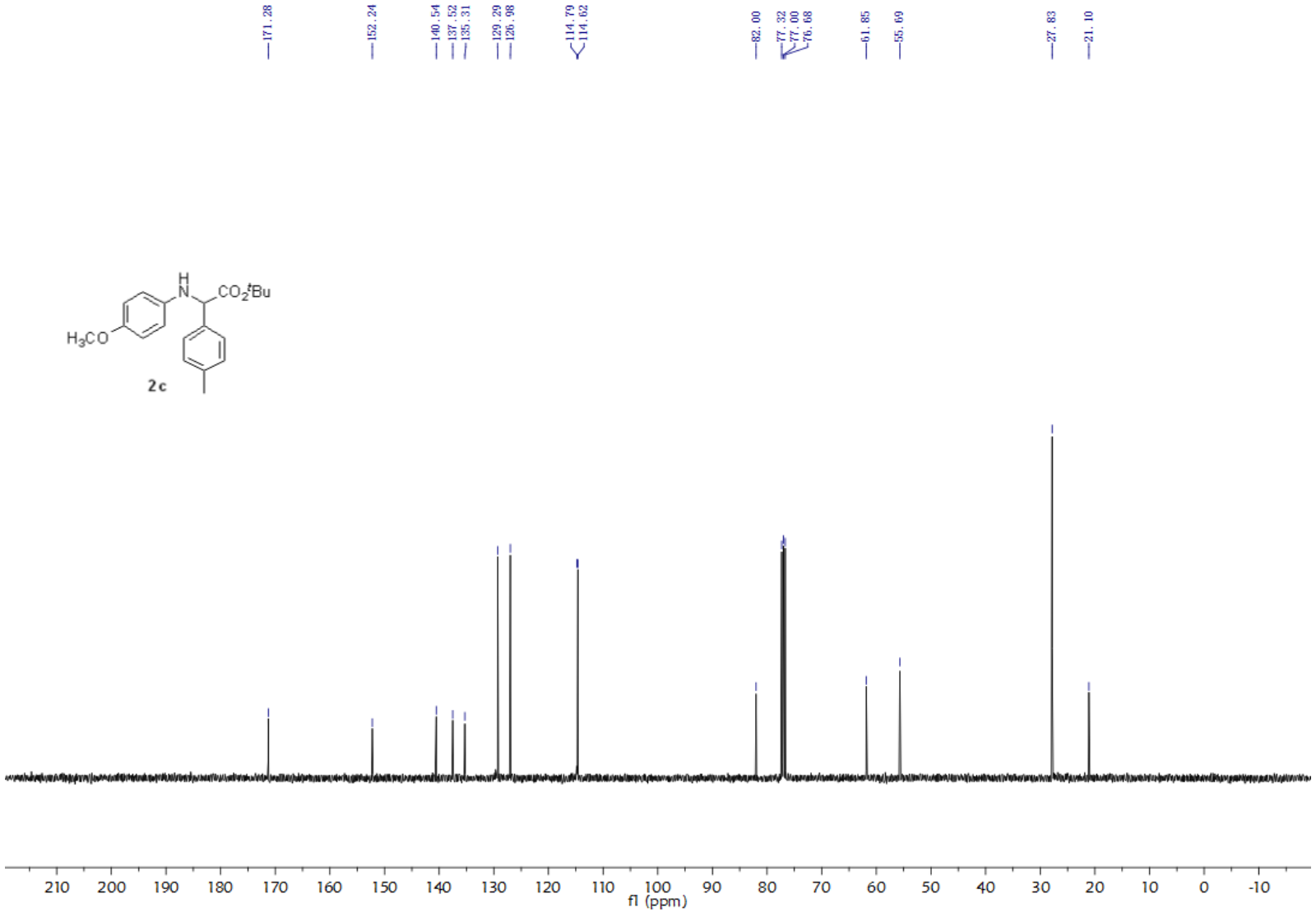
4.60
3.69
2.32
1.37
H
N
CO2tBu
H3CO
2c
2.03
1.97
1.96
2.02
1.00
0.94
2.94
2.95
9.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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77.00
76.68
61.85
55.69
27.83
21.10
H
N
CO2tBu
H3CO
2c
210
200
190
180
170
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100
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80
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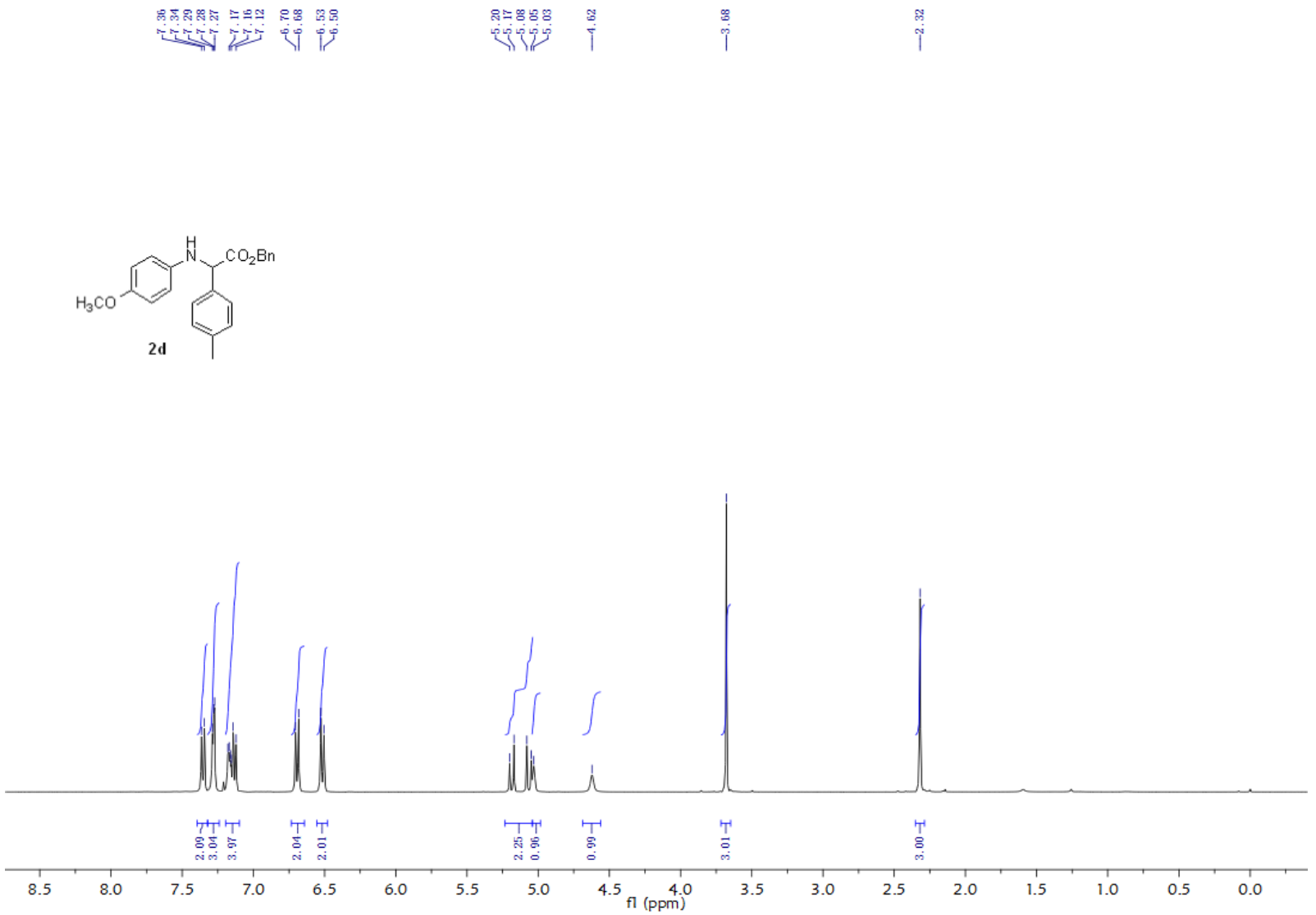
f1 (ppm)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5.08
5.05
5.03
4.62
3.68
2.32
H
N
CO2Bn
H3CO
2d
2.09
3.04
3.97
2.04
2.01
2.25
0.96
0.99
3.01
3.00
8.5
8.0
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7.0
6.5
6.0
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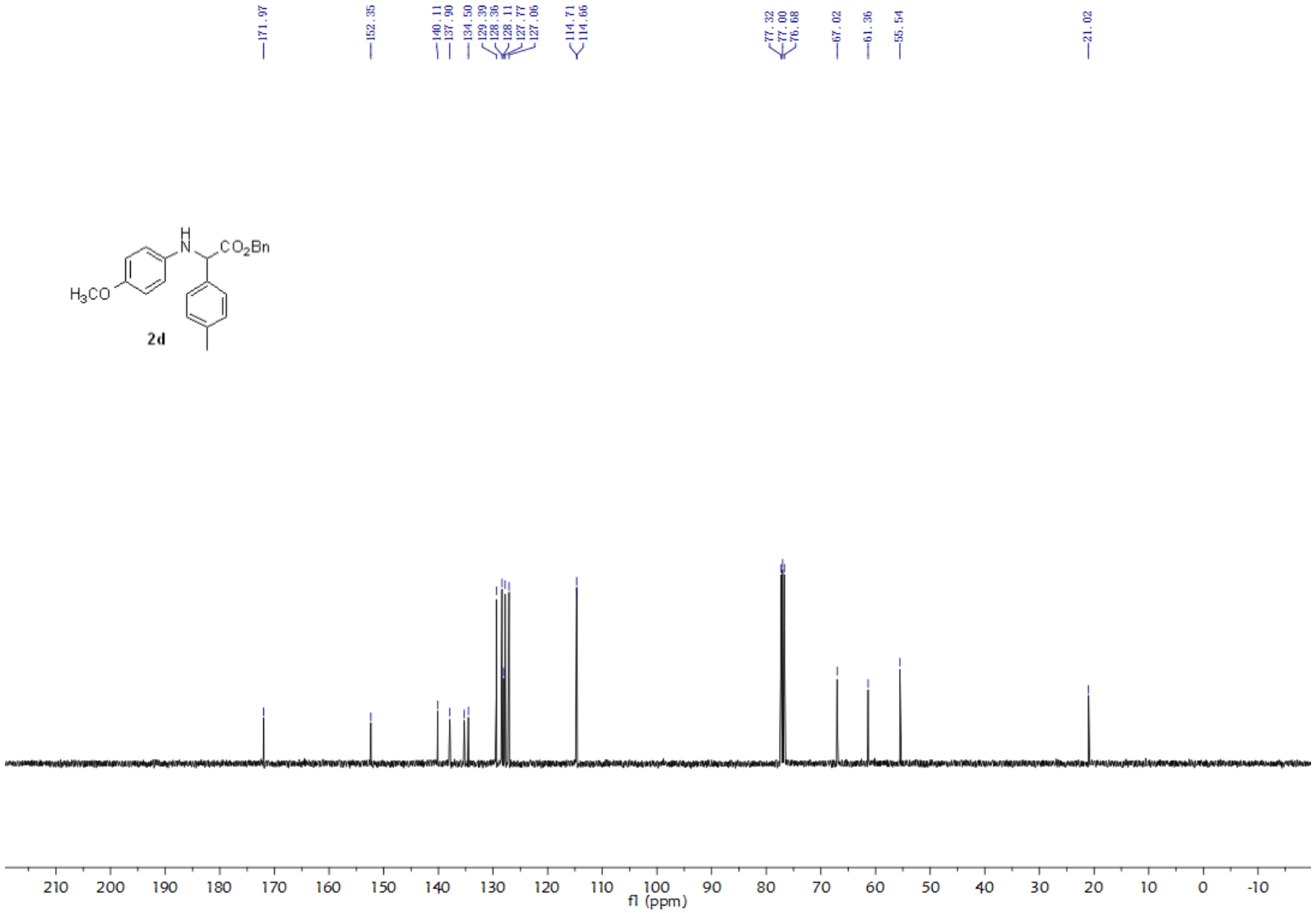
f1 (ppm)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76.68
67.02
61.36
55.54
21.02
H3CO
CO2Bn
2d
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200
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180
170
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100
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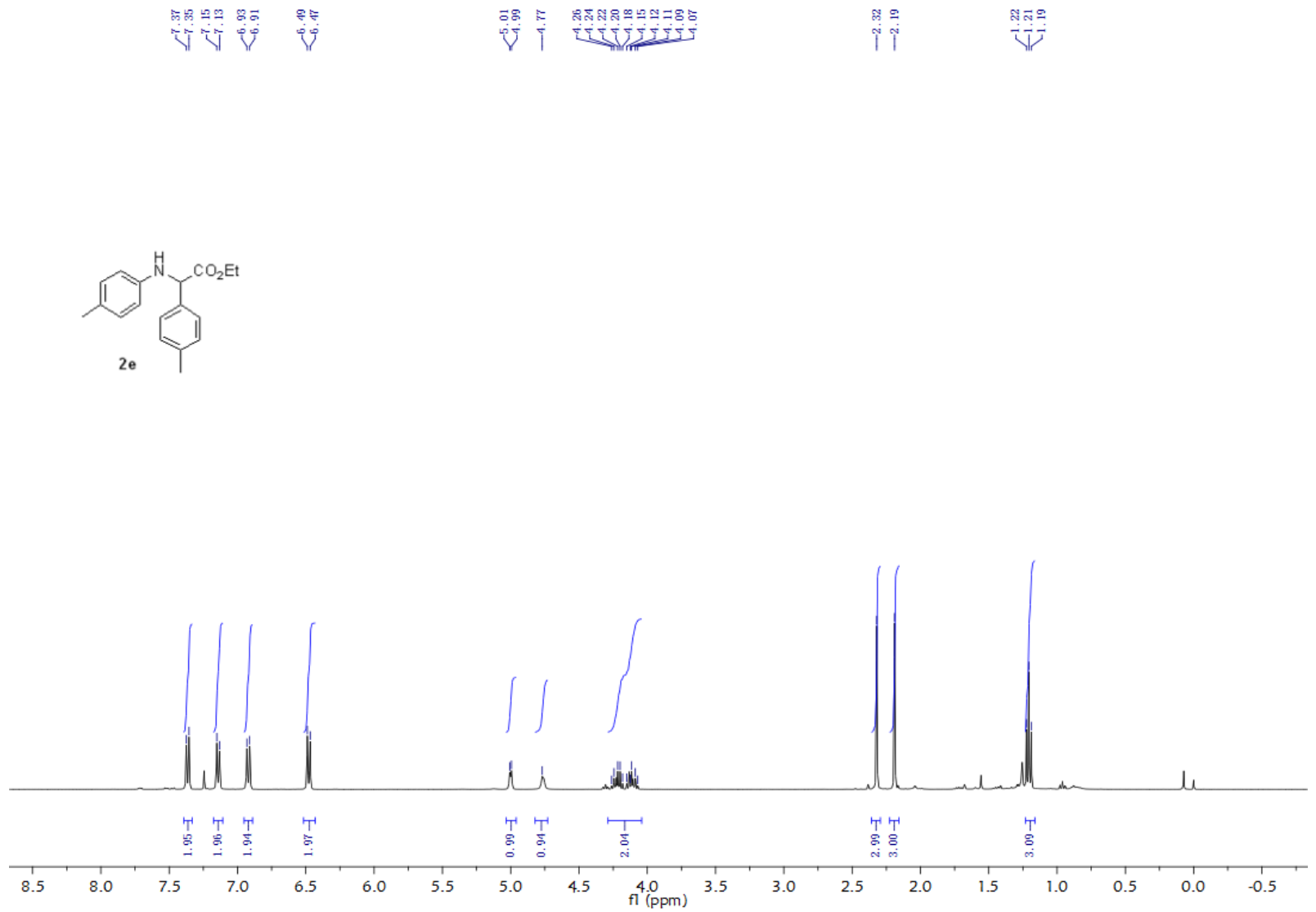
-10
f1 (ppm)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4.07
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2.19
1.22
1.21
1.19
CO2Et
2e
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1.94
1.97
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0.94
2.04
2.99
3.00
3.09
8.5
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5.0
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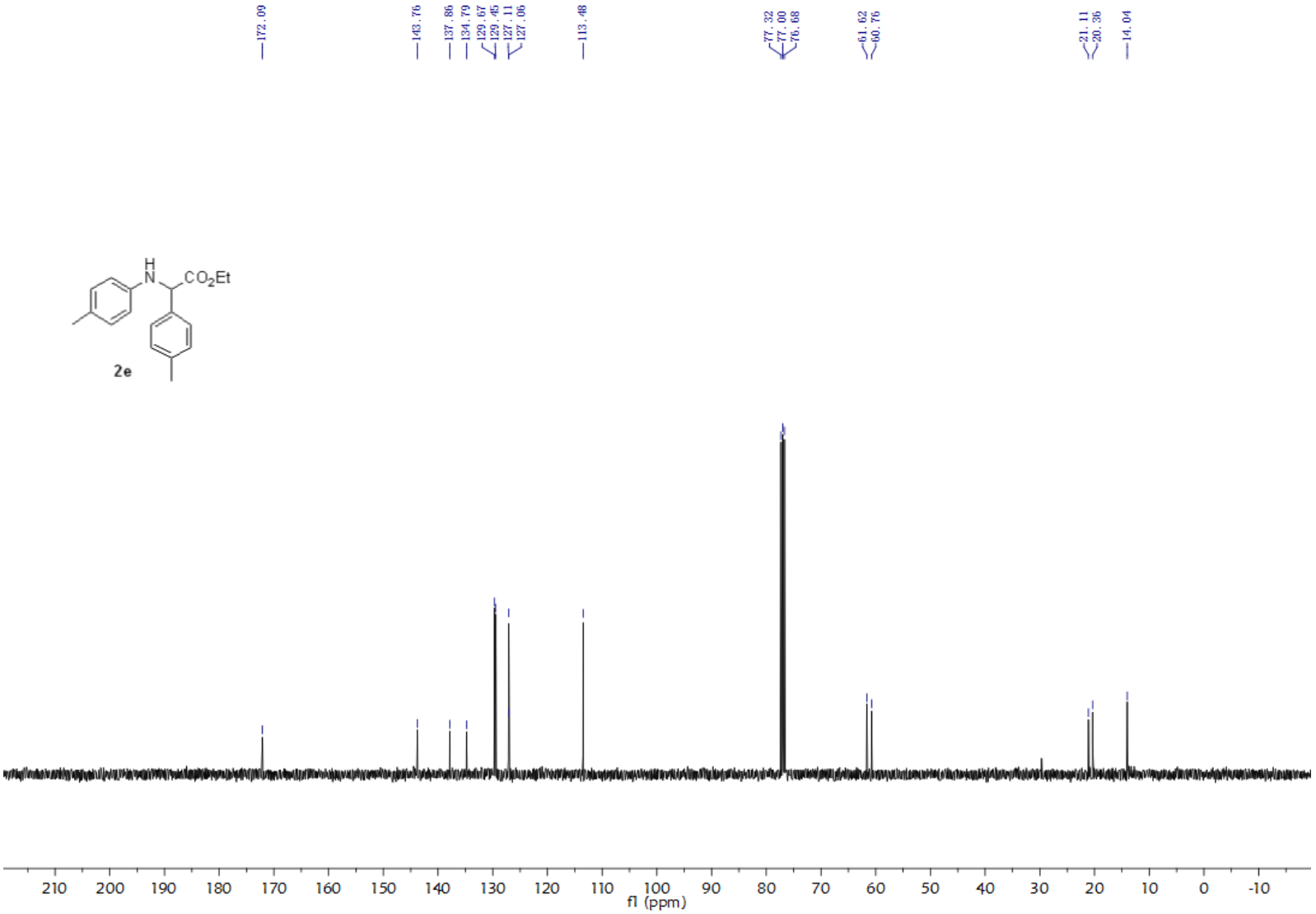
f1 (ppm)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14.04
H
N
CO2Et
2e
210
200
190
180
170
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100
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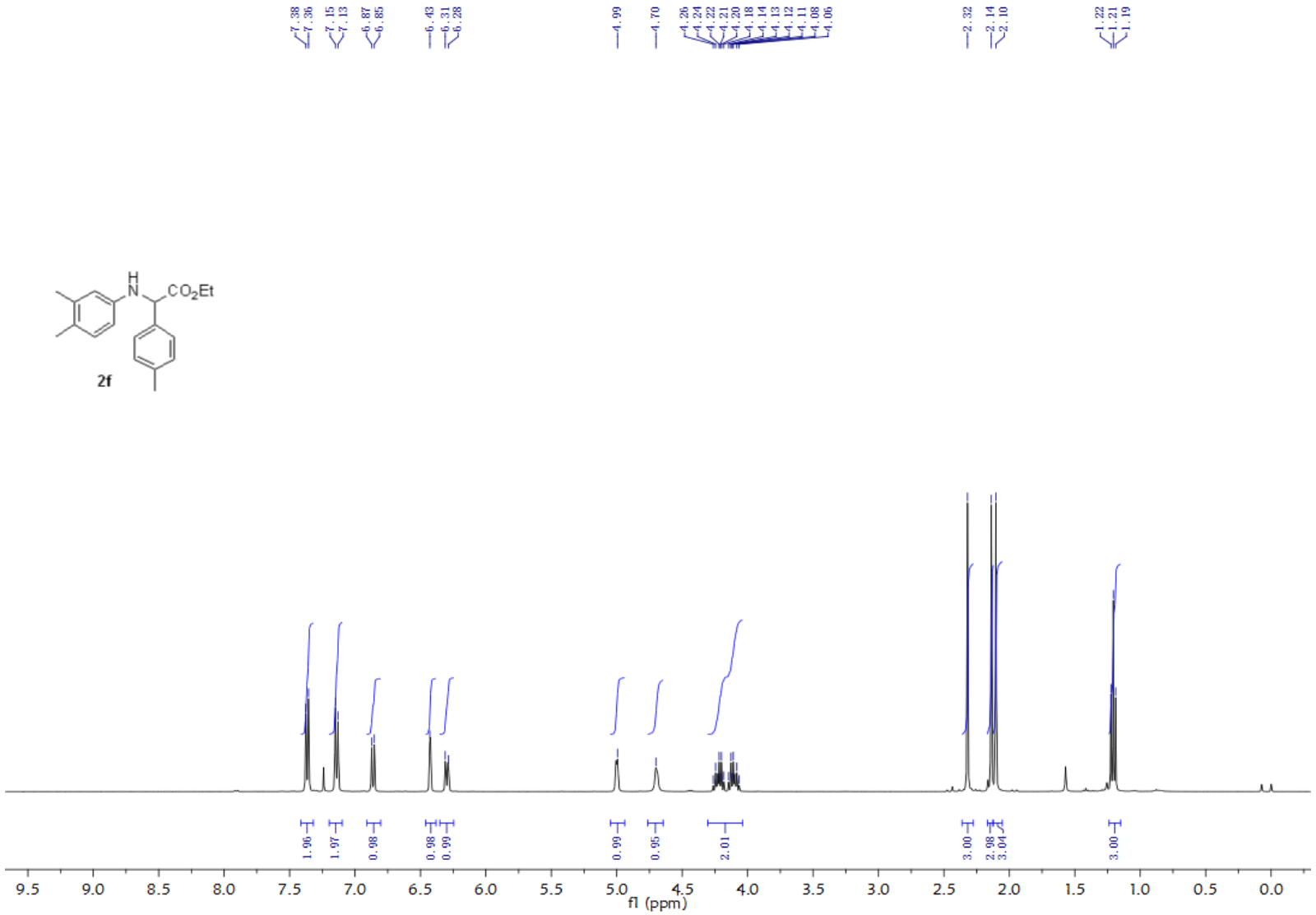
f1 (ppm)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4.08
4.06
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2.14
2.10
1.22
1.21
1.19
H
N
CO2Et
2f
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0.99
0.95
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3.00
2.98
3.04
3.00
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9.0
