Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supplementary Information for

Ligand-Enabled Silver-Catalyzed Carbene Insertion into N−H Bond of Aliphatic and Electron-rich Aromatic Amines

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1. General information

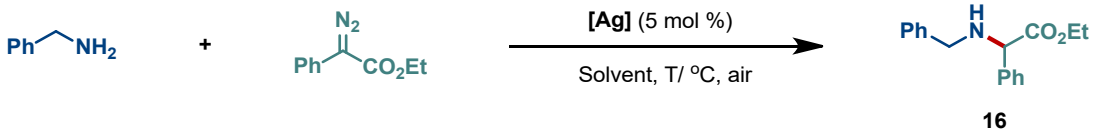
General. All reactions dealing with air- or moisture-sensitive compounds were carried out in a flame-dried, sealed Schlenk reaction tube under an atmosphere of argon. Analytical thin-layer chromatography was performed on glass plates coated with 0.25 mm 230-400 mesh silica gel containing a fluorescent indicator (Merck). Flash silica gel column chromatography was performed on silica gel 60N (spherical and neutral, 140-325 mesh) as described by Still. NMR spectra were measured on a Varian I NOVA 500 or Bruker AV-600 spectrometer and reported in parts per million. The ^{1}H NMR (500 MHz or 600 MHz) chemical shifts were measured relative to TMS, DMSO or $CDCl_3$ as the internal reference. The ^{13}C NMR (125 MHz or 150 MHz) chemical shifts are given using $CDCl_3$ and DMSO as the internal standard. High resolution mass spectra (HRMS) were recorded on the Exactive Mass Spectrometer (Agilent 1200HPLC/MicrOTOF II) equipped with ESI ionization source. Melting points were determined with XRC-1 and are uncorrected.

Materials. Unless otherwise noted, materials were purchased from Tokyo Chemical Industry Co., Aldrich Inc., Alfa Aesar, and other commercial suppliers and used as received. Solvents were dried over CaH_2 (for DCE $CHCl_3$ and DMF) or sodium (for toluene and 1,4-dioxane) by refluxing for overnight and freshly distilled prior to use.

2. Experimental Procedure

2.1 Optimization of the reaction conditions

Table S1. Optimization of the reaction conditions with diazoes and aliphatic amines[a]

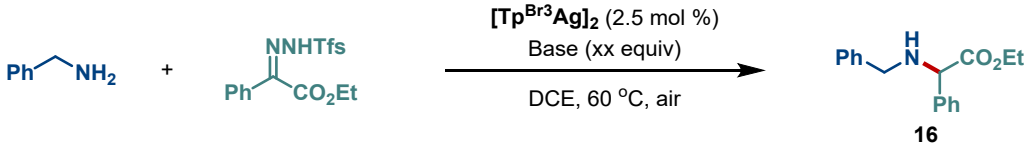


16

Entry	[Ag]	Solvent	T (°C)	Yield of 16 (%)
1	—	DCE	60	0
2	AgOTf (5 mol %)	DCE	60	15
3	$AgSbF_6$ (5 mol %)	DCE	60	29
4	$AgBF_4$ (5 mol %)	DCE	60	32
5	$Tp^{(CF3)2}Ag$ (5 mol %)	DCE	60	76
6	**$[Tp^{Br3}Ag]_2$ (2.5 mol %)**	**DCE**	**60**	**92 (91)[b]**
7	$[Tp^{Br3}Ag]_2$ (2.5 mol %)	DCE	40	52
8	$[Tp^{Br3}Ag]_2$ (2.5 mol %)	DCE	80	71
9	$[Tp^{Br3}Ag]_2$ (2.5 mol %)	$CHCl_3$	60	88
10	$[Tp^{Br3}Ag]_2$ (2.5 mol %)	1,4-dioxane	60	47
11	$[Tp^{Br3}Ag]_2$ (2.5 mol %)	$PhCF_3$	60	85
12	$[Tp^{Br3}Ag]_2$ (2.5 mol %)	PhMe	60	75

[a] Conditions: Benzylamine (0.3 mmol), $[Tp^{Br3}Ag]_2$ (2.5 mol %), **1a** (0.36 mmol) in DCE (3 mL) at 60 °C for 6 h.
[b] Isolated yields are given.

Table S2. Optimization of the reaction conditions with sulfonyl hydrazones and aliphatic amines[a]

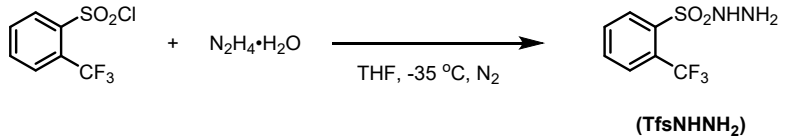


16

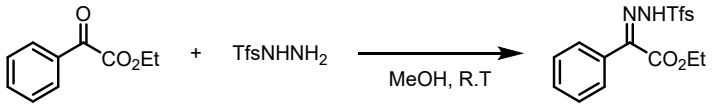
Entry	1b (mmol)	Benzylamine (mmol)	Base (mmol)	Yield of 16 (%)
1	0.2	0.24	NaH (0.24)	21
2	0.2	0.24	K_2CO_3 (0.24)	23
3	0.2	0.24	KO^{t}Bu (0.24)	20
4	0.2	0.24	LiO^{t}Bu (0.24)	45
5	0.2	0.24	DIPEA (0.24)	trace
6	0.2	0.24	DBU (0.24)	12
7	0.2	0.24	Pydine (0.24)	10
8	0.2	0.2	LiO^{t}Bu (0.2)	55
9	0.3	0.2	LiO^{t}Bu (0.2)	67
10	0.4	0.2	LiO^{t}Bu (0.2)	77
11	0.4	0.2	LiO^{t}Bu (0.4)	25
12	0.4	0.2	LiO^{t}Bu (0.6)	26
13[b]	**0.4**	**0.2**	**LiO^{t}Bu (0.2)**	**84 (82)**[c]

[a] Conditions: Benzylamine (0.2 mmol), $[Tp^{Br3}Ag]_2$ (2.5 mol %), **1b** (0.4 mmol), LiO^{t}Bu (0.2 mmol) in DCE (5 mL), 60 °C, 6 h; [b] using $[Tp^{Br3}Ag]_2$ (2.5 mol %). [c] Isolated yields are given.

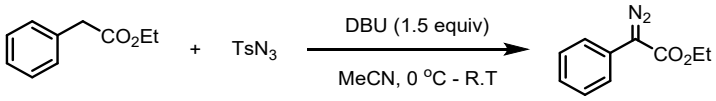
2.2 **General procedure for the synthesis of starting materials**



Add *o*-trifluoromethylbenzenesulfonyl chloride (24.4 g, 100 mmol, 1.0 equiv) to 120 mL of tetrahydrofuran (THF) solution to dissolve it. The reaction system was placed at -35 °C and hydrazine hydrate (24 mL, 250 mmol, 2.5 equiv) was added dropwise under argon atmosphere. After 4 hours of reaction, the reaction system was monitored by TLC until the raw materials disappeared. After the reaction, extract with ethyl acetate (about 60mL×3), wash with saturated sodium chloride solution, combine the organic phases, dry with anhydrous Na_2SO_4, and concentrate in vacuo; slowly drop the remaining solution into 500mL cold petroleum ether placed in a round bottom flask to precipitate the product; then the solid was filtered off with suction and dried in vacuum to obtain a white powdery solid with a yield of 85%.

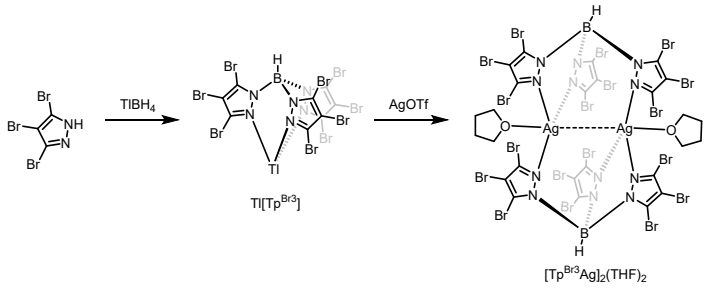


Add ethyl benzoylformate (1.81 g, 11 mmol, 1.1 equiv) to a 50 mL round bottom flask, add 15 mL of methanol, and then add $TfsNHNH_2$ (2.4 g, 10 mmol, 1.0 equiv), and stir at room temperature for approx. After 1 hour, the reaction system was monitored by TLC until $TfsNHNH_2$ disappeared. The suspension was filtered with suction and washed with ether：petroleum ether = 10:1 to obtain a white powdery solid with a yield of 80%. Use the same method for other *N*-triftosyhydrazones.

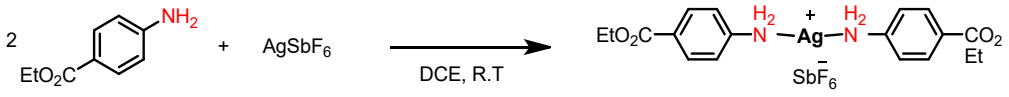


At 0 °C, *p*-toluenesulfonyl azide (2.17 g, 11 mmol, 1.1 eq) was added to ethyl phenylacetate (1.64 g, 10 mmol, 1 eq) dissolved in 30 mL of acetonitrile. Under argon atmosphere, DBU (2.28 g, 15 mmol, 1.5 eq) was slowly added dropwise to the system, and stirring was continued for about 6 hours at room temperature. The reaction system was monitored by TLC, and the reaction was stopped when the raw materials disappeared. It was quenched with saturated NH_4Cl (20 mL), extracted with DCE (30 mL × 3), and the organic phases were combined, dried over anhydrous Na_2SO_4, and then concentrated in vacuo. The product was purified by flash column chromatography (PE : EA = 100 : 1) to obtain a red oily liquid with a yield of 90%. Use the same method for other diazonium compounds.

2.3 **Synthesis of silver catalyst**

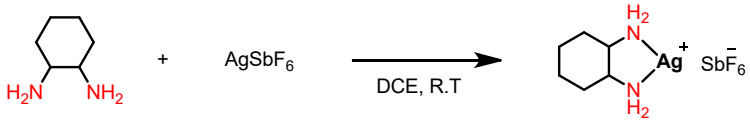


[$Tp^{Br3}Ag]_2(THF)_2$ Synthesize according to the previously reported literature[1] Previously sublimed 1*H*-3,4,5-tribromopyrazole (12.19 g, 40.0 mmol) and $TlBH_4$ (2.19 g, 10.0 mmol) were added to a 500 mL Schlenk tube. The tube was closed with a rubber septum and three vacuum/nitrogen cycles were made. The septum was replaced with a reflux condenser fitted with a bubbler on top. The nitrogen flow was stopped and the stirred solid mixture was warmed to 180-185 °C for 2 h before the temperature was increased to 200 °C and the reaction mixture stirred for an additional 2 h. After cooling to room temperature, the obtained white solid was directly purified by sublimation to remove the unreacted pyrazole (150 °C, 2 mbar) to give $TlTp^{Br3}$ as a white solid (13.4 g, 89% yield). Silver triflate (1.29 g, 5.0 mmol) was added to a solution of $TlTp^{Br3}$ (5.64 g, 5.0 mmol) in acetone. After 20 h of stirring in the dark, a white solid precipitated from the initially colorless solution. The solid was filtered off and dried under vacuum to give complex $[Tp^{Br3}Ag]_2.CH_3COCH_3$. $[Tp^{Br3}Ag]_2.CH_3COCH_3$ (5.0 mmol) was stirred in fresh distilled THF (100 mL) for 30 min in the dark. After the removal of the volatiles under reduced pressure, a white solid was obtained in quantitative yield.



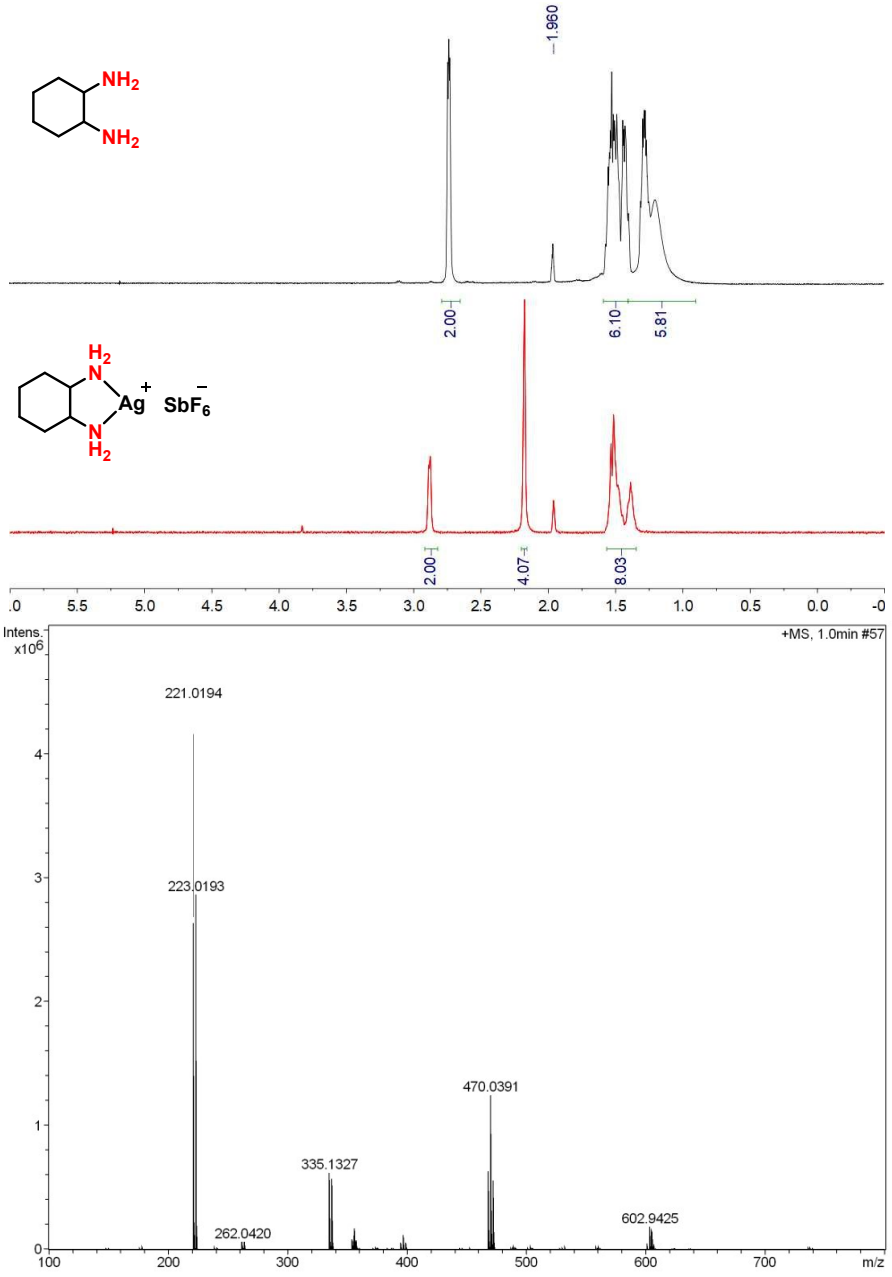
Complex A

Amine/silver complex A: To a round bottom sealed tube, $AgSbF_6$ (171.8 mg, 0.5 mmol) were added under air atmosphere. DCM (2 mL) was added to dissolve $AgSbF_6$. Ethyl 4-aminobenzoate (173 mg, 1.05 mmol) dissolved in DCM (2 mL) were added to the tube. After stirring for 5 min after the addition at room temperature, a large amount of white solid precipitated out, and the suspension was centrifuged. Wash with DCM (5 mL × 3), and then dry the solid to obtain the white solid amine/silver complex **A** (329 mg, 98% yield).



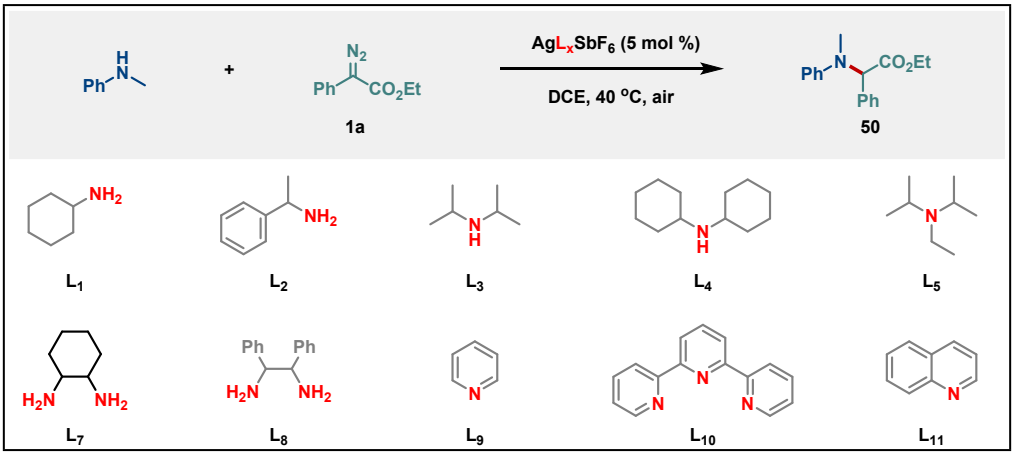
Complex B

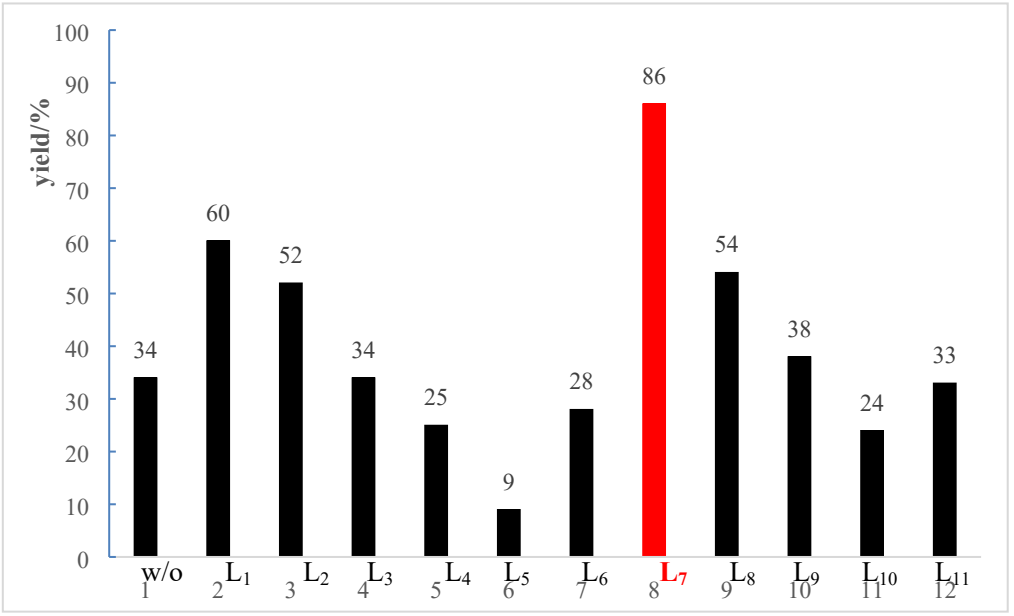
Amine/silver complex B: To a round bottom sealed tube, $AgSbF_6$ (171.8 mg, 0.5 mmol) were added under air atmosphere. DCE (2 mL) was added to dissolve $AgSbF_6$. 1,2-Diaminocyclohexane (60 mg, 0.52 mmol) dissolved in DCE (2 mL) were added to the tube. The resulting mixture was stirred at room temperature for 10 minutes, and a large amount of white solid precipitated. Then the solvent was evaporated in vacuo and washed with DCM (5 mL×3) to obtain white solid amine/silver complex **B** (211.6 mg, 95% yield).



HRMS (ESI^+) m/z calcd for $C_6H_{14}AgN_2$ $[M+H]^+$ 221.0202, found 221.0194.

Table S3. Screening of amine ligands[a]

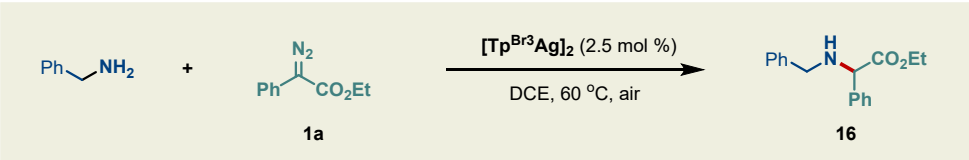




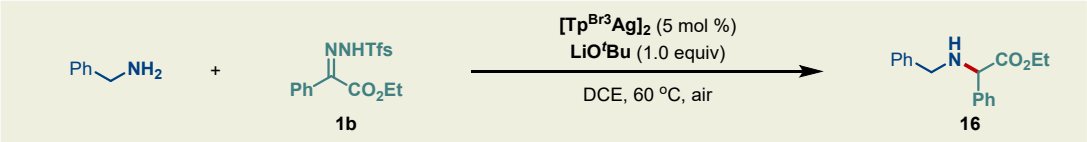
[a] Conditions: *N*-Methylaniline (0.3 mmol), amine/silver complex (5 mol %), **1a** (0.36 mmol) in DCE (3 mL), 40 °C, 1 h. Isolated yields are given.

2.4 **General procedure for the synthesis of products**

i. N-H bond insertion reaction of aliphatic amines

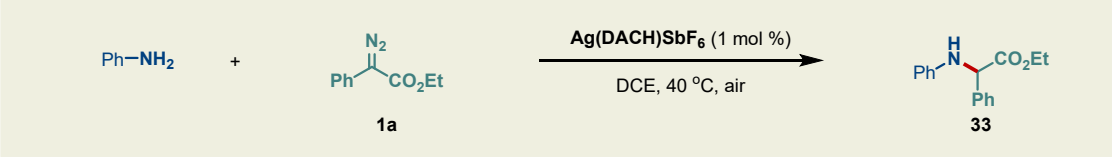


Typical synthetic procedure (with 16 as an example): Method A: To a dried Schlenk flask, $[Tp^{Br3}Ag]_2$ (16.5 mg, 0.015 mmol) were added under air atmosphere. Benzylamine (0.3 mmol) and ethyl 2-diazo-2-phenylacetate **1a** (0.36 mmol) dissolved in DCE (3 mL) were added to the Schlenk flask via a syringe. The resulting mixture was stirred at 60 ºC under sealed conditions for 6 h. After cooling to room temperature, the reaction mixture was diluted with DCM (5 mL) and filtered through a plug of celite, followed by washing with DCM (5 mL × 3). The combined residue was concentrated under reduced pressure, and then the resulting crude product was purified by column chromatography with ethyl acetate/petroleum ether (1:25 v:v) as an eluent to provide the product **16**.



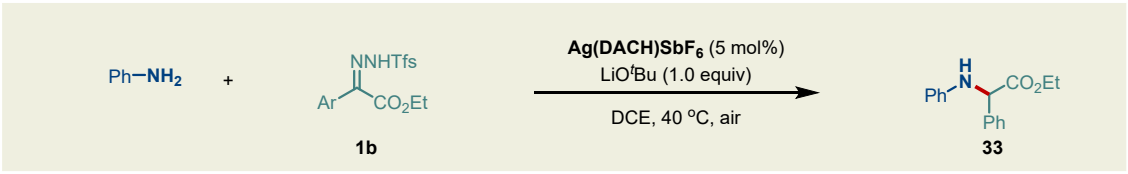
Method B: To a dried Schlenk flask, $[Tp^{Br3}Ag]_2$ (16.5 mg, 0.015mmol), ethyl 2-phenyl-2-(2-((2-(trifluoromethyl)phenyl)sulfonyl)hydrazono)acetate **1b** (0.6 mmol) and LiO^{t}Bu (1.0 equiv) were added under air atmosphere. Benzylamine (0.3 mmol) dissolved in DCE (3 mL) were added to the Schlenk flask via a syringe. The resulting mixture was stirred at 60 ºC under sealed conditions for 10 h. After cooling to room temperature, the reaction mixture was diluted with DCM (5 mL) and filtered through a plug of celite, followed by washing with DCM (5 mL × 3). The combined residue was concentrated under reduced pressure, and then the resulting crude product was purified by column chromatography with ethyl acetate/petroleum ether (1:25 v:v) as an eluent to provide the product **16**.

ii. N-H bond insertion reaction of aromatic amines



Typical synthetic procedure (with 33 as an example): Method C: To a dried sealed tube,

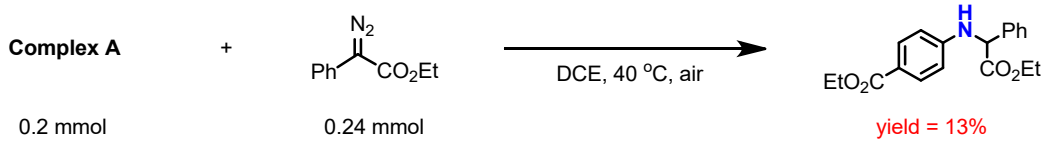
$Ag(DACH)SbF_6$ (1.4 mg, 0.003 mmol) were added under air atmosphere. Aniline (0.3 mmol) and ethyl 2-diazo-2-phenylacetate **1a** (0.36 mmol) dissolved in DCE (3 mL) were added to the sealed tube via a syringe. The resulting mixture was stirred at 40 ºC under sealed conditions for 2 h. After cooling to room temperature, the reaction mixture was diluted with DCM (5 mL) and filtered through a plug of celite, then washed with DCM (5 mL × 3). The combined residues were concentrated under reduced pressure, and then the resulting crude product was purified by column chromatography using ethyl acetate/petroleum ether (1:25 v:v) as eluent to provide product **33**.



Method D: To a dried sealed tube, $Ag(DACH)SbF_6$ (1.4 mg, 0.015 mmol), ethyl 2-phenyl-2-(2-((2-(trifluoromethyl)phenyl)sulfonyl)hydrazono)acetate **1b** (0.36 mmol) and LiO^tBu (1.0 equiv) were added under air atmosphere. Aniline (0.3 mmol) and dissolved in DCE (3 mL) were added to the sealed tube via a syringe. The resulting mixture was stirred at 40 ºC under sealed conditions for 2 h. After cooling to room temperature, the reaction mixture was diluted with DCM (5 mL) and filtered through a plug of celite, then washed with DCM (5 mL × 3). The combined residues were concentrated under reduced pressure, and then the resulting crude product was purified by column chromatography using ethyl acetate/petroleum ether (1:25 v:v) as eluent to provide product **33**.

2.5 **Mechanismtic investigations**

i. Equivalent complex A replacement catalyst and aromatic amine

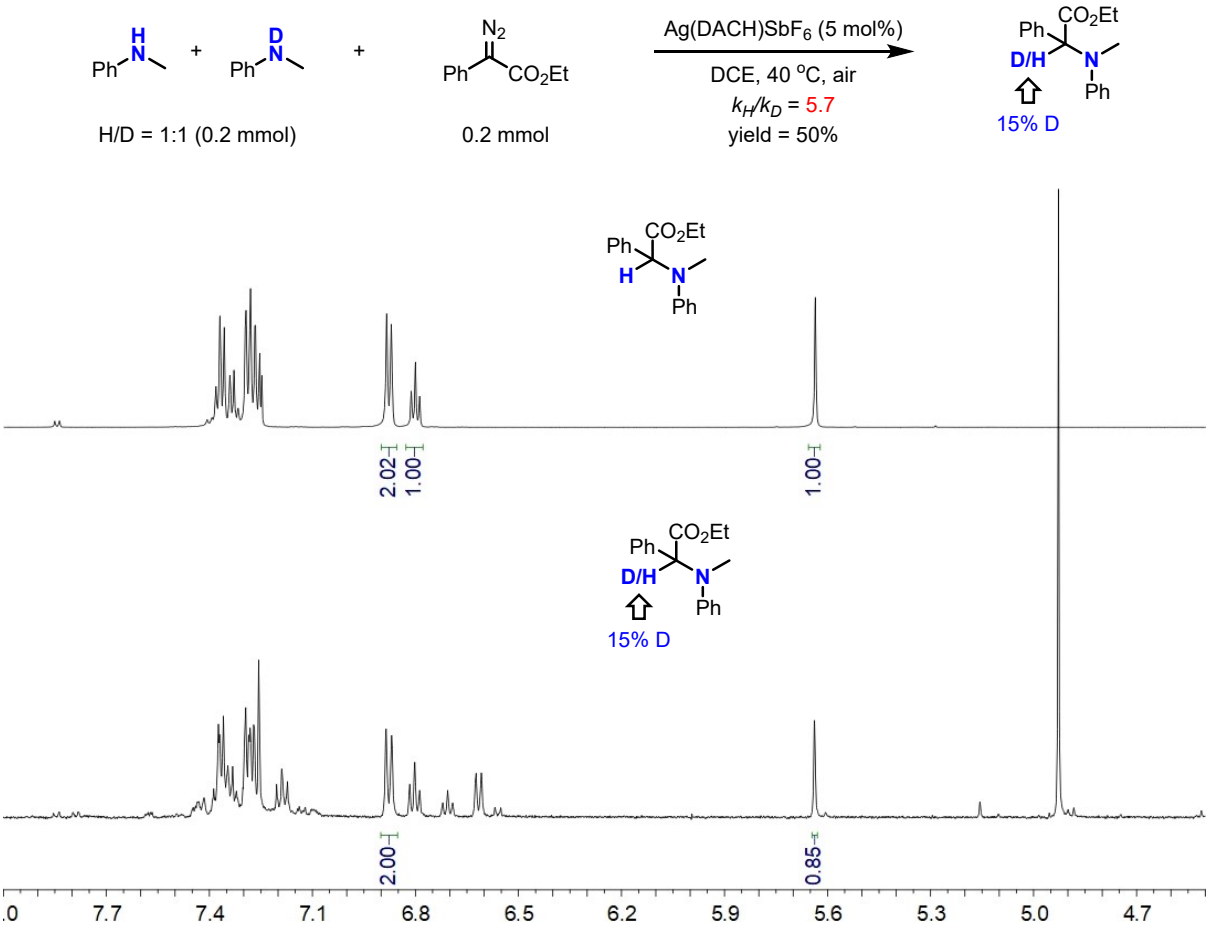


To a dried sealed tube, complex **A** (1.4 mg, 0.015 mmol) were added under air atmosphere. ethyl 2-diazo-2-phenylacetate **1a** (0.36 mmol) dissolved in DCE (3 mL) were added to the sealed tube via a syringe. The resulting mixture was stirred at 40 ºC under sealed conditions for 1 h. After cooling to room temperature, the reaction mixture was diluted with DCM (5 mL) and filtered through a plug of celite, then washed with DCM (5 mL × 3). The combined residues were concentrated under reduced pressure, and then the resulting crude product was purified by column chromatography using ethyl acetate/petroleum ether (1:25 v:v) as eluent

to provide product **33** of 13% yield.

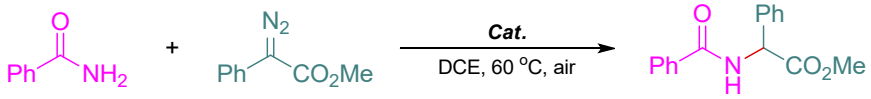
ii. KIE determined from an intermolecular competition

To a dried sealed tube, Ag(DACH)SbF_6 (7 mg, 0.01 mmol) were added under air atmosphere. *N*-Methylaniline (0.2 mmol, H/D = 1:1) and ethyl 2-diazo-2-phenylacetate **1a** (0.36 mmol) dissolved in DCE (3 mL) were added to the sealed tube via a syringe. The resulting mixture was stirred at 40 ºC under sealed conditions for 1 h. After cooling to room temperature, the deuterium content of product **33** is 15% by nuclear magnetic monitoring.



2.6 **Reaction supplement of other substrates**

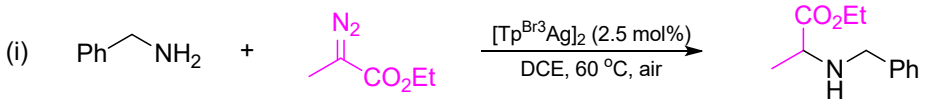
i. Amide as substrate



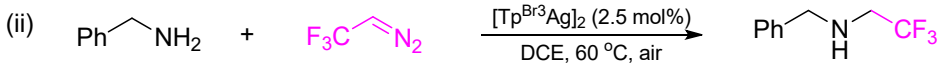
0.3 mmol 1.2 equiv. **D**

Entry	*Cat.*	Yield of C
1	$[Tp^{Br3}Ag]_2$ (2.5 mol%)	22%
2	$Ag(DACH)SbF_6$ (5 mol%)	10%
3	$AgSbF_6$ (5 mol%)	trace

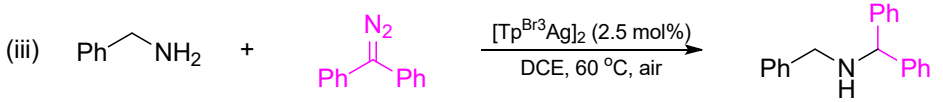
ii. Reaction of other diazo compounds with benzylamine



0.3 mmol 1.2 equiv. **D**, 0%



0.3 mmol 1.2 equiv. (in toluene) **E**, 0%



0.3 mmol 1.2 equiv. **F**, 54%

3 Computational details

In Figure 3a, all of the density functional theory (DFT) calculations were performed with the Gaussian 16 package.[2] The B97D[3] method with DEF2SVP[4] basis set has been selected for geometry optimizations under gas phase condition. The nature of the extrema (minimum) was established with analytical frequencies calculations and geometry optimizations were computed without any symmetry constraints. Intrinsic Reaction Paths (IRPs)[5,6] were traced from the various transition structures to obtain the connected intermediates.

In Figure 4，all of the density functional theory (DFT) calculations were performed with the Gaussian 16 package.[2] The B3LYP-D3[7,8] method with DEF2SVP[4] basis set has been selected for geometry optimizations. The nature of the extrema (minimum) was established with analytical frequencies calculations and geometry optimizations were computed without any symmetry constraints. Intrinsic Reaction Paths (IRPs)[5,6] were traced from the various transition structures to obtain the connected intermediates. The SMD solvation model was used to evaluate solvation energies by a self-consistent reaction field (SCRF) approach based on accurate numerical solutions of the Poisson−Boltzmann equation.[9] 1,2-dichloroethane was chosen as solvent. 3D diagrams of the computed species were generated using CYLview visualization software.[10]

Cartesian coordinates of all optimized structures

TS-int

Zero-point correction=	0.194167 (Hartree/Particle)
Thermal correction to Energy=	0.219260
Thermal correction to Enthalpy=	0.220204
Thermal correction to Gibbs Free Energy=	0.134333
Sum of electronic and zero-point Energies=	-1540.179481
Sum of electronic and thermal Energies=	-1540.154388
Sum of electronic and thermal Enthalpies=	-1540.153444
Sum of electronic and thermal Free Energies=	-1540.239315

Sb	3.37083600	-0.65230100	0.07083000
F	2.94286200	0.89718000	-1.17787400
F	3.89312100	-1.68740200	-1.46231500
F	5.12831100	0.08628700	0.31826300

F	3.63376200	-2.09112300	1.31835900
F	2.65088000	0.51544700	1.49122900
F	1.48081200	-1.16515500	-0.20168600
Ag	0.92457900	1.75982000	-0.55337000
C	-4.03374200	0.75332700	0.77119800
C	-2.75919000	1.20666900	1.13347300
C	-1.62601000	0.42736800	0.83182400
C	-1.76529300	-0.80474000	0.16117900
C	-3.04192000	-1.24995000	-0.19618900
C	-4.18854500	-0.47967300	0.10054900
H	-4.91803800	1.35352000	1.00851600
H	-2.64065800	2.16641200	1.65416000
H	-0.87211900	-1.39553700	-0.07177700
H	-3.17512900	-2.20667800	-0.71402100
N	-0.31481600	0.90757100	1.15692200
H	-0.32034100	1.55267400	1.95054900
H	0.34585100	0.14623400	1.36331800
C	-5.52545300	-1.01796600	-0.31605600
O	-5.68709400	-2.07362600	-0.89889400
O	-6.54130600	-0.18966300	0.03173800
C	-7.87704900	-0.61967300	-0.32538700
H	-7.92272900	-0.76145600	-1.42291000
H	-8.06797400	-1.60719000	0.13823600
C	-8.85252500	0.44138600	0.15874500
H	-9.88562300	0.14189400	-0.09982100
H	-8.78803000	0.56424200	1.25628400
H	-8.64151000	1.41739300	-0.31748400

TS

Zero-point correction=	0.200212 (Hartree/Particle)
Thermal correction to Energy=	0.223956
Thermal correction to Enthalpy=	0.224900
Thermal correction to Gibbs Free Energy=	0.141994
Sum of electronic and zero-point Energies=	-1540.246047
Sum of electronic and thermal Energies=	-1540.222303
Sum of electronic and thermal Enthalpies=	-1540.221359
Sum of electronic and thermal Free Energies=	-1540.304265

Sb	3.04982200	-1.06519600	0.06592100
F	3.32761000	0.95431000	-0.31478400
F	4.42064000	-1.61378100	-1.17026600
F	4.09779200	-0.81298200	1.69246800

F	2.42210900	-2.82680700	0.60499100
F	1.16000400	-0.18156400	1.69462500
F	1.53571700	-0.86377100	-1.21141600
Ag	1.39035200	2.06523900	-0.37752200
C	-4.04961000	1.16629600	0.47366300
C	-2.93758100	1.97773000	0.66756700
C	-1.63017700	1.55172500	0.24819500
C	-1.51322600	0.25050800	-0.34994300
C	-2.63150000	-0.55166400	-0.53229600
C	-3.92059500	-0.11226900	-0.13031300
H	-5.04055900	1.51040400	0.78817400
H	-3.04666200	2.96839200	1.12865200
H	-0.51724200	-0.11320500	-0.63124800
H	-2.53807500	-1.54696100	-0.98181300
N	-0.53324000	2.33407000	0.41912600
H	-0.74538900	3.20045800	0.91786900
H	0.42537400	0.32076700	1.38260100
C	-5.07767600	-1.02796400	-0.35451000
O	-4.99434400	-2.12739800	-0.87346000
O	-6.24762600	-0.49549000	0.08622000
C	-7.43145200	-1.30737600	-0.08989500
H	-7.55016300	-1.53546700	-1.16743200
H	-7.28173800	-2.27355300	0.43091300
C	-8.61509500	-0.53185000	0.46689300
H	-9.53974300	-1.12736400	0.34705600
H	-8.47386800	-0.31698800	1.54292100
H	-8.74438500	0.42744000	-0.06885100

1a

Zero-point correction=	0.408414 (Hartree/Particle)
Thermal correction to Energy=	0.443414
Thermal correction to Enthalpy=	0.444359
Thermal correction to Gibbs Free Energy=	0.336009
Sum of electronic and zero-point Energies=	-1978.668855
Sum of electronic and thermal Energies=	-1978.633854
Sum of electronic and thermal Enthalpies=	-1978.632910
Sum of electronic and thermal Free Energies=	-1978.741260

Sb	2.29662700	-1.62724100	-0.31513700
F	2.91310300	0.08209300	-1.00265700
F	3.11228400	-2.52332000	-1.80749500
F	3.91039200	-1.80503000	0.71372100

F	1.63286700	-3.30775500	0.36403800
F	1.45476200	-0.70012800	1.16071300
F	0.66170300	-1.42111700	-1.35295000
Ag	-0.86870800	0.79971500	-0.56498900
N	-2.32693300	-1.71968000	-1.46604500
C	-2.67530300	-0.89168500	-0.47271800
N	-2.01870900	-2.40796000	-2.29989100
C	-3.72237900	0.06165600	-0.94984800
O	-4.13472200	0.07015000	-2.09120500
O	-4.10622500	0.91634200	0.00315900
C	-5.12969000	1.88747900	-0.33480800
H	-4.92061700	2.28672200	-1.33812200
H	-4.99281300	2.68820300	0.40482300
C	-6.51561900	1.28001300	-0.25309900
H	-7.26955700	2.05890300	-0.45052300
H	-6.63972400	0.48212800	-1.00052300
H	-6.70325100	0.86267700	0.74886900
C	-2.31431900	-1.34091000	0.91075100
C	-1.30488600	-2.30948800	1.08225200
C	-2.93341700	-0.80554800	2.05721700
C	-0.91347500	-2.71629200	2.35663900
H	-0.78168100	-2.72563900	0.22206700
C	-2.53783200	-1.22477200	3.33048400
H	-3.71556700	-0.05738300	1.95489100
C	-1.52650300	-2.17683100	3.49160600
H	-0.10510400	-3.44476900	2.44952500
H	-3.03077300	-0.79488100	4.20660200
H	-1.21626200	-2.49138200	4.49117800
C	3.24258800	4.04642900	1.52736300
C	3.13050900	4.71887900	0.15618300
C	2.59299500	3.73455500	-0.88565800
C	1.24349700	3.11844200	-0.48356400
C	1.33658800	2.46543300	0.91352800
C	1.89660300	3.45142600	1.94863700
H	2.48516000	4.22239400	-1.86914100
H	2.44858300	5.58601700	0.22834900
H	4.10889800	5.11191100	-0.16638000
H	3.99650200	3.24014600	1.47728200
H	3.59480500	4.76437800	2.28657000
H	0.47996700	3.91577300	-0.43042200
H	2.02581800	1.61290700	0.81850200
H	1.16072600	4.26649300	2.08611300
H	1.98268800	2.93372600	2.91867300
H	3.31406100	2.90689700	-1.01576100

N	0.03673400	1.90628200	1.32900600
H	0.17559400	1.21982600	2.07185600
H	-0.55924900	2.64101700	1.71779000
N	0.78083900	2.13737700	-1.48739000
H	0.55972800	2.60952900	-2.36534800
H	1.54526900	1.48761500	-1.69390300

TS1

Zero-point correction=	0.406009 (Hartree/Particle)
Thermal correction to Energy=	0.441068
Thermal correction to Enthalpy=	0.442012
Thermal correction to Gibbs Free Energy=	0.334063
Sum of electronic and zero-point Energies=	-1978.644761
Sum of electronic and thermal Energies=	-1978.609703
Sum of electronic and thermal Enthalpies=	-1978.608759
Sum of electronic and thermal Free Energies=	-1978.716708

Sb	-2.30031700	-1.84238200	-0.04420500
F	-3.35521500	-0.25899000	0.34035400
F	-3.38226900	-2.86469200	1.17370300
F	-3.46350100	-2.28915000	-1.50760700
F	-1.19971500	-3.38939900	-0.39128200
F	-1.19246100	-0.79982300	-1.24288800
F	-1.12421600	-1.34617600	1.42285200
Ag	0.71793300	0.97210300	0.54198200
N	2.89093800	-0.38860300	2.35212600
C	2.63920800	0.02493400	0.59202700
N	2.63262800	-0.75728500	3.36122000
C	3.65984000	1.11518100	0.48617800
O	4.23251700	1.66214500	1.40371000
O	3.76795200	1.46958500	-0.80202000
C	4.62625600	2.59190600	-1.12498300
H	4.50014300	3.36921800	-0.35654400
H	4.23618000	2.96783300	-2.08101200
C	6.07398900	2.15831400	-1.24376300
H	6.69342400	3.01876400	-1.54420800
H	6.45020300	1.78241100	-0.28037400
H	6.18637000	1.36943300	-2.00414500
C	2.85578200	-1.26131500	-0.09385200
C	1.79455600	-2.18721700	-0.18064400
C	4.09731800	-1.59010300	-0.68409400
C	1.95693200	-3.39498500	-0.85560900

H	0.84537700	-1.95458000	0.29952200
C	4.25359500	-2.79315900	-1.36980600
H	4.93587900	-0.89431500	-0.61855000
C	3.18490700	-3.69598000	-1.45706100
H	1.11570000	-4.08764900	-0.91777600
H	5.21255800	-3.03284200	-1.83570200
H	3.31242900	-4.63893200	-1.99536400
C	-3.89037100	3.63975100	-1.43518600
C	-3.98406700	4.10416700	0.02163500
C	-3.31759400	3.09218700	0.95804800
C	-1.85704300	2.80991800	0.57509500
C	-1.74828900	2.37224400	-0.89919700
C	-2.43323300	3.38216000	-1.82990400
H	-3.35445900	3.44113800	2.00398300
H	-3.48505200	5.08528200	0.12507500
H	-5.03658500	4.25253400	0.31498100
H	-4.46926200	2.70649700	-1.55736300
H	-4.34118900	4.38503300	-2.11143100
H	-1.26559200	3.73642600	0.69292300
H	-2.26148400	1.40330400	-0.98106900
H	-1.86748600	4.33251700	-1.79268700
H	-2.36681600	3.01230000	-2.86696300
H	-3.86644800	2.13471300	0.91732100
N	-0.34065700	2.13270000	-1.26004600
H	-0.28910500	1.57822800	-2.11575500
H	0.12794500	3.01915000	-1.46377200
N	-1.24388600	1.78939100	1.44934400
H	-1.16480400	2.14642700	2.40303800
H	-1.86586400	0.97860100	1.50563700

int1

Zero-point correction=	0.517841 (Hartree/Particle)
Thermal correction to Energy=	0.557841
Thermal correction to Enthalpy=	0.558785
Thermal correction to Gibbs Free Energy=	0.439561
Sum of electronic and zero-point Energies=	-2156.571263
Sum of electronic and thermal Energies=	-2156.531263
Sum of electronic and thermal Enthalpies=	-2156.530318
Sum of electronic and thermal Free Energies=	-2156.649542

Ag	0.52546900	0.43722100	-0.69670600
C	-1.36708600	0.34407000	-1.46796000

C	-2.34822900	1.09036400	-0.65913900
O	-3.00866500	0.55157200	0.21675500
O	-2.36877400	2.39133600	-0.93485700
C	-3.15523500	3.26001400	-0.07557000
H	-4.09751300	2.75404300	0.18052100
H	-3.37862700	4.13458300	-0.70177400
C	-2.36973000	3.64076700	1.16342500
H	-2.96459200	4.33348200	1.78007700
H	-2.13843700	2.75205600	1.77055500
H	-1.42641900	4.14083600	0.89219300
C	-1.83097300	-0.42026900	-2.57772400
C	-0.88947600	-1.12453900	-3.38402400
C	-3.21694900	-0.52858700	-2.90598500
C	-1.30806900	-1.90458900	-4.45209400
H	0.16992400	-1.04081800	-3.14513200
C	-3.62858300	-1.31121300	-3.97464200
H	-3.96069800	-0.00935700	-2.29726800
C	-2.67626800	-1.99980800	-4.74572700
H	-0.57238900	-2.45232300	-5.04338900
H	-4.69057400	-1.39714900	-4.21527800
H	-3.00781900	-2.61936500	-5.58332600
C	5.72202100	1.56020500	1.19689000
C	5.61344800	0.12152000	1.71390200
C	4.15242300	-0.26268700	1.96771200
C	3.28146000	-0.05513600	0.72345500
C	3.39793400	1.37839300	0.18186700
C	4.86508000	1.75786100	-0.05826900
H	4.07066500	-1.31532800	2.28435800
H	6.04367100	-0.56761000	0.96486000
H	6.20388300	-0.00445200	2.63649600
H	5.38212800	2.25790500	1.98404400
H	6.77228200	1.81611500	0.98002000
H	3.63256000	-0.73279900	-0.06986800
H	2.96877800	2.06148800	0.93732300
H	5.25542500	1.12255500	-0.87489600
H	4.91829700	2.80166200	-0.41117100
H	3.74243100	0.35296900	2.79015100
N	2.56899400	1.50191900	-1.03216400
H	2.52862700	2.47363000	-1.34462200
H	2.99754900	0.97078900	-1.79616600
N	1.86768300	-0.39127000	0.96048900
H	1.75874500	-1.40464000	1.02630600
H	1.55473900	-0.02027500	1.86085700
C	-0.17227000	-1.06612800	3.74714300

C	-1.05368100	-1.11528600	2.66533900
C	-0.96188700	-2.15116300	1.70605900
C	0.05111800	-3.12508400	1.87270900
C	0.92928500	-3.05941200	2.95475900
C	0.83006700	-2.03298700	3.90424600
H	-0.26453600	-0.25241700	4.47279800
H	-1.82089000	-0.34669300	2.53919200
H	0.15835200	-3.91372800	1.12522700
H	1.71433400	-3.81541300	3.04627800
N	-1.84508000	-2.21872300	0.64917900
H	-2.37995700	-1.37415900	0.45493700
H	-1.50067500	-2.68867600	-0.18248000
H	1.52366800	-1.98518500	4.74705000
Sb	2.11592600	-3.27552400	-1.85337000
F	1.41207800	-3.47527500	-3.63924000
F	1.76612600	-5.12654900	-1.46373100
F	3.88611200	-3.69129600	-2.47717400
F	2.80086200	-3.02885600	-0.05858100
F	2.43219600	-1.39013200	-2.21879000
F	0.33746500	-2.82591100	-1.22867200

TS2

Zero-point correction=	0.517669 (Hartree/Particle)
Thermal correction to Energy=	0.555882
Thermal correction to Enthalpy=	0.556827
Thermal correction to Gibbs Free Energy=	0.443396
Sum of electronic and zero-point Energies=	-2156.568762
Sum of electronic and thermal Energies=	-2156.530549
Sum of electronic and thermal Enthalpies=	-2156.529605
Sum of electronic and thermal Free Energies=	-2156.643035

Sb	2.19341400	-2.20213900	-0.53864900
F	3.66204700	-0.94319200	-0.38207300
F	3.12090200	-3.11563400	-1.95457900
F	3.00258200	-3.34876200	0.77495300
F	0.69015800	-3.39862300	-0.72531700
F	1.23849300	-1.27501700	0.87529100
F	1.39011600	-1.00109900	-1.83479200
Ag	0.05491700	1.38139500	-0.35473600
C	-2.00502900	1.01331900	-0.51555700
C	-2.80381900	2.26493400	-0.50718700
O	-3.01628000	2.99182400	0.45178100