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7.0
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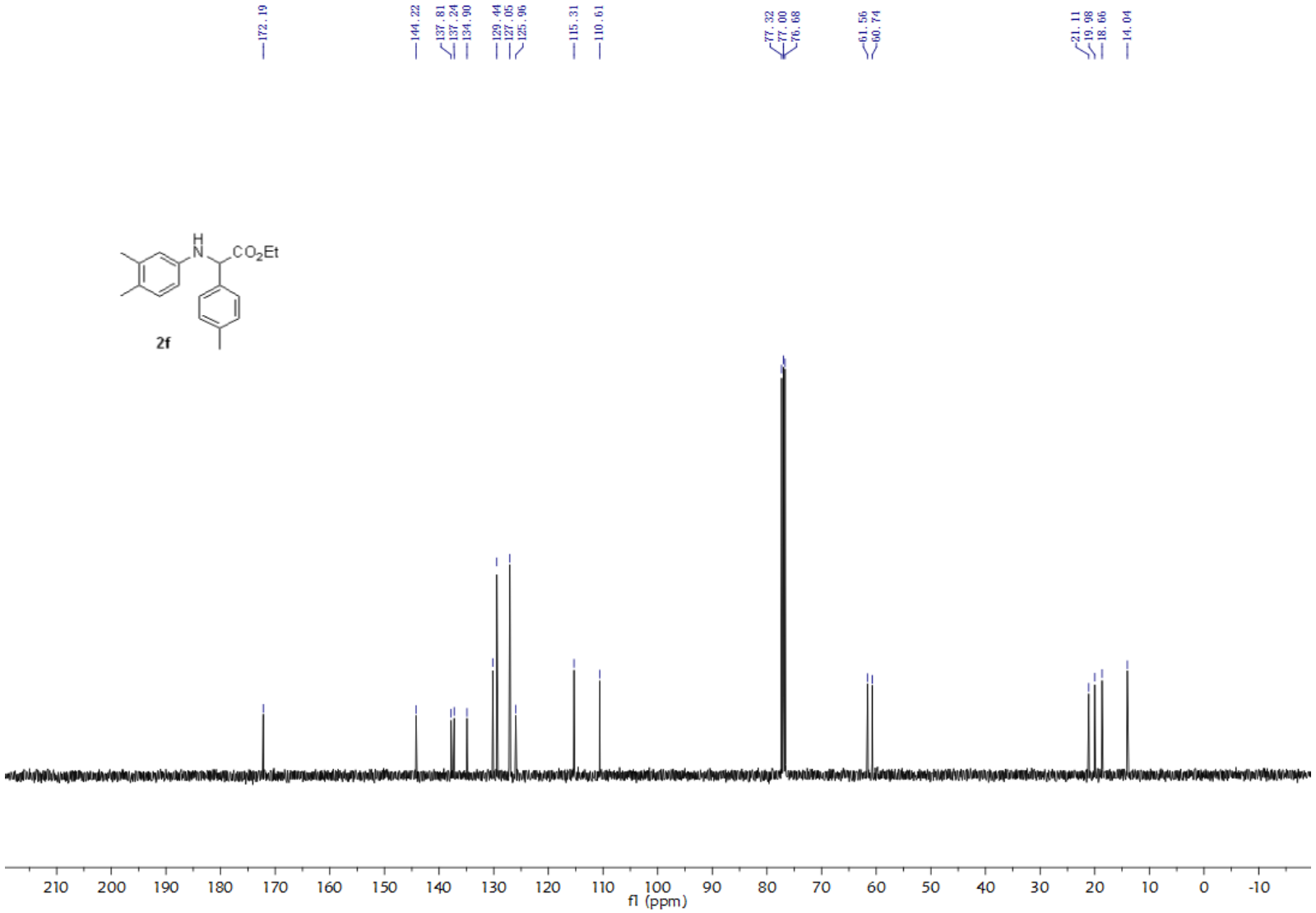
f1 (ppm)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61.56
60.74
21.11
19.98
18.66
14.04
H
N
CO2Et
2f
210
200
190
180
170
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100
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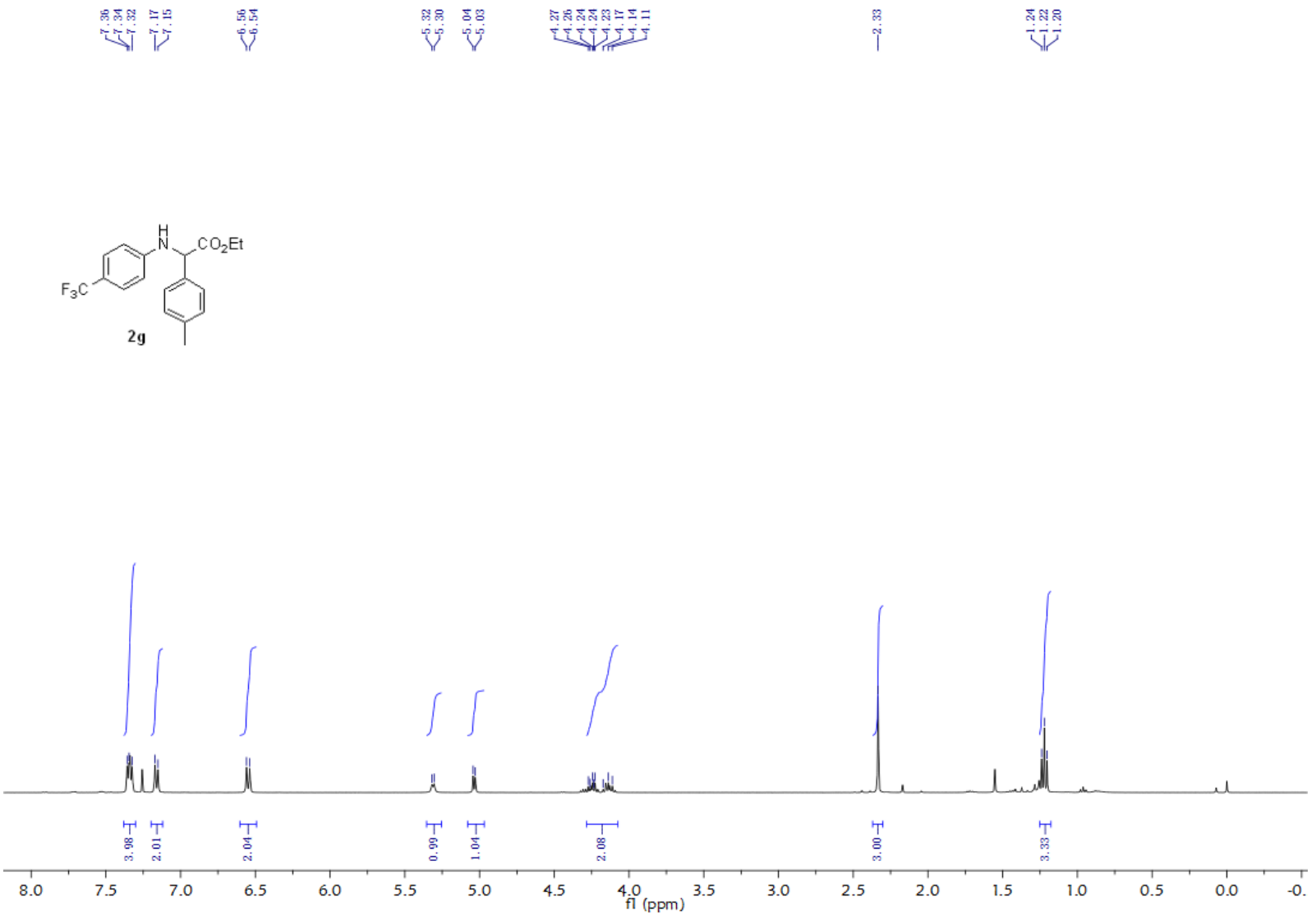
f1 (ppm)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4.24
4.23
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4.14
4.11
2.33
1.24
1.22
1.20
H
N
CO2Et
F3C
2g
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2.01
2.04
0.99
1.04
2.08
3.00
3.33
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7.0
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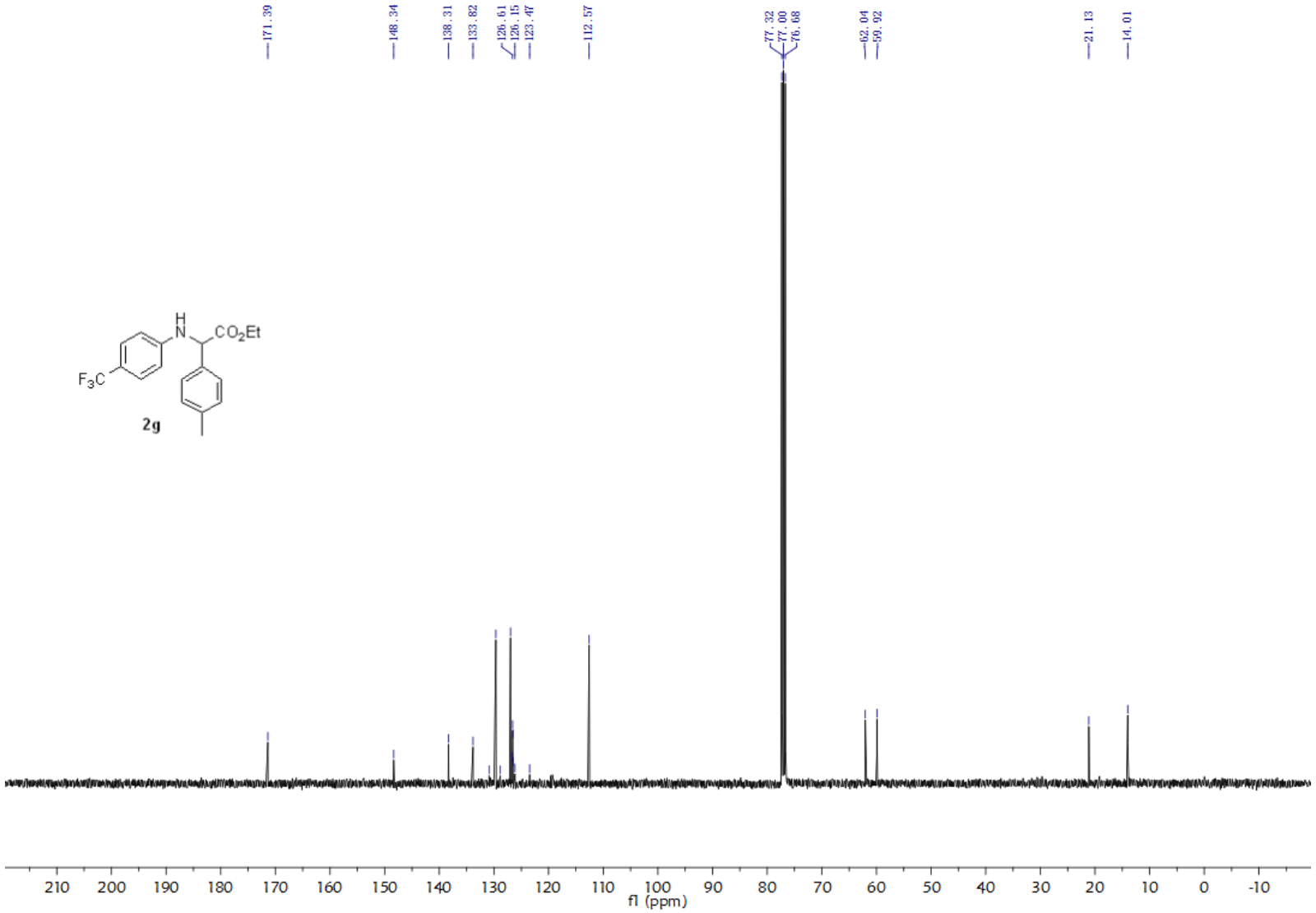
f1 (ppm)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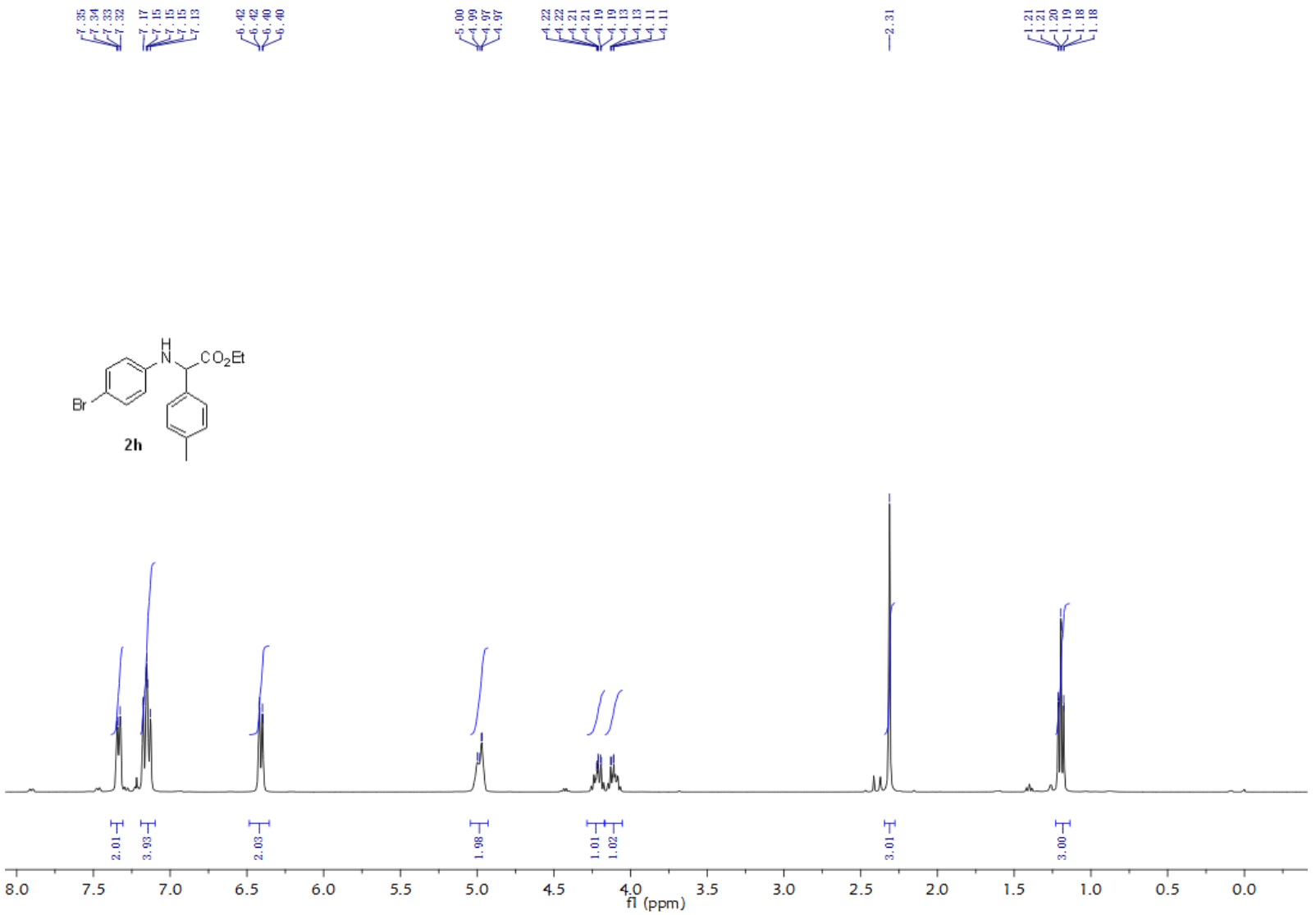
N
CO2Et
F3C
2g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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4.13
4.13
4.11
4.11
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1.21
1.20
1.19
1.18
1.18
Br
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H
CO2Et
2h
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2.03
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1.01
1.02
3.01
3.00
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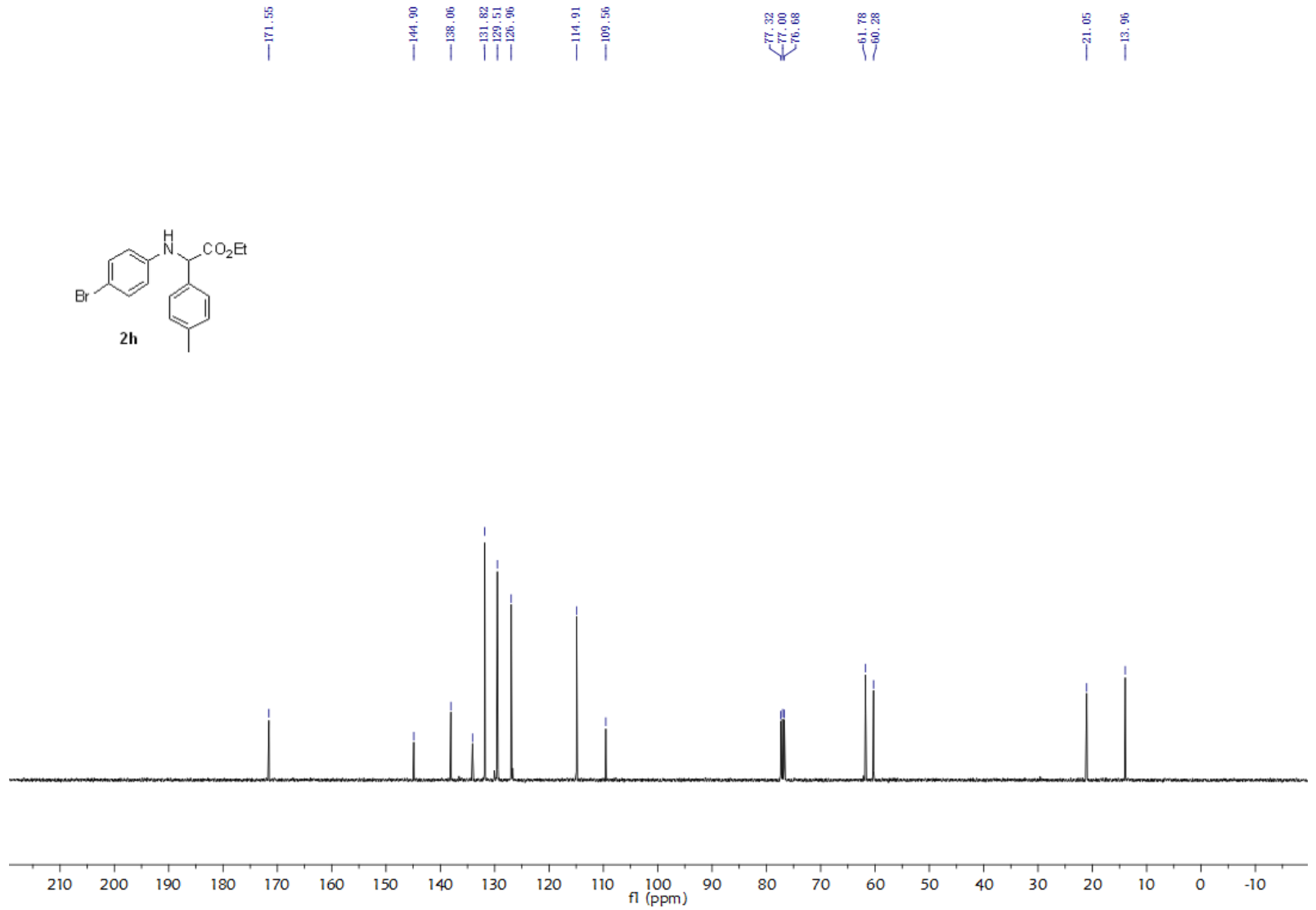
f1 (ppm)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76.68
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13.96
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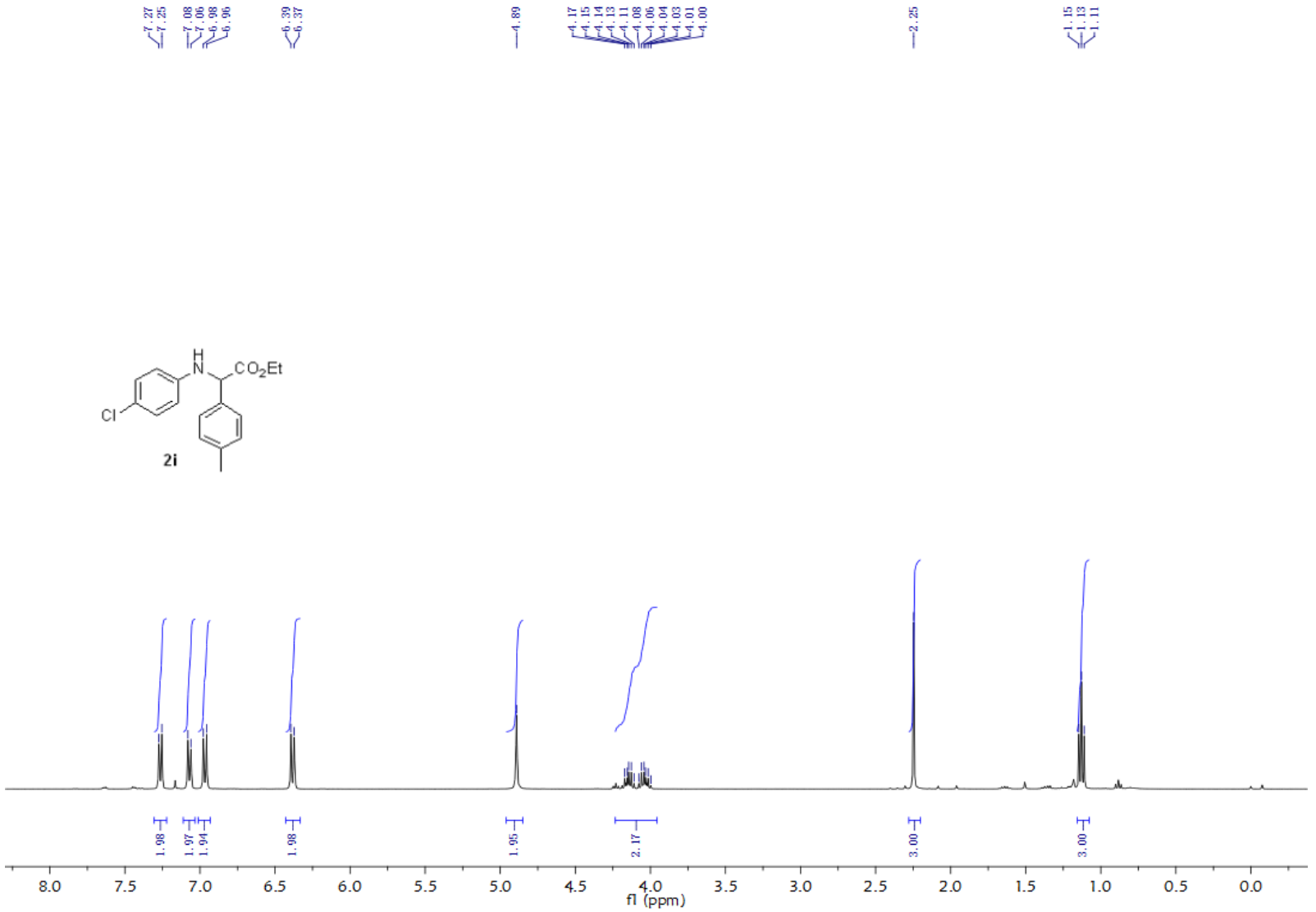
2h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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4.03
4.01
4.00
2.25
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1.13
1.11
Cl
H
N
CO2Et
2i
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1.98
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3.00
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2.0
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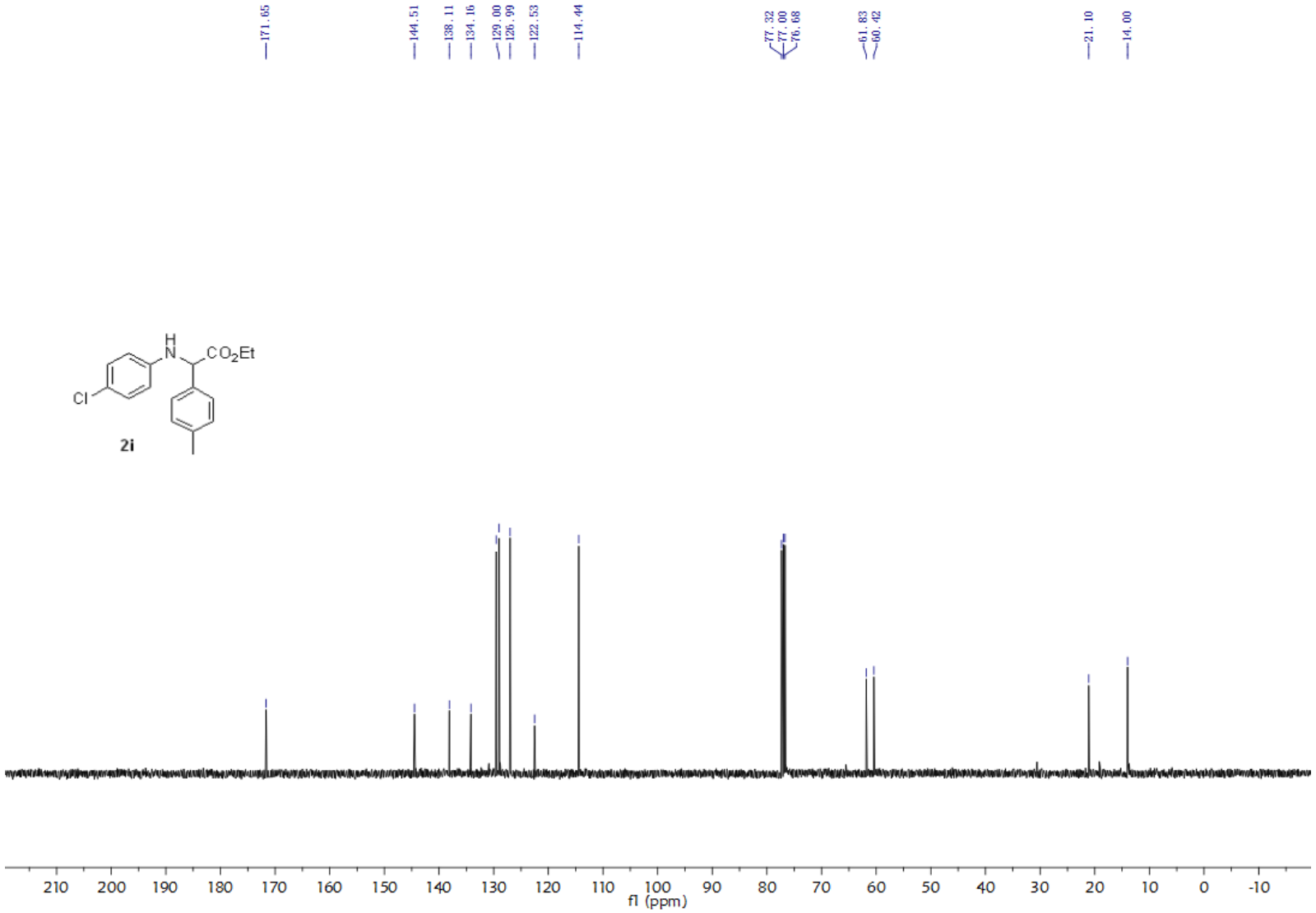
f1 (ppm)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60.42
21.10
14.00
Cl
H
N
CO2Et
2i
210
200
190
180
170
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140