O	-3.20047900	2.55824000	-1.75412500
C	-3.80180600	3.85455500	-1.99106300
H	-4.51155100	4.07425400	-1.17961500
H	-4.36107400	3.72673300	-2.92838600
C	-2.74598700	4.93581700	-2.11399000
H	-3.22698400	5.89891600	-2.34924900
H	-2.19105400	5.04992900	-1.17032400
H	-2.03341500	4.69800300	-2.91969400
C	-2.64168300	-0.23047500	-0.86519200
C	-1.85057800	-1.38830100	-1.07908200
C	-4.05413100	-0.36974700	-0.94295500
C	-2.43039700	-2.61739000	-1.37093000
H	-0.76883300	-1.29982100	-1.02031600
C	-4.63342000	-1.60205700	-1.23196800
H	-4.69353700	0.49981400	-0.78211100
C	-3.82540700	-2.72675400	-1.44656600
H	-1.78983800	-3.48735400	-1.52876800
H	-5.72099600	-1.69346500	-1.28137400
H	-4.28660100	-3.69222700	-1.67082700
C	5.12482500	2.19302000	2.20572800
C	5.35273000	3.00958000	0.92989700
C	4.49671400	2.47161500	-0.22022600
C	3.00246300	2.43007700	0.13288200
C	2.76771700	1.62274900	1.42499900
C	3.63785700	2.15733600	2.57154900
H	4.63651600	3.07908300	-1.13048900
H	5.08863200	4.06613600	1.12009100
H	6.41808800	2.99660500	0.64584500
H	5.48223600	1.15988900	2.04463500
H	5.71276900	2.60624400	3.04217300
H	2.64197900	3.45984600	0.31022400
H	3.06505500	0.58693700	1.20775800
H	3.29460300	3.17849500	2.82498700
H	3.46952000	1.53330400	3.46535200
H	4.81272000	1.44198400	-0.46686900
N	1.33718600	1.58515100	1.76661000
H	1.15215000	0.77510700	2.35887800
H	1.07520100	2.41138700	2.30924200
N	2.19411700	1.87200100	-0.97009700
H	2.26331900	2.47457700	-1.79210900
H	2.58487600	0.96780900	-1.25046800
C	-3.60956000	-2.67535600	2.31291600
C	-2.68691500	-1.64759200	2.12684800
C	-3.12452900	-0.30719300	2.09289600

C	-4.49821600	-0.02248300	2.24500100
C	-5.40761300	-1.06044500	2.44288700
C	-4.97253200	-2.39131600	2.47150200
H	-3.26114100	-3.71126300	2.32651000
H	-1.62505900	-1.86610900	1.98641400
H	-4.83601300	1.01582100	2.20252100
H	-6.46895700	-0.82834700	2.56432600
N	-2.22711800	0.70326700	1.82926100
H	-1.23718100	0.51827500	1.94294300
H	-2.51879400	1.67945900	1.86699100
H	-5.68986700	-3.20236500	2.61803900

int2

Zero-point correction=	0.521873 (Hartree/Particle)
Thermal correction to Energy=	0.560669
Thermal correction to Enthalpy=	0.561613
Thermal correction to Gibbs Free Energy=	0.444886
Sum of electronic and zero-point Energies=	-2156.604719
Sum of electronic and thermal Energies=	-2156.565924
Sum of electronic and thermal Enthalpies=	-2156.564979
Sum of electronic and thermal Free Energies=	-2156.681707

Sb	-1.39085300	-2.47676200	-0.13281400
F	-3.26762300	-2.02787000	-0.14952200
F	-1.69361400	-4.03571800	0.94463600
F	-1.56078000	-3.53082200	-1.72845600
F	0.53672000	-2.76524000	-0.09814900
F	-1.00261300	-0.92037200	-1.23088700
F	-1.17853200	-1.42533800	1.48328800
Ag	-0.31796400	1.43341000	0.39846400
C	1.85125400	0.94092800	-0.05387300
C	2.02493600	2.14910200	-0.86145000
O	1.91370700	2.17429200	-2.08854000
O	2.24393600	3.26664300	-0.13440600
C	2.05030800	4.53413000	-0.79163500
H	2.54139800	4.51599300	-1.77621000
H	2.57076500	5.26032500	-0.15098800
C	0.57431700	4.86710600	-0.91993600
H	0.45351000	5.86955000	-1.36141100
H	0.06639200	4.13950800	-1.57053900
H	0.08365000	4.86027600	0.06673600
C	2.58781900	0.66504300	1.22053700

C	2.17439500	-0.41522700	2.03001400
C	3.72321300	1.39223500	1.62366300
C	2.86616000	-0.75250800	3.19390500
H	1.29605400	-0.99635400	1.73931200
C	4.40214200	1.06782500	2.80318600
H	4.07738100	2.22105600	1.01054600
C	3.98199600	-0.00621700	3.59319100
H	2.52395500	-1.59697100	3.79838700
H	5.27738000	1.65409700	3.09716700
H	4.51873300	-0.26166900	4.51066200
C	-5.81143100	1.04877000	-0.92531700
C	-6.01099600	1.33874400	0.56540400
C	-4.74941400	0.98627000	1.35793100
C	-3.49478600	1.70008000	0.83059800
C	-3.30618600	1.43392200	-0.67769600
C	-4.58086600	1.78803600	-1.45831800
H	-4.87594900	1.22356500	2.42769200
H	-6.24353400	2.41089200	0.70178800
H	-6.87292200	0.77539300	0.95999800
H	-5.66913300	-0.03783300	-1.06786500
H	-6.70785700	1.33255200	-1.50144500
H	-3.61519300	2.79134200	0.95840800
H	-3.11323400	0.35571000	-0.79437300
H	-4.74385900	2.88025700	-1.38759600
H	-4.41833300	1.55939000	-2.52527400
H	-4.56717300	-0.10179100	1.28758400
N	-2.11426900	2.13613500	-1.17226200
H	-1.91537200	1.85794200	-2.13431900
H	-2.28450200	3.14474900	-1.19925500
N	-2.29180300	1.30351900	1.59106700
H	-2.29173600	1.75305900	2.50791500
H	-2.32015400	0.29753600	1.77663500
C	4.86179100	-2.56112900	-0.84175000
C	3.57803500	-2.04057400	-0.64962800
C	3.24524900	-0.82328800	-1.24487500
C	4.16365400	-0.11701600	-2.02614700
C	5.44196700	-0.64934100	-2.21161100
C	5.79406300	-1.86764600	-1.61896000
H	5.12942200	-3.51363100	-0.37818000
H	2.84163100	-2.57556100	-0.04944500
H	3.87681600	0.83103500	-2.48188600
H	6.16553900	-0.10720800	-2.82528200
N	1.91030200	-0.25082900	-1.00139000
H	1.27863100	-0.99842800	-0.68608100

H	1.52056100	0.10069000	-1.89095700
H	6.79648300	-2.27733600	-1.76589300

int3

Zero-point correction= 0.639891 (Hartree/Particle)
Thermal correction to Energy= 0.685971
Thermal correction to Enthalpy= 0.686915
Thermal correction to Gibbs Free Energy= 0.552481
Sum of electronic and zero-point Energies= -2443.920957
Sum of electronic and thermal Energies= -2443.874878
Sum of electronic and thermal Enthalpies= -2443.873934
Sum of electronic and thermal Free Energies= -2444.008367

C	-2.32062600	-0.13187800	-0.34197100
C	-2.20817500	-0.60247700	0.96817100
O	-1.41667700	-1.47743700	1.41173800
O	-3.07566800	0.00020300	1.84410400
C	-2.87139400	-0.21349300	3.24523500
H	-1.84998000	0.10177900	3.51839400
H	-2.95692700	-1.28790400	3.47643600
C	-3.91442700	0.59781200	3.98454700
H	-3.77404800	0.49171200	5.07180900
H	-3.83423500	1.66557200	3.72539900
H	-4.93287400	0.25468900	3.73755800
C	-1.50579200	-0.57097600	-1.46527200
C	-1.10312600	0.31668200	-2.49388300
C	-1.06996700	-1.91738700	-1.56937300
C	-0.30002100	-0.11222900	-3.55158900
H	-1.37864700	1.37271000	-2.44503400
C	-0.26298000	-2.33797900	-2.62826200
H	-1.40258700	-2.63950400	-0.82329100
C	0.13499300	-1.44072800	-3.62660500
H	0.01104800	0.61023900	-4.31127200
H	0.05305200	-3.38430100	-2.67536700
H	0.77255000	-1.77098700	-4.45064500
C	-1.17212400	3.88751600	0.72392100
C	-1.52502700	2.60881100	0.28226100
C	-2.84669600	2.34855900	-0.05639200
C	-3.83592300	3.32846300	0.04954000
C	-3.47838300	4.60163400	0.50380900
C	-2.14747000	4.88329800	0.83856000
H	-0.12703300	4.09338100	0.96689400

H	-0.77926600	1.82341100	0.19462600
H	-4.87046000	3.09782900	-0.21754100
H	-4.24360800	5.37660400	0.59510100
N	-3.23411100	1.00799200	-0.55010700
H	-6.51928200	0.79967900	0.24789100
H	-3.42849400	1.08256500	-1.55742200
C	-6.65669700	-2.56117300	-1.89792900
C	-6.59640300	-1.29903300	-1.30036200
C	-5.87564600	-1.11305700	-0.10824200
C	-5.21799100	-2.21319100	0.47195800
C	-5.28329700	-3.46967700	-0.13303100
C	-6.00069500	-3.65425000	-1.32142200
H	-7.22314000	-2.68830000	-2.82464200
H	-7.10624300	-0.44658700	-1.75858300
H	-4.64943900	-2.07272100	1.39342200
H	-4.76491700	-4.31307400	0.33128700
N	-5.73754800	0.17660900	0.44840100
H	-5.52893400	0.17688900	1.44591100
H	-4.18981700	0.76758500	-0.13775200
Sb	2.42334900	1.98501500	-0.55497500
F	3.90469000	1.28824700	0.48914400
F	2.41728200	3.59587300	0.50871700
F	3.66491300	2.77542700	-1.79258800
F	0.93252900	2.65565200	-1.57577000
F	2.39208500	0.35919900	-1.60194700
F	1.22128300	1.17815300	0.74205400
Ag	0.76801100	-1.60302300	0.96414200
C	6.26920800	-2.47274300	-0.28751700
C	6.38731700	-2.55108800	1.23787500
C	5.30128600	-1.70668800	1.91053400
C	3.88389100	-2.10154700	1.46515500
C	3.76653100	-2.04368500	-0.07305100
C	4.86534600	-2.87805800	-0.74573000
H	5.36816300	-1.78440000	3.00915800
H	6.28361700	-3.60409800	1.55858000
H	7.38531300	-2.21741100	1.56787600
H	6.47147000	-1.43685700	-0.61486000
H	7.02685800	-3.11234800	-0.77039100
H	3.68376600	-3.14258900	1.77959600
H	3.90031700	-0.98997500	-0.35566800
H	4.69206300	-3.94443600	-0.50530400
H	4.76592400	-2.77801100	-1.83969000
H	5.44936200	-0.64175700	1.65444300
N	2.41752900	-2.42605400	-0.52174800

H	2.21596500	-2.00513500	-1.42962600
H	2.35173700	-3.43865700	-0.64682700
N	2.85097600	-1.25261100	2.08351900
H	2.86104600	-1.36791300	3.09791200
H	3.07255900	-0.26916900	1.90569000
H	-1.87254900	5.88182100	1.18773100
H	-6.04810600	-4.63926700	-1.79207000

TS3

Zero-point correction=	0.635546 (Hartree/Particle)
Thermal correction to Energy=	0.680863
Thermal correction to Enthalpy=	0.681807
Thermal correction to Gibbs Free Energy=	0.550692
Sum of electronic and zero-point Energies=	-2443.887506
Sum of electronic and thermal Energies=	-2443.842189
Sum of electronic and thermal Enthalpies=	-2443.841245
Sum of electronic and thermal Free Energies=	-2443.972361

Sb	1.36549400	1.68761100	2.49047200
F	3.26602200	1.62501900	2.13870600
F	1.69129600	2.36570900	4.25945700
F	1.28203100	3.48203700	1.78997700
F	-0.54541300	1.72965500	2.82597200
F	1.01516500	0.96298400	0.72630300
F	1.44389900	-0.12757400	3.17122500
Ag	0.74330800	-1.47074600	-1.25158500
C	-2.46648900	-0.92819400	-0.37273800
C	-2.33402300	-1.28938000	-1.78394400
O	-1.28009000	-1.69223500	-2.28958600
O	-3.42884000	-1.07660600	-2.52354100
C	-3.33875800	-1.19192700	-3.96774500
H	-2.38333600	-0.75564300	-4.29377500
H	-4.16163300	-0.56589000	-4.33928100
C	-3.48478200	-2.63200000	-4.41462800
H	-3.48238100	-2.67555400	-5.51559500
H	-2.65162100	-3.24578400	-4.04137800
H	-4.43380200	-3.05972600	-4.05415600
C	-1.87930100	-1.88397300	0.62498100
C	-1.90452400	-3.27300800	0.40003400
C	-1.29467300	-1.40564800	1.80889200
C	-1.34154500	-4.15682600	1.32343700
H	-2.36103100	-3.66495400	-0.51223400

C	-0.74104400	-2.28931200	2.73943000
H	-1.25646800	-0.33461700	2.00223900
C	-0.75880300	-3.66625200	2.49835400
H	-1.36353900	-5.23230300	1.12846300
H	-0.26846700	-1.88887100	3.63798700
H	-0.31724200	-4.35665400	3.22194600
C	5.88743700	-0.27421600	0.77546800
C	5.65557900	-1.54238100	1.60297300
C	4.15784200	-1.79050300	1.79995600
C	3.38506300	-1.86464900	0.47237500
C	3.64707300	-0.60693100	-0.38494300
C	5.15207300	-0.36405100	-0.56529700
H	3.98300200	-2.72169700	2.36526200
H	6.10889300	-2.40701500	1.08370500
H	6.15607200	-1.46364500	2.58253600
H	5.50655500	0.59738700	1.33579300
H	6.96465500	-0.10759000	0.60846100
H	3.74218200	-2.73712000	-0.10574300
H	3.21635500	0.24672900	0.15634600
H	5.57375100	-1.19316100	-1.16505500
H	5.29514500	0.55902300	-1.15225600
H	3.72493000	-0.96888700	2.39464700
N	2.93482400	-0.69466000	-1.67469900
H	2.94899000	0.21484800	-2.13987800
H	3.43000200	-1.33432600	-2.30211300
N	1.93959400	-2.04897700	0.69110500
H	1.75072100	-2.97287900	1.08151600
H	1.61187200	-1.38314200	1.39412900
C	-5.19278900	-1.05122200	3.38997900
C	-4.48758400	-0.44358900	2.34673900
C	-4.59421700	-0.97364000	1.06048700
C	-5.38037100	-2.09682100	0.79638700
C	-6.08229600	-2.69573700	1.84524200
C	-5.98823000	-2.17451900	3.14117100
H	-5.11603900	-0.64405900	4.40088600
H	-3.85522100	0.42811000	2.52842900
H	-5.43435600	-2.49637800	-0.21943900
H	-6.70274100	-3.57338600	1.64876500
N	-3.83709500	-0.36470600	-0.02187100
H	-3.54937900	0.66268600	0.17327800
H	-6.53637000	-2.64701500	3.95996000
C	-0.67513000	3.35724500	-0.99942800
C	-0.29526200	4.05964900	-2.14253200
C	-0.91571300	3.82736300	-3.37981600

C	-1.94046400	2.87353500	-3.44156800
C	-2.33729800	2.17028500	-2.30305300
C	-1.71186800	2.38224600	-1.04145800
H	-0.16379200	3.54168000	-0.05214100
H	0.50711000	4.80081000	-2.06698200
H	-0.60954600	4.37937100	-4.27208300
H	-2.44639100	2.67623900	-4.39233200
H	-3.14990500	1.44344700	-2.37413000
N	-2.09748900	1.64351300	0.05025600
H	-1.93678500	0.26755100	-0.23840300
H	-1.55442800	1.88051200	0.87989000
H	-4.40046800	-0.35159800	-0.88240200

Pr

Zero-point correction=	0.638959 (Hartree/Particle)
Thermal correction to Energy=	0.685702
Thermal correction to Enthalpy=	0.686646
Thermal correction to Gibbs Free Energy=	0.549843
Sum of electronic and zero-point Energies=	-2443.942567
Sum of electronic and thermal Energies=	-2443.895824
Sum of electronic and thermal Enthalpies=	-2443.894880
Sum of electronic and thermal Free Energies=	-2444.031683

C	-2.80917000	-1.12865300	0.09554400
C	-2.70542400	-0.57437700	1.53908400
O	-1.68339600	-0.27503700	2.12719400
O	-3.90548100	-0.47102800	2.09544700
C	-3.98445200	0.02428500	3.46416400
H	-3.66586700	1.07861900	3.46015900
H	-3.27100400	-0.54606000	4.07774200
C	-5.40801600	-0.14522000	3.94030700
H	-5.48914800	0.23095700	4.97207600
H	-6.11217300	0.41547600	3.30785900
H	-5.70000600	-1.20709200	3.93636600
C	-1.45721600	-1.50878100	-0.50807500
C	-1.13117900	-1.15771100	-1.82430600
C	-0.54000300	-2.28386700	0.23246800
C	0.08775500	-1.55280700	-2.38640600
H	-1.83459600	-0.57087800	-2.41561100
C	0.67896500	-2.67979800	-0.33467800
H	-0.79187500	-2.60957600	1.24485000
C	0.99782700	-2.30914000	-1.64541000

H	0.32912500	-1.25775800	-3.41091700
H	1.39114800	-3.26597400	0.24882800
H	1.96011500	-2.59715500	-2.06812700
C	-2.22407900	3.14708700	-0.85003500
C	-2.36052800	1.79184400	-0.53230500
C	-3.46175900	1.05002600	-1.01038200
C	-4.41247900	1.71674800	-1.81963000
C	-4.26324400	3.06735900	-2.12733100
C	-3.16839900	3.80037700	-1.64632400
H	-1.35683400	3.69208500	-0.46581900
H	-1.59588000	1.31634800	0.07853900
H	-5.26923900	1.15622300	-2.20288400
H	-5.01454600	3.55491800	-2.75515200
N	-3.64517300	-0.29213500	-0.72952100
H	-4.48350500	-0.72662300	-1.09633600
H	-3.37567200	-2.06496900	0.23084000

TS4

Zero-point correction=	0.517074 (Hartree/Particle)
Thermal correction to Energy=	0.555378
Thermal correction to Enthalpy=	0.556323
Thermal correction to Gibbs Free Energy=	0.441578
Sum of electronic and zero-point Energies=	-2156.596867
Sum of electronic and thermal Energies=	-2156.558563
Sum of electronic and thermal Enthalpies=	-2156.557619
Sum of electronic and thermal Free Energies=	-2156.672363

Sb	-1.09124900	-2.58904900	-0.03909600
F	-2.89684000	-1.90522400	0.11471200
F	-1.50764700	-4.06094000	1.12215300
F	-1.58061500	-3.62420500	-1.58089200
F	0.74829300	-3.16729500	-0.18688500
F	-0.65089200	-1.09656400	-1.21856000
F	-0.60831800	-1.50363700	1.49036800
Ag	-0.39714500	1.38521300	0.37116100
C	1.88344700	1.13029000	-0.04661000
C	1.89928800	2.38712200	-0.73333700
O	1.83308600	2.33168300	-2.01481000
O	1.97627900	3.54010000	-0.09810800
C	1.67323100	4.75852800	-0.82979300
H	2.24437800	4.76193100	-1.76958400
H	2.05398300	5.55722300	-0.17939500

C	0.18385100	4.89746400	-1.07585800
H	-0.01716600	5.87145800	-1.54974800
H	-0.17953100	4.10650400	-1.74797200
H	-0.37721600	4.84896900	-0.12914200
C	2.43426300	0.81400800	1.29255600
C	2.43071000	-0.52790400	1.73484200
C	2.97673400	1.79136200	2.15439200
C	2.94330900	-0.87430200	2.98515100
H	1.99968200	-1.30499600	1.10303000
C	3.48025200	1.43758300	3.40921500
H	3.00418300	2.83408900	1.83986700
C	3.46994300	0.10516400	3.83544100
H	2.92284000	-1.92163700	3.29886300
H	3.89355100	2.21600700	4.05702500
H	3.86748900	-0.16704900	4.81655800
C	-5.86675800	0.95445300	-1.10005000
C	-6.08314100	1.16387800	0.40159400
C	-4.84375800	0.73511500	1.19130300
C	-3.56520300	1.44999700	0.72716400
C	-3.35505500	1.27602100	-0.79252700
C	-4.61131600	1.69277800	-1.57193300
H	-4.98313500	0.91546200	2.27060400
H	-6.29200600	2.23209700	0.59529900
H	-6.96493200	0.60104600	0.75019100
H	-5.75158600	-0.12547000	-1.30412300
H	-6.74602900	1.29455700	-1.67209000
H	-3.66226200	2.53336300	0.92381300
H	-3.16389700	0.20487500	-0.96730200
H	-4.75443100	2.78254500	-1.44379400
H	-4.43519600	1.51971500	-2.64709300
H	-4.68370900	-0.35044400	1.06369200
N	-2.15249700	2.00355200	-1.22748600
H	-1.92340000	1.76101300	-2.19275500
H	-2.33352200	3.01071500	-1.22694200
N	-2.38177500	0.97815300	1.47460300
H	-2.42413400	1.30184700	2.44236100
H	-2.39754800	-0.04355200	1.52430500
C	4.57243600	-2.50473800	-1.83495100
C	3.33994300	-1.88779100	-1.60066300
C	3.29378200	-0.51653100	-1.32781000
C	4.47397500	0.23565200	-1.27900900
C	5.70118100	-0.39106800	-1.50926000
C	5.75623400	-1.76111500	-1.79039100
H	4.60422500	-3.57735000	-2.04310600

H	2.41569700	-2.46851100	-1.60238600
H	4.43699400	1.30383500	-1.05594900
H	6.62081400	0.19830400	-1.46838200
N	2.01734800	0.12814000	-1.13322400
H	1.24764000	-0.54523300	-1.16273000
H	1.86273000	1.11434700	-2.00429700
H	6.71863600	-2.24738500	-1.96827600

int4

Zero-point correction=	0.520555 (Hartree/Particle)
Thermal correction to Energy=	0.559367
Thermal correction to Enthalpy=	0.560311
Thermal correction to Gibbs Free Energy=	0.443474
Sum of electronic and zero-point Energies=	-2156.602272
Sum of electronic and thermal Energies=	-2156.563460
Sum of electronic and thermal Enthalpies=	-2156.562516
Sum of electronic and thermal Free Energies=	-2156.679353

Sb	1.56786200	2.41363900	-0.24378400
F	3.35236300	1.71228200	-0.48876400
F	2.25332800	3.96446100	0.65781400
F	1.65902900	3.31642700	-1.93786500
F	-0.25319300	3.01912500	0.01025500
F	0.83736800	0.84841400	-1.14820900
F	1.45984400	1.47789900	1.45127700
Ag	-0.00538200	-1.74349000	-0.37124000
C	-2.17172800	-0.80326000	-0.06299500
C	-2.64006500	-1.87188400	-0.84194200
O	-2.90252800	-1.69650500	-2.13253900
O	-2.92430200	-3.06365100	-0.35035400
C	-2.99544300	-4.21436900	-1.23682900
H	-3.68788700	-3.99116600	-2.06123200
H	-3.44041900	-4.99615700	-0.60728300
C	-1.62496700	-4.61900300	-1.74116900
H	-1.71700100	-5.54217600	-2.33516100
H	-1.18836800	-3.84182000	-2.38736500
H	-0.93788300	-4.81411200	-0.90237900
C	-2.08661200	-0.75452900	1.42722100
C	-1.55985600	0.41175600	2.02504000
C	-2.47636700	-1.81121000	2.27947700
C	-1.40294700	0.50633800	3.40808300