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120
110
100
90
80
70
60
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40
30
20
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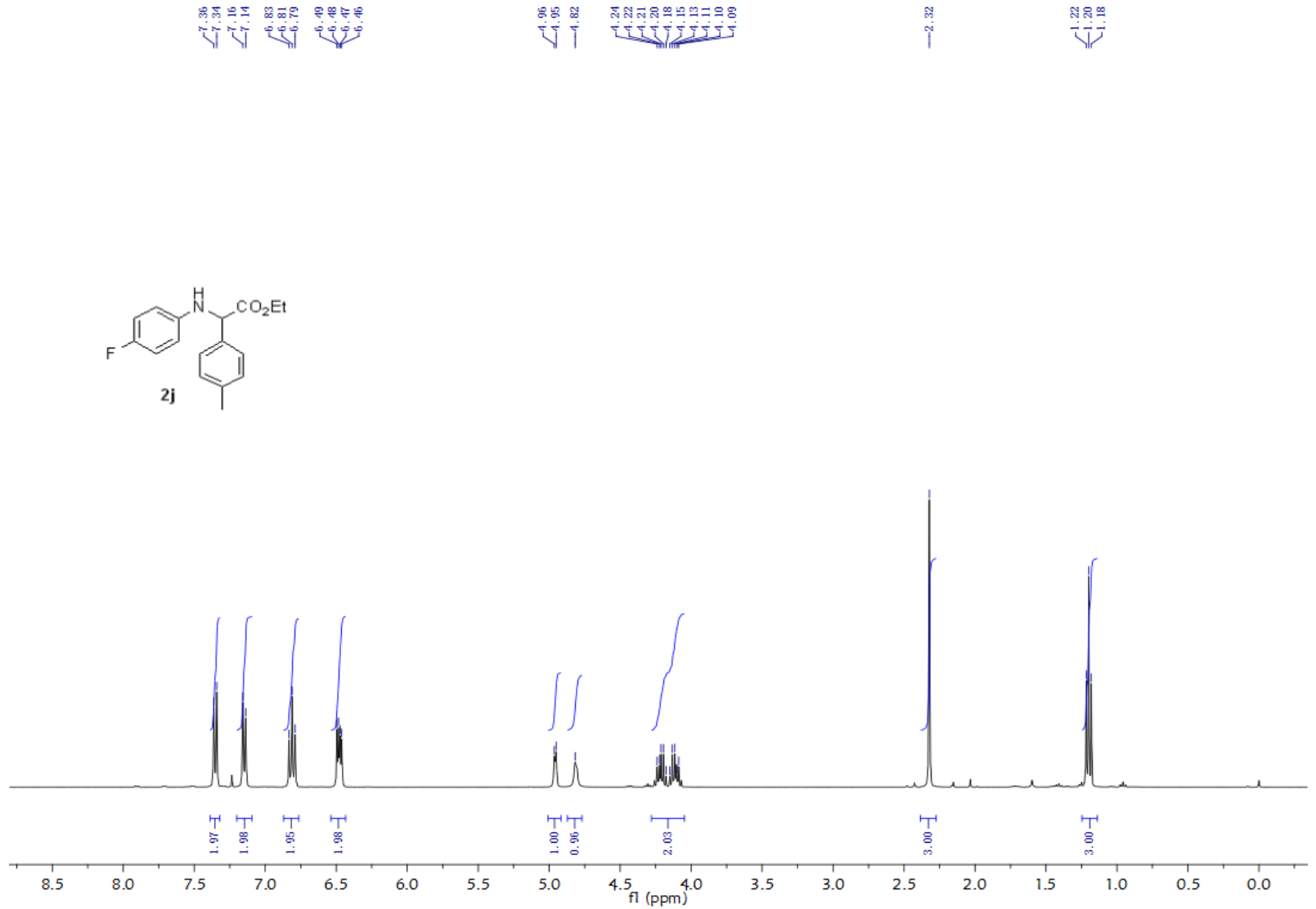
0
-10
f1 (ppm)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1.20
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1.13
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1.10
1.09
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1.22
1.20
1.18
F
H
N
CO2Et
2j
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1.95
1.98
1.00
0.96
2.03
3.00
3.00
8.5
8.0
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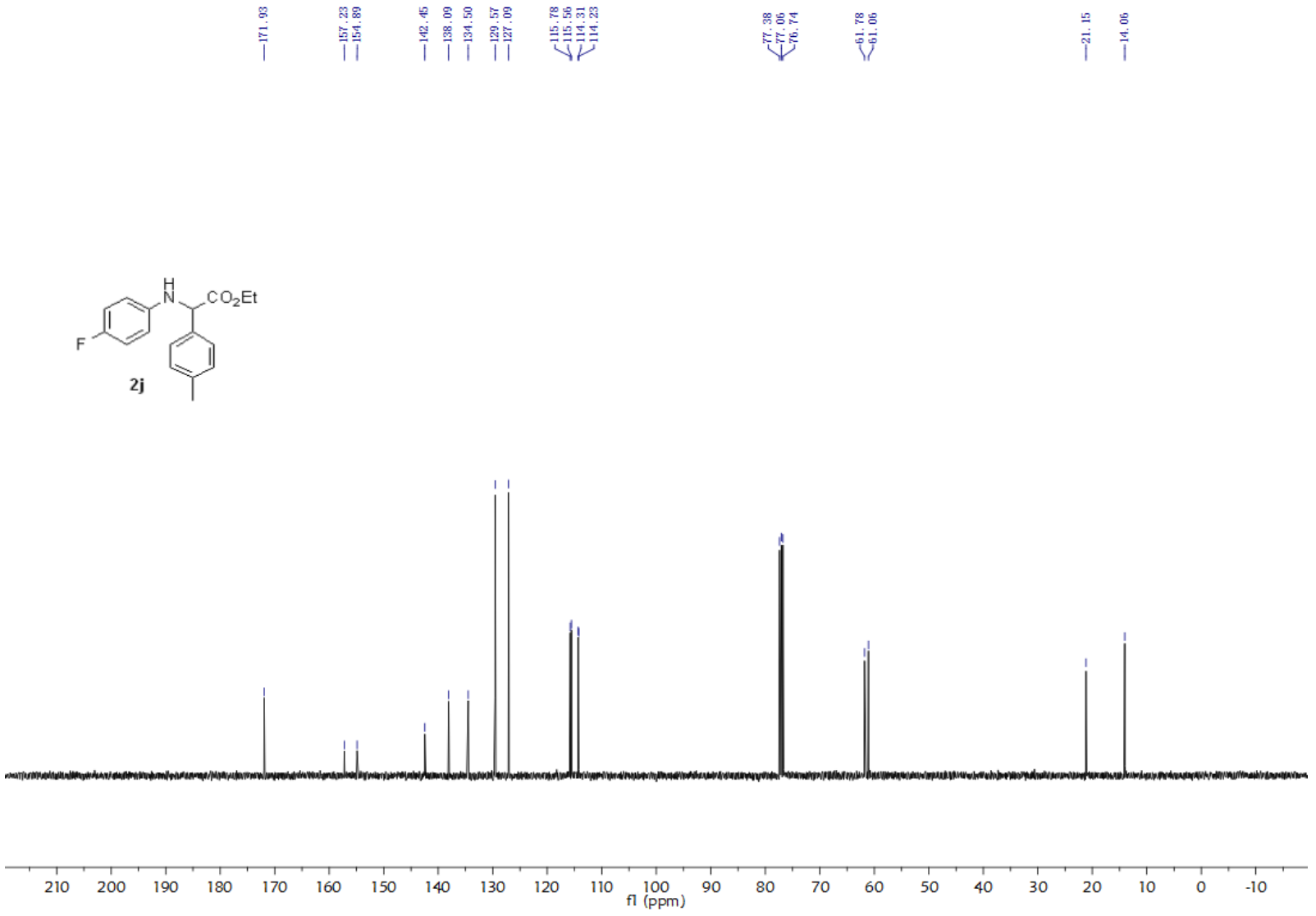
f1 (ppm)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14.06
H
N
CO2Et
F
2j
210
200
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180
170
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80
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40
30
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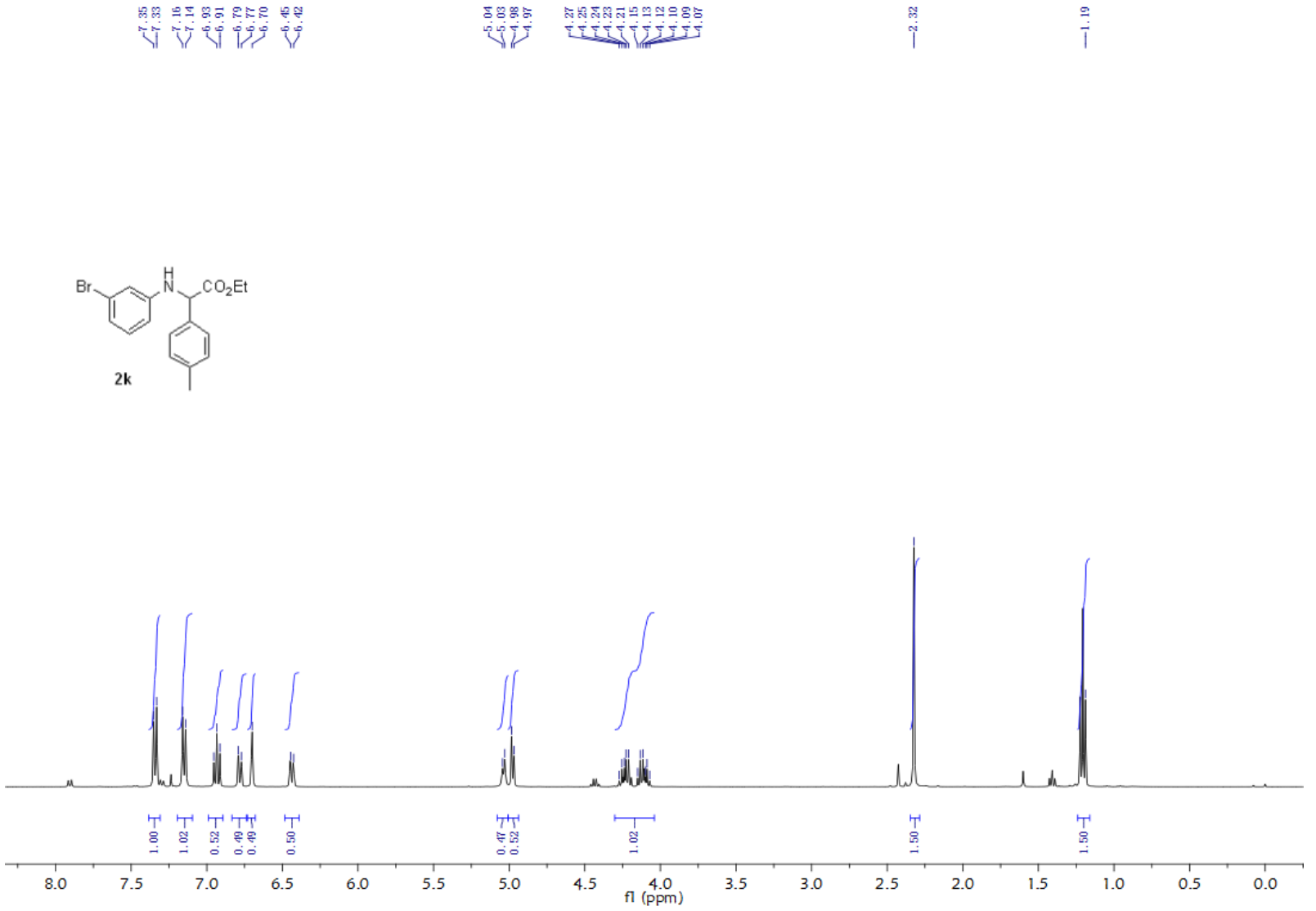
0
-10
f1 (ppm)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4.09
4.07
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CO2Et
2k
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0.52
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6.0
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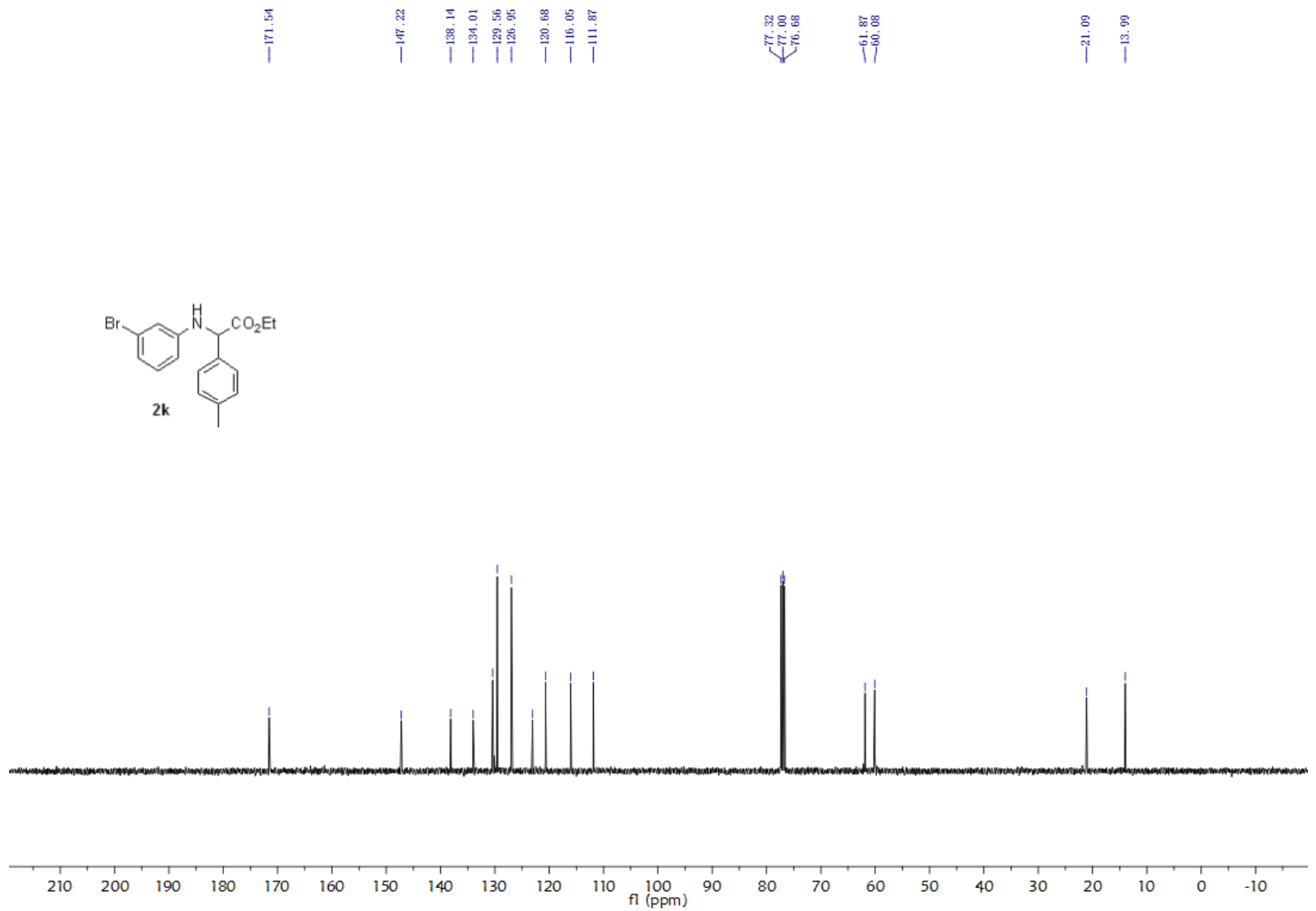
f1 (ppm)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76.68
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60.08
21.09
13.99
Br
H
N
CO2Et
2k
210
200
190
180
170
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120
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100
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80
70
60
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40
30
20
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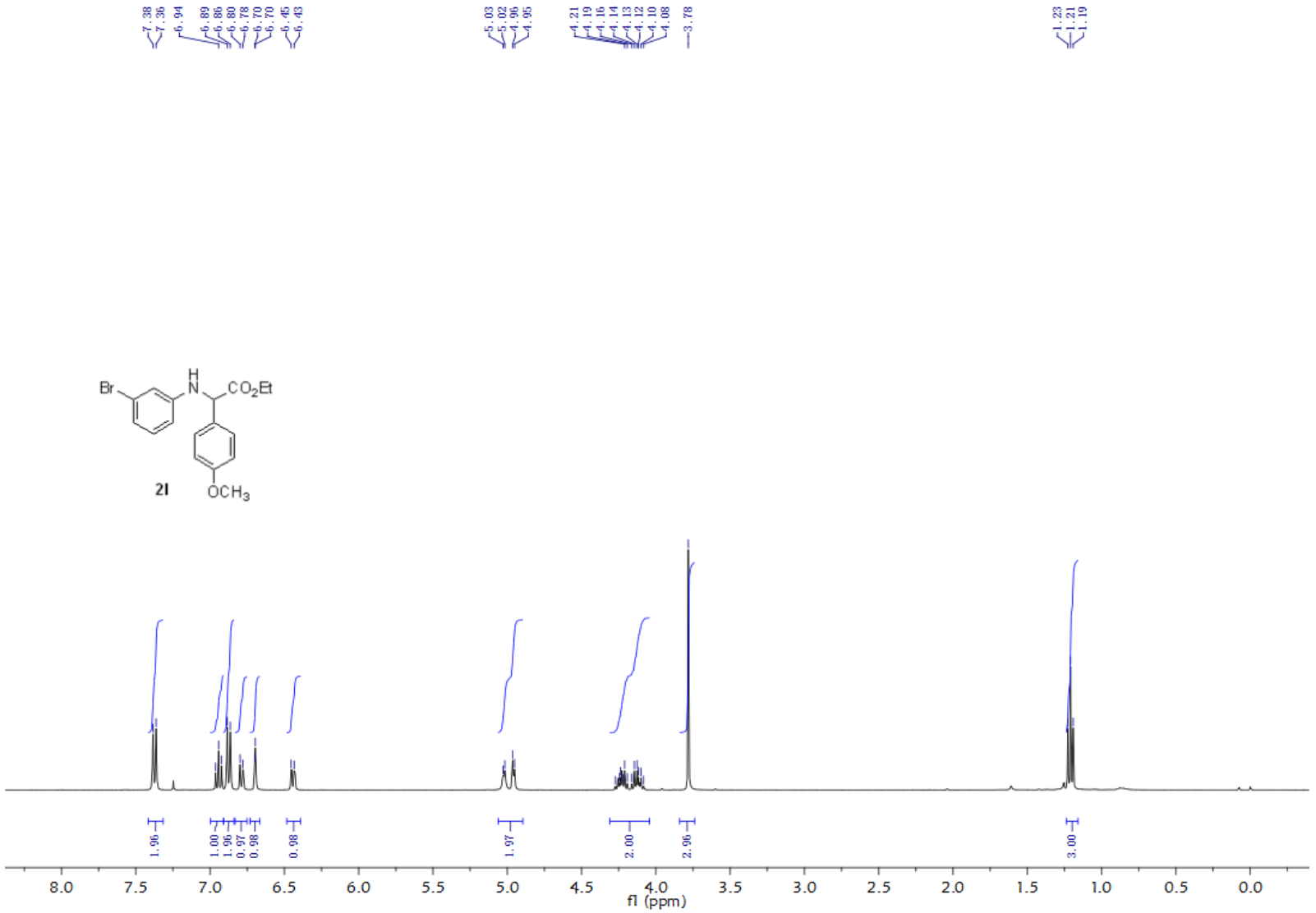
f1 (ppm)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H
CO2Et
OCH3
2l
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1.96
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0.98
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2.00
2.96
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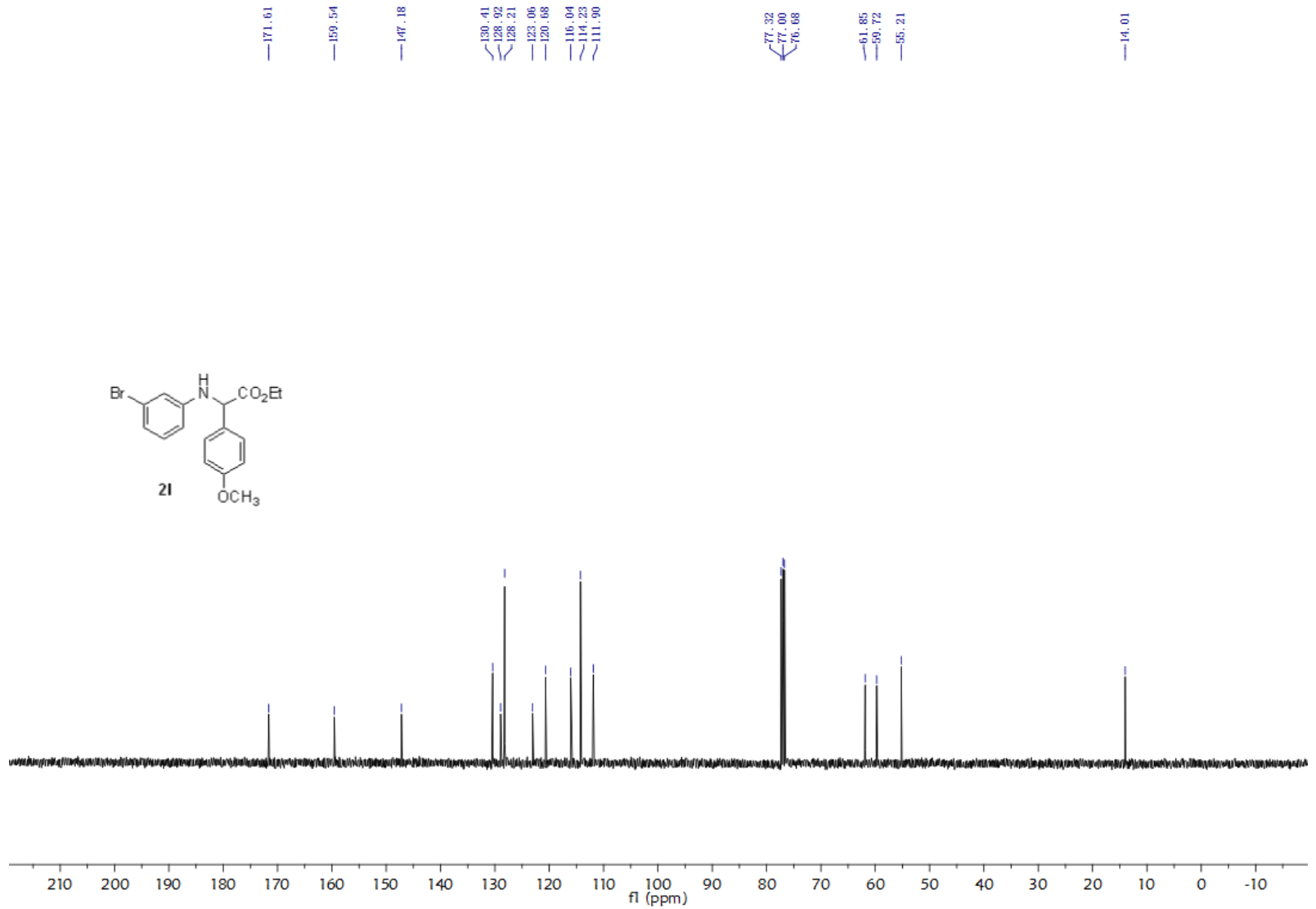