H	-1.24107300	1.24633900	1.40188500
C	-2.32081900	-1.70728500	3.66446900
H	-2.89955000	-2.72051700	1.85754600
C	-1.77895000	-0.55337100	4.24060700
H	-0.97432600	1.41770700	3.83352300
H	-2.63174700	-2.54171900	4.29952900
H	-1.65458000	-0.47981800	5.32407700
C	5.55094800	-1.26090600	-0.51904000
C	5.49369200	-1.49914100	0.99307400
C	4.11162200	-1.14084000	1.54553300
C	2.96983400	-1.88768000	0.83602700
C	3.04996500	-1.66782100	-0.69094400
C	4.43823300	-2.03690700	-1.23036000
H	4.05305200	-1.34653000	2.62750900
H	5.71051600	-2.56249600	1.20441400
H	6.26984100	-0.90942700	1.50862600
H	5.42233200	-0.18277600	-0.72129200
H	6.53519800	-1.54990900	-0.92332800
H	3.08129000	-2.97328600	1.01381300
H	2.87665100	-0.59750500	-0.87707100
H	4.59453800	-3.12364800	-1.09300600
H	4.46201400	-1.84523800	-2.31657900
H	3.93258000	-0.05931900	1.41222500
N	1.96586200	-2.39963200	-1.37971900
H	1.98067800	-2.17861300	-2.37747100
H	2.13166300	-3.40828300	-1.31667300
N	1.64965500	-1.49207800	1.35751600
H	1.47014800	-1.93702300	2.25812800
H	1.63175600	-0.48425900	1.53472500
C	-4.29341600	3.51873100	-0.91578100
C	-3.19516400	2.66204700	-0.99715400
C	-3.32685700	1.30244700	-0.65381600
C	-4.57858600	0.82775400	-0.22128800
C	-5.67091500	1.69701500	-0.14279500
C	-5.54117100	3.04544200	-0.48995900
H	-4.16874500	4.57198600	-1.18270400
H	-2.21961100	3.04083300	-1.30769000
H	-4.70027900	-0.21981200	0.06066800
H	-6.63516700	1.30963300	0.19816400
N	-2.21838600	0.44033600	-0.79581800
H	-1.33085400	0.92969600	-0.87978000
H	-2.68125900	-0.74916300	-2.30371200
H	-6.39808100	3.72044700	-0.42491700

TS5

Zero-point correction=	0.514869 (Hartree/Particle)
Thermal correction to Energy=	0.553518
Thermal correction to Enthalpy=	0.554462
Thermal correction to Gibbs Free Energy=	0.440091
Sum of electronic and zero-point Energies=	-2156.529485
Sum of electronic and thermal Energies=	-2156.490836
Sum of electronic and thermal Enthalpies=	-2156.489892
Sum of electronic and thermal Free Energies=	-2156.604262

Sb	-0.20317500	-2.42902300	0.01488900
F	-2.08578600	-2.49031600	-0.44351400
F	-0.31579500	-4.19971700	0.75398600
F	0.26899700	-3.13255700	-1.71443900
F	1.66251400	-2.32185800	0.48495700
F	-0.10188300	-0.63330200	-0.74233100
F	-0.69985500	-1.66207100	1.72294900
Ag	-1.21693500	1.43129600	1.27758400
C	2.35869900	1.70193700	0.12290300
C	1.81282900	2.74441600	-0.77704400
O	2.77657600	3.39353000	-1.30502500
O	0.57051800	2.99329100	-1.01448800
C	0.18250800	4.08195300	-1.91987600
H	0.90657000	4.90045800	-1.80109600
H	-0.79647800	4.40175300	-1.53913600
C	0.11054300	3.57699700	-3.34296500
H	-0.21872200	4.39852400	-3.99848100
H	1.09661400	3.23187200	-3.68949200
H	-0.61245700	2.75132700	-3.43287200
C	1.74504100	1.47297300	1.44163300
C	2.04616000	0.30590800	2.17511400
C	0.85235700	2.41254100	2.04223600
C	1.52780000	0.09479400	3.45520100
H	2.68857100	-0.45080800	1.72538500
C	0.31933800	2.17759200	3.33046200
H	0.68454100	3.38557700	1.57232800
C	0.66251200	1.02015200	4.04572300
H	1.79312300	-0.82059500	3.99096600
H	-0.31756700	2.93866500	3.78994700
H	0.25404400	0.84841600	5.04400900
C	-5.02984400	-0.28869500	-2.57964700
C	-5.91384700	-0.42276700	-1.33568200

C	-5.06168000	-0.67643600	-0.08904600
C	-3.99492600	0.40821600	0.12653400
C	-3.11492700	0.56391600	-1.13289100
C	-3.97490100	0.80348500	-2.38145800
H	-5.69436800	-0.74378100	0.81223700
H	-6.49659300	0.50683400	-1.19935200
H	-6.64508700	-1.23786900	-1.46514700
H	-4.52193200	-1.25141500	-2.76968700
H	-5.64158100	-0.06976900	-3.47064000
H	-4.49428400	1.37779400	0.30779100
H	-2.57081000	-0.38343400	-1.25409400
H	-4.47431300	1.78585500	-2.27967200
H	-3.31206900	0.87195900	-3.26053800
H	-4.53885400	-1.64447100	-0.18994500
N	-2.09806000	1.60816000	-0.93834600
H	-1.30409500	1.45124100	-1.55750000
H	-2.47574600	2.53063000	-1.16544500
N	-3.15502700	0.12601100	1.30638100
H	-3.71767400	0.16976200	2.15766500
H	-2.80153800	-0.83305000	1.25431000
C	5.12323800	-1.96424400	-1.75795600
C	3.90750900	-1.32867600	-1.51517200
C	3.86561300	-0.06983400	-0.86731100
C	5.08634900	0.51011400	-0.46270100
C	6.29838600	-0.13901300	-0.71452900
C	6.33465600	-1.37673400	-1.36558800
H	5.12343400	-2.93703200	-2.25852600
H	2.96794700	-1.80567500	-1.80534000
H	5.07906600	1.46932100	0.05824100
H	7.22972700	0.33442300	-0.38940000
N	2.63373200	0.52915100	-0.66428500
H	1.83008700	-0.06624800	-0.85054100
H	3.39674500	2.74622700	-0.49507600
H	7.28610100	-1.87823200	-1.55896600

TS6

Zero-point correction=	0.515974 (Hartree/Particle)
Thermal correction to Energy=	0.554528
Thermal correction to Enthalpy=	0.555472
Thermal correction to Gibbs Free Energy=	0.441511
Sum of electronic and zero-point Energies=	-2156.533211
Sum of electronic and thermal Energies=	-2156.494658

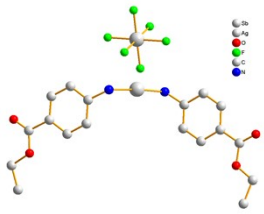
Sum of electronic and thermal Enthalpies= -2156.493714
Sum of electronic and thermal Free Energies= -2156.607675

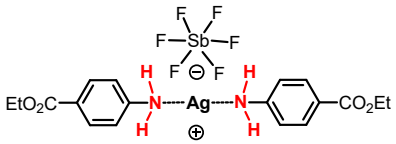
Sb	0.11588500	-2.70048800	-0.03814400
F	-1.47315300	-3.06808700	-1.06948800
F	-0.00426500	-4.41322800	0.82729600
F	1.23205900	-3.45864400	-1.41759500
F	1.66419500	-2.23382600	1.01816400
F	0.24315300	-0.97631800	-0.92833900
F	-1.00059100	-1.92582300	1.34821000
Ag	-0.67970100	1.07167100	1.27755100
C	1.78575600	2.07651700	-1.15804800
C	0.65173300	2.40032400	-2.00777300
O	0.33874000	1.77407300	-3.01637800
O	-0.03860500	3.47564500	-1.57099000
C	-1.11917900	3.96029100	-2.38684800
H	-1.67026700	3.10962300	-2.81597800
H	-0.69608800	4.53412900	-3.22961800
C	-2.00524600	4.82265200	-1.51466100
H	-2.83084100	5.23839300	-2.11351700
H	-2.43715700	4.23229300	-0.69001700
H	-1.43679200	5.65942300	-1.07894800
C	1.77160400	2.34744700	0.28890500
C	1.69855700	1.27902600	1.22910300
C	1.77177100	3.66435800	0.78201000
C	1.61438200	1.54804100	2.61190600
H	1.80979200	0.24538300	0.89507900
C	1.68825400	3.92014500	2.15520100
H	1.83212100	4.49285500	0.07486300
C	1.60567300	2.87269700	3.07727500
H	1.61204900	0.71323100	3.31760500
H	1.69513700	4.95518300	2.50756300
H	1.55156100	3.07778900	4.14888900
C	-5.21166200	-1.00459500	-1.34779400
C	-5.92056300	-0.63525600	-0.04112900
C	-4.92559200	-0.58991000	1.12201200
C	-3.74621600	0.35909400	0.86094600
C	-3.04961500	0.01559700	-0.47318300
C	-4.05986200	-0.03652300	-1.62804500
H	-5.42773900	-0.29129500	2.05773200
H	-6.39982600	0.35466000	-0.15285900
H	-6.72709100	-1.35331700	0.18181900
H	-4.80806600	-2.03031100	-1.26845800
H	-5.92297700	-1.00606800	-2.19030500

H	-4.12536700	1.39387600	0.77677000
H	-2.60095700	-0.98291700	-0.36204300
H	-4.46090500	0.98202800	-1.78972400
H	-3.52405900	-0.31946300	-2.54955300
H	-4.51331000	-1.60244900	1.28927200
N	-1.95059800	0.95666000	-0.73290100
H	-1.36860100	0.62557100	-1.50373600
H	-2.33059600	1.86141700	-1.01650300
N	-2.77985000	0.34367800	1.97993900
H	-3.19351700	0.78069300	2.80512500
H	-2.58482000	-0.62662400	2.23960700
C	4.77999200	-1.90171600	-0.68228800
C	3.66636400	-1.24996700	-1.21408600
C	3.53778400	0.13991900	-1.07590400
C	4.52915800	0.87099000	-0.40066600
C	5.64036600	0.20521700	0.12337300
C	5.77325400	-1.18099100	-0.01013300
H	4.85988000	-2.98683500	-0.78706400
H	2.88543100	-1.82096900	-1.71733800
H	4.43494100	1.95111000	-0.28163400
H	6.40709700	0.78181200	0.64758600
N	2.40554200	0.76623500	-1.65909000
H	1.72209800	0.13711800	-2.09055200
H	2.70482400	1.86484300	-2.09703300
H	6.64023900	-1.69540300	0.41144900

4 X-ray Crystallographic Data of Complex A

Crystallography data and structure refinement for **Complex A (**CCDC 2105536**)**





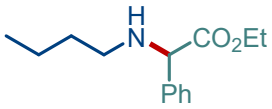
Complex A

Empirical formula	$AgC_{18}F_6N_2O_4SbH_{22}$
Temperature	293(2) K
Formula weight	673.99
Unit cell dimensions	a = 8.2459(6) Å alpha = 90 deg b = 20.336(2) Å beta = 90 deg. c = 13.7102(12) Å gamma = 90 deg.
Volume	2299.0 (3) $Å^3$
Z	4
ρcalc	1.947 g/cm^3
μ/mm^{-1}	2.102
F(000)	1312.0
Crystal size	0.1 x 0.1x 0.1 mm
Radiation	MoKα (λ = 0.71073 Å)
2θrange for data collection	7.17 to 58.672/°
Reflections collected	4990
Independent reflections	2622[R_{int} = 0.0296, R_{sigma} = 0.0419]
Data/restraints/parameters	2622/0/152
Goodness-of-fit on F^2	0.979
Final R indexes [I>=2σ (I)]	R_1 = 0.0347, wR_2 = 0.0697
Final R indexes [all data]	R_1 = 0.0495, wR_2 = 0.0803

Complex **A** was crystallized as a colourless crystal via vaporization of a hexane/ EtOAc solution, and its structure was determined by x-ray structure analysis. The crystallographic data that can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data request/cif.

5 Characterization data for the products

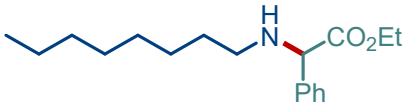
*Known compounds have been marked with references



ethyl 2-(butylamino)-2-phenylacetate (1)[11]

Light yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.39-7.27 (m, 5H), 4.34 (s, 1H), 4.23-4.16 (m, 1H), 4.15-4.09 (m, 1H), 2.61-2.56 (m, 1H), 2.52-2.47 (m, 1H), 1.97 (s, 1H), 1.53-1.47 (m, 2H), 1.38-1.29 (m, 2H), 1.21 (t, *J* = 7.5 Hz, 3H), 0.89 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 173.2, 138.4, 128.6, 127.9, 127.3, 65.7, 61.0, 47.5, 32.1, 20.4, 14.1, 13.9; **HRMS** (ESI^+) m/z calcd for $C_{14}H_{21}NNaO_2$ $[M+Na]^+$ 258.1464, found 258.1467.

……



ethyl 2-(octylamino)-2-phenylacetate (2)

Light yellow oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.40-7.25 (m, 5H), 4.34 (s, 1H), 4.21-4.17 (m, 1H), 4.15-4.10 (m, 1H), 2.59-2.55 (m, 1H), 2.51-2.47 (m, 1H), 2.01 (s, 1H), 1.55-1.46 (m, 2H), 1.35-1.23 (m, 10H), 1.21 (t, *J* = 7.2 Hz, 3H), 0.87 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.2, 138.4, 128.6, 127.9, 127.3, 65.7, 61.0, 47.8, 31.8, 30.0, 29.4, 29.2, 27.2, 22.6, 14.07, 14.02; **HRMS** (ESI^+) m/z calcd for $C_{18}H_{29}NNaO_2$ $[M+Na]^+$ 314.2090, found 314.2098.

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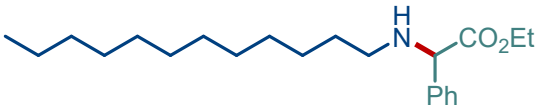

ethyl 2-(dodecylamino)-2-phenylacetate (3)

Light yellow oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.37 (d, *J* = 7.2 Hz, 2H), 7.33 (t, *J* = 7.2 Hz, 2H), 7.28 (t, *J* = 7.2 Hz, 1H), 4.34 (s, 1H), 4.22-4.17 (m, 1H), 4.15-4.09 (m, 1H), 2.59-2.55 (m, 1H), 2.51-2.47 (m, 1H), 1.99 (s, 1H), 1.55-1.46 (m, 2H), 1.33-1.25 (m, 18H), 1.20 (t, *J* = 7.2 Hz, 3H), 0.88 (t, *J* = 6.6 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.1, 138.4, 128.6, 127.9, 127.3, 65.6, 61.0, 47.8, 31.9, 30.0, 29.62, 29.59, 29.57, 29.53, 29.47, 29.3, 27.2, 22.7, 14.1; **HRMS** (ESI^+) m/z calcd for $C_{22}H_{38}NO_2$ $[M+H]^+$ 348.2897, found 348.2906.

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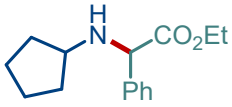
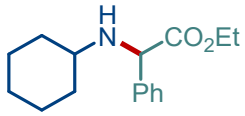


ethyl 2-(cyclopentylamino)-2-phenylacetate (4)

Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.39-7.26 (m, 5H), 4.23-4.16 (m, 1H), 4.14-4.08 (m, 1H), 2.99-2.95 (m, 1H), 2.04 (br, 1H), 1.85-1.73 (m, 2H), 1.73-1.64 (m, 2H), 1.55-1.44 (m, 2H), 1.41-1.37 (m, 2H), 1.21 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.5, 138.7, 128.6, 127.9, 127.4, 64.3, 61.1, 57.4, 33.2, 33.0, 24.0, 23.96, 14.1; **HRMS** (ESI^+) m/z calcd for $C_{15}H_{22}NO_2$ $[M+H]^+$ 248.1645, found 248.1655.

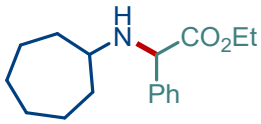
……



ethyl 2-(cyclohexylamino)-2-phenylacetate (5)[12]

Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.37 (d, *J* = 7.0 Hz, 2H), 7.33 (t, *J* = 7.5 Hz, 2H), 7.28 (t, *J* = 7.0 Hz, 1H), 4.51 (s, 1H), 4.22-4.15 (m, 1H), 4.14-4.08 (m, 1H), 2.41-2.30 (m, 1H), 2.09 (s, 1H), 1.87-1.81 (m, 2H), 1.74-1.66 (m, 2H), 1.59-1.56 (m, 1H), 1.23-1.10 (m, 8H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 173.6, 138.8, 128.6, 127.8, 127.3, 62.4, 61.0, 54.4, 33.4, 33.2, 26.0, 24.8, 14.1; **HRMS** (ESI^+) m/z calcd for $C_{16}H_{23}NNaO_2$ $[M+Na]^+$ 284.1621, found 284.1626.

……



ethyl 2-(cycloheptylamino)-2-phenylacetate (6)

Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.38-7.30 (m, 4H), 7.30-7.25 (m, 1H), 4.45 (s, 1H), 4.22-4.07 (m, 2H), 2.57-2.52 (m, 1H), 2.07 (s, 1H), 1.86-1.74 (m, 2H), 1.69-1.60 (m, 2H), 1.55-1.30 (m, 8H), 1.20 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 173.5, 138.6, 128.6, 127.8, 127.2, 62.8, 61.0, 56.4, 34.73, 34.67, 28.2, 28.1, 24.1, 14.0; **HRMS** (ESI^+) m/z calcd for $C_{17}H_{26}NO_2$ $[M+H]^+$ 276.1958, found 276.1968.

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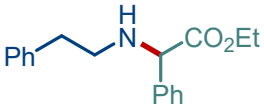
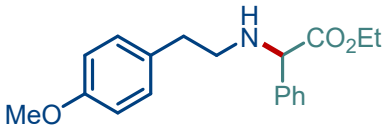


ethyl 2-(phenethylamino)-2-phenylacetate (7)

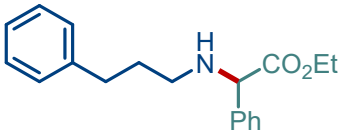
Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.35-7.30 (m, 4H), 7.30-7.24 (m, 3H), 7.21-7.15 (m, 3H), 4.37 (s, 1H), 4.20-4.04 (m, 2H), 2.88-2.71 (m, 4H), 2.13 (br, 1H), 1.17 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.8, 139.7, 138.1, 128.63, 128.58, 128.4, 127.9, 127.3, 126.1, 65.5, 61.0, 49.0, 36.4, 14.0; **HRMS** (ESI^+) m/z calcd for $C_{18}H_{21}NNaO_2$ $[M+Na]^+$

306.1464, found 306.1481.



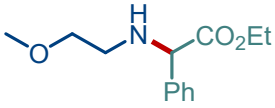
ethyl 2-((3-(4-methoxyphenyl)propyl)amino)-2-phenylacetate (8)

Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.36-7.27 (m, 5H), 7.09 (d, *J* = 8.5 Hz, 2H), 6.81 (d, *J* = 8.5 Hz, 2H), 4.38 (s, 1H), 4.21-4.14 (m, 1H), 4.13-4.05 (m, 1H), 3.76 (s, 3H), 2.86-2.72 (m, 4H), 2.07 (br, 1H), 1.18 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.9, 158.0, 138.0, 131.5, 129.5, 128.6, 128.0, 127.3, 113.8, 65.5, 61.1, 55.1, 49.1, 35.3, 14.0; **HRMS** (ESI^+) m/z calcd for $C_{19}H_{23}NNaO_3$ $[M+Na]^+$ 336.1570, found 336.1575.



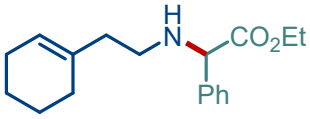
ethyl 2-phenyl-2-((3-phenylpropyl)amino)acetate (9)

Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.38-7.24 (m, 7H), 7.19-7.14 (m, 3H), 4.33 (s, 1H), 4.25-4.06 (m, 2H), 2.71-2.58 (m, 3H), 2.56-2.51 (m, 1H), 1.94 (s, 1H), 1.87-1.80 (m, 2H), 1.20 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 173.2, 142.1, 138.4, 128.7, 128.4, 128.3, 128.0, 127.4, 125.8, 65.6, 61.1, 47.3, 33.5, 31.6, 14.1; **HRMS** (ESI^+) m/z calcd for $C_{19}H_{23}NNaO_2$ $[M+Na]^+$ 320.1621, found 320.1627.



ethyl 2-((2-methoxyethyl)amino)-2-phenylacetate (10)

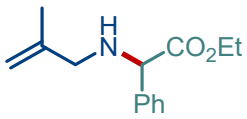
Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.44-7.28 (m, 5H), 4.40 (s, 1H), 4.25-4.09 (m, 2H), 3.55-3.47 (m, 2H), 3.25 (s, 3H), 2.85-2.69 (m, 2H), 2.23 (s, 1H), 1.21 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 172.0, 136.8, 127.7, 127.2, 126.4, 70.7, 64.7, 60.4, 57.6, 46.4, 13.1; **HRMS** (ESI^+) m/z calcd for $C_{13}H_{19}NNaO_3$ $[M+Na]^+$ 260.1257, found 260.1254.



ethyl 2-((2-(cyclohex-1-en-1-yl)ethyl)amino)-2-phenylacetate (11)

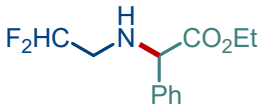
Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.38-7.31 (m, 4H), 7.30-7.27 (m, 1H), 5.51-5.42

(m, 1H), 4.36 (s, 1H), 4.22-4.08 (m, 2H), 2.67-2.53 (m, 2H), 2.16 (t, *J* = 7.0 Hz, 2H), 2.09 (s, 1H), 2.01-1.95 (m, 2H), 1.93-1.78 (m, 2H), 1.63-1.57 (m, 2H), 1.56-1.52 (m, 2H), 1.20 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.0, 138.3, 135.1, 128.6, 127.9, 127.3, 122.8, 65.5, 61.0, 45.3, 38.2, 28.0, 25.2, 22.9, 22.4, 14.1; **HRMS** (ESI^+) m/z calcd for $C_{18}H_{25}NNaO_2$ $[M+Na]^+$ 310.1777, found 310.1787.



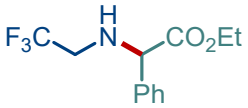
ethyl 2-((2-methylallyl)amino)-2-phenylacetate (12)

Light yellow oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.38 (d, *J* = 7.2 Hz, 2H), 7.34 (t, *J* = 7.2 Hz, 2H), 7.29 (t, *J* = 7.2 Hz, 1H), 4.89-4.85 (m, 2H), 4.35 (s, 1H), 4.22-4.09 (m, 2H), 3.12 (ABq, *J* = 13.8 Hz, 2H), 2.11 (s, 1H), 1.75 (s, 3H), 1.20 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 173.0, 143.2, 138.3, 128.6, 127.9, 127.4, 111.5, 64.2, 61.0, 53.3, 20.7, 14.1; **HRMS** (ESI^+) m/z calcd for $C_{14}H_{19}NNaO_2$ $[M+Na]^+$ 256.1308, found 256.1309.



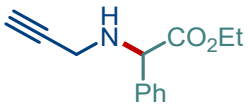
ethyl 2-((2,2-difluoroethyl)amino)-2-phenylacetate (13)

Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.39-7.29 (m, 5H), 5.82 (tt, *J* = 56.5, 4.5 Hz, 1H), 4.42 (s, 1H), 4.24-4.07 (m, 2H), 3.02-2.78 (m, 2H), 2.22 (s, 1H), 1.20 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.4, 137.5, 128.8, 128.4, 127.5, 116.0 (t, *J* = 238.5 Hz), 65.1, 61.4, 49.2 (t, *J* = 24.0 Hz), 14.1; **^{19}F NMR** (564 MHz, $CDCl_3$) δ -(121.40)-(-121.62) (m); **HRMS** (ESI^+) m/z calcd for $C_{12}H_{16}F_2NO_2$ $[M+H]^+$ 260.1281, found 260.1278.



ethyl 2-phenyl-2-((2,2,2-trifluoroethyl)amino)acetate (14)

Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.35-7.21 (m, 5H), 4.43 (s, 1H), 4.17-3.99 (m, 2H), 3.10-2.95 (m, 2H), 2.37 (s, 1H), 1.12 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.1, 137.0, 128.8, 128.4, 127.5, 125.4 (q, *J* = 276.0 Hz), 64.4, 61.5, 47.8 (q, *J* = 31.5 Hz), 14.0; **^{19}F NMR** (564 MHz, $CDCl_3$) δ -71.72 (t, *J* = 9.6 Hz); **HRMS** (ESI^+) m/z calcd for $C_{12}H_{14}F_3NNaO_2$ $[M+Na]^+$ 284.0869, found 284.0873.



ethyl 2-phenyl-2-(prop-2-yn-1-ylamino)acetate (15)

Colorless oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.40 (d, *J* = 8.4 Hz, 2H), 7.35 (t, *J* = 7.8 Hz, 2H), 7.33-7.29 (m, 1H), 4.61 (s, 1H), 4.23-4.11 (m, 2H), 3.48-3.45 (m, 1H), 3.32-3.25 (m, 1H), 2.25 (s, 1H), 2.05 (s, 1H), 1.21 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.4, 137.5, 128.7, 128.2, 127.8, 81.2, 72.0, 63.7, 61.3, 35.9, 14.1; **HRMS** (ESI^+) m/z calcd for $C_{13}H_{15}NNaO_2$ $[M+Na]^+$ 240.0995, found 240.1000.

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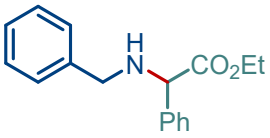

ethyl 2-(benzylamino)-2-phenylacetate (16)[12]

Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.41-7.24 (m, 10H), 4.37 (s, 1H), 4.23-4.07 (m, 2H), 3.74 (s, 2H), 2.29 (br, 1H), 1.20 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 173.0, 139.5, 138.2, 128.7, 128.44, 128.36, 128.0, 127.6, 127.2, 64.5, 61.2, 51.4, 14.1; **HRMS** (ESI^+) m/z calcd for $C_{17}H_{19}NNaO_2$ $[M+Na]^+$ 292.1308, found 292.1313.

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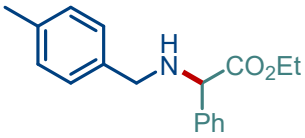

ethyl 2-((4-methylbenzyl)amino)-2-phenylacetate (17)

Light yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.38 (d, *J* = 7.5 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.29 (t, *J* = 7.0 Hz, 1H), 7.21 (d, *J* = 7.5 Hz, 2H), 7.12 (d, *J* = 7.5 Hz, 2H), 4.37 (s, 1H), 4.22-4.15 (m, 1H), 4.14-4.07 (m, 1H), 3.70 (br, 1H), 2.36 (s, 1H), 2.33 (s, 3H), 1.19 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.9, 138.2, 136.7, 136.4, 129.1, 128.6, 128.3, 128.0, 127.5, 64.3, 61.1, 51.1, 21.1, 14.1; **HRMS** (ESI^+) m/z calcd for $C_{18}H_{21}NNaO_2$ $[M+Na]^+$ 306.1464, found 306.1471.

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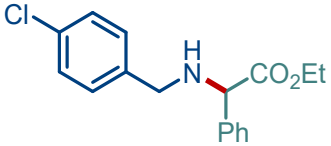

ethyl 2-((4-chlorobenzyl)amino)-2-phenylacetate (18)

Brown oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.38-7.24 (m, 9H), 4.33 (s, 1H), 4.23-4.06 (m, 2H),

3.70 (s, 2H), 2.01 (s, 1H), 1.20 (t, J = 7.0 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.8, 138.0, 137.9, 132.7, 129.6, 128.6, 128.5, 128.0, 127.4, 64.3, 61.1, 50.5, 14.0; **HRMS** (ESI^+) m/z calcd for $C_{17}H_{18}ClNNaO_2$ $[M+Na]^+$ 326.0918, found 326.0923.

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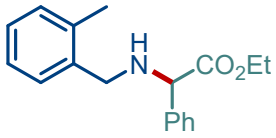

ethyl 2-((2-methylbenzyl)amino)-2-phenylacetate (19)

Light yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.40 (d, J = 7.5 Hz, 2H), 7.34 (t, J = 7.0 Hz, 2H), 7.31-7.26 (m, 2H), 7.18-7.11 (m, 3H), 4.40 (s, 1H), 4.22-4.08 (m, 2H), 3.72 (q, J = 13.0 Hz, 2H), 2.31 (s, 3H), 2.19 (s, 1H), 1.20 (t, J = 7.5 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 172.0, 137.3, 136.5, 135.7, 129.3, 127.8, 127.6, 127.0, 126.5, 126.2, 124.9, 63.9, 60.1, 48.3, 17.9, 13.1; **HRMS** (ESI^+) m/z calcd for $C_{18}H_{21}NNaO_2$ $[M+Na]^+$ 306.1464, found 306.1464.

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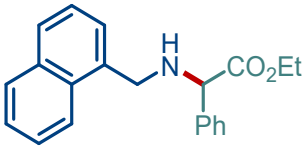

ethyl 2-((naphthalen-1-ylmethyl)amino)-2-phenylacetate (20)

Yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.13 (d, J = 8.0 Hz, 1H), 7.84 (d, J = 7.5 Hz, 1H), 7.77 (d, J = 8.0 Hz, 1H), 7.53-7.39 (m, 6H), 7.35 (t, J = 7.5 Hz, 2H), 7.30 (t, J = 7.2 Hz, 1H), 4.48 (s, 1H), 4.23-4.12 (m, 4H), 2.35 (s, 1H), 1.20 (t, J = 7.0 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.0, 138.2, 135.1, 133.9, 131.9, 128.61, 128.58, 128.02, 127.96, 127.6, 126.4, 126.1, 125.6, 125.3, 123.9, 65.1, 61.1, 49.3, 14.1; **HRMS** (ESI^+) m/z calcd for $C_{21}H_{21}NNaO_2$ $[M+Na]^+$ 342.1464, found 342.1427.

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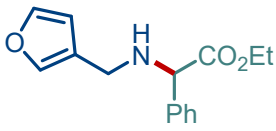

ethyl 2-((furan-3-ylmethyl)amino)-2-phenylacetate (21)

Yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.40-7.36 (m, 3H), 7.35 (d, J = 1.5 Hz, 1H), 7.34-7.28 (m, 2H), 6.31 (dd, J = 3.0, 2.0 Hz, 1H), 6.16 (d, J = 2.5 Hz, 1H), 4.38 (s, 1H), 4.21-4.05 (m, 2H), 3.74 (q, J = 14.5 Hz, 2H), 1.68 (s, 1H), 1.19 (t, J = 7.0 Hz, 3H); **^{13}C NMR** (125MHz, $CDCl_3$) δ 172.6, 153.0, 142.0, 137.8, 128.7, 128.1, 127.6, 110.1, 107.5, 64.2, 61.2, 43.8, 14.1; **HRMS** (ESI^+) m/z calcd for $C_{15}H_{18}NO_3$ $[M+H]^+$ 260.1281, found 260.1278.

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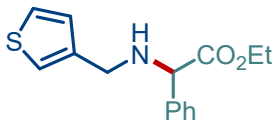

ethyl 2-phenyl-2-((thiophen-3-ylmethyl)amino)acetate (22)

Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.40-7.27 (m, 6H), 7.13 (d, *J* = 1.5 Hz, 1H), 7.06 (d, *J* = 5.0 Hz, 1H), 4.38 (s, 1H), 4.23-4.08 (m, 2H), 3.76 (s, 2H), 2.14 (s, 1H), 1.20 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.9, 140.6, 138.1, 128.7, 128.0, 127.7, 127.5, 125.8, 122.0, 64.4, 61.2, 46.4, 14.1; **HRMS** (ESI^+) m/z calcd for $C_{15}H_{17}NNaO_2S$ $[M+Na]^+$ 298.0872, found 298.0864.

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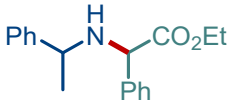

ethyl 2-phenyl-2-(((R)-1-phenylethyl)amino)acetate (23)[13]

Colorless oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.36-7.30 (m, 5H), 7.29-7.24 (m, 5H), 4.18 (d, *J* = 2.5 Hz, 1H), 4.13-3.98 (m, 2H), 3.58-3.54 (m, 1H), 2.36 (s, 1H), 1.34 (dd, *J* = 5.5, 2.5 Hz, 3H), 1.14-1.11 (m, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.8, 144.5, 138.4, 128.6, 128.5, 127.9, 127.7, 127.1, 126.9, 62.6, 61.1, 54.7, 24.3, 13.9; **HRMS** (ESI^+) m/z calcd for $C_{18}H_{21}NNaO_2$ $[M+Na]^+$ 306.1464, found 306.1459.

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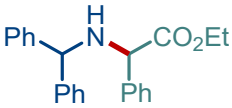

ethyl 2-(benzhydrylamino)-2-phenylacetate (24)

White solid; mp: 122-123 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.40 (d, *J* = 7.5 Hz, 2H), 7.37-7.26 (m, 11H), 7.24-7.18 (m, 2H), 4.74 (s, 1H), 4.31 (s, 1H), 4.23-4.07 (m, 2H), 2.70 (s, 1H), 1.18 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 173.2, 143.3, 143.2, 138.3, 128.7, 128.6, 128.5, 128.0, 127.6, 127.48, 127.47, 127.3, 127.2, 64.5, 62.9, 61.2, 14.1; **HRMS** (ESI^+) m/z calcd for $C_{23}H_{23}NNaO_2$ $[M+Na]^+$ 368.1261, found 368.1271.

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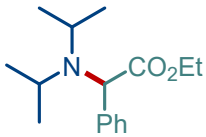

ethyl 2-(diisopropylamino)-2-phenylacetate (25)

Light yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.31-7.28 (m, 4H), 7.26-7.22 (m, 1H), 4.75 (s, 1H), 4.29-4.14 (m, 2H), 3.31-3.24 (m, 2H), 1.28 (t, *J* = 7.0 Hz, 3H), 1.12 (d, *J* = 6.5 Hz, 6H), 0.96 (d, *J* = 7.0 Hz, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 175.6, 139.5, 128.4, 128.0,

127.0, 61.6, 60.2, 45.7, 23.1, 21.6, 14.1; **HRMS** (ESI^+) m/z calcd for $C_{16}H_{26}NO_2$ $[M+H]^+$ 264.1958, found 264.1960.

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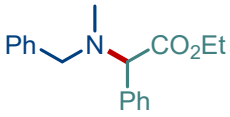

ethyl 2-(benzyl(methyl)amino)-2-phenylacetate (26)

Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.48 (d, *J* = 7.5 Hz, 2H), 7.36-7.28 (m, 7H), 7.22 (t, *J* = 7.0 Hz, 1H), 4.31 (s, 1H), 4.26-4.13 (m, 2H), 3.65 (d, *J* = 13.5 Hz, 1H), 3.53 (d, *J* = 13.5 Hz, 1H), 2.21 (s, 3H), 1.24 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 171.8, 138.9, 136.7, 128.8, 128.7, 128.4, 128.1, 128.0, 126.9, 72.2, 60.6, 58.5, 39.0, 14.2; **HRMS** (ESI^+) m/z calcd for $C_{18}H_{21}NNaO_2$ $[M+Na]^+$ 306.1464, found 306.1474.

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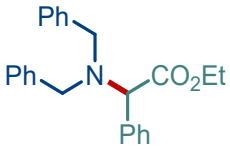

ethyl 2-(dibenzylamino)-2-phenylacetate (27)[12]

Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.38-7.25 (m, 13H), 7.22-7.19 (m, 2H), 4.60 (s, 1H), 4.35-4.18 (m, 2H), 3.82-3.72 (m, 4H), 1.28 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.1, 139.5, 136.8, 128.8, 128.3, 128.2, 127.7, 127.0, 65.8, 60.4, 54.2, 14.4; **HRMS** (ESI^+) m/z calcd for $C_{24}H_{26}NO_2$ $[M+H]^+$ 360.1958, found 360.1955.

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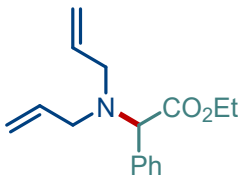

ethyl 2-(diallylamino)-2-phenylacetate (28)

Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.39 (d, *J* = 7.5 Hz, 2H), 7.33 (t, *J* = 7.0 Hz, 2H), 7.28 (t, *J* = 7.0 Hz, 1H), 5.87-5.79 (m, 2H), 5.18-5.12 (m, 4H), 4.59 (s, 1H), 4.27-4.11 (m, 2H), 3.22 (d, *J* = 6.5 Hz, 4H), 1.25 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 172.1, 136.8, 135.7, 128.7, 128.3, 127.9, 117.5, 67.7, 60.5, 53.2, 14.3; **HRMS** (ESI^+) m/z calcd for $C_{16}H_{21}NNaO_2$ $[M+Na]^+$ 282.1464, found 282.1468.

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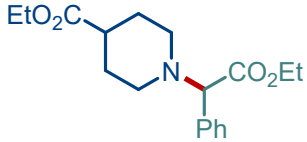

ethyl 1-(2-ethoxy-2-oxo-1-phenylethyl)piperidine-4-carboxylate (29)

Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.43 (d, *J* = 7.0 Hz, 2H), 7.36-7.28 (m, 3H), 4.22-4.15 (m, 1H), 4.14-4.09 (m, 3H), 4.01 (s, 1H), 2.90 (d, *J* = 11.0 Hz, 1H), 2.76 (d, *J* = 11.0 Hz, 1H), 2.32-2.25 (m, 1H), 2.21 (td, *J* = 11.0, 3.0 Hz, 1H), 2.01 (td, *J* = 11.0, 3.0 Hz, 1H), 1.92-1.76 (m, 4H), 1.23 (t, *J* = 7.5 Hz, 3H), 1.20 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 175.0, 171.5, 136.1, 128.7, 128.4, 128.1, 74.1, 60.7, 60.2, 50.6, 50.5, 41.1, 28.1, 28.1, 14.2, 14.1; **HRMS** (ESI^+) m/z calcd for $C_{18}H_{25}NNaO_4$ $[M+Na]^+$ 342.1676, found 342.1671.

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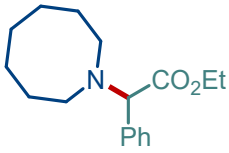

ethyl 2-(azocan-1-yl)-2-phenylacetate (30)

Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.5 Hz, 2H), 7.32 (t, *J* = 7.0 Hz, 2H), 7.28 (t, *J* = 7.0 Hz, 1H), 4.40 (s, 1H), 4.22-4.12 (m, 2H), 2.70-2.57 (m, 4H), 1.74-1.65 (m, 2H), 1.61-1.50 (m, 4H), 1.49-1.40 (m, 4H), 1.24 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.7, 138.0, 129.0, 128.1, 127.6, 73.3, 60.3, 51.5, 27.9, 27.5, 25.7, 14.2; **HRMS** (ESI^+) m/z calcd for $C_{17}H_{26}NO_2$ $[M+H]^+$ 276.1958, found 276.1960.

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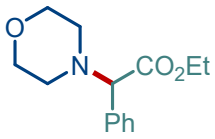

ethyl 2-morpholino-2-phenylacetate (31)[14]

Light yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.45 (d, *J* = 7.0 Hz, 2H), 7.38-7.29 (m, 3H), 4.23-4.06 (m, 2H), 3.96 (s, 1H), 3.73 (t, *J* = 4.5 Hz, 4H), 2.46-2.43 (m, 4H), 1.20 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.1, 135.4, 128.8, 128.5, 128.4, 74.4, 66.8, 60.9, 51.5, 14.0; **HRMS** (ESI^+) m/z calcd for $C_{14}H_{20}NO_3$ $[M+H]^+$ 250.1438, found 250.1446.

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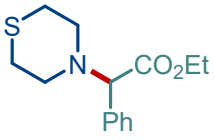

ethyl 2-phenyl-2-thiomorpholinoacetate (32)

Light yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.39 (d, *J* = 7.0 Hz, 2H), 7.37-7.29 (m, 3H), 4.24-4.10 (m, 3H), 2.84-2.78 (m, 2H), 2.77-2.71 (m, 2H), 2.70-2.66 (m, 4H), 1.22 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 171.4, 135.6, 128.7, 128.5, 128.2, 73.9, 60.8, 52.7,

27.9, 14.1; **HRMS** (ESI$^+$) m/z calcd for $C_{14}H_{19}NNaO_2S$ $[M+Na]^+$ 288.1029, found 288.1036.

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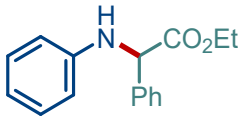

ethyl 2-phenyl-2-(phenylamino)acetate (33)[12]

White solid; mp: 86-87 °C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.2 Hz, 2H), 7.34 (t, *J* = 7.2 Hz, 2H), 7.28 (t, *J* = 7.2 Hz, 1H), 7.13-7.09 (m, 2H), 6.68 (t, *J* = 7.2 Hz, 1H), 6.55 (d, *J* = 7.2 Hz, 2H), 5.06 (s, 1H), 4.95 (s, 1H), 4.25-4.19 (m, 1H), 4.15-4.10 (m, 1H), 1.20 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.9, 146.1, 137.8, 129.3, 128.8, 128.2, 127.2, 118.1, 113.5, 61.8, 60.9, 14.1; **HRMS** (ESI$^+$) m/z calcd for $C_{16}H_{18}NO_2$ $[M+H]^+$ 256.1332, found 256.1334.

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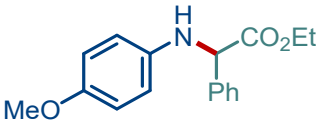

ethyl 2-((4-methoxyphenyl)amino)-2-phenylacetate (34)[12]

Yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.48 (d, *J* = 7.0 Hz, 2H), 7.34 (t, *J* = 7.0 Hz, 2H), 7.29 (t, *J* = 7.0 Hz, 1H), 6.71 (d, *J* = 9.0 Hz, 2H), 6.53 (d, *J* = 9.0 Hz, 2H), 5.00 (s, 1H), 4.67 (s, 1H), 4.24-4.19 (m, 1H), 4.15-4.10 (m, 1H), 3.69 (s, 3H), 1.20 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.0, 152.5, 140.2, 137.9, 128.7, 128.1, 127.2, 114.8, 114.7, 61.7, 61.6, 55.7, 14.0; **HRMS** (ESI$^+$) m/z calcd for $C_{17}H_{20}NO_3$ $[M+H]^+$ 286.1438, found 286.1442.

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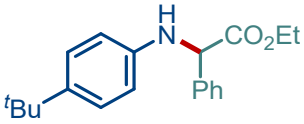

ethyl 2-((4-(tert-butyl)phenyl)amino)-2-phenylacetate (35)[15]

White solid; mp: 94-95 °C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.8 Hz, 2H), 7.34 (t, *J* = 7.8 Hz, 2H), 7.28 (t, *J* = 7.2 Hz, 1H), 7.15 (d, *J* = 8.4, 2H), 6.52 (d, *J* = 8.4 Hz, 2H), 5.02 (s, 1H), 4.85 (s, 1H), 4.25-4.20 (m, 1H), 4.16-4.10 (m, 1H), 1.23 (s, 9H), 1.20 (t, *J* = 6.6 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.0, 143.7, 140.8, 138.0, 128.8, 128.1, 127.2, 126.0, 113.0, 61.7, 61.1, 33.8, 31.5, 14.0; **HRMS** (ESI$^+$) m/z calcd for $C_{20}H_{25}NNaO_2$ $[M+Na]^+$ 334.1778, found 334.1780.

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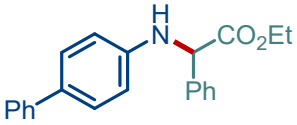

ethyl 2-([1,1'-biphenyl]-4-ylamino)-2-phenylacetate (36)[15]

White solid; mp: 95-97 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.53-7.45 (m, 4H), 7.41-7.28 (m, 7H), 7.23 (t, *J* = 7.0 Hz, 1H), 6.63 (d, *J* = 10.5 Hz, 2H), 5.10 (s, 1H), 5.06 (br, 1H), 4.28-4.22 (m, 1H), 4.18-4.12 (m, 1H), 1.22 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 171.7, 145.4, 141.1, 137.6, 130.9, 128.9, 128.6, 128.3, 127.9, 127.2, 126.3, 126.1, 113.6, 61.9, 60.8, 14.0; **HRMS** (ESI^+) m/z calcd for $C_{22}H_{21}NNaO_2$ $[M+Na]^+$ 354.1465, found 354.1466.

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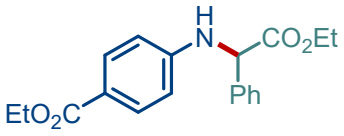

ethyl 4-((2-ethoxy-2-oxo-1-phenylethyl)amino)benzoate (37)

White solid; mp: 120-121 °C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.81 (d, *J* = 9.0 Hz, 2H), 7.46 (d, *J* = 7.2 Hz, 2H), 7.34 (t, *J* = 7.2 Hz, 2H), 7.29 (t, *J* = 7.2 Hz, 1H), 6.51 (d, *J* = 9.0 Hz, 2H), 5.47 (s, 1H), 5.11 (s, 1H), 4.30-4.20 (m, 3H), 4.16-4.10 (m, 1H), 1.31 (t, *J* = 7.2 Hz, 3H), 1.20 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.1, 166.6, 149.4, 136.8, 131.3, 128.9, 128.4, 127.0, 119.6, 112.3, 62.0, 60.1, 60.0, 14.3, 13.9; **HRMS** (ESI^+) m/z calcd for $C_{19}H_{21}NNaO_4$ $[M+Na]^+$ 350.1363, found 350.1365.

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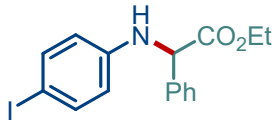

ethyl 2-((4-iodophenyl)amino)-2-phenylacetate (38)[12]

White solid; mp: 122-123 °C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.45 (d, *J* = 7.2 Hz, 2H), 7.37-7.33 (m, 4H), 7.30 (t, *J* = 7.2 Hz, 1H), 6.33 (d, *J* = 8.4 Hz, 2H), 5.04 (s, 1H), 5.00 (s, 1H), 4.26-4.21 (m, 1H), 4.16-4.10 (m, 1H), 1.21 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.4, 145.4, 137.8, 137.1, 128.9, 128.4, 127.1, 115.6, 78.9, 62.0, 60.5, 14.0; **HRMS** (ESI^+) m/z calcd for $C_{16}H_{17}INO_2$ $[M+H]^+$ 382.0299, found 382.0295.

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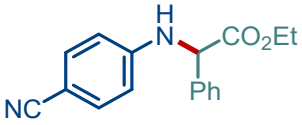

ethyl 2-((4-cyanophenyl)amino)-2-phenylacetate (39)[16]

Yellow solid; mp: 100-102 °C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.45 (d, *J* = 7.2 Hz, 2H), 7.38-7.29 (m, 5H), 6.51 (d, *J* = 9.0 Hz, 2H), 5.59 (d, *J* = 5.4 Hz, 1H), 5.07 (d, *J* = 6.0 Hz, 1H), 4.27-4.22 (m, 1H), 4.17-4.12 (m, 1H), 1.21 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$)

δ 170.8, 148.9, 136.3, 133.6, 129.0, 128.6, 126.9, 120.0, 113.0, 99.8, 62.2, 59.8, 13.9; **HRMS** (ESI$^+$) m/z calcd for $C_{17}H_{17}N_2O_2$ $[M+H]^+$ 281.1285, found 382.0292.

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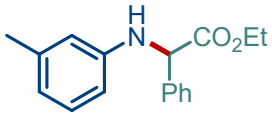

ethyl 2-phenyl-2-(*m*-tolylamino)acetate (40)[12]

White solid; mp: 108-109 °C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.8 Hz, 2H), 7.33 (t, *J* = 7.2 Hz, 2H), 7.28 (t, *J* = 7.2 Hz, 1H), 6.99 (t, *J* = 7.8 Hz, 1H), 6.51 (d, *J* = 7.2 Hz, 1H), 6.41 (s, 1H), 6.35 (d, *J* = 8.4 Hz, 1H), 5.05 (s, 1H), 4.88 (s, 1H), 4.25-4.20 (m, 1H), 4.15-4.10 (m, 1H), 2.21 (s, 3H), 1.20 (t, *J* = 6.6 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.8, 146.0, 138.9, 137.8, 129.1, 128.7, 128.1, 127.1, 119.0, 114.3, 110.4, 61.7, 60.8, 21.5, 14.0; **HRMS** (ESI$^+$) m/z calcd for $C_{17}H_{20}NO_2$ $[M+H]^+$ 270.1489, found 270.1492.

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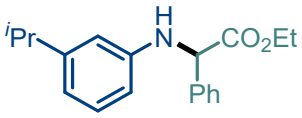

ethyl 2-((3-isopropylphenyl)amino)-2-phenylacetate (41)

White solid; mp: 115-116 °C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.50 (d, *J* = 7.8 Hz, 2H), 7.34 (t, *J* = 7.2 Hz, 2H), 7.29 (t, *J* = 7.8 Hz, 1H), 7.04 (t, *J* = 7.8 Hz, 1H), 6.58 (d, *J* = 7.2 Hz, 1H), 6.47 (t, *J* = 2.4 Hz, 1H), 6.36 (dd, *J* = 7.8, 2.4 Hz, 1H), 5.05 (s, 1H), 4.91 (s, 1H), 4.26-4.21 (m, 1H), 4.16-4.10 (m, 1H), 2.78-2.74 (m, 1H), 1.21 (t, *J* = 7.2 Hz, 3H), 1.19-1.15 (m, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.9, 150.0, 146.1, 137.9, 129.1, 128.8, 128.1, 127.2, 116.4, 112.0, 110.7, 61.7, 61.0, 34.1, 23.9, 23.8, 14.0; **HRMS** (ESI$^+$) m/z calcd for $C_{19}H_{23}NNaO_2$ $[M+Na]^+$ 320.1621, found 320.1631.