f1 (ppm)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77.00
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14.01
Br
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N
CO2Et
OCH3
2l
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200
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180
170
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120
110
100
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80
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50
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30
20
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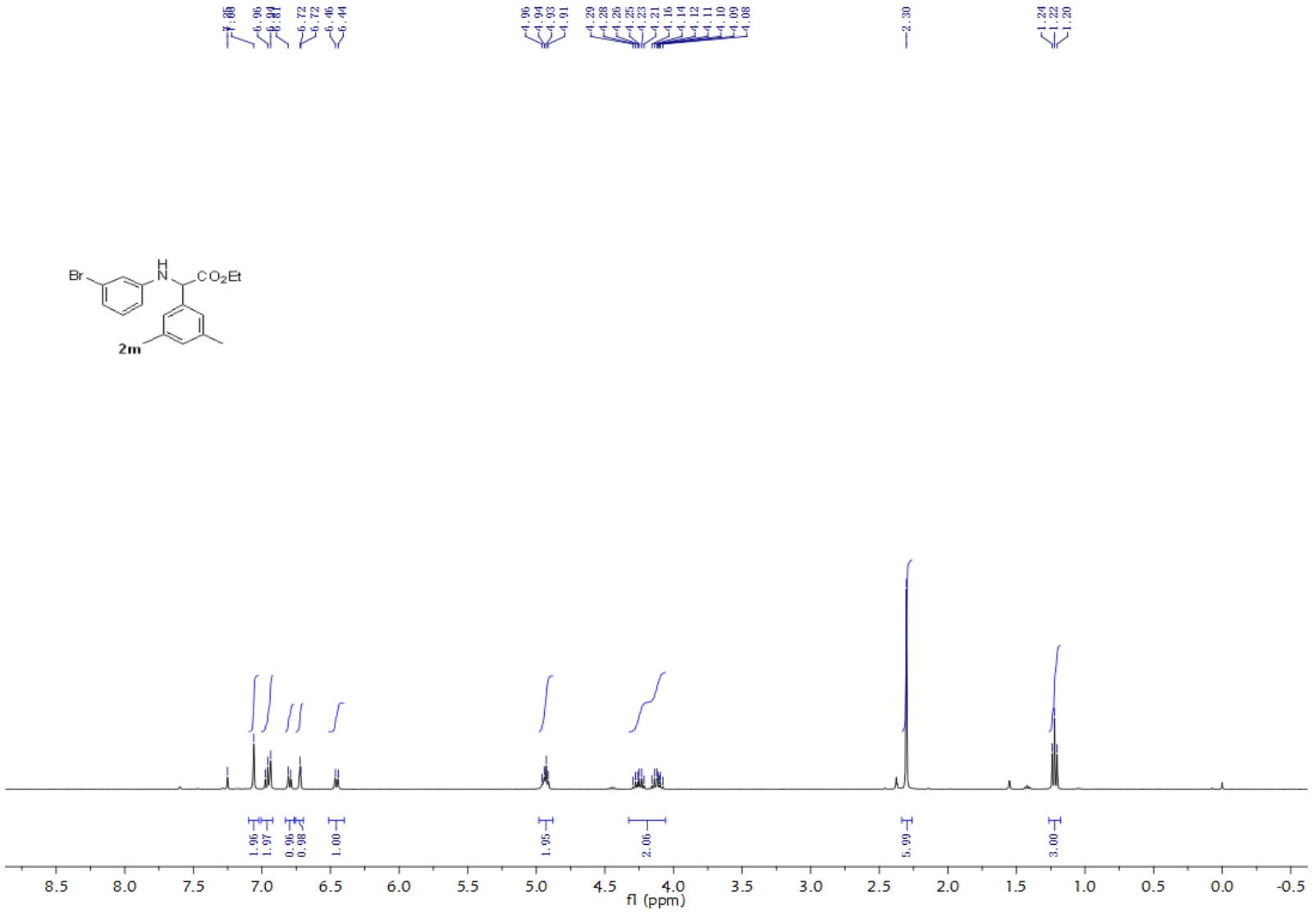
-10
f1 (ppm)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CO2Et
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3.00
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5.0
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3.0
2.5
2.0
1.5
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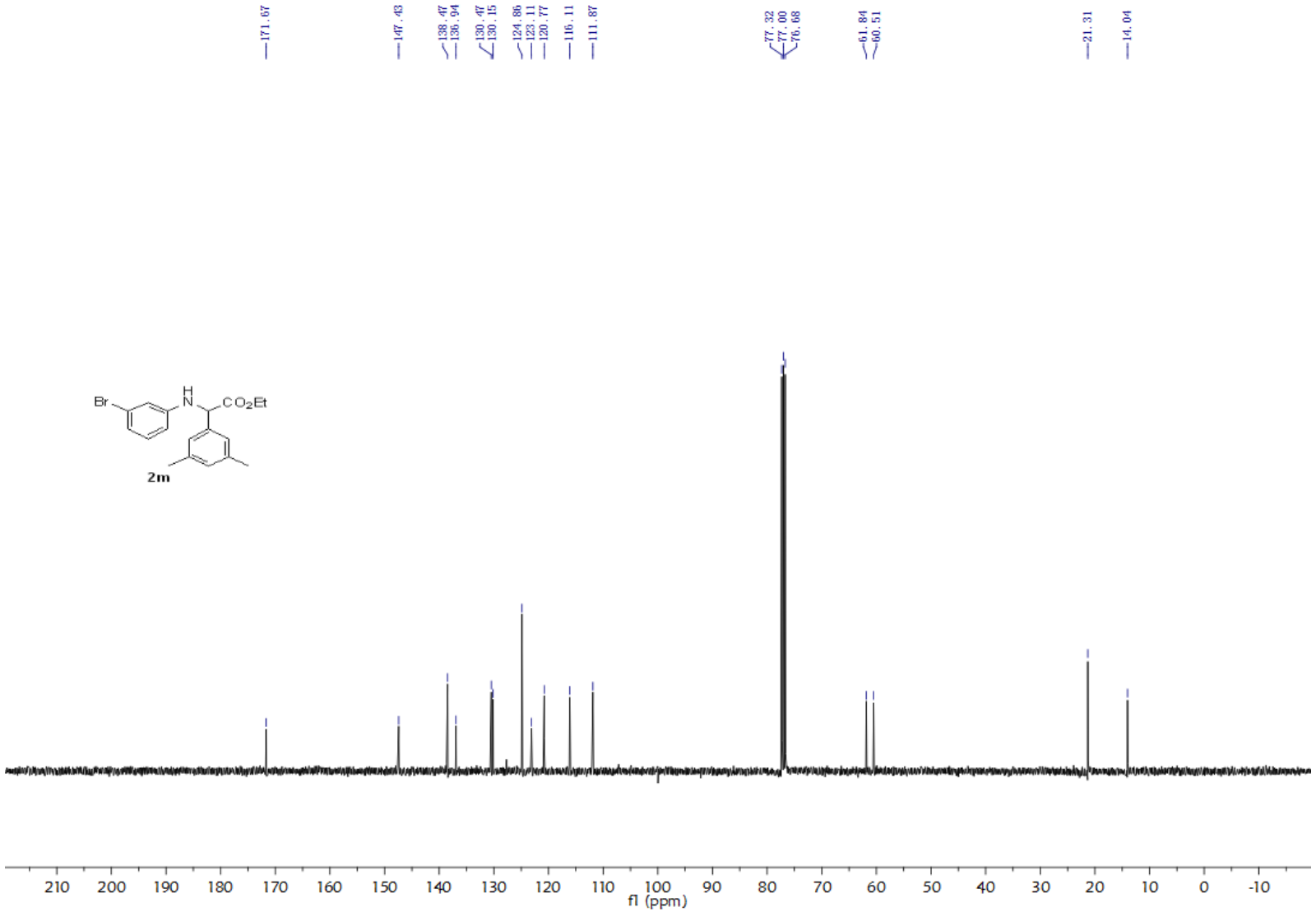
-0.5
f1 (ppm)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60.51
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CO2Et
2m
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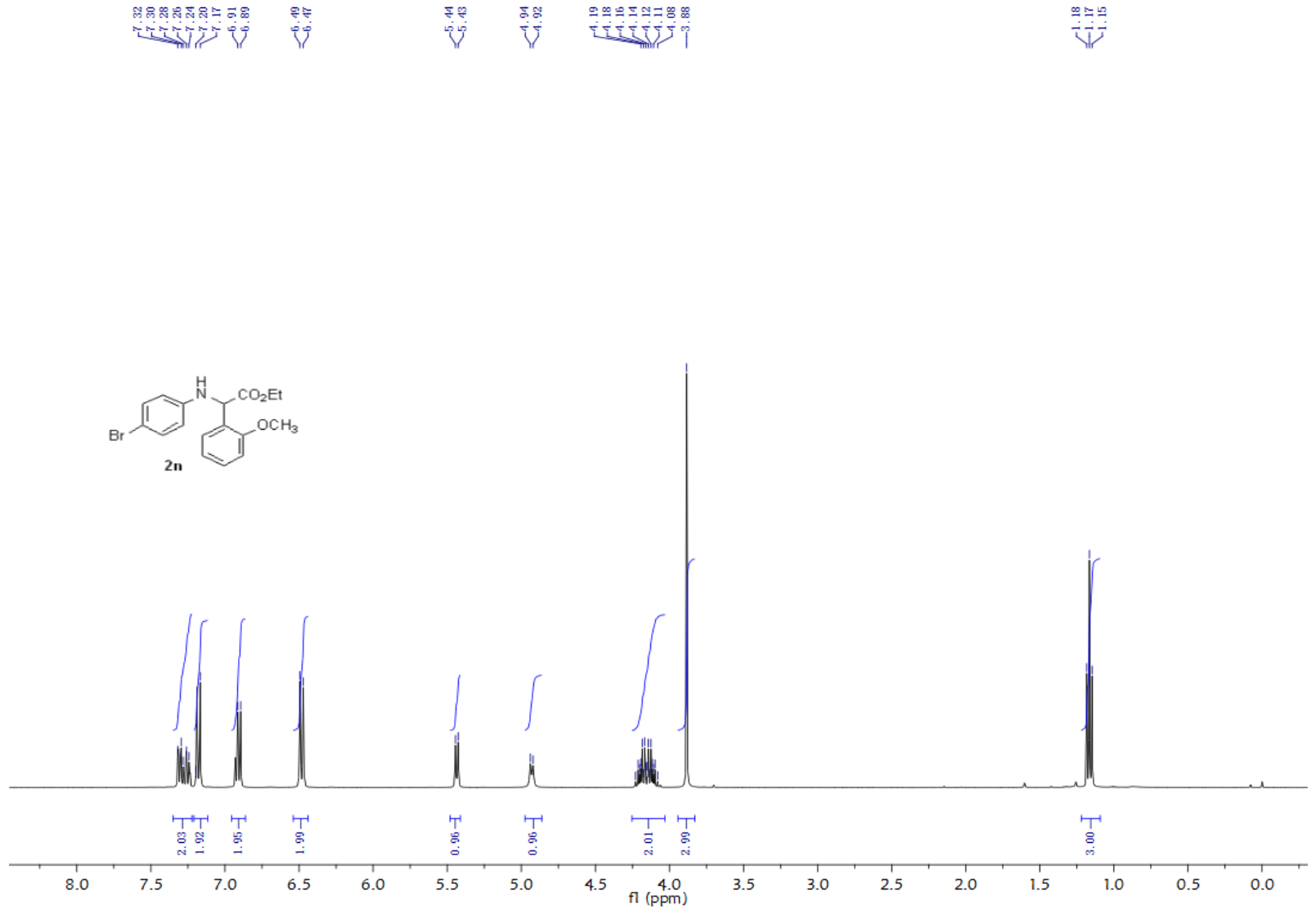
f1 (ppm)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OCH3
2n
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1.99
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2.01
2.99
3.00
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2.0
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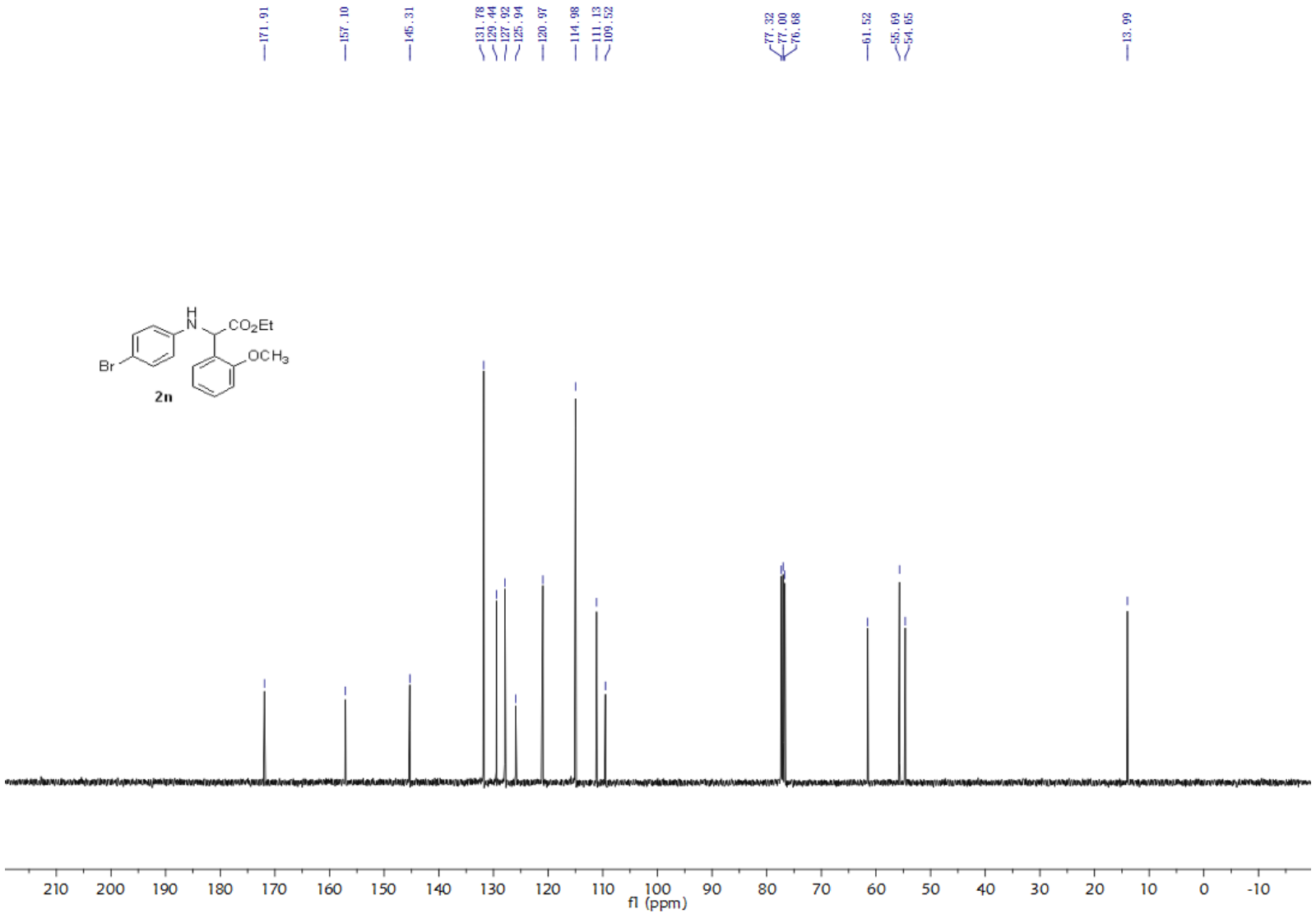
0.0
f1 (ppm)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OCH3
2n
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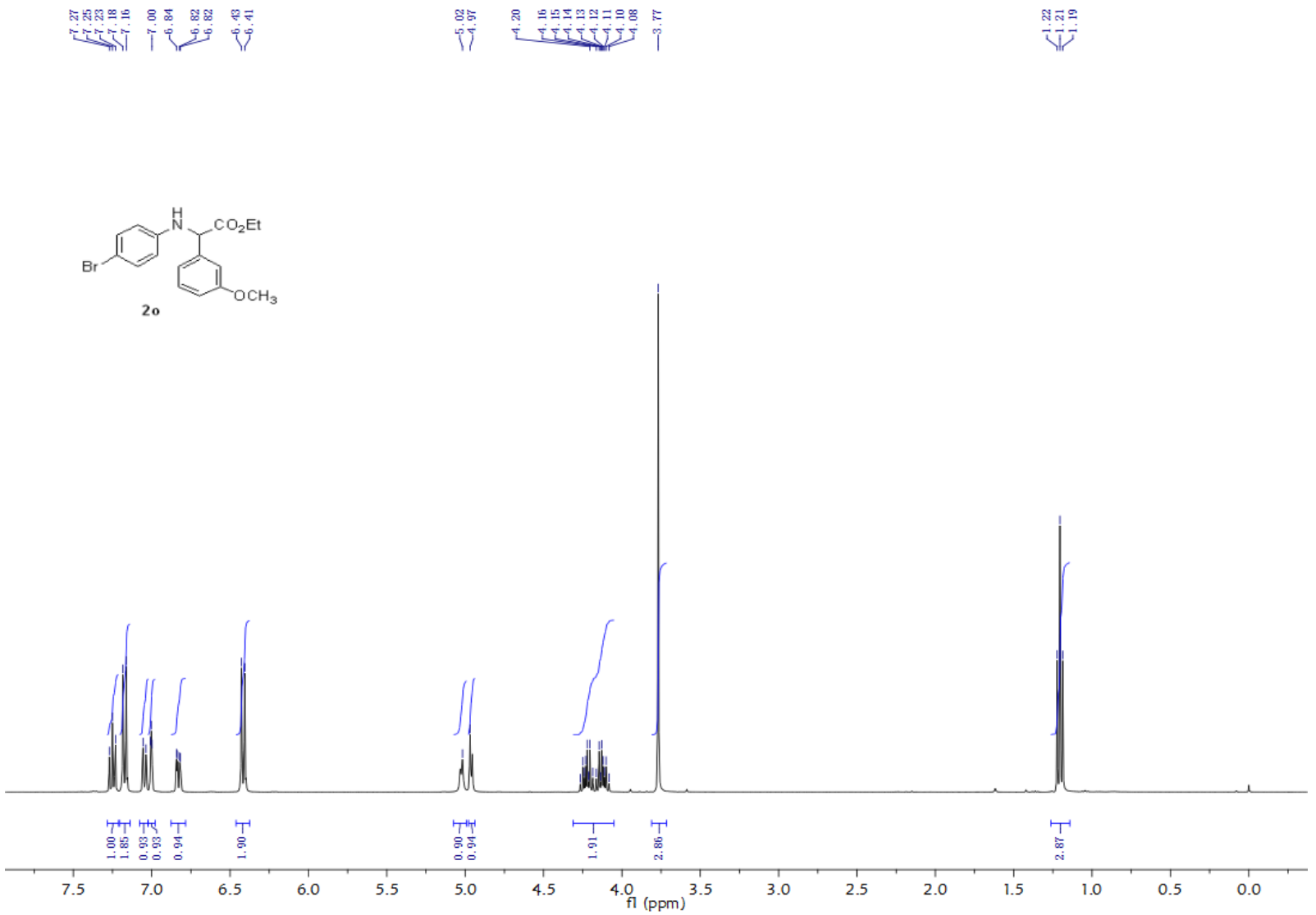
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4.13
4.12
4.11
4.10
4.08
3.77
1.22
1.21
1.19
Br
H
N
CO2Et
OCH3
2o
1.00
1.85
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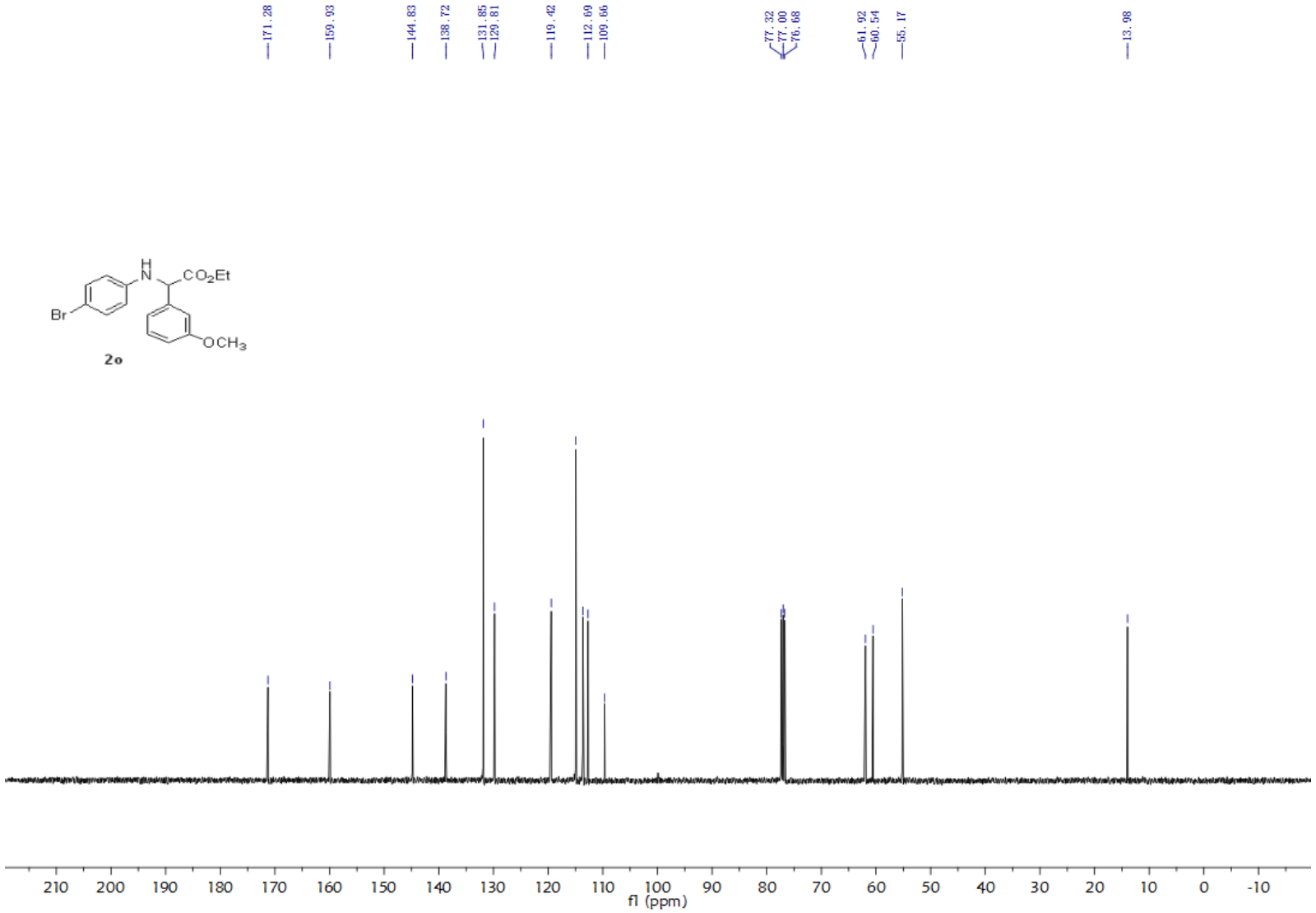
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55.17
13.98
Br
H
N
CO2Et
OCH3
2o
210
200
190
180
170
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100
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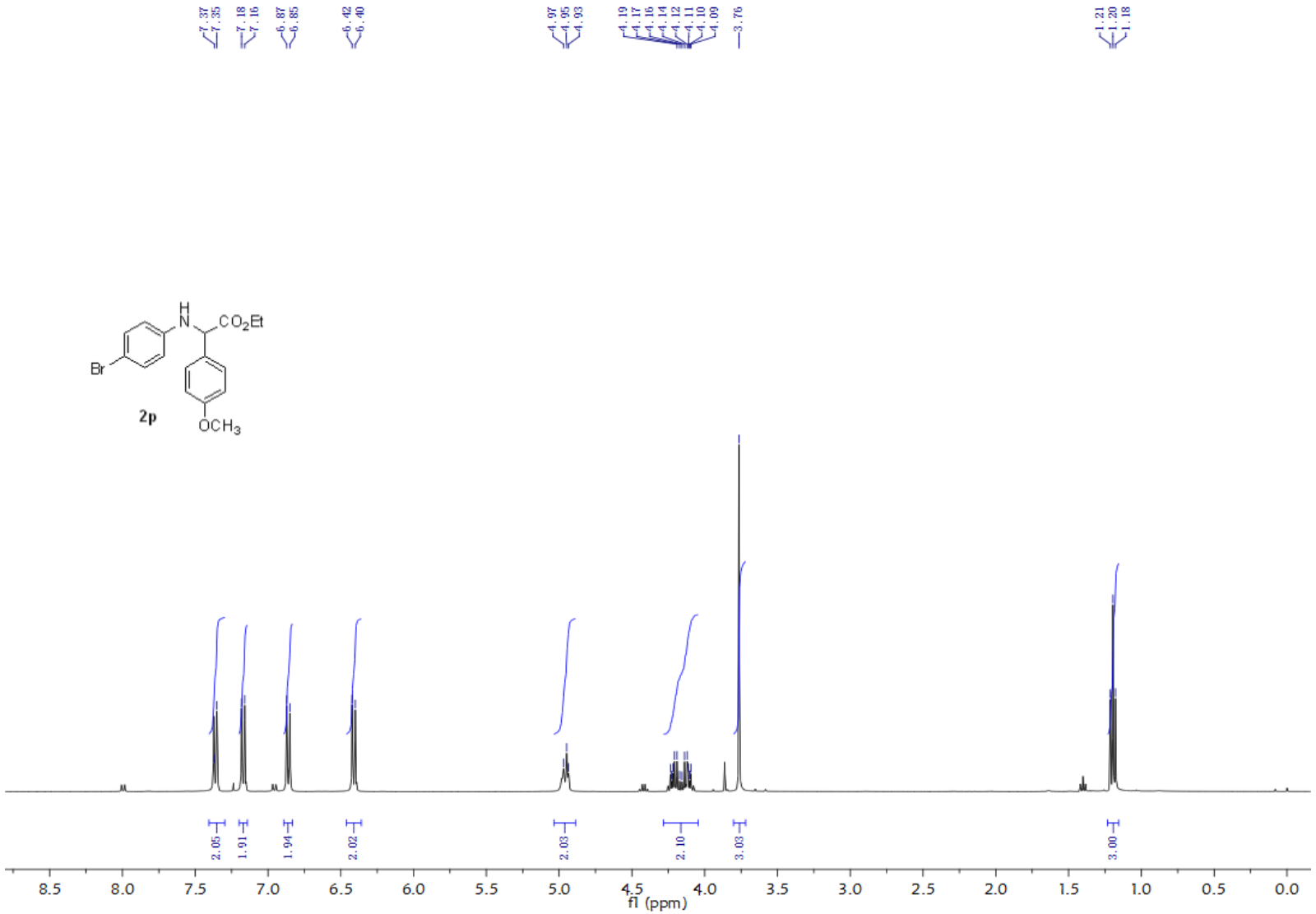
f1 (ppm)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4.14