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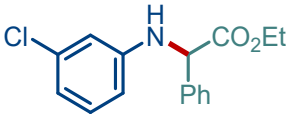

ethyl 2-((3-chlorophenyl)amino)-2-phenylacetate (42)[12]

Light yellow solid; mp: 86-87 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.47 (d, *J* = 7.5 Hz, 2H), 7.35 (t, *J* = 7.0 Hz, 2H), 7.30 (t, *J* = 7.0 Hz,, 1H), 7.00 (t, *J* = 8.0 Hz, 1H), 6.64 (d, *J* = 8.0 Hz, 1H), 6.53 (s, 1H), 6.40 (dd, *J* = 8.0, 2.0 Hz, 1H), 5.09 (s, 1H), 5.02 (s, 1H), 4.27-4.19 (m, 1H), 4.16-4.08 (m, 1H), 1.20 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.4, 147.1, 137.2, 134.9, 130.2, 128.9, 128.4, 127.1, 117.9, 113.2, 111.6, 62.0, 60.5, 14.0; **HRMS** (ESI$^+$) m/z calcd for $C_{16}H_{17}ClNO_2$ $[M+H]^+$ 290.0948, found 290.0948.

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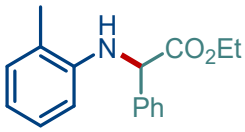

ethyl 2-phenyl-2-(*o*-tolylamino)acetate (43)[12]

Colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50 (d, *J* = 7.5 Hz, 2H), 7.34 (t, *J* = 7.0 Hz, 2H), 7.29 (t, *J* = 7.5 Hz, 1H), 7.06 (d, *J* = 7.5 Hz, 1H), 6.96 (t, *J* = 7.5 Hz, 1H), 6.64 (t, *J* = 7.5 Hz, 1H), 6.33 (d, *J* = 8.0 Hz, 1H), 5.09 (s, 1H), 4.90 (s, 1H), 4.28-4.19 (m, 1H), 4.18-4.10 (m, 1H), 2.28 (s, 3H), 1.21 (t, *J* = 7.5 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.0, 144.0, 137.8, 130.2, 128.8, 128.1, 127.1, 127.0, 122.4, 117.6, 110.7, 61.8, 60.7, 17.5, 14.0. **HRMS** (ESI^+) m/z calcd for $C_{17}H_{20}NO_2$ $[M+H]^+$ 270.1489, found 270.1488.

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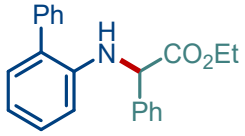

ethyl 2-([1,1'-biphenyl]-2-ylamino)-2-phenylacetate (44)

White solid; mp: 121-122 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.55-7.47 (m, 4H), 7.44 (d, *J* = 7.0 Hz, 2H), 7.38 (t, *J* = 7.0 Hz, 1H), 7.33 (t, *J* = 7.0 Hz, 2H), 7.28 (t, *J* = 7.0 Hz, 1H), 7.13 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.09 (t, *J* = 7.5 Hz, 1H), 6.76 (dd, *J* = 7.5, 6.5 Hz, 1H), 6.43 (d, *J* = 8.0 Hz, 1H), 5.33 (s, 1H), 5.07 (s, 1H), 4.18-4.11 (m, 1H), 4.11-4.04 (m, 1H), 1.15 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.5, 142.8, 139.2, 137.6, 130.3, 129.2, 129.0, 128.8, 128.5, 128.2, 128.1, 127.4, 127.1, 117.7, 111.3, 61.7, 60.9, 13.9; **HRMS** (ESI^+) m/z calcd for $C_{22}H_{22}NO_2$ $[M+H]^+$ 332.1645, found 332.1648.

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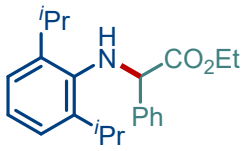

ethyl 2-((2,6-diisopropylphenyl)amino)-2-phenylacetate (45)[16]

Yellow oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.39 (d, *J* = 7.2 Hz, 2H), 7.33 (t, *J* = 7.2 Hz, 2H), 7.29 (t, *J* = 7.2 Hz, 1H), 7.06-6.99 (m, 3H), 4.64 (s, 1H), 4.33 (s, 1H), 4.21-4.09 (m, 2H), 3.20-3.11 (m, 2H), 1.19-1.16 (m, 9H), 1.09 (d, *J* = 7.2 Hz, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.3, 141.9, 141.5, 138.7, 128.6, 128.0, 126.9, 123.6, 123.5, 66.9, 61.4, 27.7, 24.3, 24.0, 14.0; **HRMS** (ESI^+) m/z calcd for $C_{22}H_{30}NO_2$ $[M+H]^+$ 340.2271, found 340.2276.

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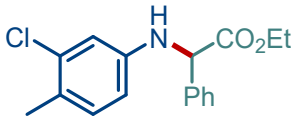

ethyl 2-((3-chloro-4-methylphenyl)amino)-2-phenylacetate (46)

White solid; mp: 109-110 °C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.47 (d, *J* = 7.8 Hz, 2H), 7.35 (t, *J* = 7.2 Hz, 2H), 7.30 (t, *J* = 7.2 Hz, 1H), 6.93 (d, *J* = 8.4 Hz, 1H), 6.57 (d, *J* = 2.4 Hz, 1H), 6.37 (dd, *J* = 8.4, 2.4 Hz, 1H), 5.00 (s, 1H), 4.90 (s, 1H), 4.26-4.21 (m, 1H), 4.16-4.10 (m, 1H), 2.20 (s, 3H), 1.21 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.6, 145.0, 137.3, 134.7, 131.3, 128.9, 128.3, 127.1, 124.9, 113.8, 112.0, 61.9, 60.7, 18.9, 14.0; **HRMS** (ESI^+) m/z calcd for $C_{17}H_{19}ClNO_2$ $[M+H]^+$ 304.1099, found 304.1101.

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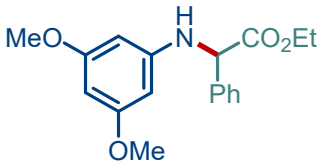

ethyl 2-((3,5-dimethoxyphenyl)amino)-2-phenylacetate (47)

Brown oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.47 (d, *J* = 7.2 Hz, 2H), 7.34 (t, *J* = 7.2 Hz, 2H), 7.29 (t, *J* = 7.2 Hz, 1H), 5.86 (s, 1H), 5.75 (s, 2H), 5.03 (s, 1H), 4.98 (s, 1H), 4.29-4.06 (m, 2H), 3.69 (s, 6H), 1.21 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.7, 161.6, 147.9, 137.7, 128.8, 128.2, 127.1, 92.3, 90.5, 61.8, 60.8, 55.1, 14.0; **HRMS** (ESI^+) m/z calcd for $C_{18}H_{22}NO_4$ $[M+H]^+$ 316.1543, found 316.1545.

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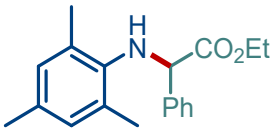

methyl 2-(mesitylamino)-2-phenylacetate (48)[12]

Colorless oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.42 (d, *J* = 7.2 Hz, 2H), 7.32 (t, *J* = 7.2 Hz, 2H), 7.28 (t, *J* = 7.2 Hz, 1H), 6.76 (s, 2H), 4.85 (s, 1H), 4.28 (s, 1H), 4.22-4.05 (m, 2H), 2.20 (s, 6H), 2.19 (s, 3H), 1.17 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.4, 141.8, 138.8, 131.0, 129.5, 128.9, 128.6, 127.9, 127.0, 64.2, 61.4, 20.5, 18.8, 14.0; **HRMS** (ESI^+) m/z calcd for $C_{19}H_{24}INO_2$ $[M+H]^+$ 298.1802, found 298.1803.

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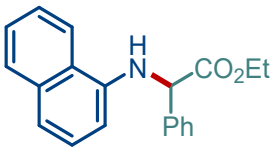

ethyl 2-(naphthalen-1-ylamino)-2-phenylacetate (49)[12]

Brown oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.4 Hz, 1H), 7.78 (d, *J* = 7.8 Hz, 1H), 7.57 (d, *J* = 7.2 Hz, 2H), 7.52-7.43 (m, 2H), 7.35 (t, *J* = 7.2 Hz, 2H), 7.31 (t, *J* = 7.2 Hz, 1H), 7.23-7.15 (m, 2H), 6.34 (d, *J* = 7.2 Hz, 1H), 5.80 (br, 1H), 5.23 (s, 1H), 4.31-4.25 (m, 1H), 4.21-4.16 (m, 1H), 1.24 (t, *J* = 6.6 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.9, 141.0, 137.5, 134.3, 128.8, 128.6, 128.3, 127.2, 126.3, 125.8, 124.9, 123.4, 120.1, 118.0, 105.6, 62.0, 60.9, 14.0; **HRMS** (ESI^+) m/z calcd for $C_{20}H_{19}NNaO_2$ $[M+Na]^+$ 328.1308, found 328.1309.

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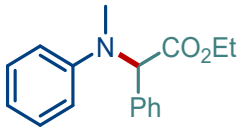

ethyl 2-(methyl(phenyl)amino)-2-phenylacetate (50)[12]

White solid; mp: 72-73 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.40-7.31 (m, 3H), 7.30-7.25 (m, 4H), 6.88 (d, *J* = 8.0 Hz, 2H), 6.80 (t, *J* = 7.0 Hz, 1H), 5.64 (s, 1H), 4.32-4.20 (m, 2H), 2.80 (s, 3H), 1.27 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.8, 150.0, 136.0, 129.2, 128.6, 128.4, 128.0, 118.0, 113.5, 65.8, 61.0, 34.6, 14.3. **HRMS** (ESI^+) m/z calcd for $C_{17}H_{20}NO_2$ $[M+H]^+$ 270.1489, found 270.1490.

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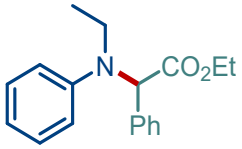

ethyl 2-(ethyl(phenyl)amino)-2-phenylacetate (51)

White solid; mp: 75-76 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.40-7.31 (m, 5H), 7.25 (t, *J* = 7.5 Hz, 2H), 6.85 (d, *J* = 8.0 Hz, 2H), 6.79 (t, *J* = 7.5 Hz, 1H), 5.52 (s, 1H), 4.30-4.14 (m, 2H), 3.32 (q, *J* = 7.0 Hz, 2H), 1.24 (t, *J* = 7.5 Hz, 3H), 0.91 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.1, 148.6, 136.1, 129.2, 128.9, 128.6, 128.1, 118.1, 114.5, 66.2, 61.1, 42.5, 14.2, 13.5; **HRMS** (ESI^+) m/z calcd for $C_{18}H_{22}NO_2$ $[M+H]^+$ 284.1645, found 284.1648.

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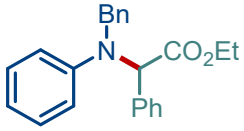

methyl 2-(benzyl(phenyl)amino)-2-phenylacetate (52)

White solid; mp: 103-104 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.33 (d, *J* = 7.0 Hz, 2H), 7.30-7.23 (m, 3H), 7.21-7.09 (m, 7H), 6.84-6.76 (m, 3H), 5.72 (s, 1H), 4.55 (ABq, *J* = 17.5 Hz, 2H), 4.19 (q, *J* = 7.0 Hz, 2H), 1.21 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.9, 149.2, 139.5, 135.5, 129.1, 128.9, 128.5, 128.2, 128.0, 126.5, 126.3, 118.7, 114.9, 66.4, 61.2,

52.4, 14.1; **HRMS** (ESI$^+$) m/z calcd for $C_{23}H_{24}NO_2$ $[M+H]^+$ 346.1802, found 346.1804.

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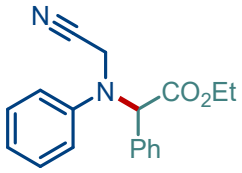

ethyl 2-((cyanomethyl)(phenyl)amino)-2-phenylacetate (53)

White solid; mp: 137-138 °C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.47-7.30 (m, 7H), 7.03-6.99 (m, 3H), 5.53 (s, 1H), 4.29-4.18 (m, 2H), 4.06 (s, 2H), 1.23 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.0, 147.2, 134.1, 129.6, 129.2, 129.1, 128.6, 121.5, 116.2, 116.1, 65.7, 61.5, 38.0, 14.0; **HRMS** (ESI$^+$) m/z calcd for $C_{18}H_{19}N_2O_2$ $[M+H]^+$ 295.1441, found 295.1444.

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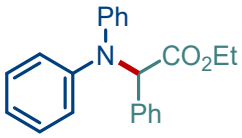

ethyl 2-(diphenylamino)-2-phenylacetate (54)

White solid; mp: 110-112 °C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.56-7.42 (m, 7H), 7.41-7.24 (m, 4H), 7.13-7.07 (m, 2H), 6.76 (t, *J* = 7.2 Hz, 1H), 6.43 (d, *J* = 7.8 Hz, 1H), 5.34 (s, 1H), 5.07 (s, 1H), 4.23-3.99 (m, 2H), 1.14 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.5, 142.8, 139.1, 137.6, 130.3, 129.2, 128.9, 128.7, 128.5, 128.1, 127.4, 127.1, 117.7, 111.2, 61.7, 60.8, 13.9; **HRMS** (ESI$^+$) m/z calcd for $C_{22}H_{22}NO_2$ $[M+H]^+$ 332.1645, found 332.1646.

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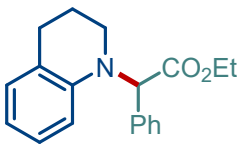

ethyl 2-(3,4-dihydroquinolin-1(*2H*)-yl)-2-phenylacetate (56)

Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.39-7.27 (m, 5H), 7.06 (t, *J* = 7.5 Hz, 1H), 7.00 (d, *J* = 7.5 Hz, 1H), 6.67 (dd, *J* = 13.0, 7.5 Hz, 2H), 5.63 (s, 1H), 4.34-4.19 (m, 2H), 3.33-3.29 (m, 1H), 2.98-2.89 (m, 1H), 2.87-2.77 (m, 1H), 2.73-2.68 (m, 1H), 1.88-1.75 (m, 2H), 1.27 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 172.1, 145.5, 135.6, 129.4, 128.7, 128.6, 128.0, 127.0, 123.8, 117.0, 110.4, 64.4, 61.0, 44.6, 28.2, 22.4, 14.3; **HRMS** (ESI$^+$) m/z calcd for $C_{19}H_{22}NO_2$ $[M+H]^+$ 296.1645, found 296.1648.

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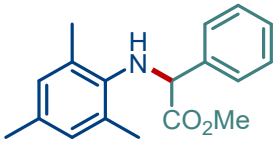

methyl 2-(mesitylamino)-2-phenylacetate (57)[17]

Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.0 Hz, 2H), 7.36-7.28 (m, 3H), 6.76 (s, 2H), 4.87 (d, *J* = 10.0 Hz, 1H), 4.25 (d, *J* = 10.0 Hz, 1H), 3.68 (s, 3H), 2.20 (s, 6H), 2.19 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 174.0, 141.6, 138.7, 131.2, 129.6, 129.0, 128.7, 128.1, 127.0, 64.1, 52.4, 20.5, 18.8; **HRMS** (ESI^+) m/z calcd for $C_{18}H_{22}NO_2$ $[M+H]^+$ 284.1645, found 284.1649.

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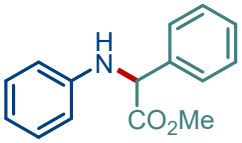

methyl 2-phenyl-2-(phenylamino)acetate (58)[18]

White solid; mp: 80-82 °C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.8 Hz, 2H), 7.34 (t, *J* = 7.2 Hz, 2H), 7.30 (t, *J* = 7.2 Hz, 1H), 7.11 (t, *J* = 7.8 Hz, 2H), 6.69 (t, *J* = 7.6 Hz, 2H), 6.55 (d, *J* = 7.8 Hz, 2H), 5.07 (s, 1H), 4.95 (s, 1H), 3.72 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.4, 146.0, 137.7, 129.3, 128.9, 128.4, 127.3, 118.2, 113.4, 60.8, 52.8; **HRMS** (ESI^+) m/z calcd for $C_{15}H_{16}NO_2$ $[M+H]^+$ 242.1176, found 242.1180.

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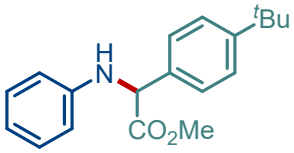

methyl 2-(4-(*tert*-butyl)phenyl)-2-(phenylamino)acetate (59)[19]

White solid; mp: 115-116 °C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.40 (d, *J* = 8.4 Hz, 2H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.12 (t, *J* = 7.8 Hz, 2H), 6.70 (t, *J* = 7.2 Hz, 1H), 6.57 (d, *J* = 7.8 Hz, 2H), 5.06 (s, 1H), 4.86 (br, 1H), 3.72 (s, 3H), 1.30 (s, 9H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.6, 151.3, 146.2, 134.4, 129.3, 126.9, 125.9, 118.1, 113.4, 60.5, 52.7, 31.3; **HRMS** (ESI^+) m/z calcd for $C_{19}H_{23}NNaO_2$ $[M+Na]^+$ 320.1621, found 320.1626.

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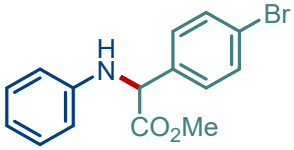

methyl 2-(4-bromophenyl)-2-(phenylamino)acetate (60)

White solid; mp: 115-116 °C; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.47 (d, *J* = 8.4 Hz, 2H), 7.38

(d, J = 8.4 Hz, 2H), 7.11 (t, J = 7.8 Hz, 2H), 6.71 (t, J = 7.2 Hz, 1H), 6.52 (d, J = 7.8 Hz, 2H), 5.03 (s, 1H), 4.98 (s, 1H), 3.73 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.7, 145.6, 136.8, 132.0, 129.3, 129.0, 122.3, 118.4, 113.5, 60.2, 53.0; **HRMS** (ESI^+) m/z calcd for $C_{15}H_{14}BrNNaO_2$ $[M+Na]^+$ 342.0100, found 342.0102.

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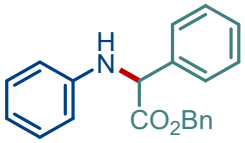

benzyl 2-phenyl-2-(phenylamino)acetate (61)

Colorless oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.49 (d, J = 7.0 Hz, 2H), 7.36-7.27 (m, 6H), 7.18-7.15 (m, 2H), 7.11 (dd, J = 8.5, 7.5 Hz, 2H), 6.69 (t, J = 7.0 Hz, 1H), 6.56 (d, J = 7.5 Hz, 2H), 5.22-5.09 (m, 3H), 4.95 (d, J = 5.5 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.7, 145.9, 137.5, 135.3, 129.2, 128.8, 128.5, 128.30, 128.29, 127.9, 127.3, 118.2, 113.5, 67.3, 60.9; **HRMS** (ESI^+) m/z calcd for $C_{21}H_{20}NO_2$ $[M+H]^+$ 318.1489, found 318.1490.

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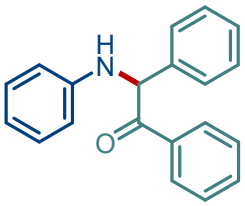

1,2-diphenyl-2-(phenylamino)ethan-1-one (62)

White solid; mp: 89-90 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.99 (d, J = 7.5 Hz, 2H), 7.52 (t, J = 7.5 Hz, 1H), 7.43 (dd, J = 15.0, 7.5 Hz, 4H), 7.27 (t, J = 7.5 Hz, 2H), 7.19 (t, J = 7.5 Hz, 1H), 7.12 (t, J = 7.5 Hz, 2H), 6.68 (t, J = 8.5 Hz, 3H), 6.02 (s, 1H), 5.41 (s, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 197.0, 146.1, 137.7, 135.0, 133.5, 129.2, 129.0, 128.8, 128.7, 128.09, 128.07, 117.8, 113.5, 62.7; **HRMS** (ESI^+) m/z calcd for $C_{20}H_{18}NO$ $[M+H]^+$ 288.1383, found 288.1380.

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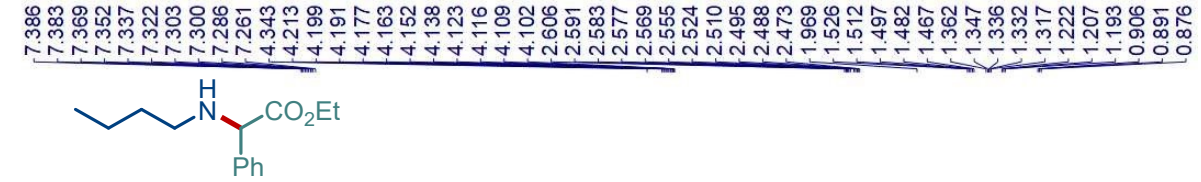
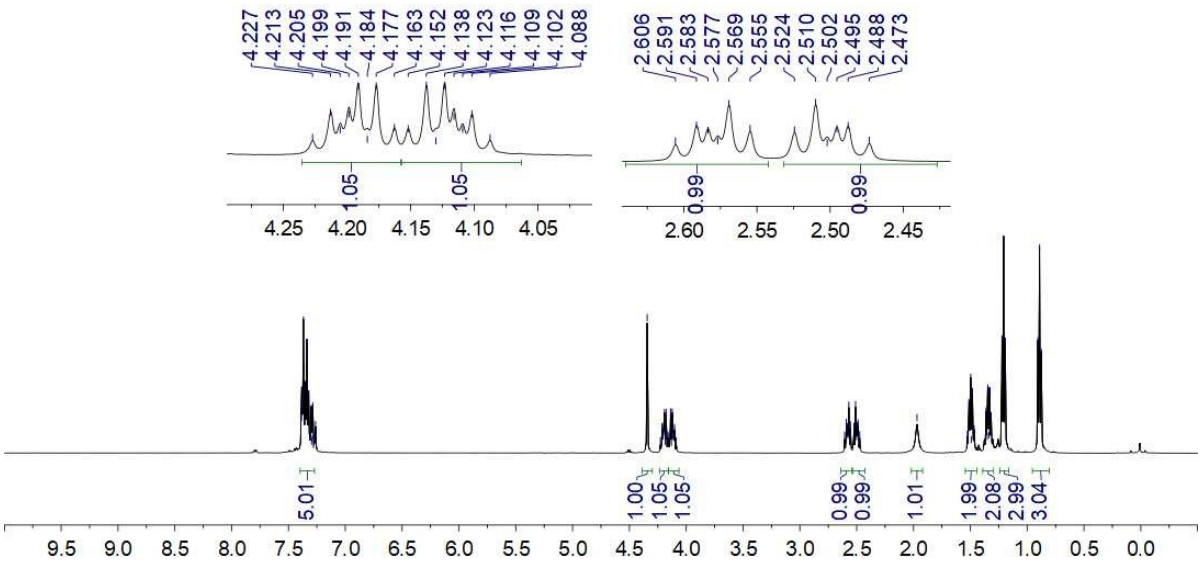
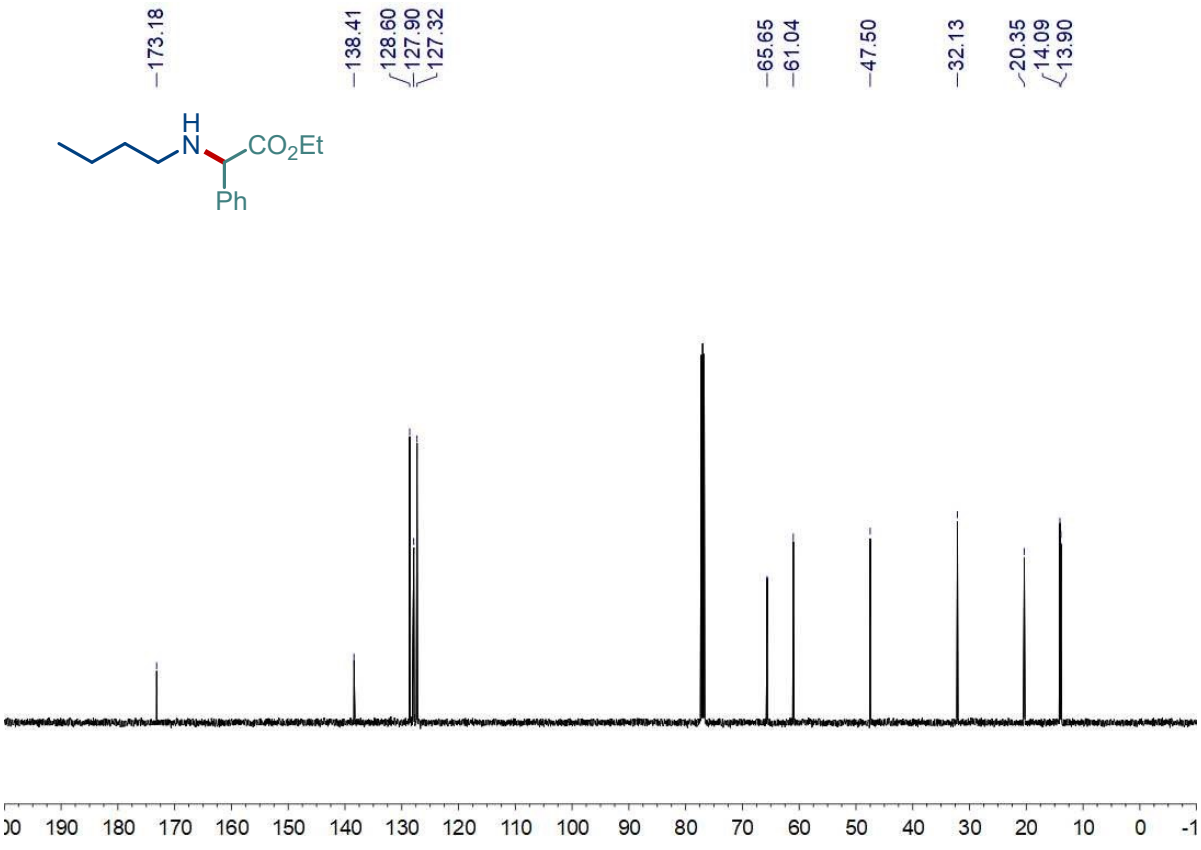
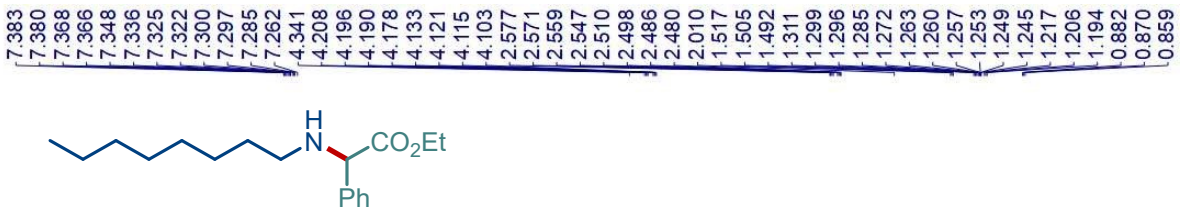
7 Copies of ^{1}H-, ^{13}C- and ^{19}F- Spectra





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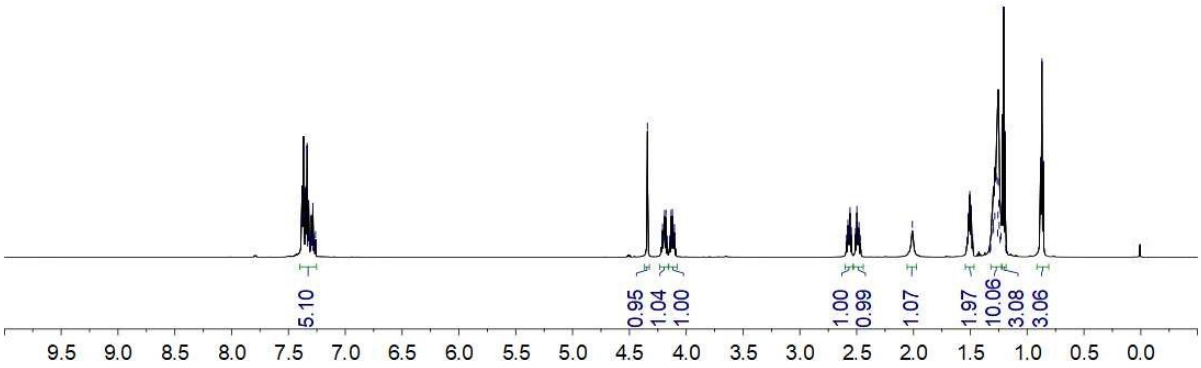
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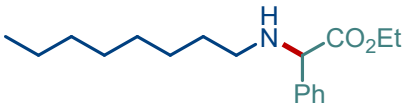
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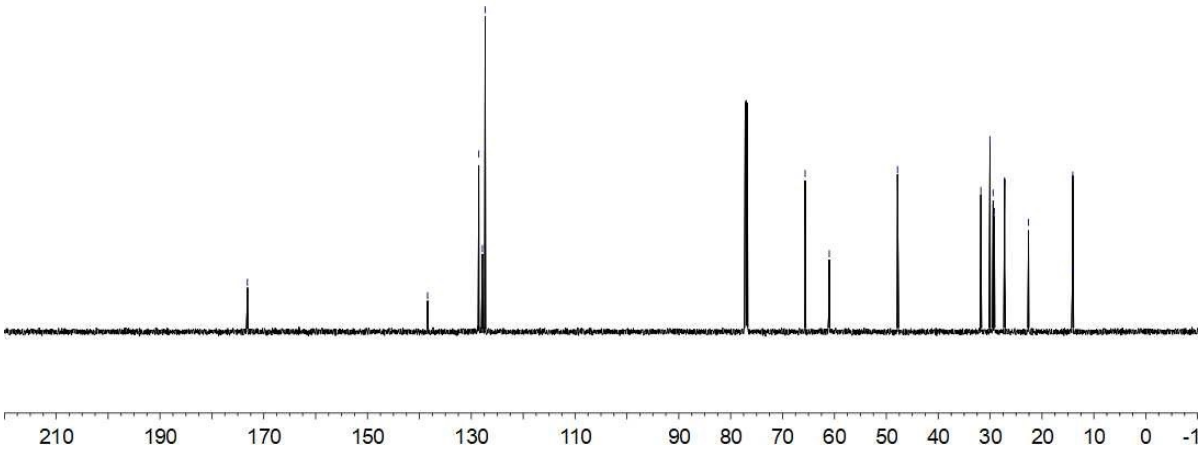
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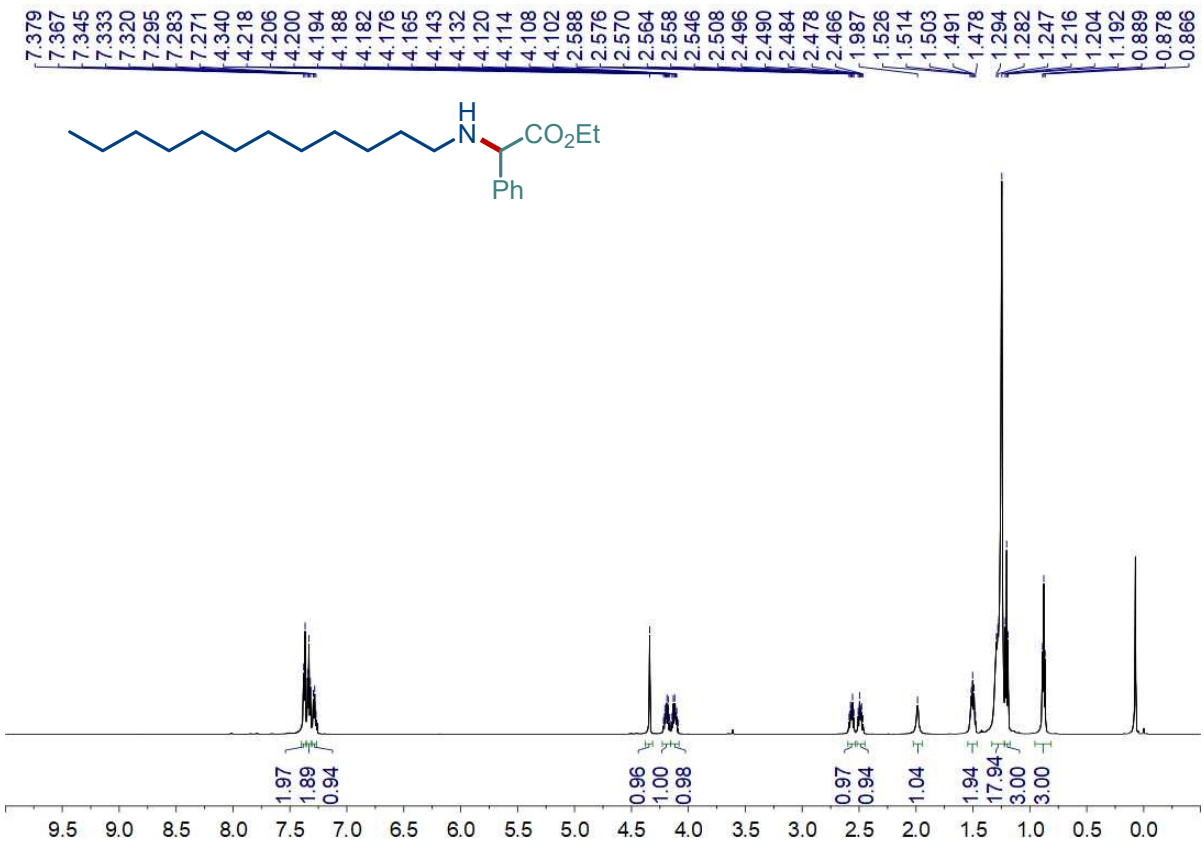
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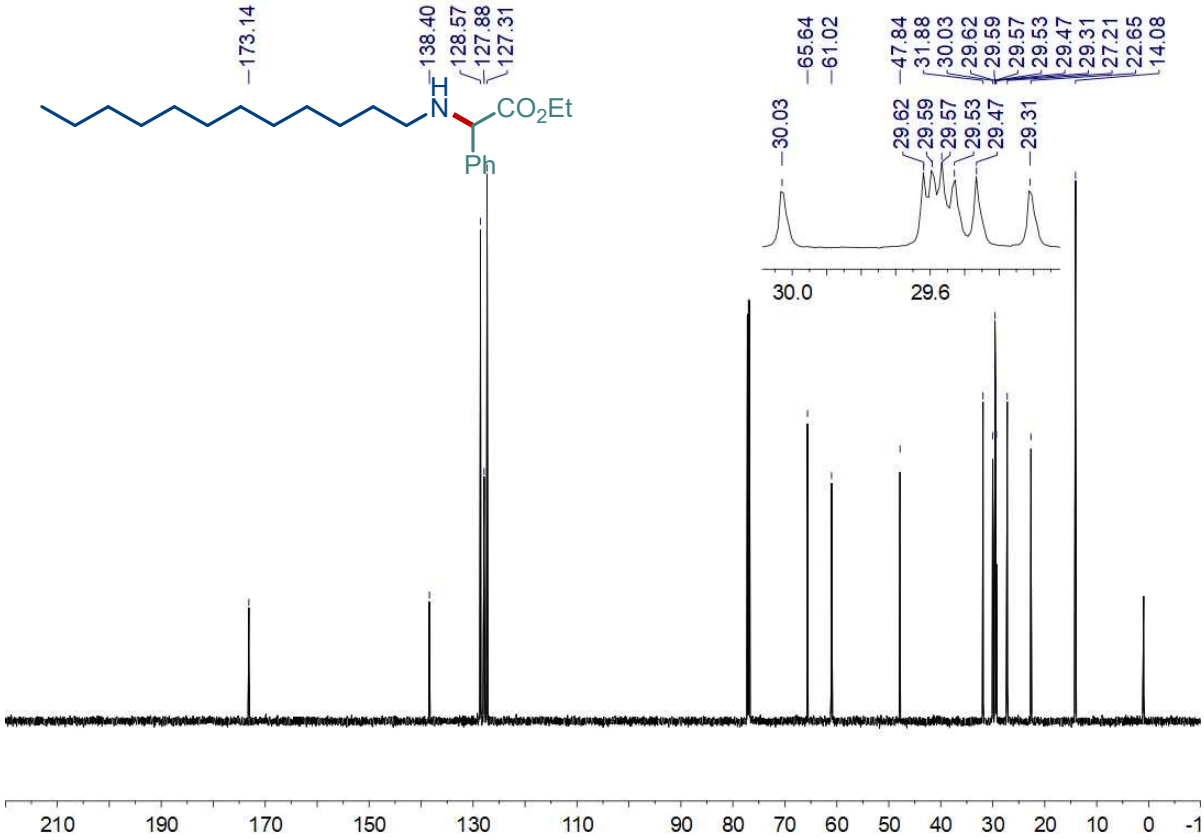
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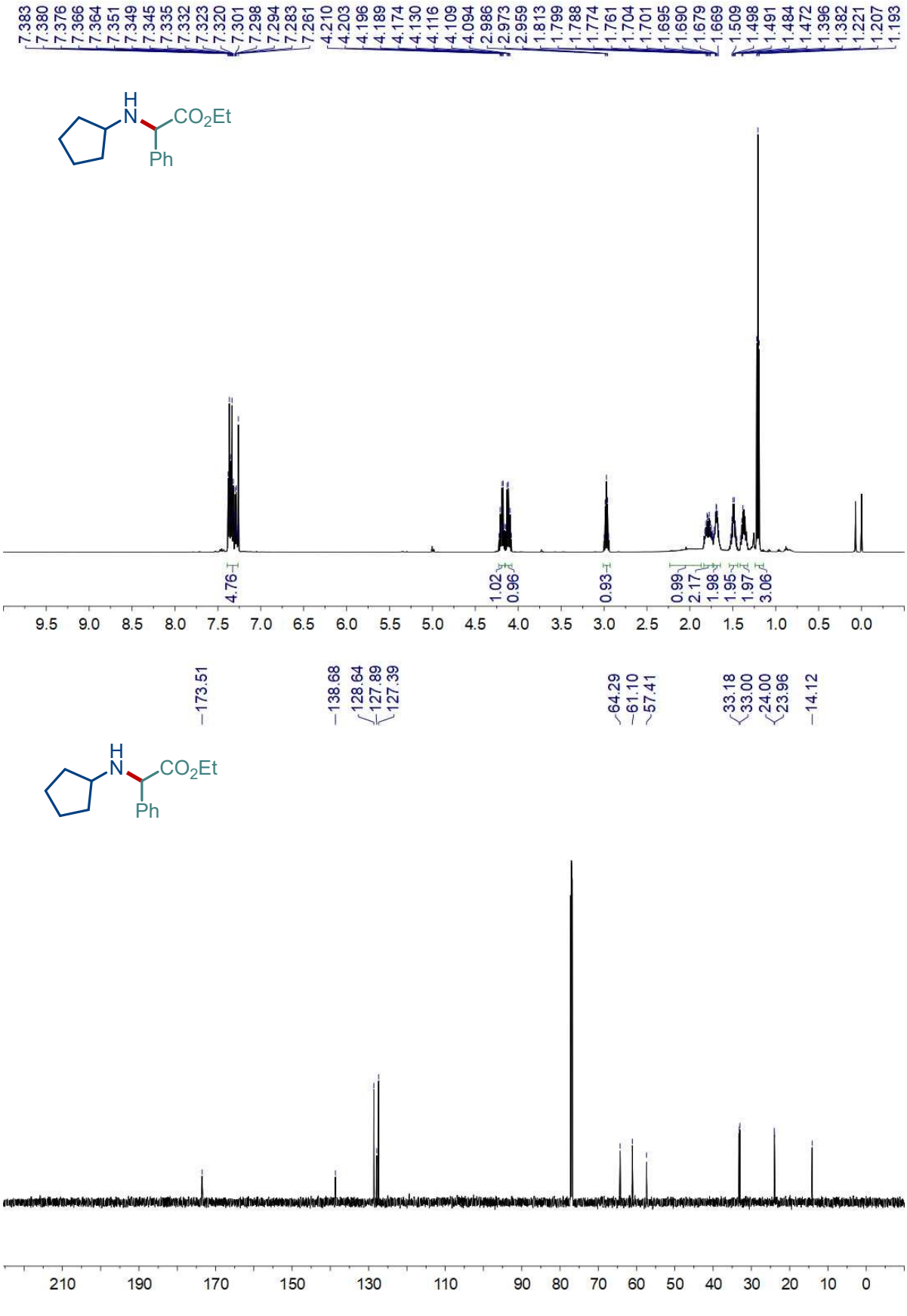
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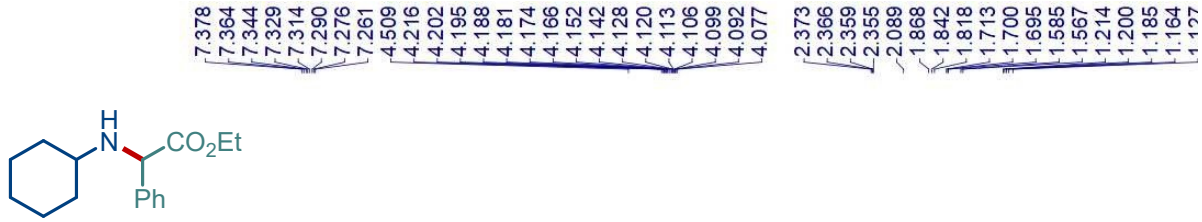
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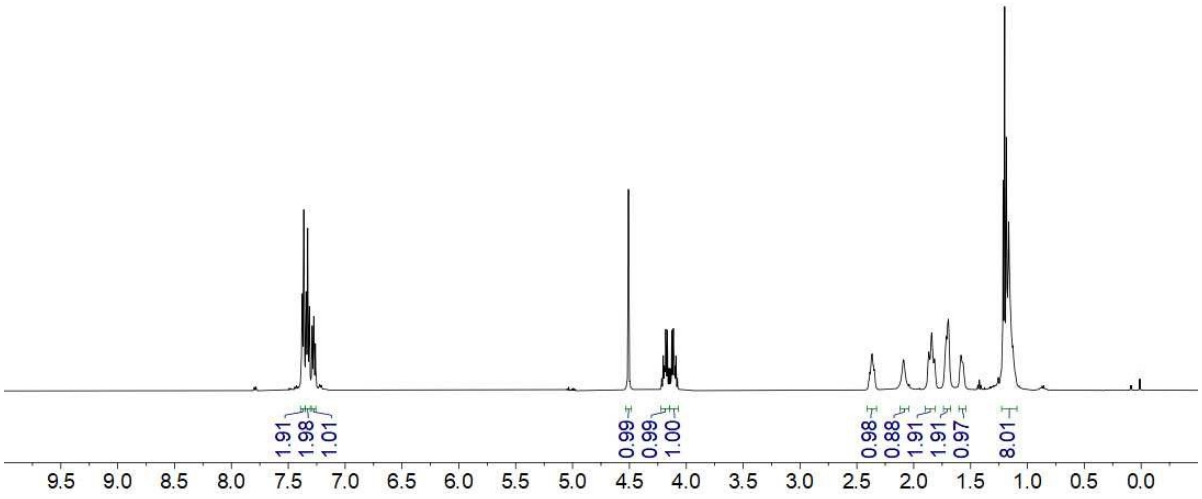
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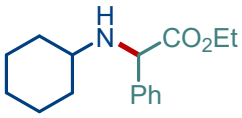
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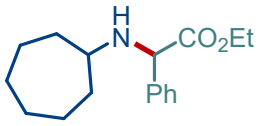
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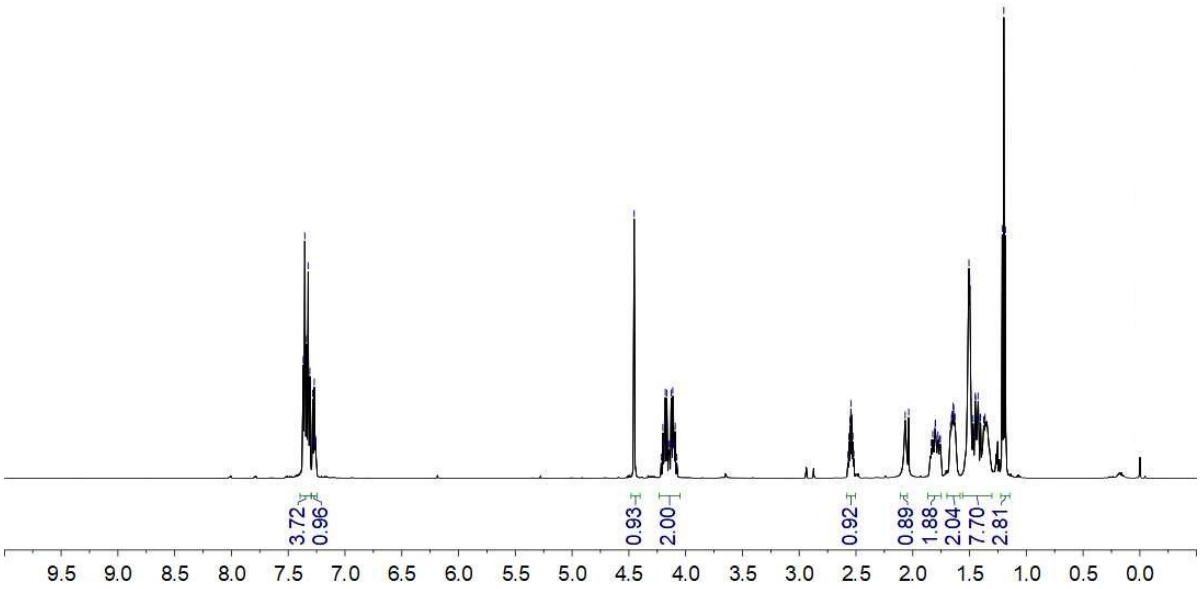