4.12
4.11
4.10
4.09
3.76
1.21
1.20
1.18
Br
H
N
CO2Et
OCH3
2p
2.05
1.91
1.94
2.02
2.03
2.10
3.03
3.00
8.5
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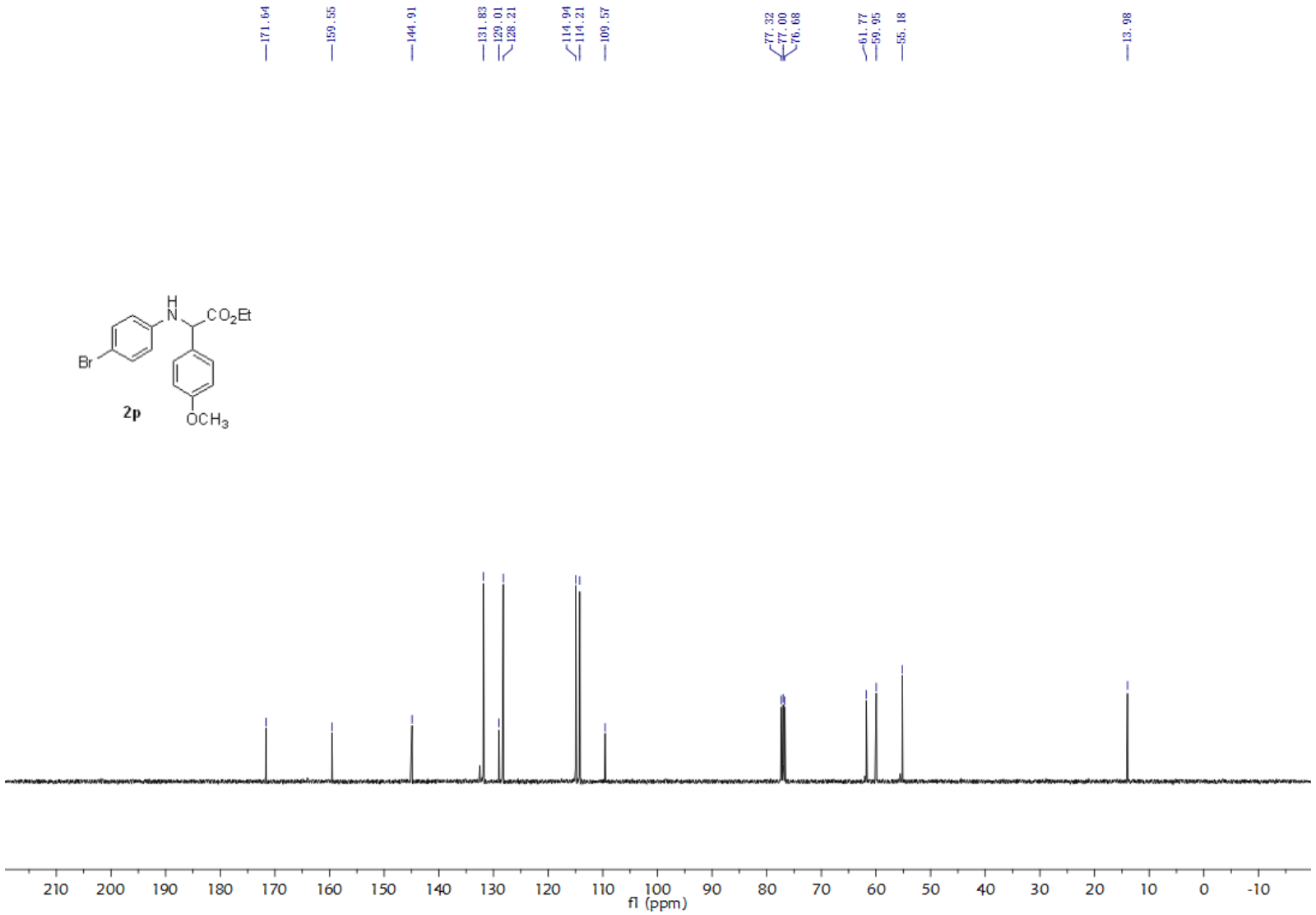
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13.98
H
N
CO2Et
Br
OCH3
2p
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200
190
180
170
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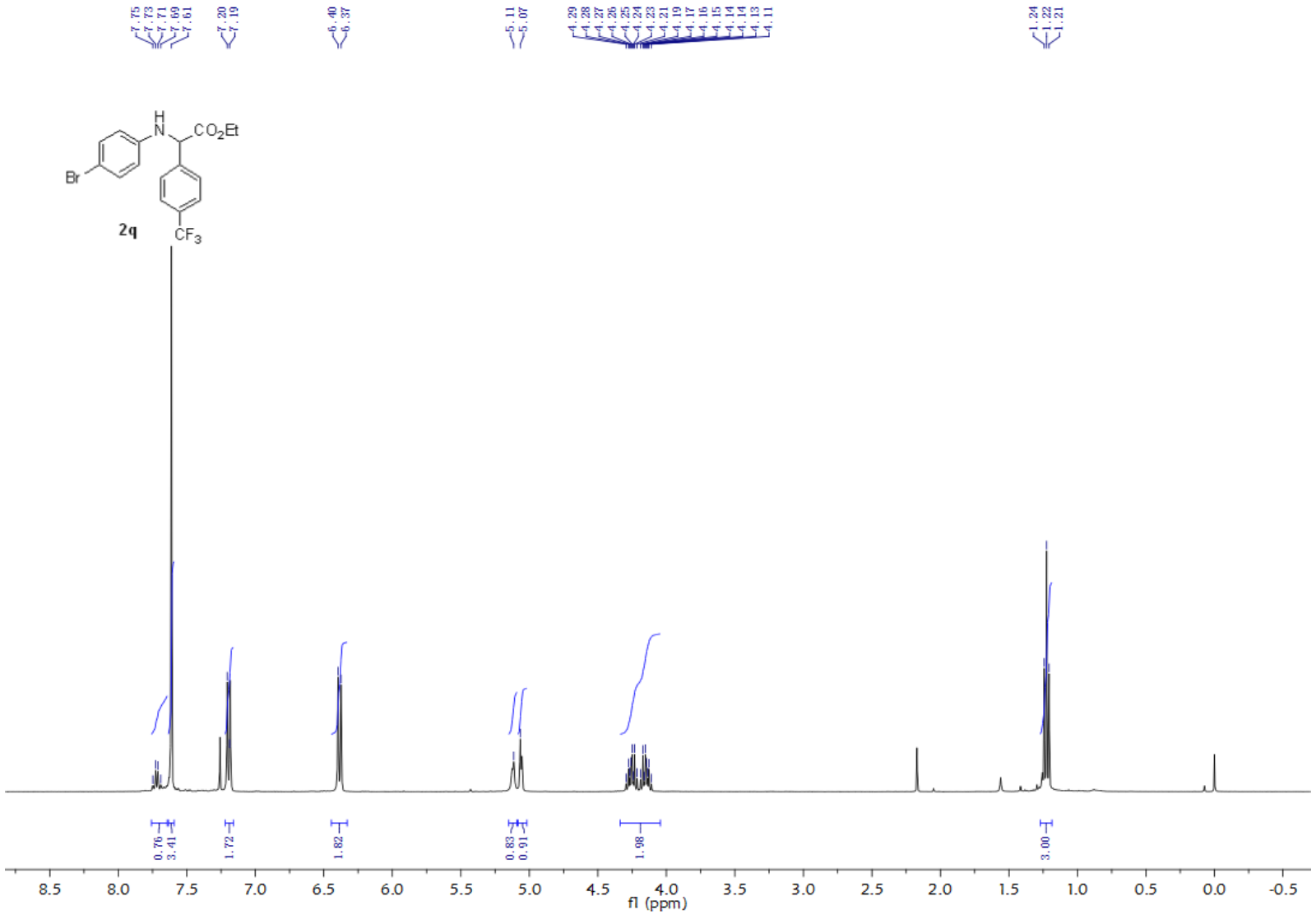
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1.15
1.14
1.14
1.13
1.11
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1.22
1.21
H
N
CO2Et
Br
CF3
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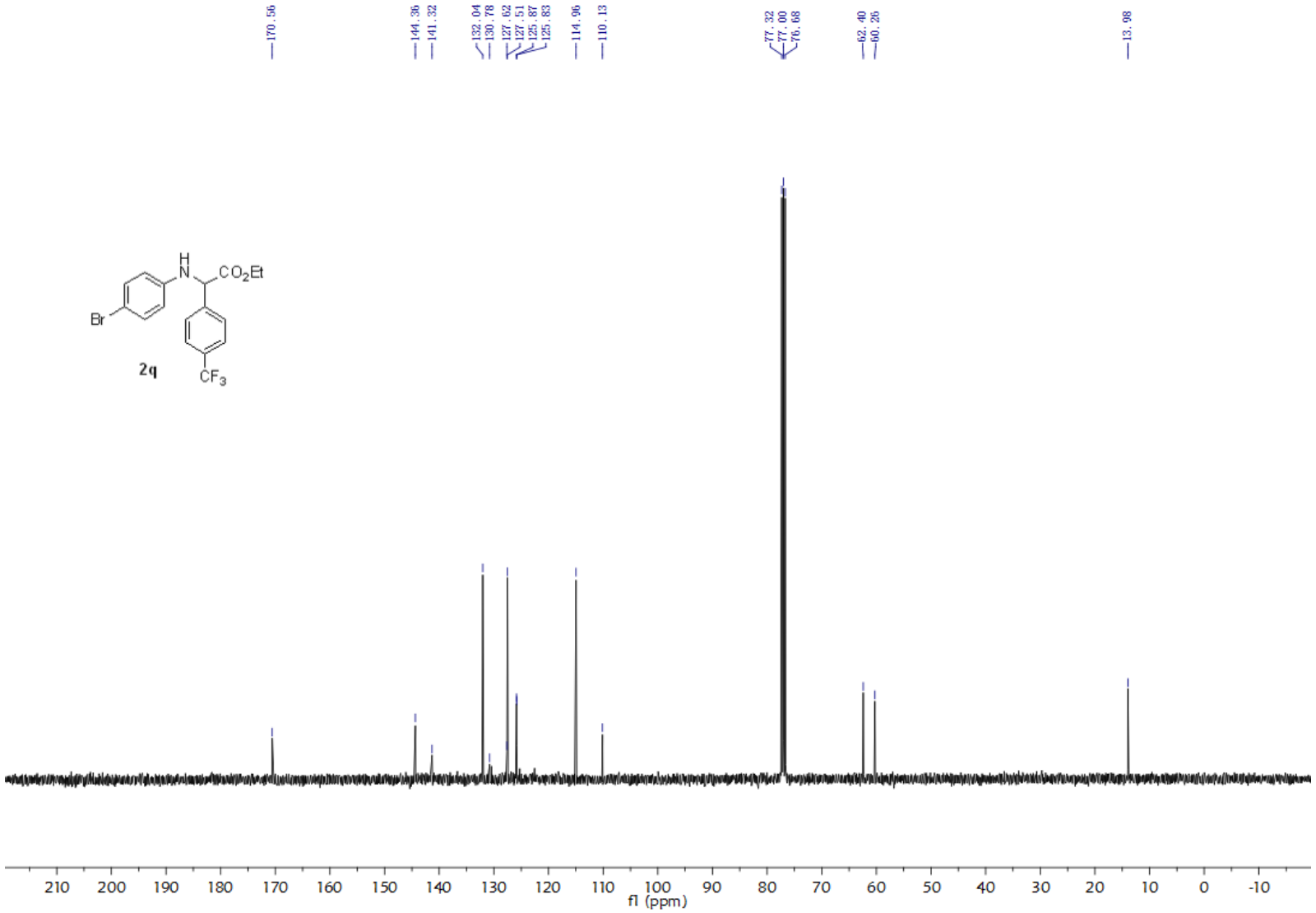
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60.26
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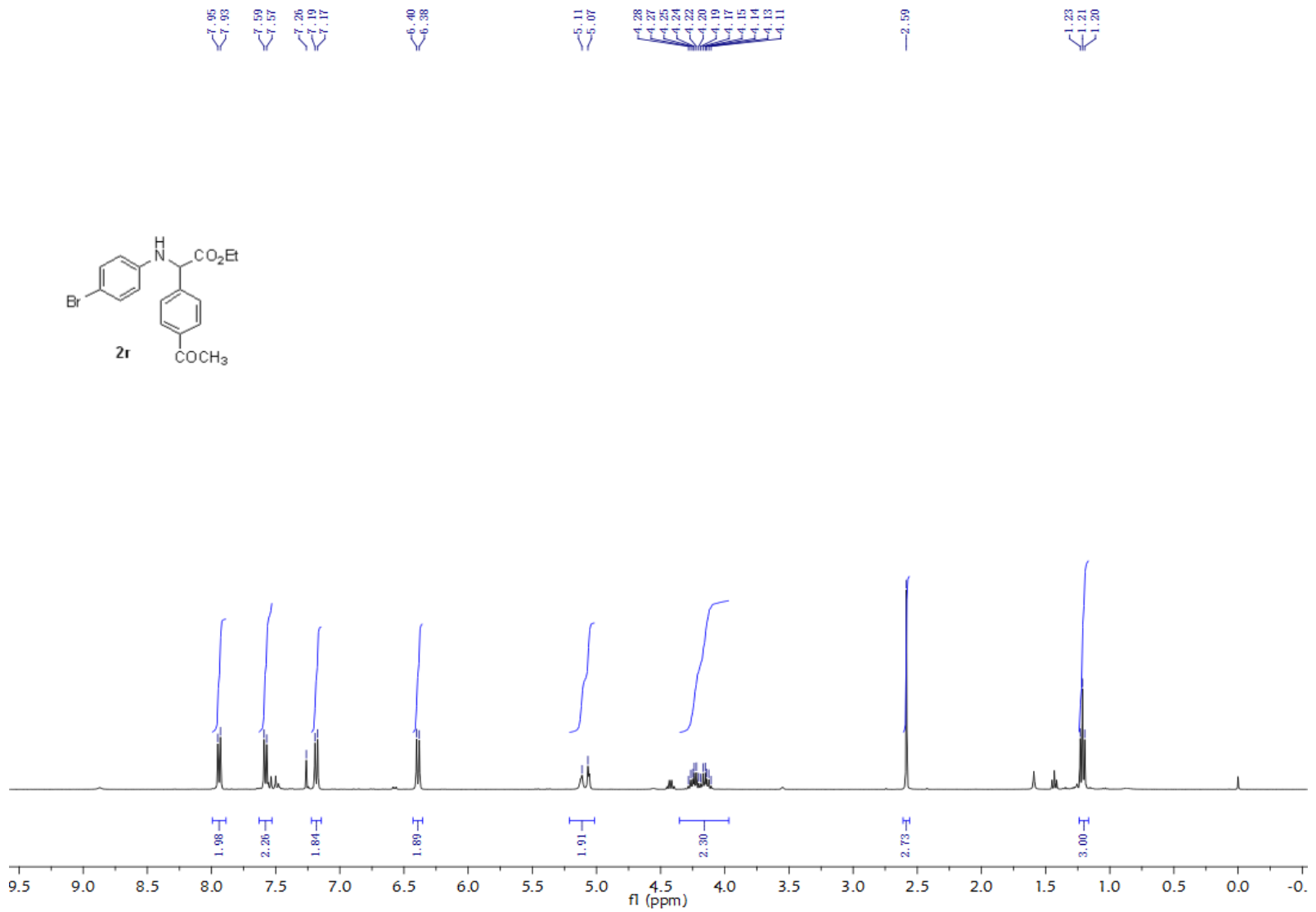
CO2Et
Br
CF3
2q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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4.20
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4.15
4.14
4.13
4.11
2.59
1.23
1.21
1.20
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N
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Br
COCH3
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1.91
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5.0
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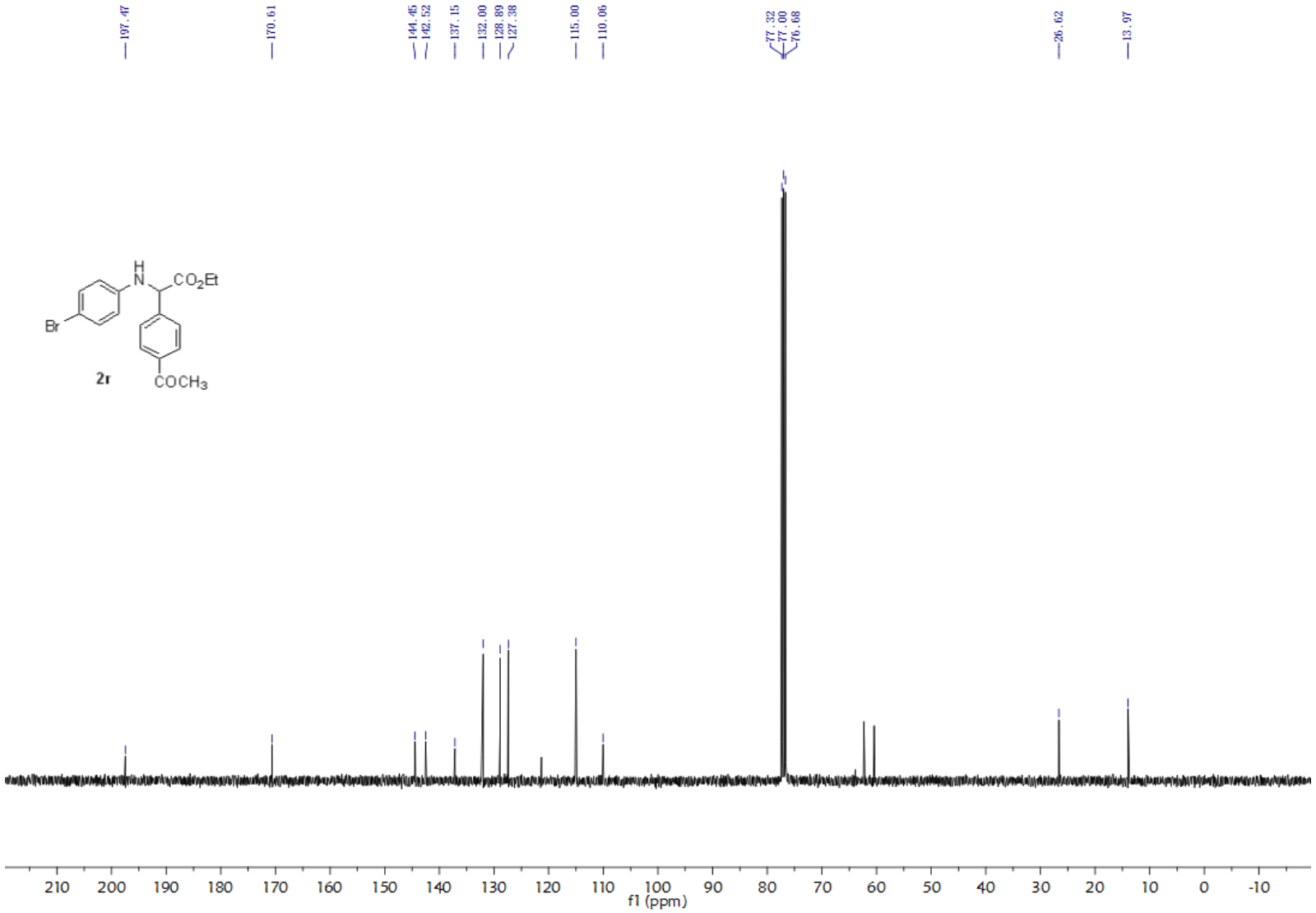
f1 (ppm)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Br
H
N
CO2Et
COCH3
2r
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200
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180
170
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100
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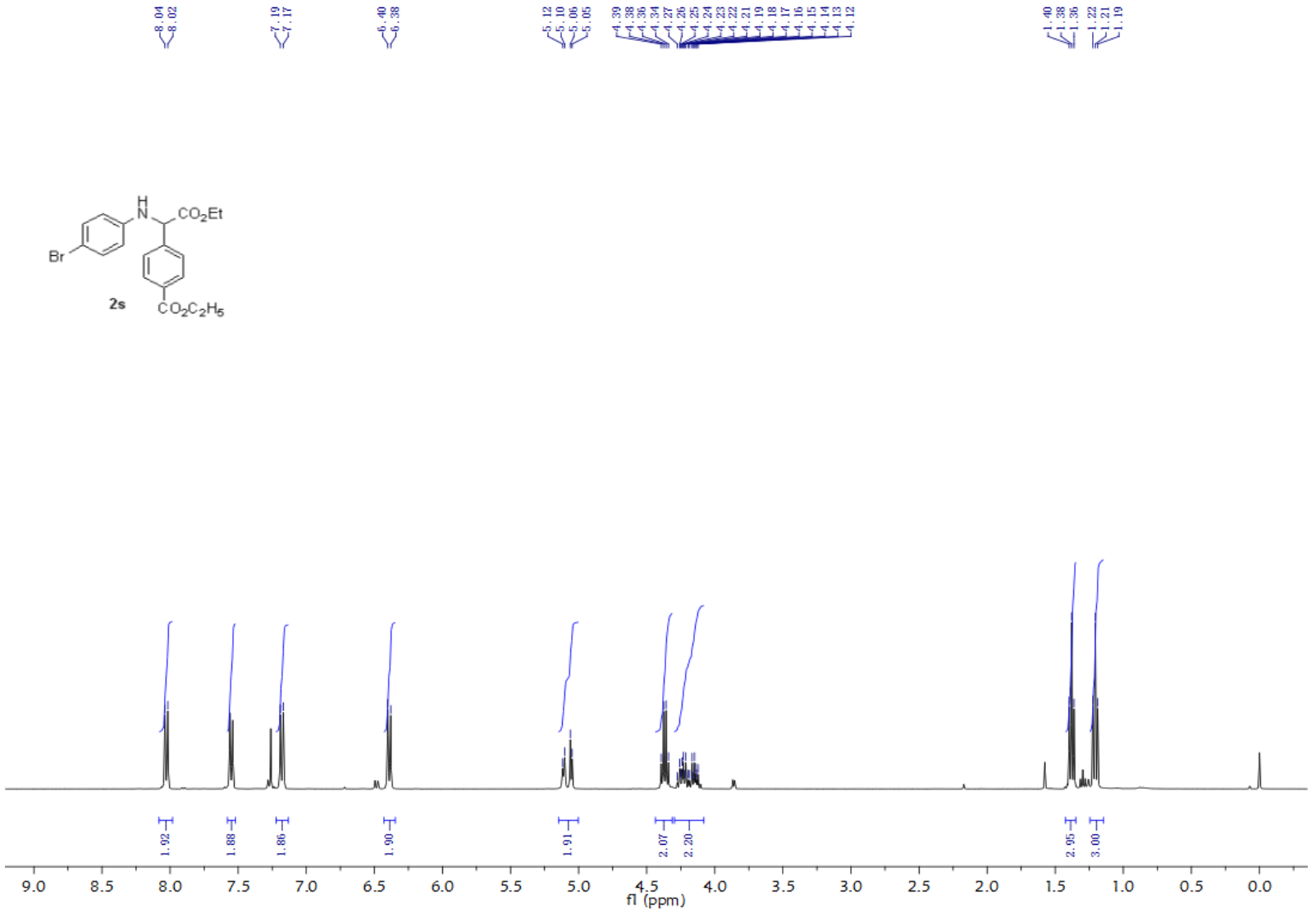
-10
f1 (ppm)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4.23
4.22
4.21
4.19
4.18
4.17
4.16
4.15
4.14
4.13
4.12
1.40
1.38
1.36
1.22
1.21
1.19
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Br
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CO2C2H5
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1.86
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1.91
2.07
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2.95
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6.0
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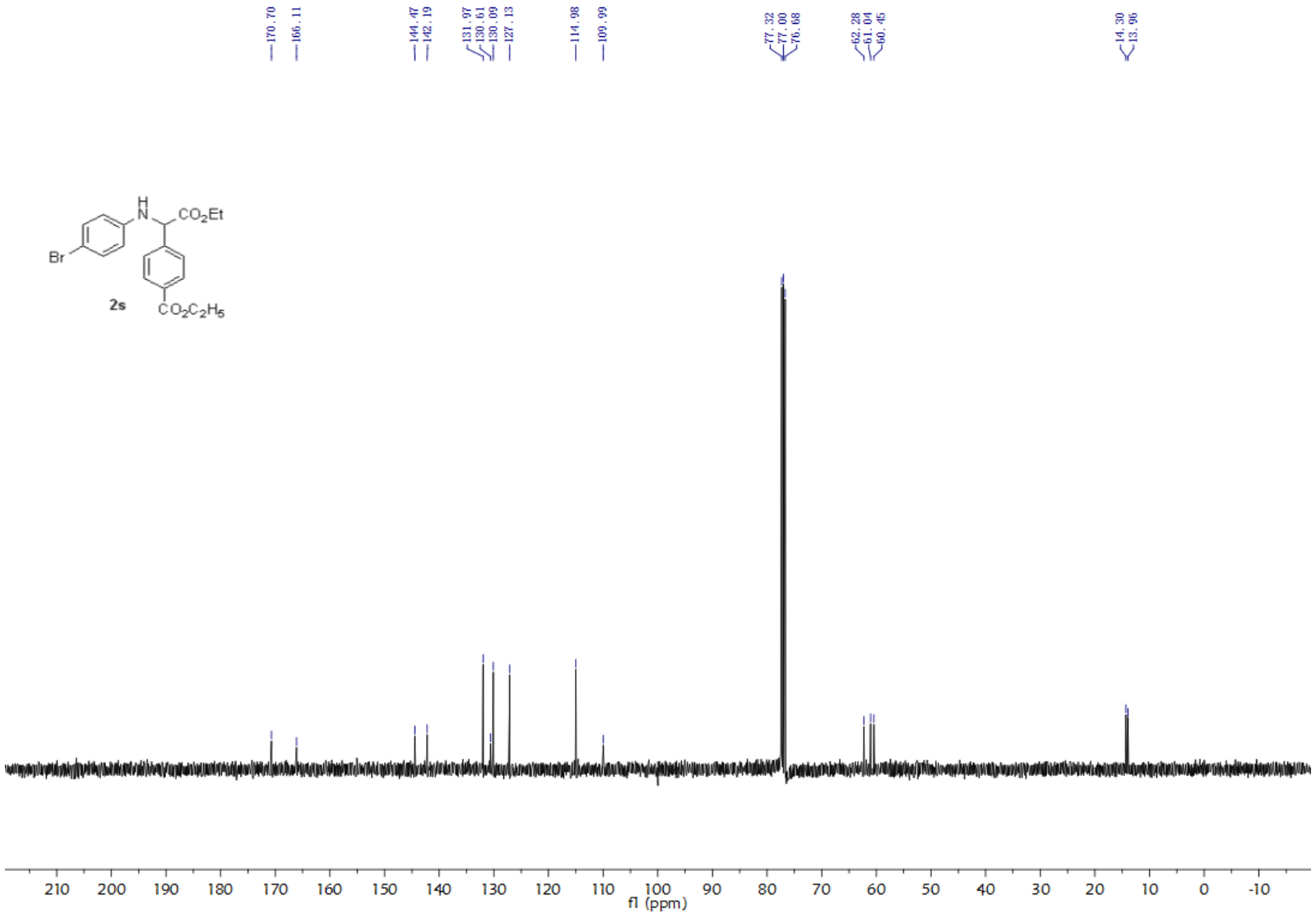
f1 (ppm)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62.28
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13.96
Br
H
N
CO2Et
CO2C2H5
2s
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200
190
180
170
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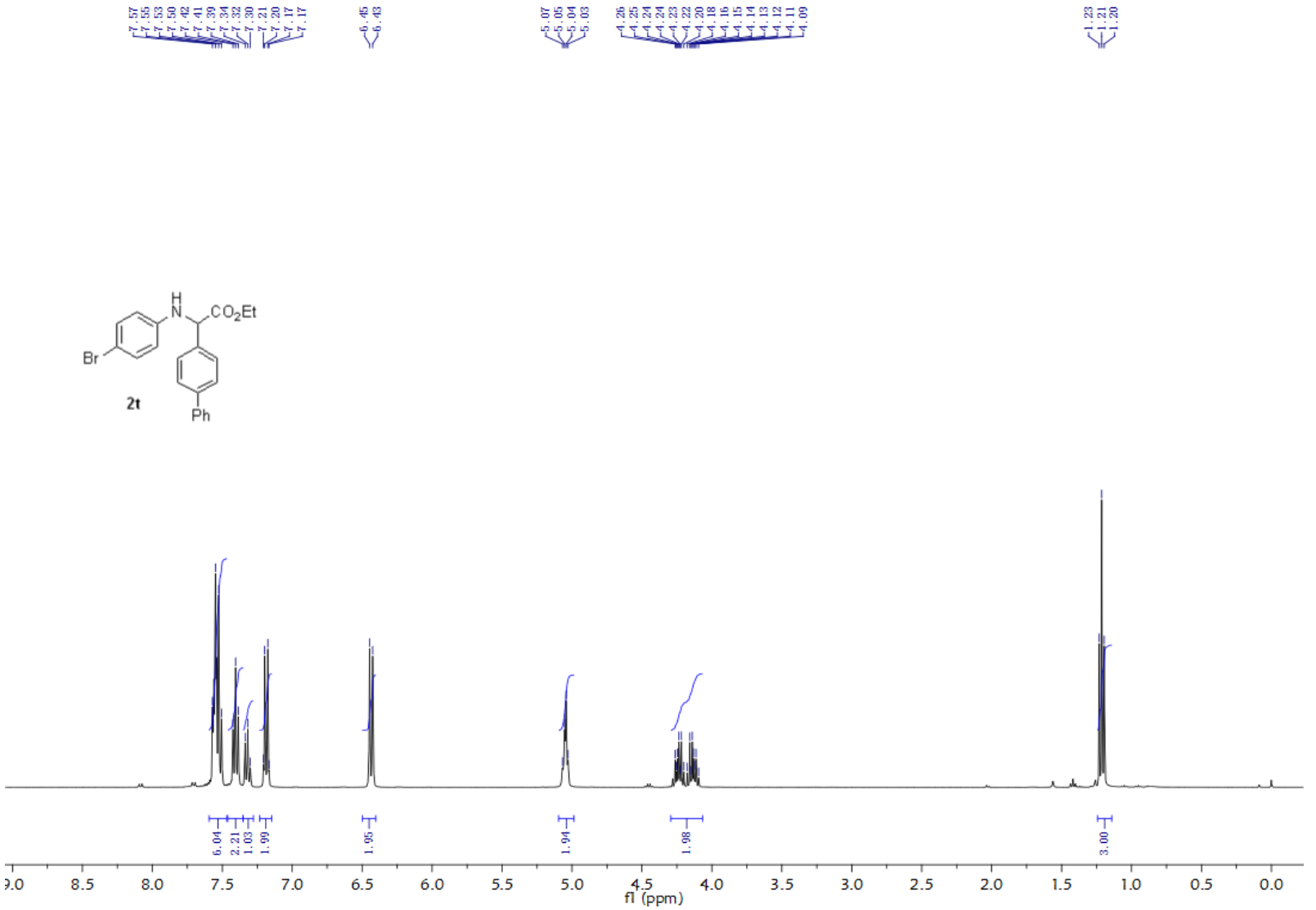
f1 (ppm)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6.43
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5.03
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1.24
1.24
1.23
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1.18
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1.20
Br
N
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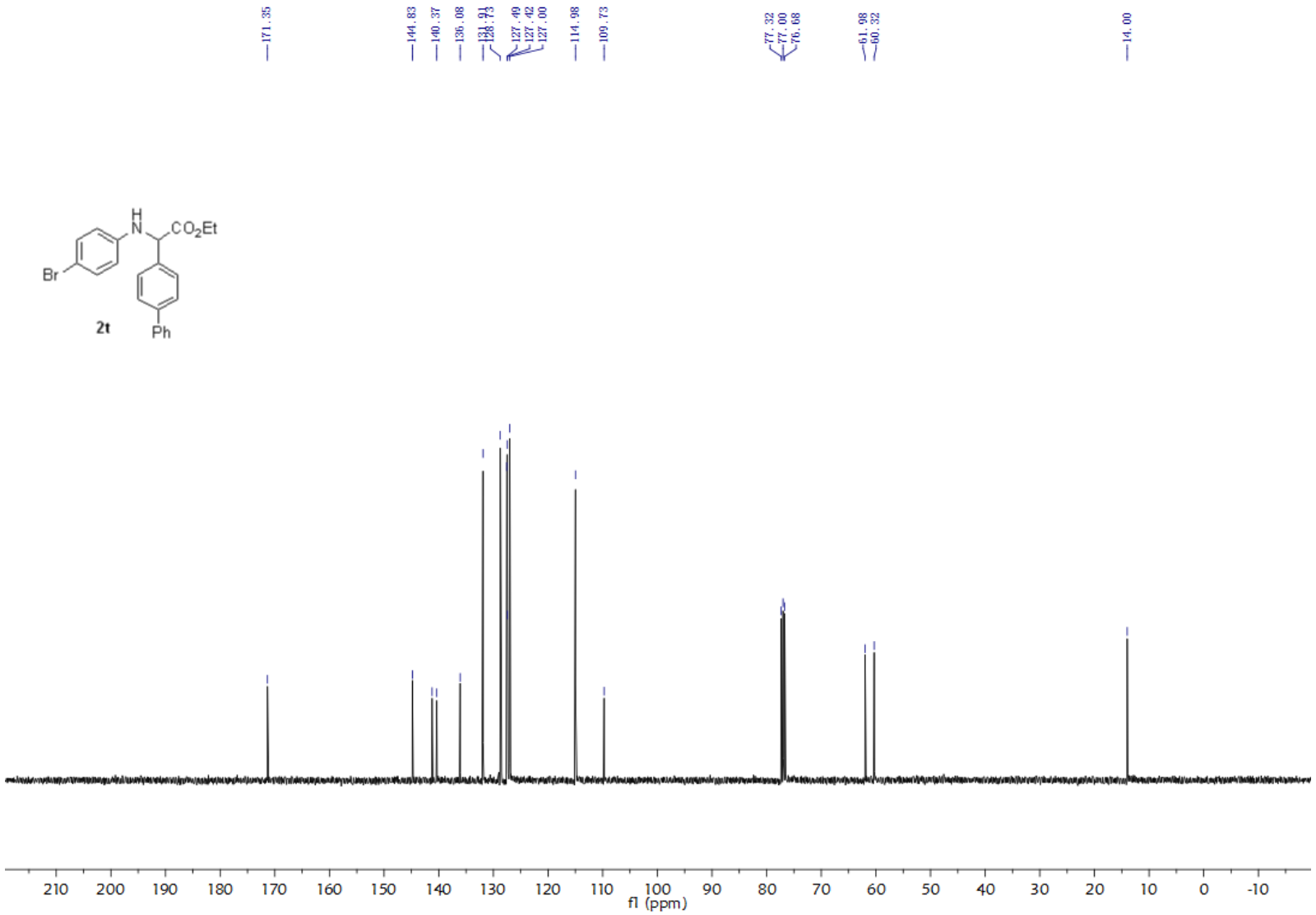
3.00
f1 (ppm)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H
N
CO2Et
Ph
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180
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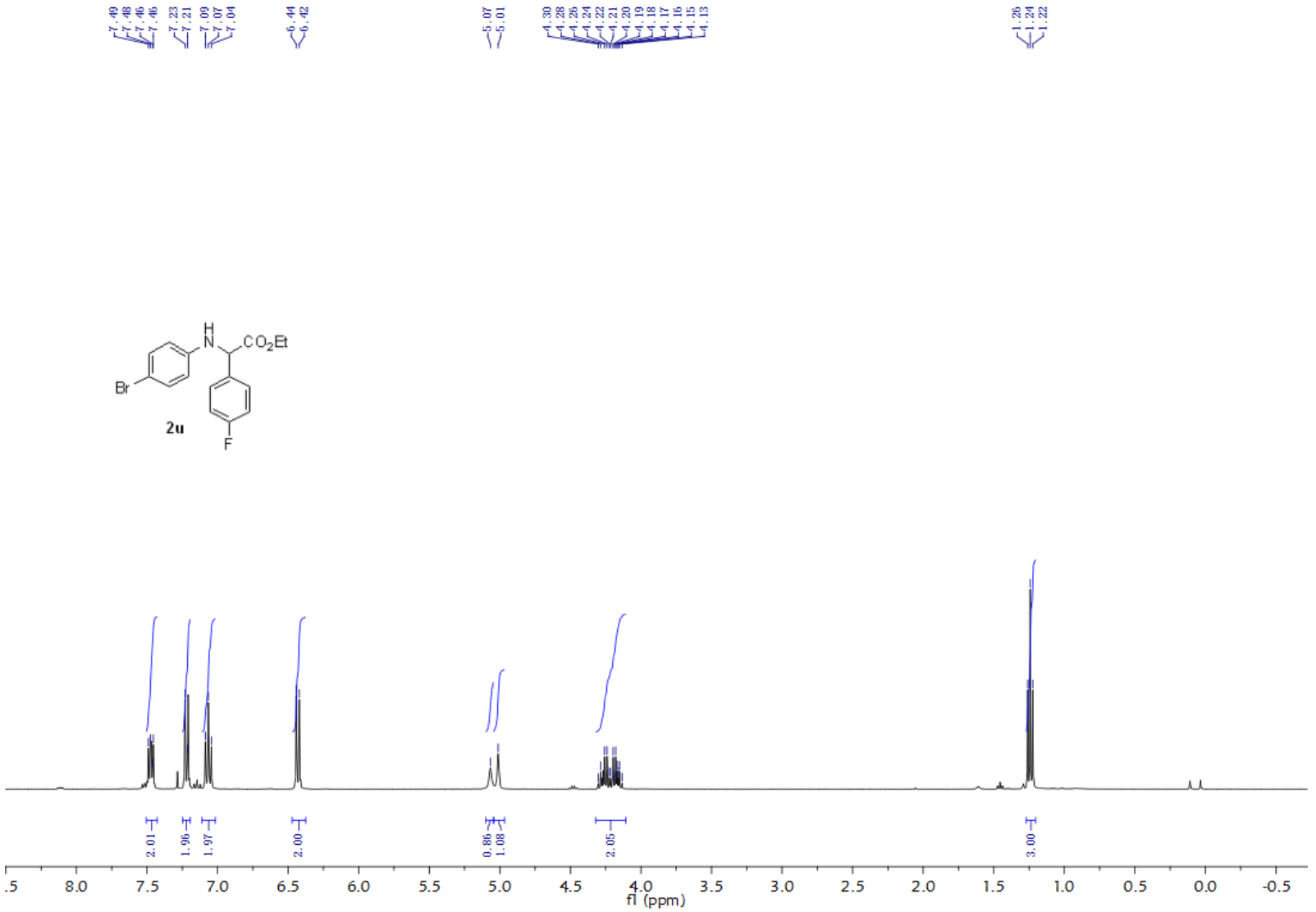
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1.22
1.21
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1.18
1.17
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1.13
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1.22
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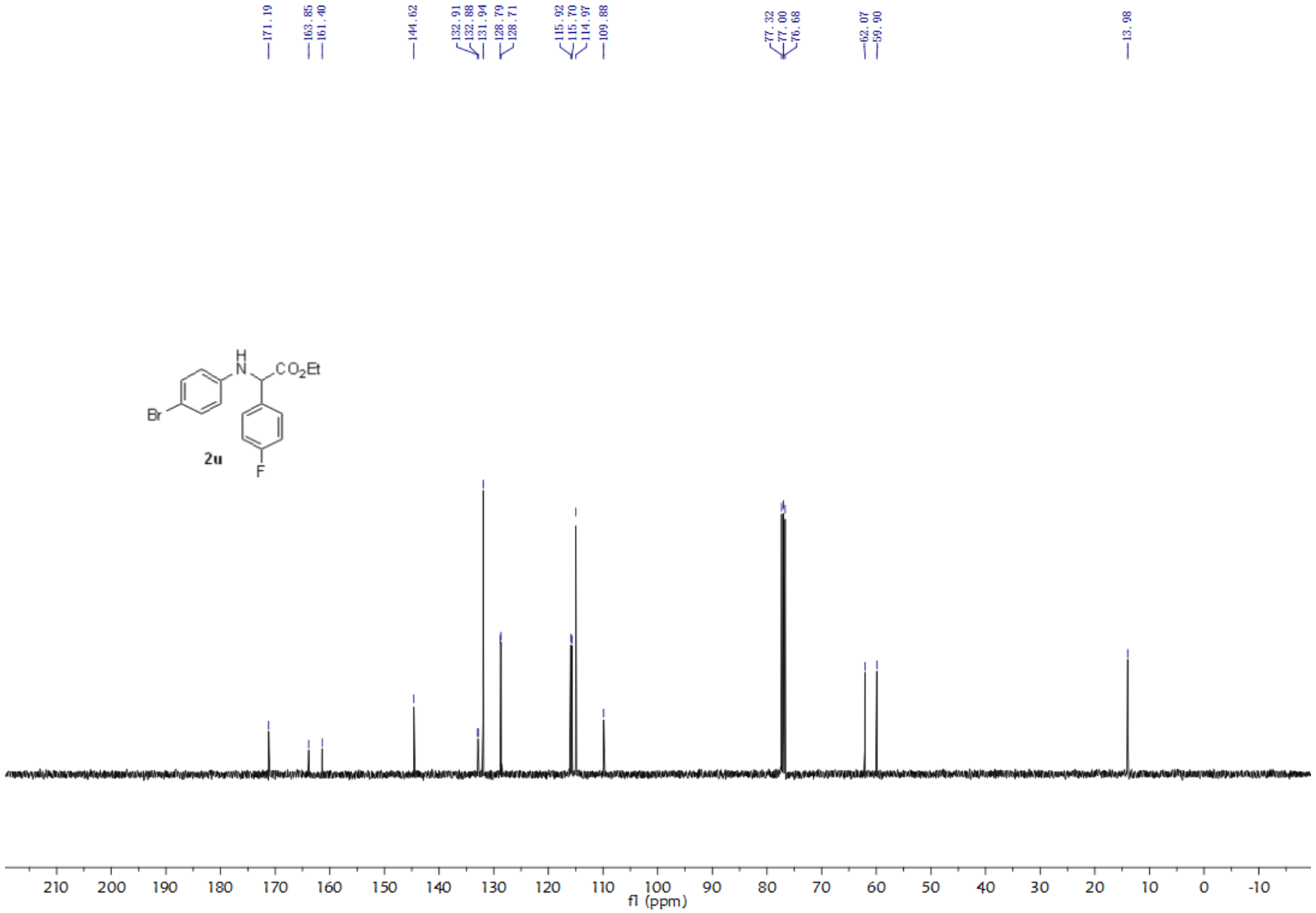
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76.68
62.07
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H
N
CO2Et
Br
F
2u
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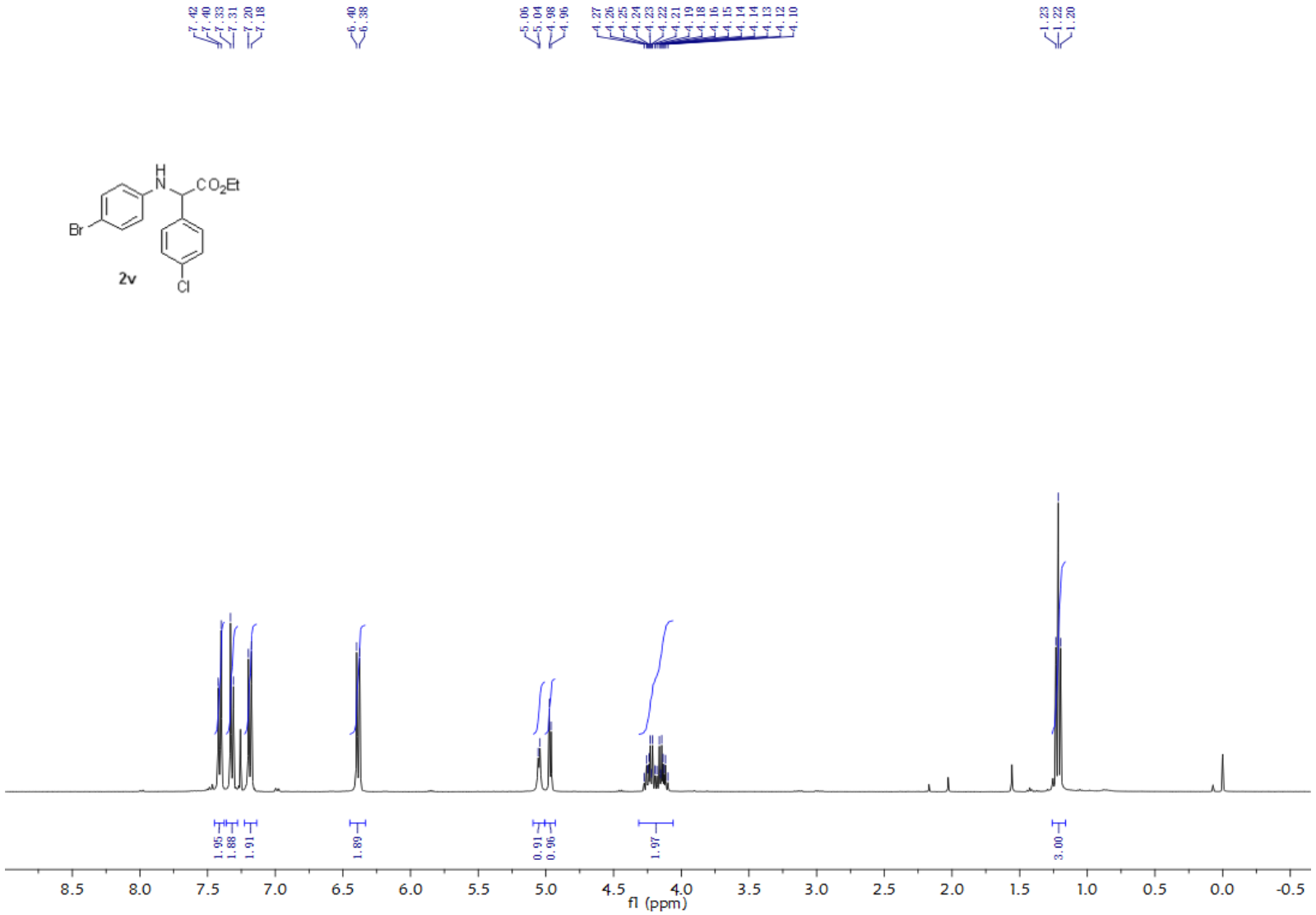
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4.15
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4.14
4.13
4.12
4.10
1.23
1.22
1.20
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Br
Cl
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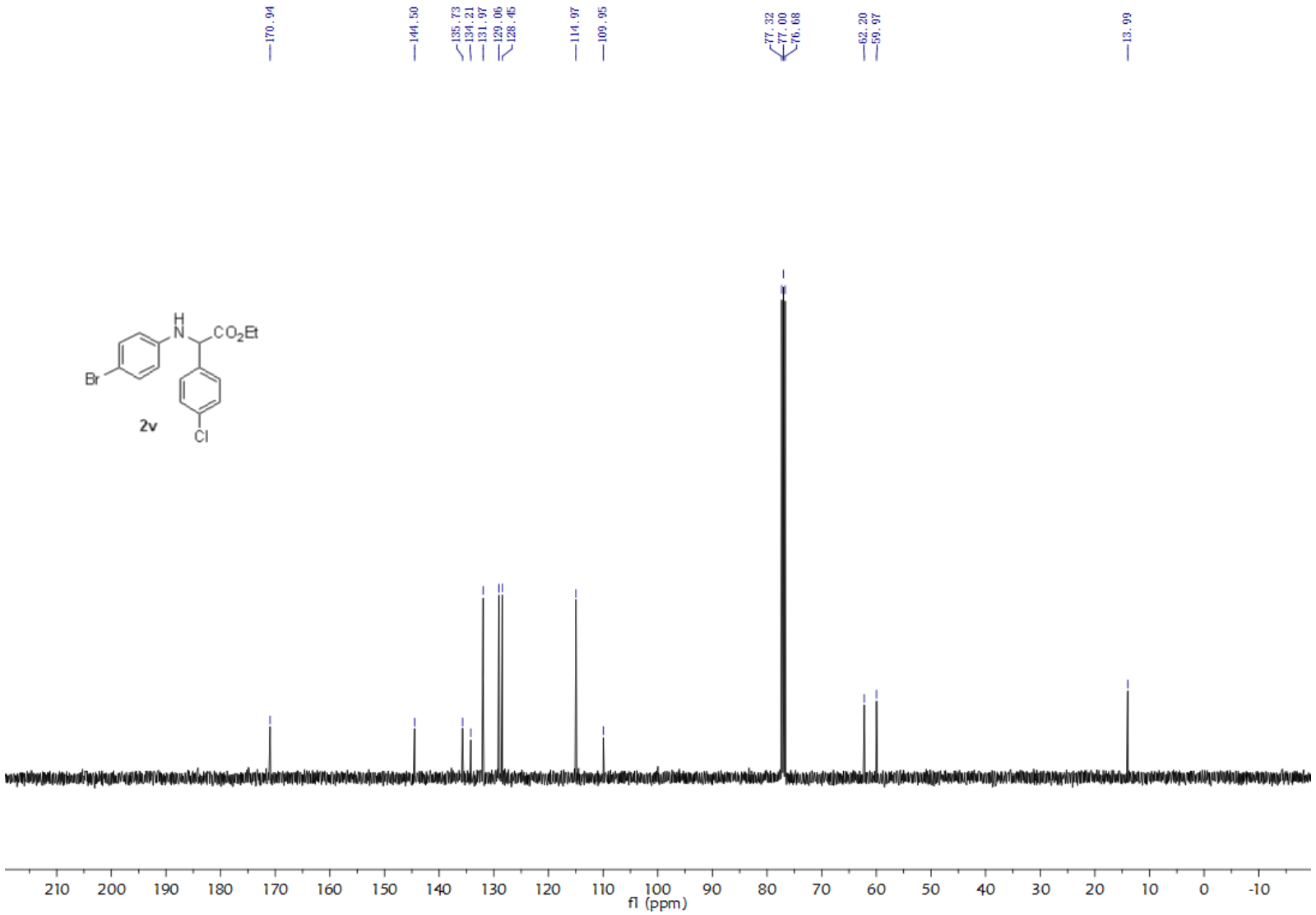
f1 (ppm)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76.68
62.20
59.97
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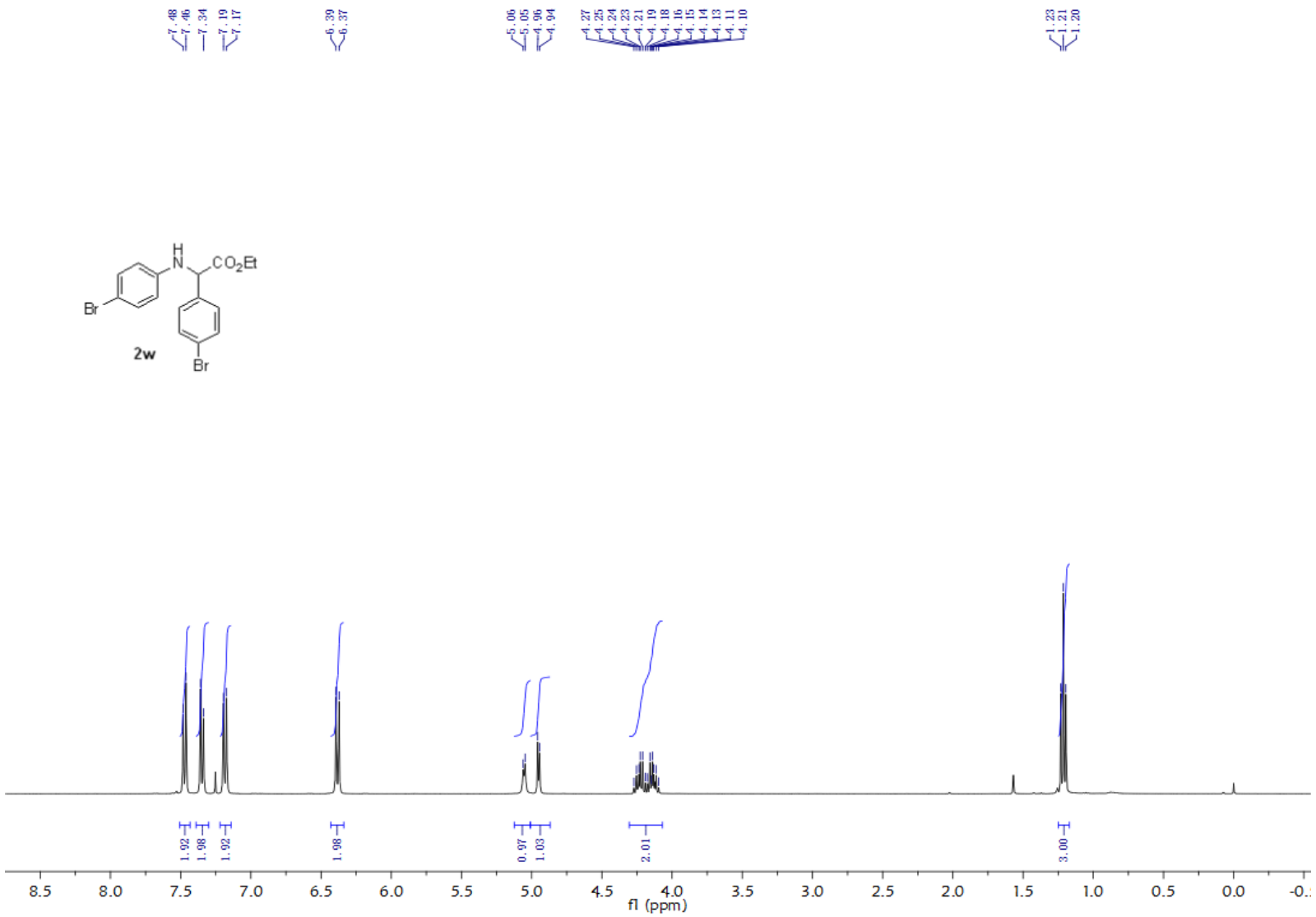
CO2Et
Br
Cl
2v
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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1.10
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1.20
H
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CO2Et
Br
Br
2w
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1.98
1.92
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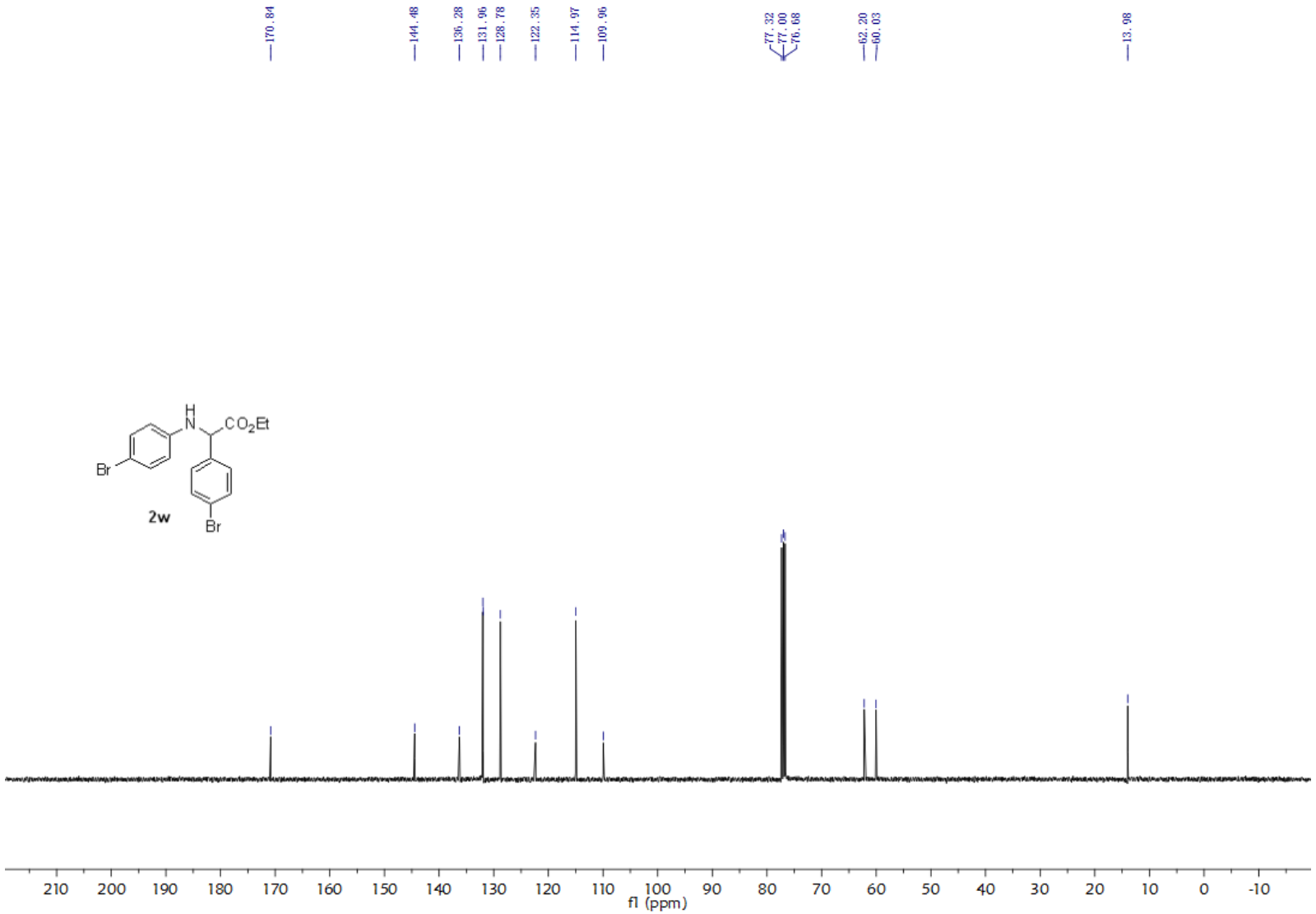
f1 (ppm)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CO2Et
Br
Br
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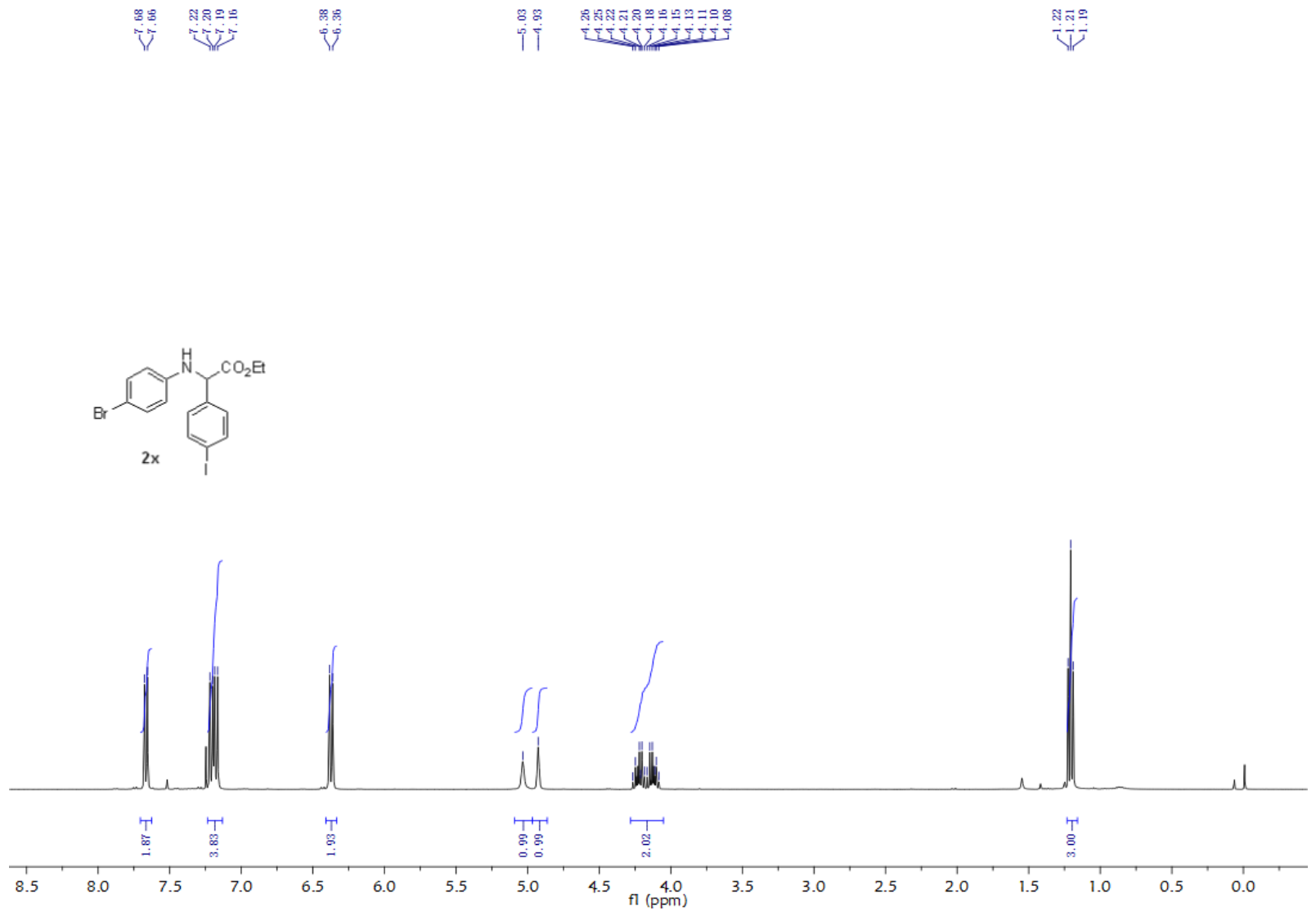
f1 (ppm)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1.21
1.19
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1.0
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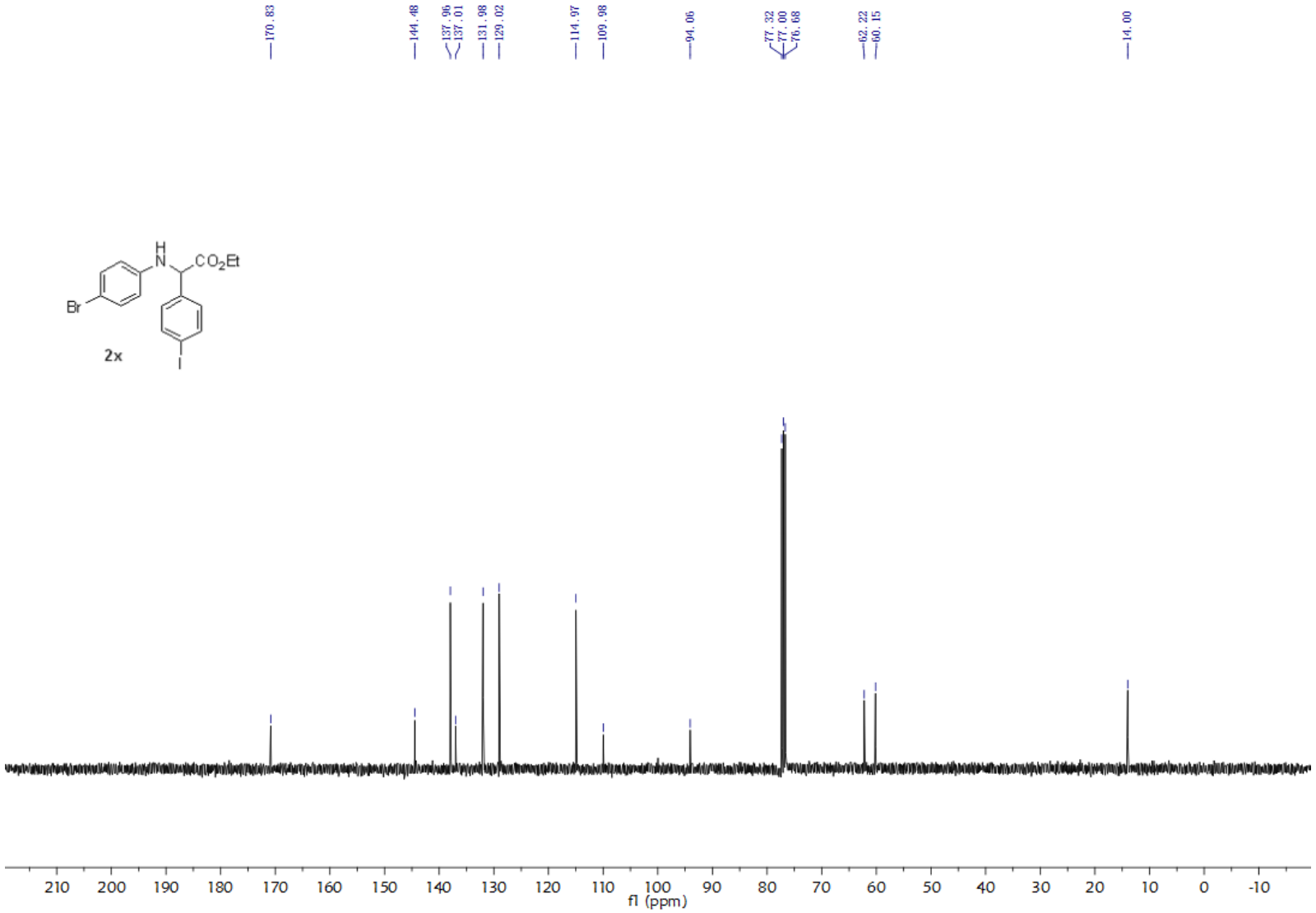
f1 (ppm)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62.22
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14.00
H
N
CO2Et
Br
I
2x
210
200
190
180
170
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100
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80
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60
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20
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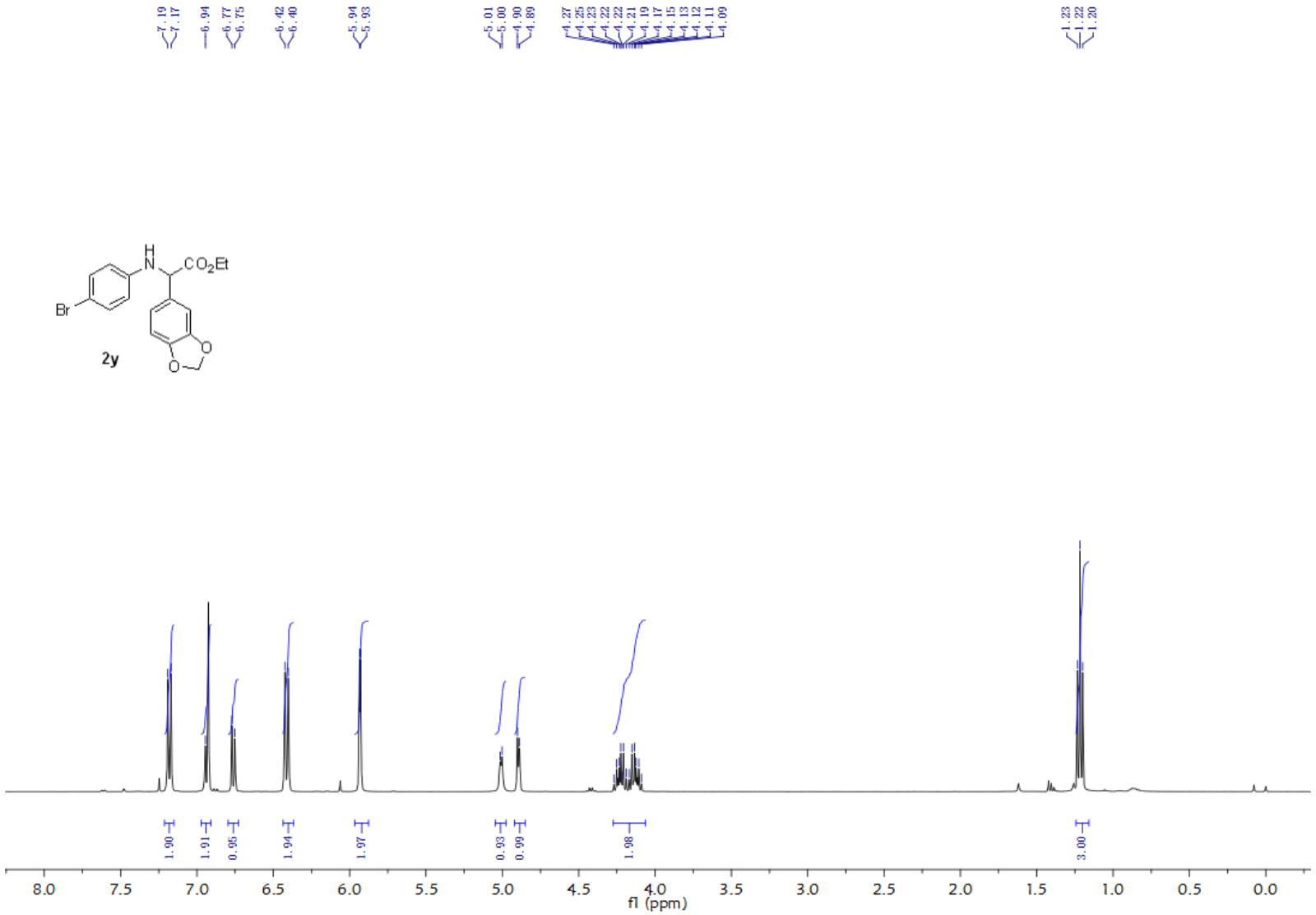
-10
f1 (ppm)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1.23
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1.19
1.17
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1.12
1.11
1.09
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1.22
1.20
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O
O
O
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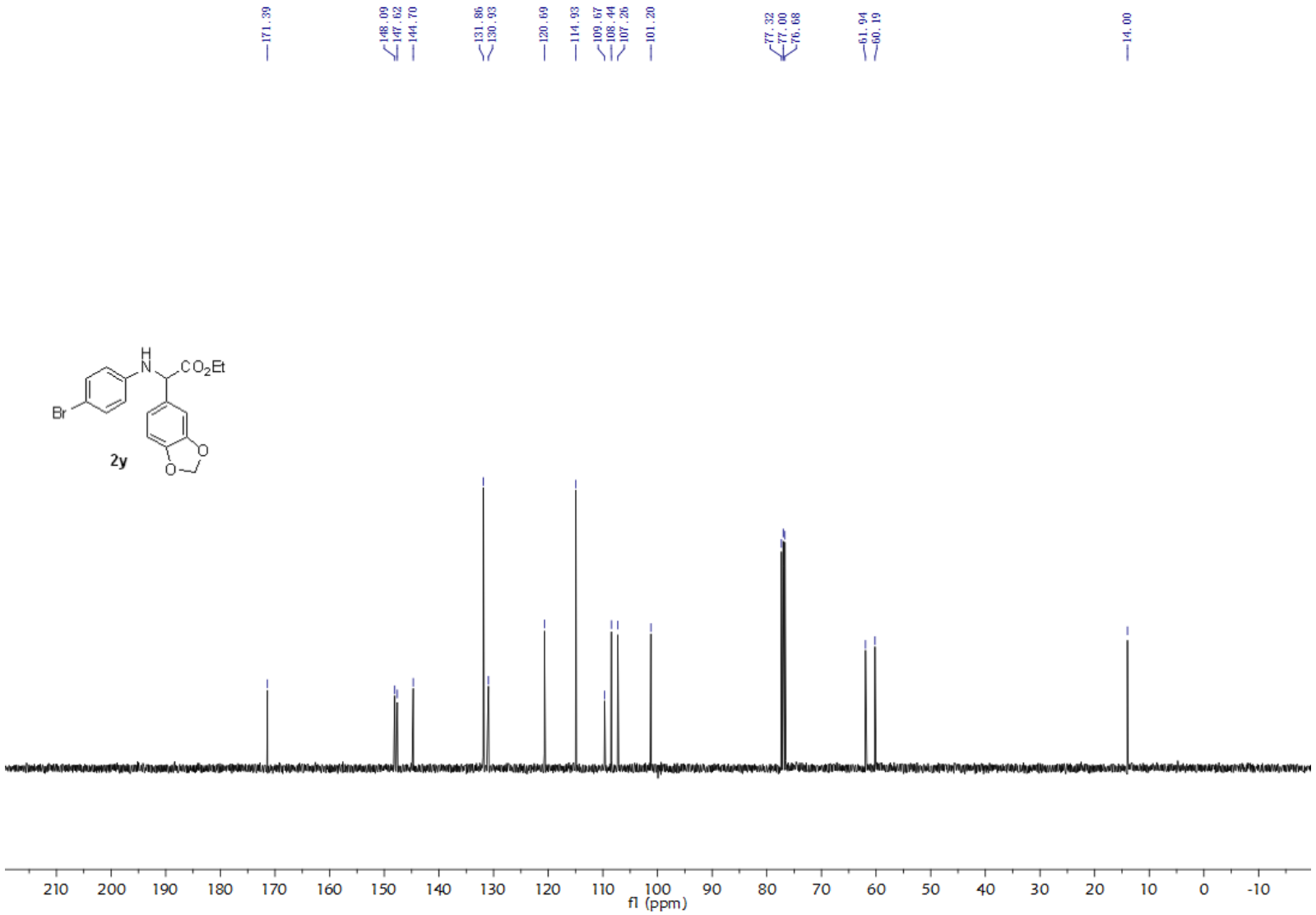
0.0
f1 (ppm)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107.26
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76.68
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60.19
14.00
Br
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CO2Et
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O
O
2y
210
200
190
180
170
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100
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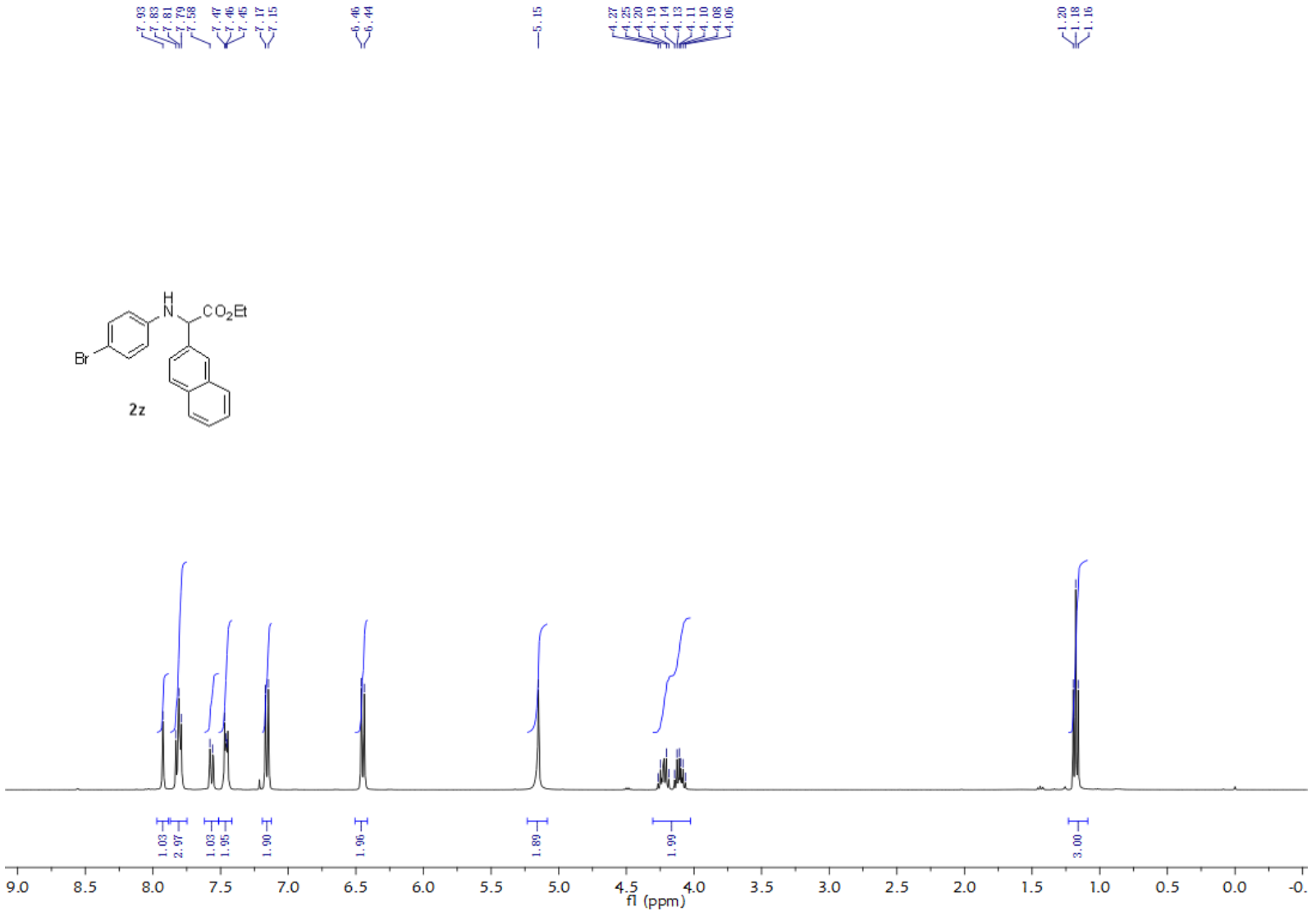
f1 (ppm)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4.27
4.25
4.20
4.19
4.14
4.13
4.11
4.10
4.08
4.06
1.20
1.18
1.16
Br
N
H
CO2Et
2z
1.03
2.97
1.03
1.95
1.90
1.96
1.89
1.99
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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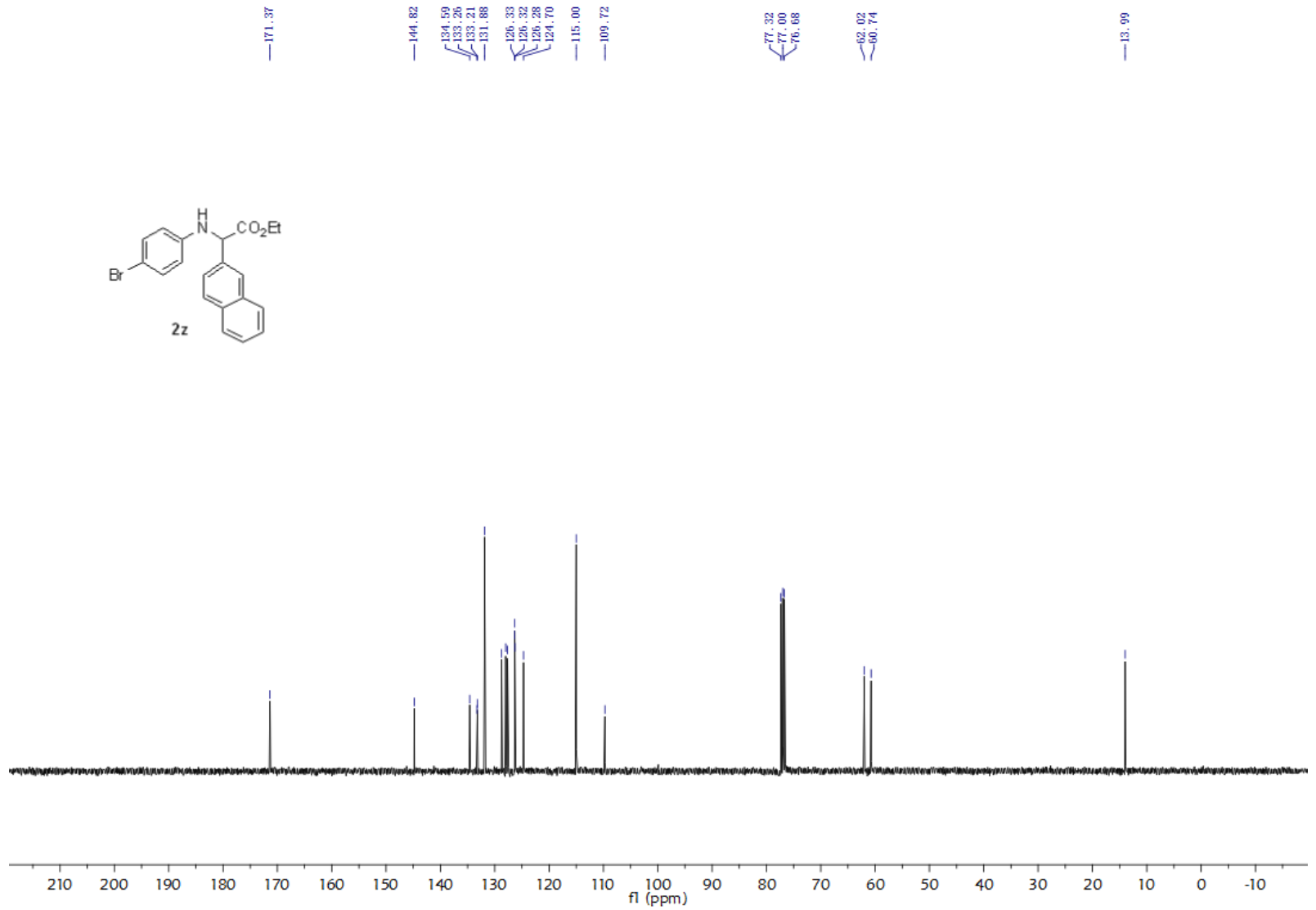
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131.88
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126.32
126.28
124.70
115.00
109.72
77.32
77.00
76.68
62.02
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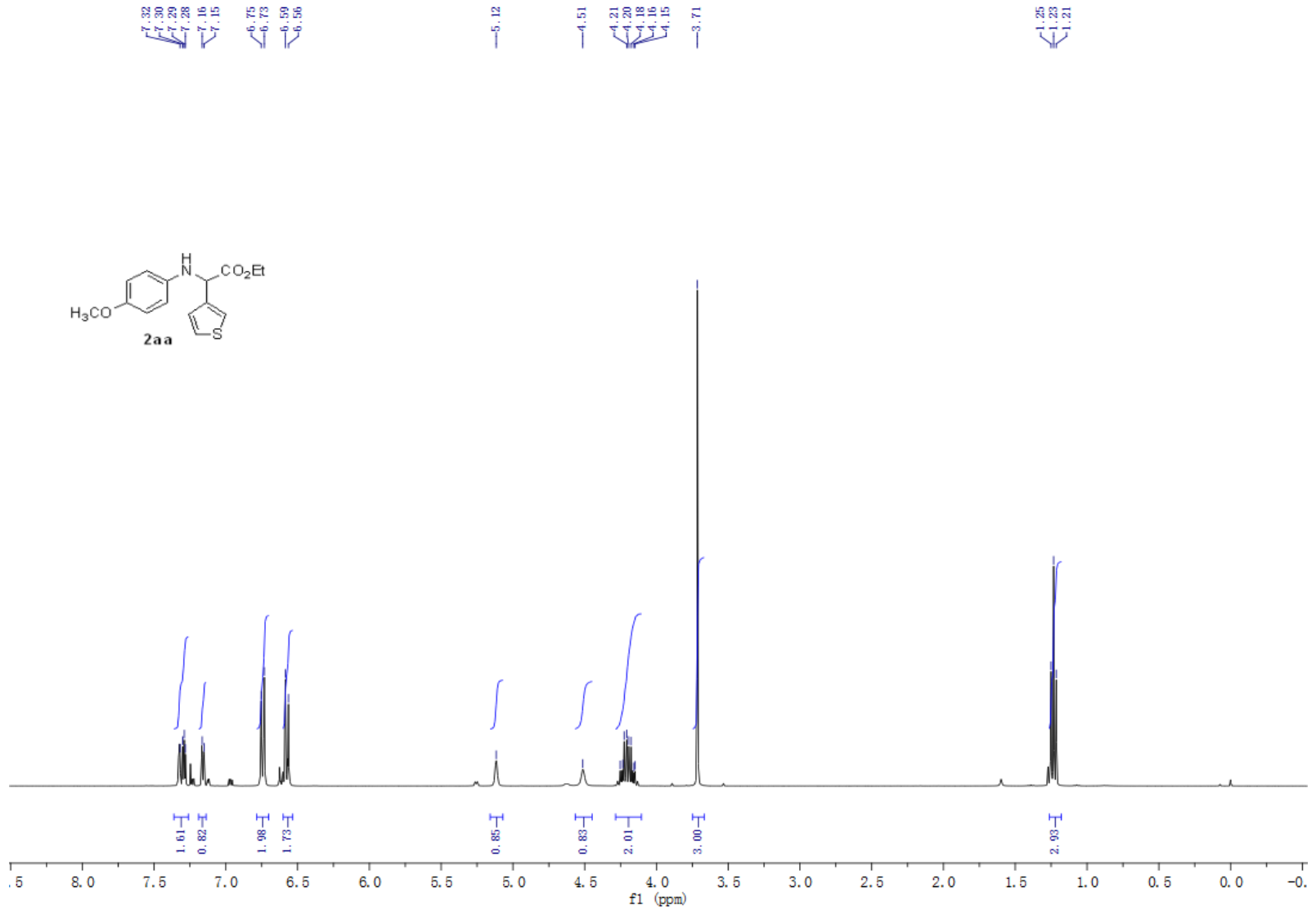
H
N
CO2Et
Br
2z
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.29
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7.16
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6.73
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6.56
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4.21
4.20
4.18
4.16
4.15
3.71
1.25
1.23
1.21
H
N
CO2Et
H3CO
S
2aa
1.61
0.82
1.98
1.73
0.85
0.83
2.01
3.00
2.93
8.0
7.5
7.0
6.5
6.0
5.5
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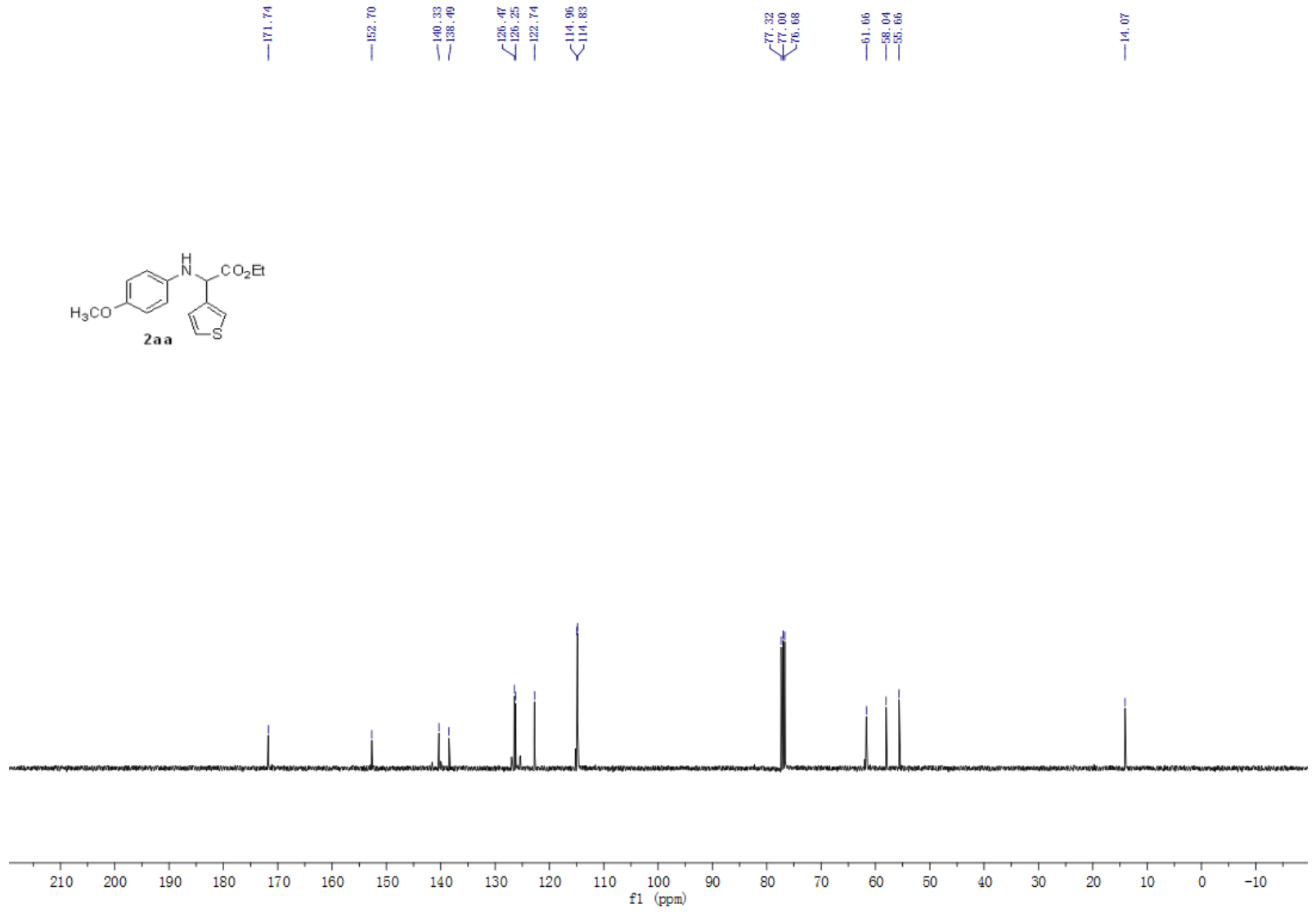
f1 (ppm)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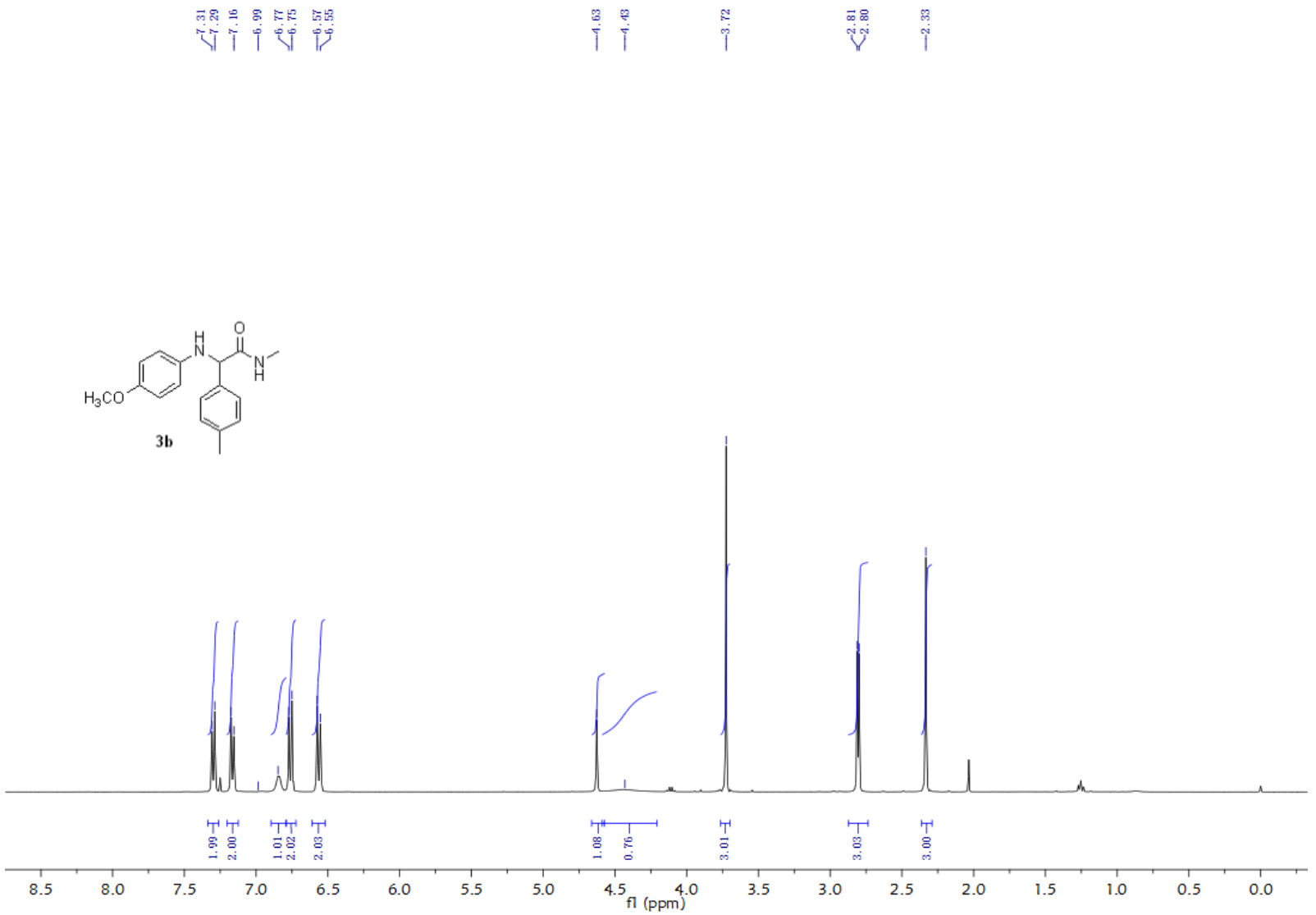
126.25
122.74
114.96
114.83
77.32
77.00
76.68
61.66
58.04
55.66
14.07
H
N
CO2Et
H3CO
S
2aa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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6.77
6.75
6.57
6.55
4.63
4.43
3.72
2.81
2.80
2.33
H3CO
3b
1.99
2.00
1.01
2.02
2.03
1.08
0.76
3.01
3.03
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
3.5
3.0
2.5
2.0
1.5
1.0
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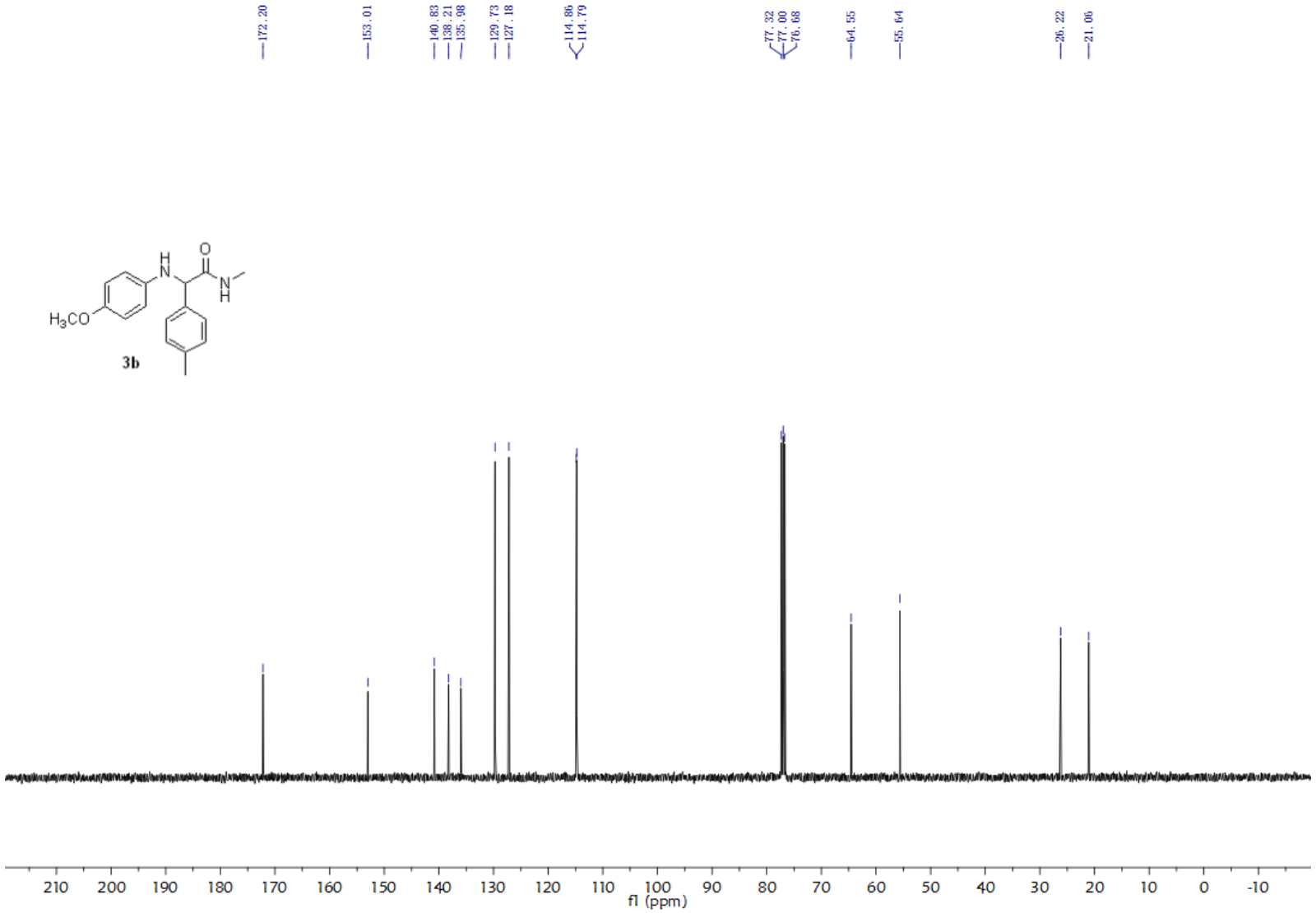
0.0
f1 (ppm)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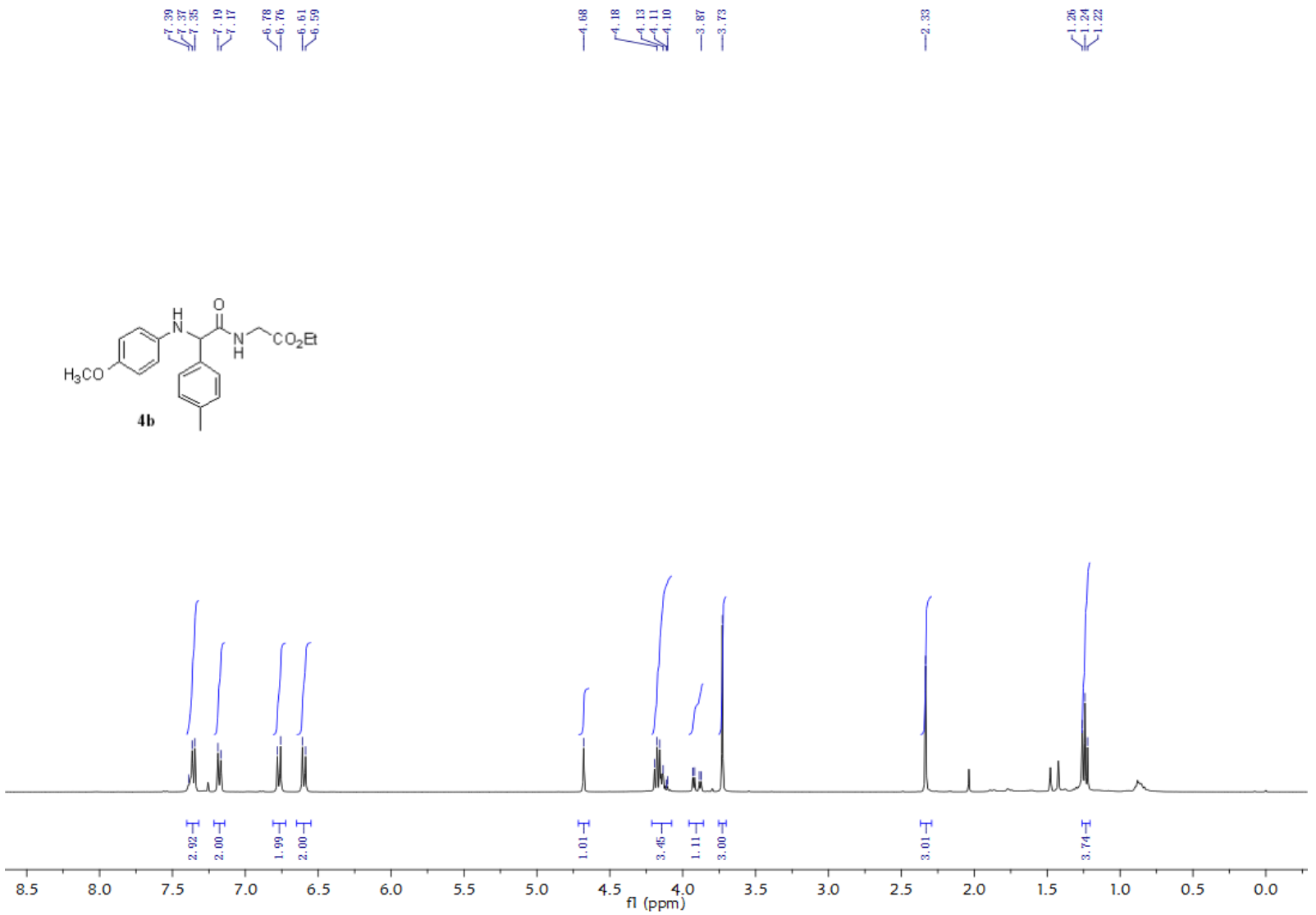
138.21
135.98
129.73
127.18
114.86
114.79
77.32
77.00
76.68
64.55
55.64
26.22
21.06
H3CO
3b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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6.61
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4.68
4.18
4.13
4.11
4.10
3.87
3.73
2.33
1.26
1.24
1.22
H3CO
H
N
O
N
H
CO2Et
4b
2.92
2.00
1.99
2.00
1.01
3.45
1.11
3.00
3.01
3.74
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
3.0
2.5
2.0
1.5
1.0
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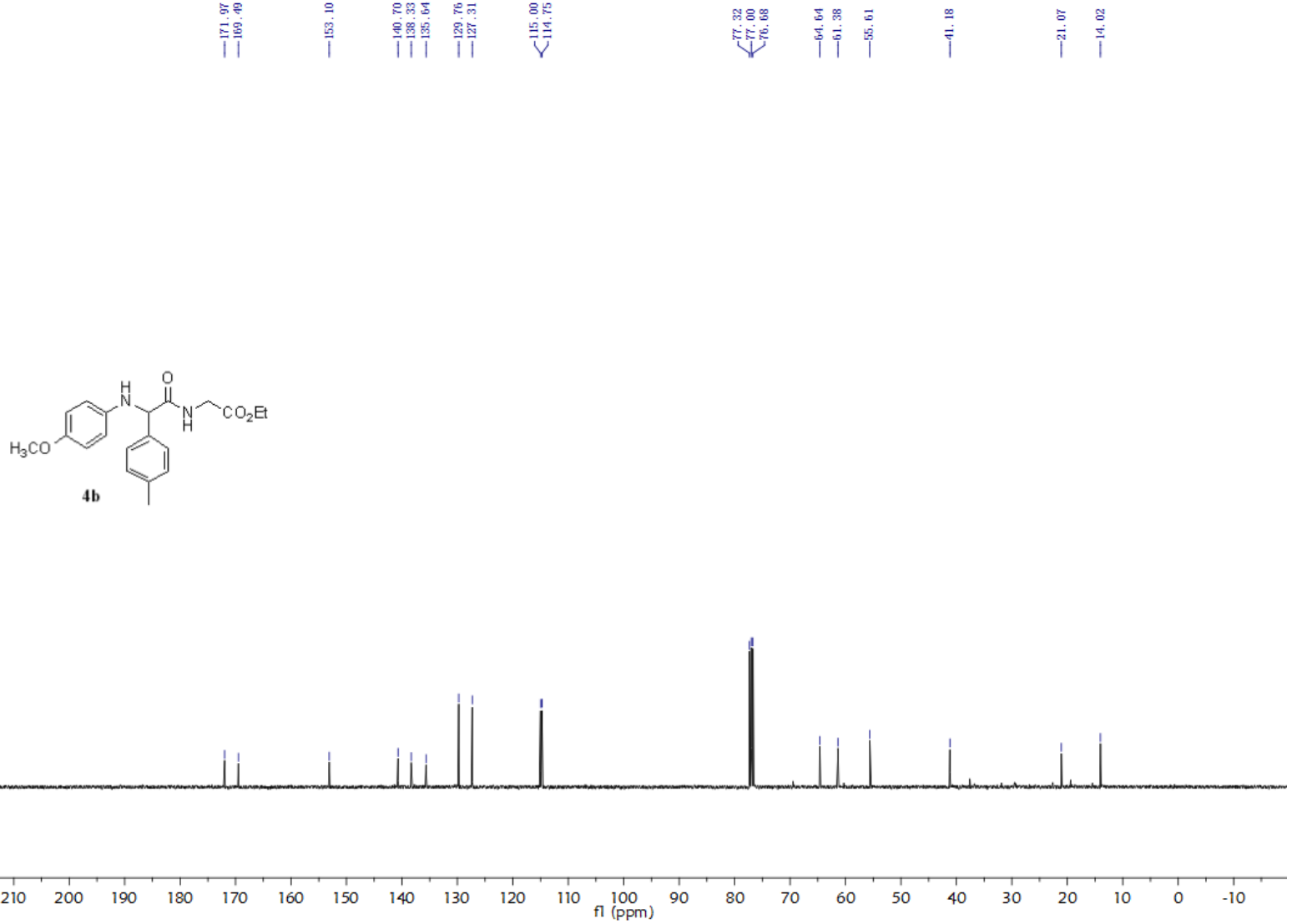
f1 (ppm)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169.49
153.10
140.70
138.33
135.64
129.76
127.31
115.00
114.75
77.32
77.00
76.68
64.64
61.38
55.61
41.18
21.07
14.02
H3CO
N
H
O
N
H
CO2Et
4b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)