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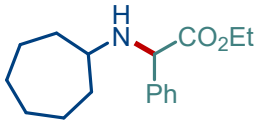
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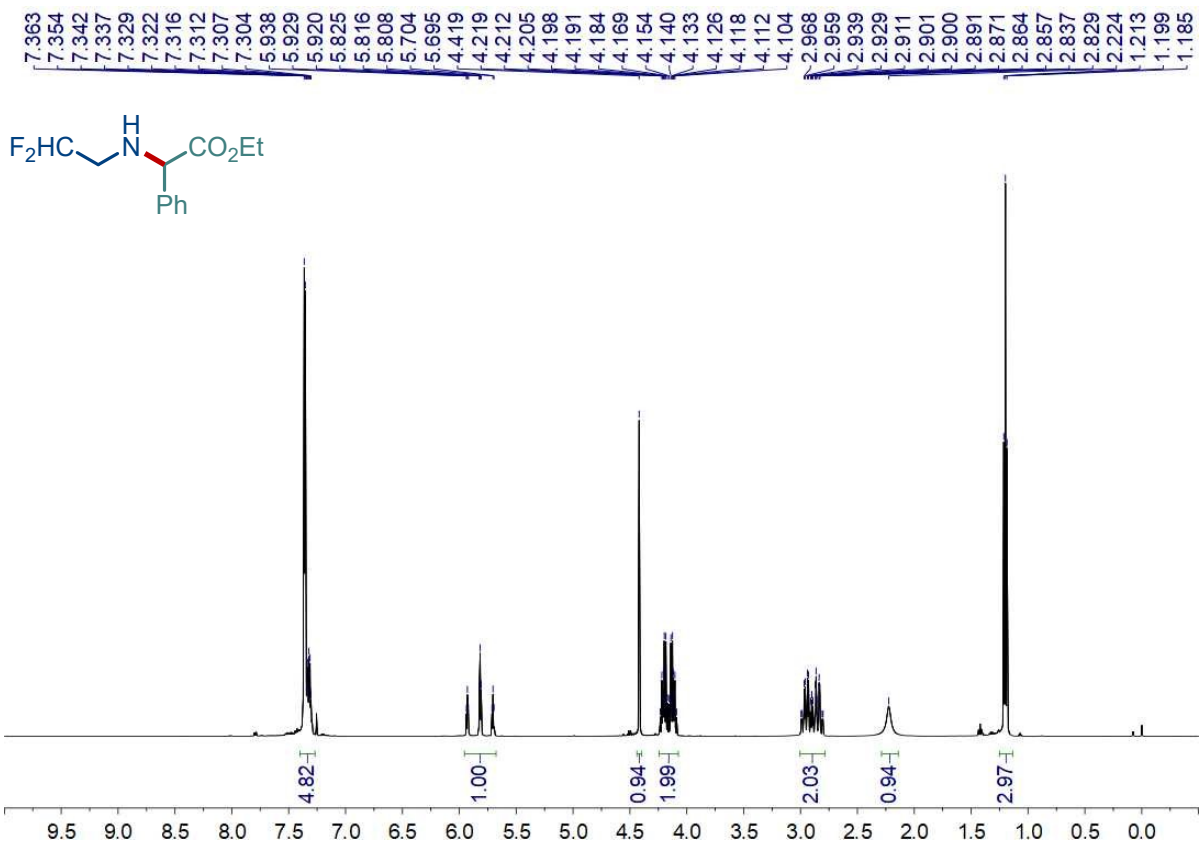
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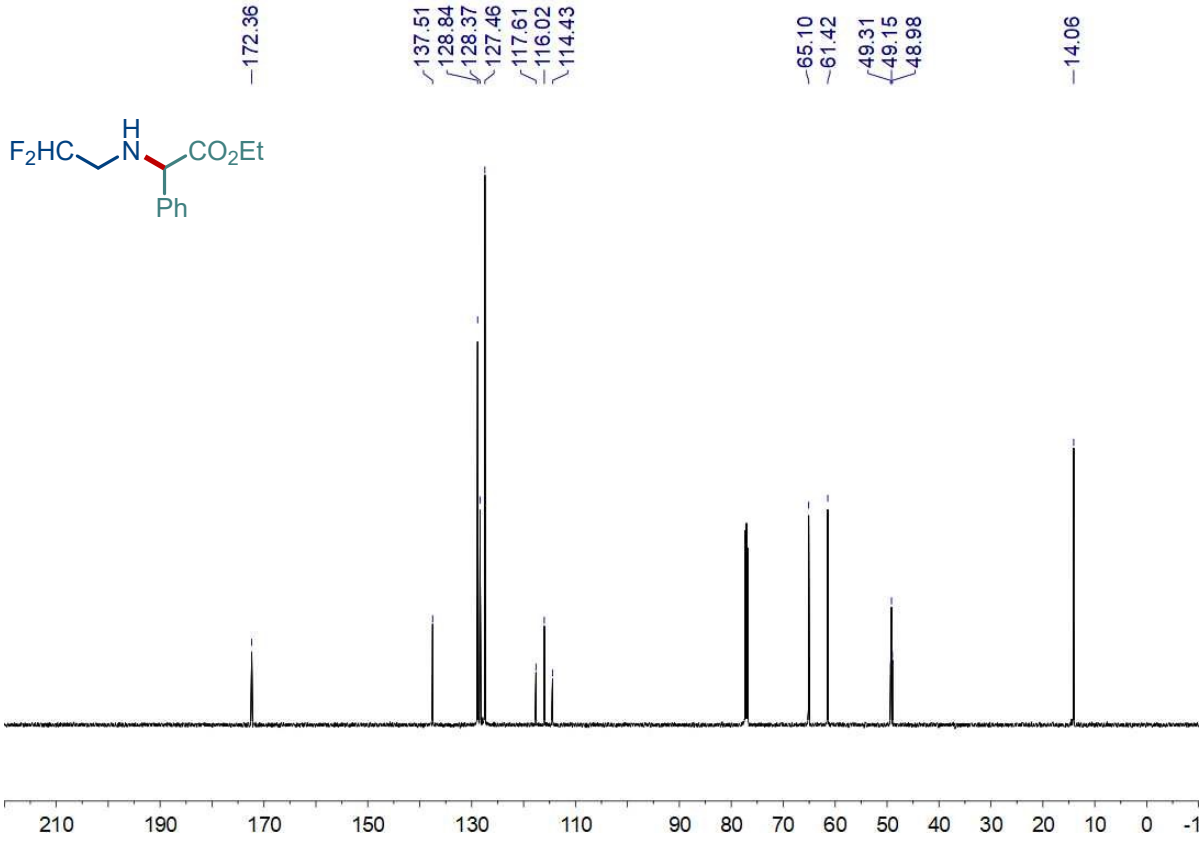
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H
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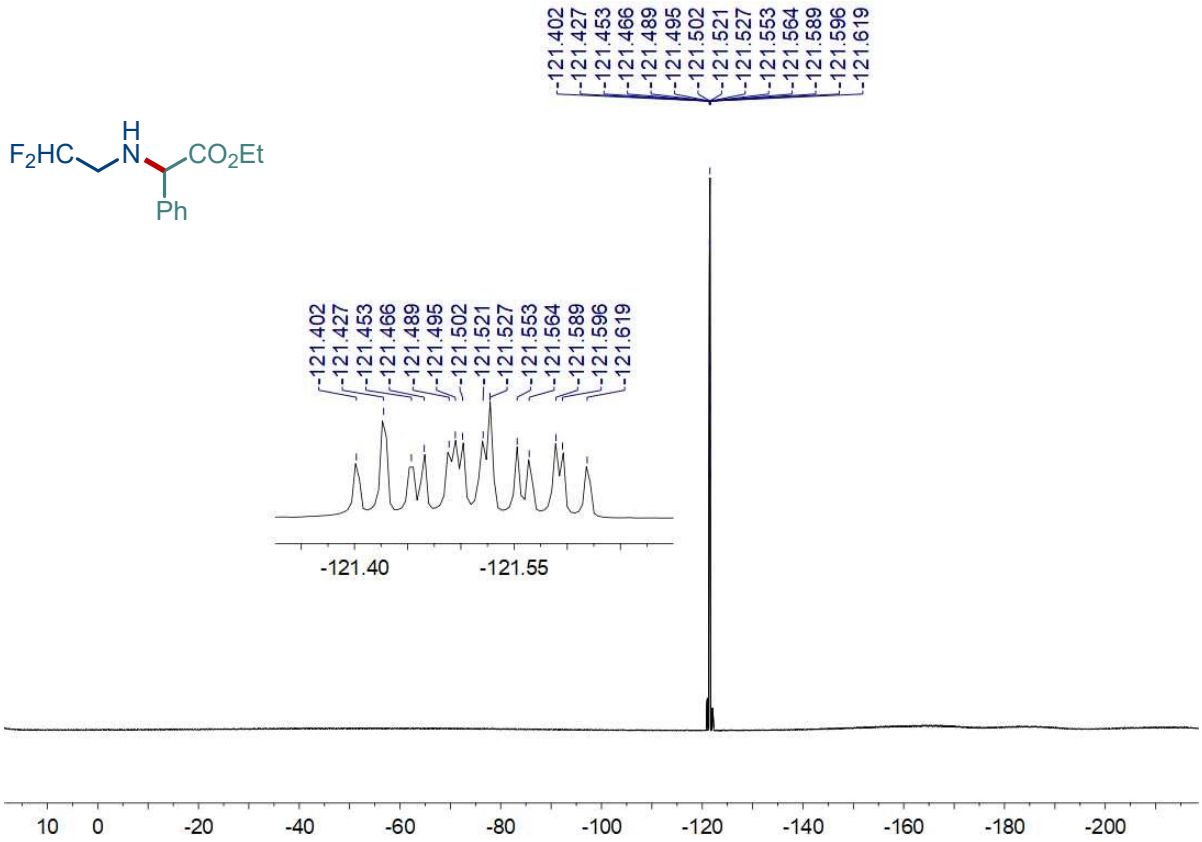
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H
N
CO2Et
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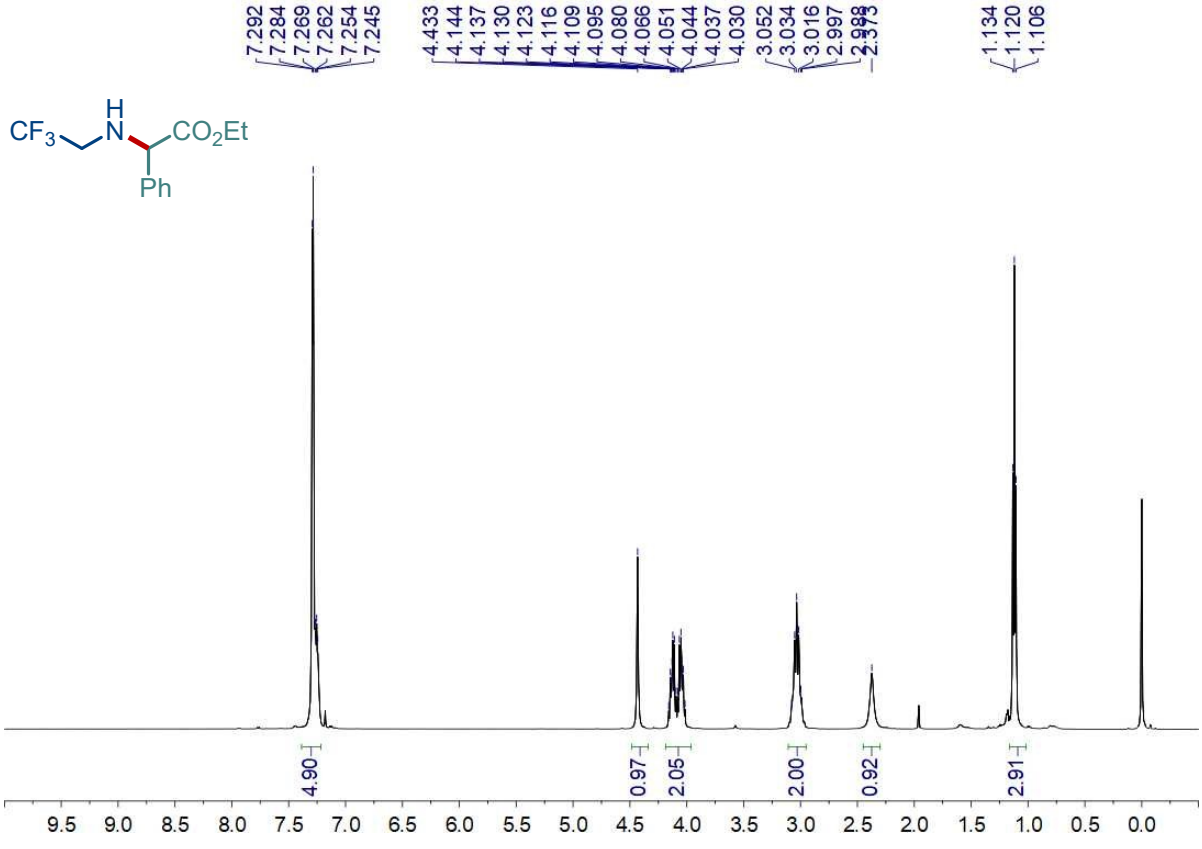
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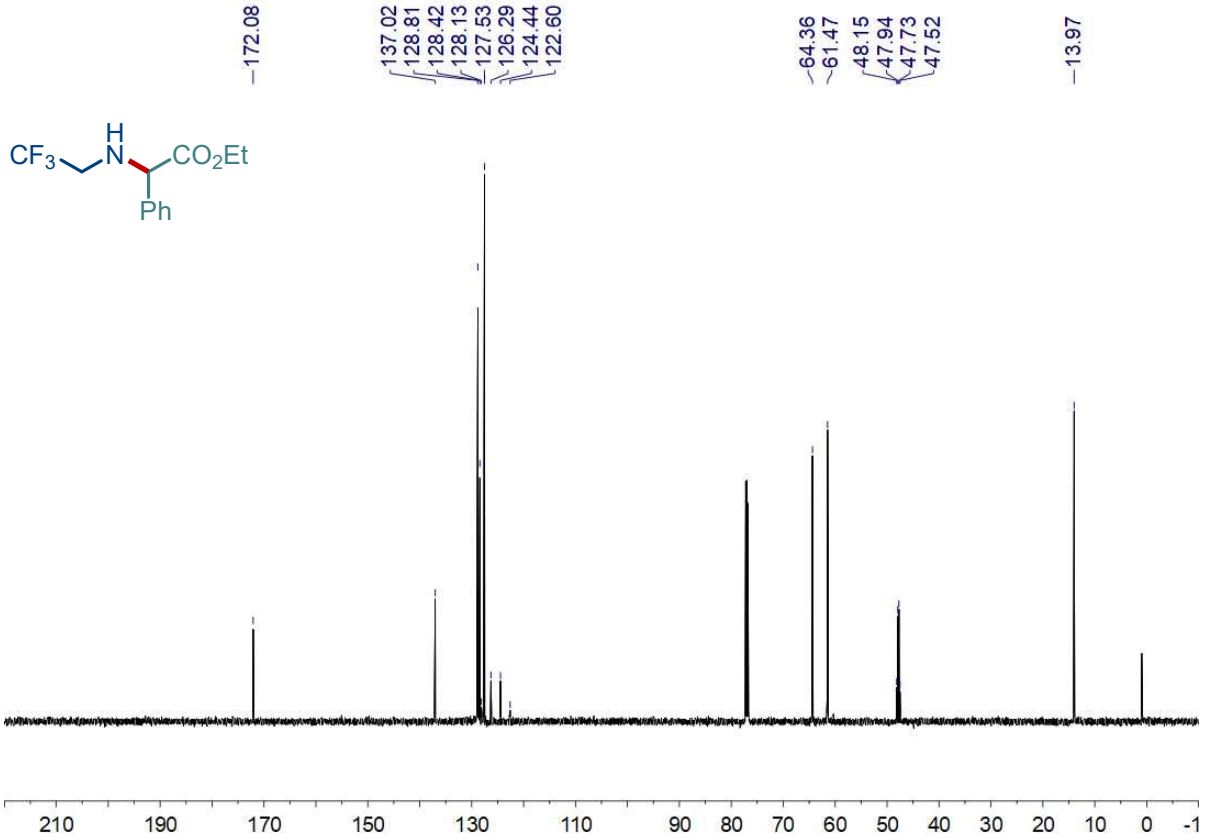
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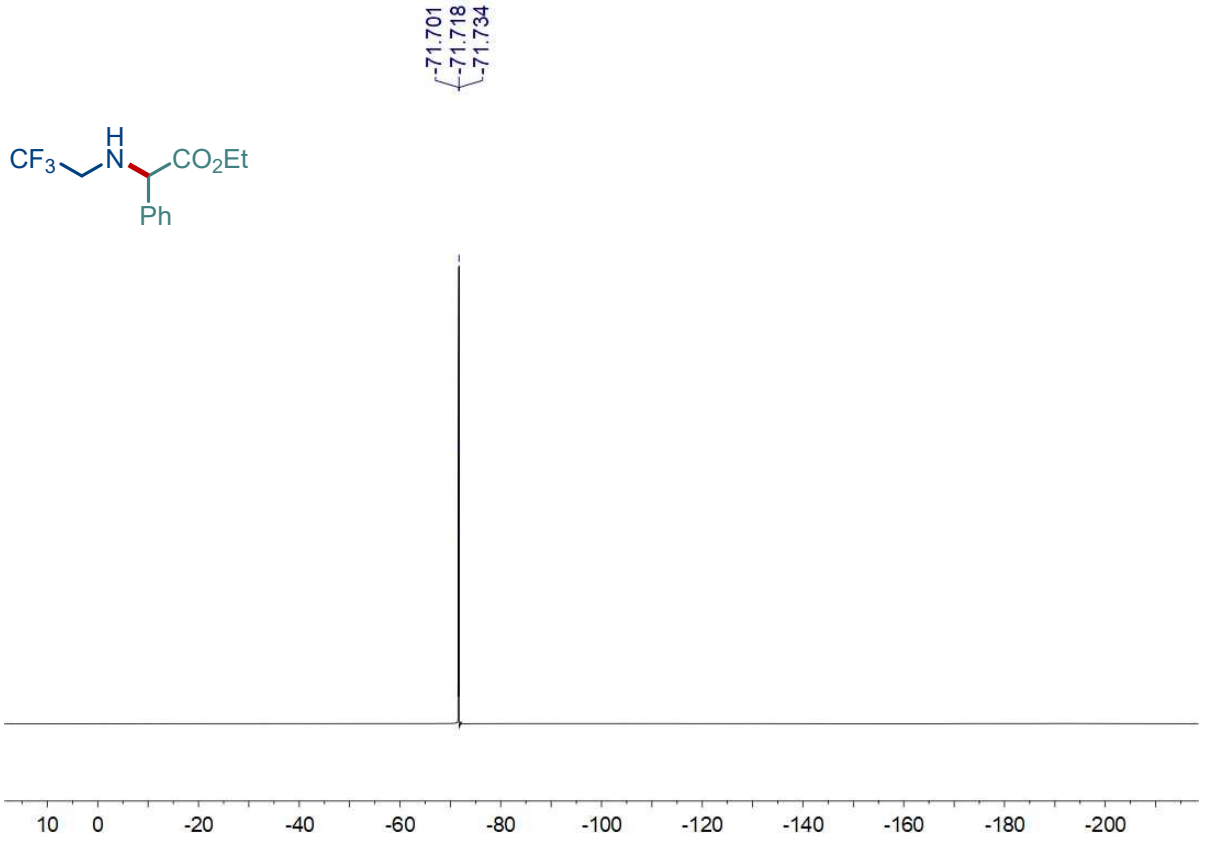
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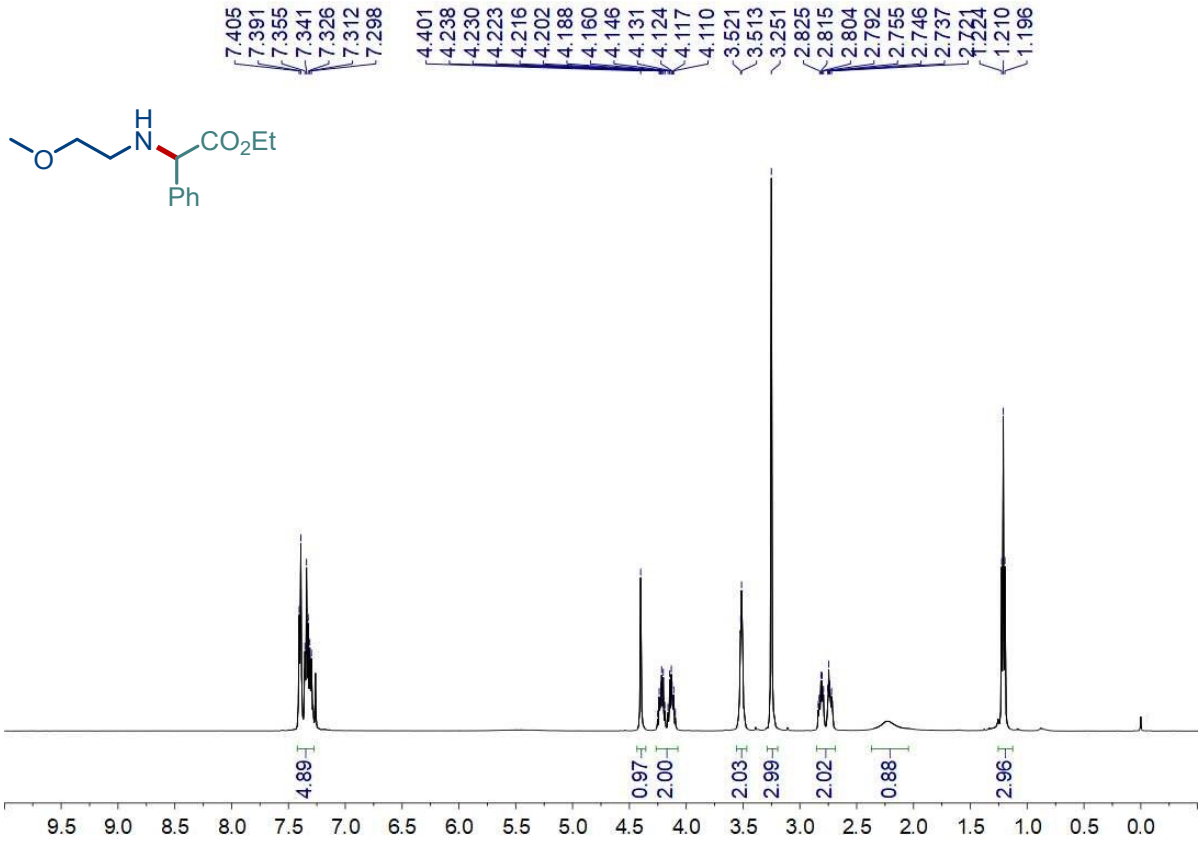
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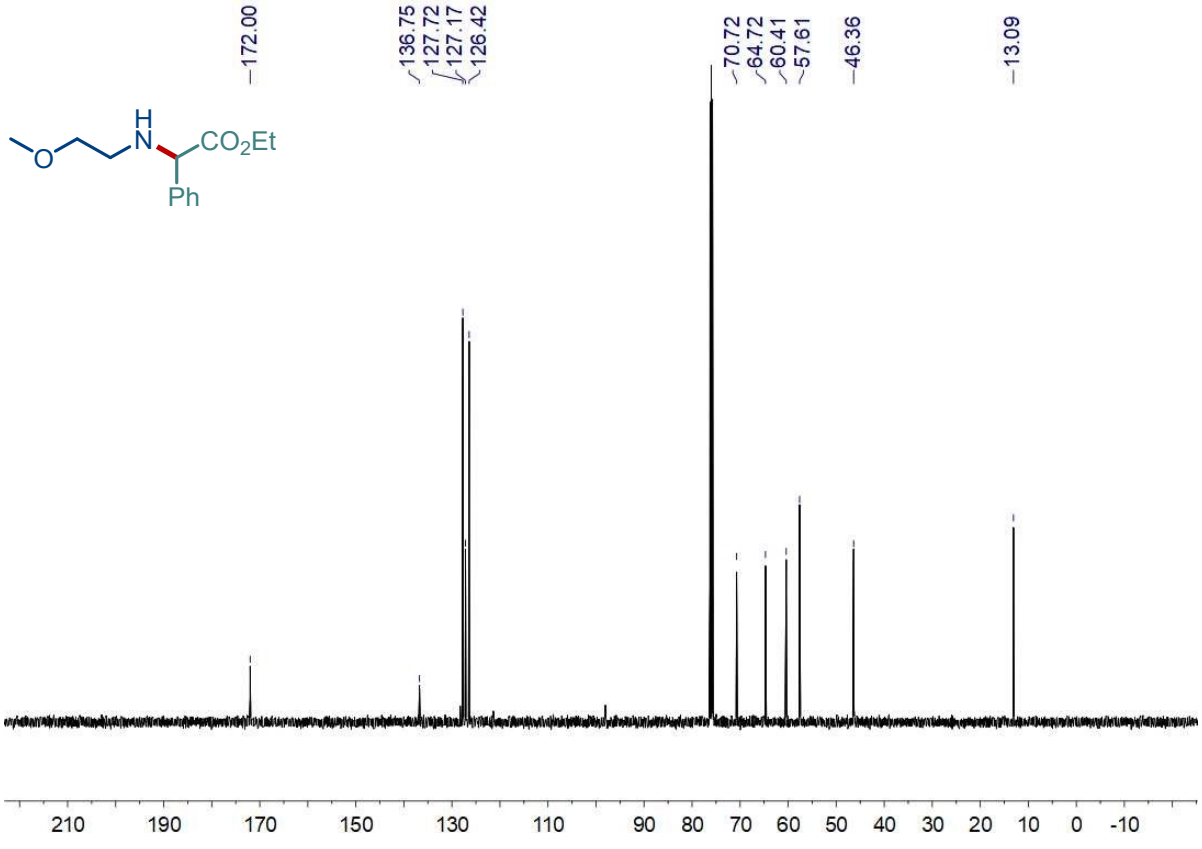
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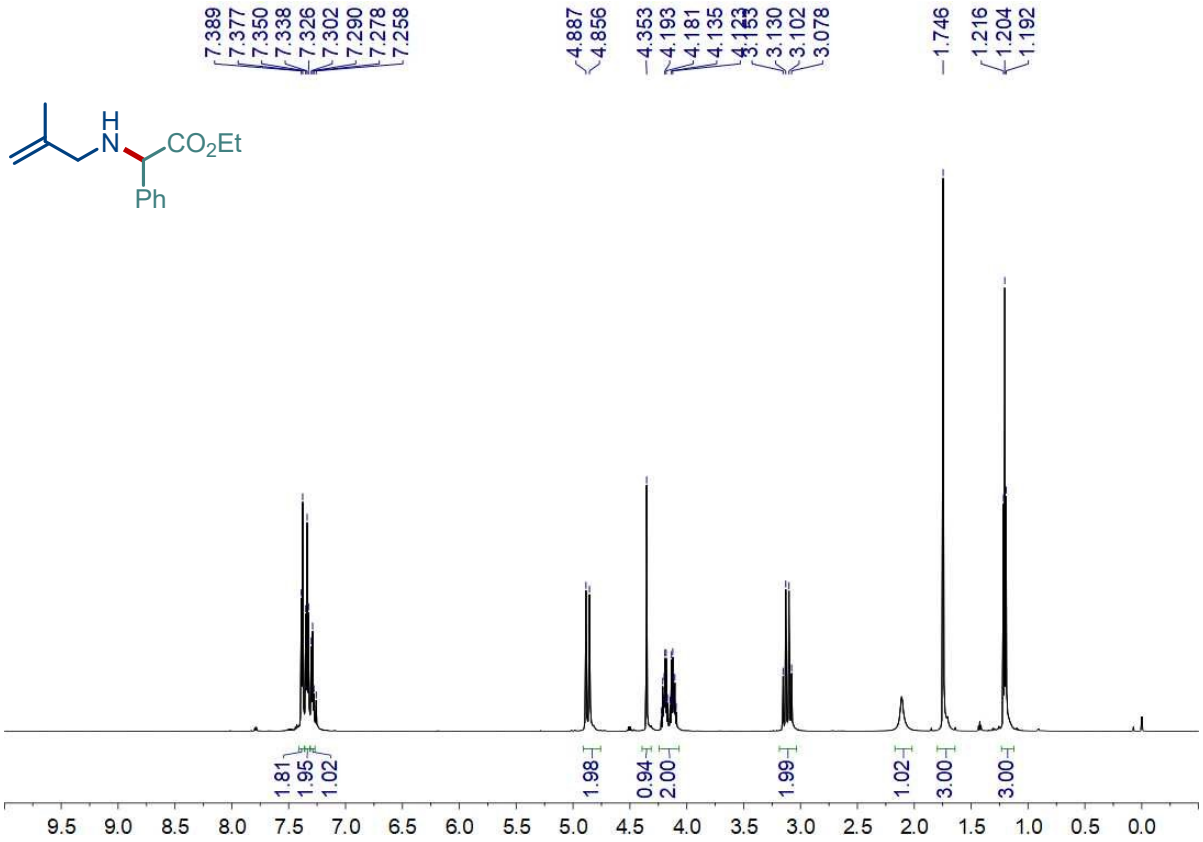
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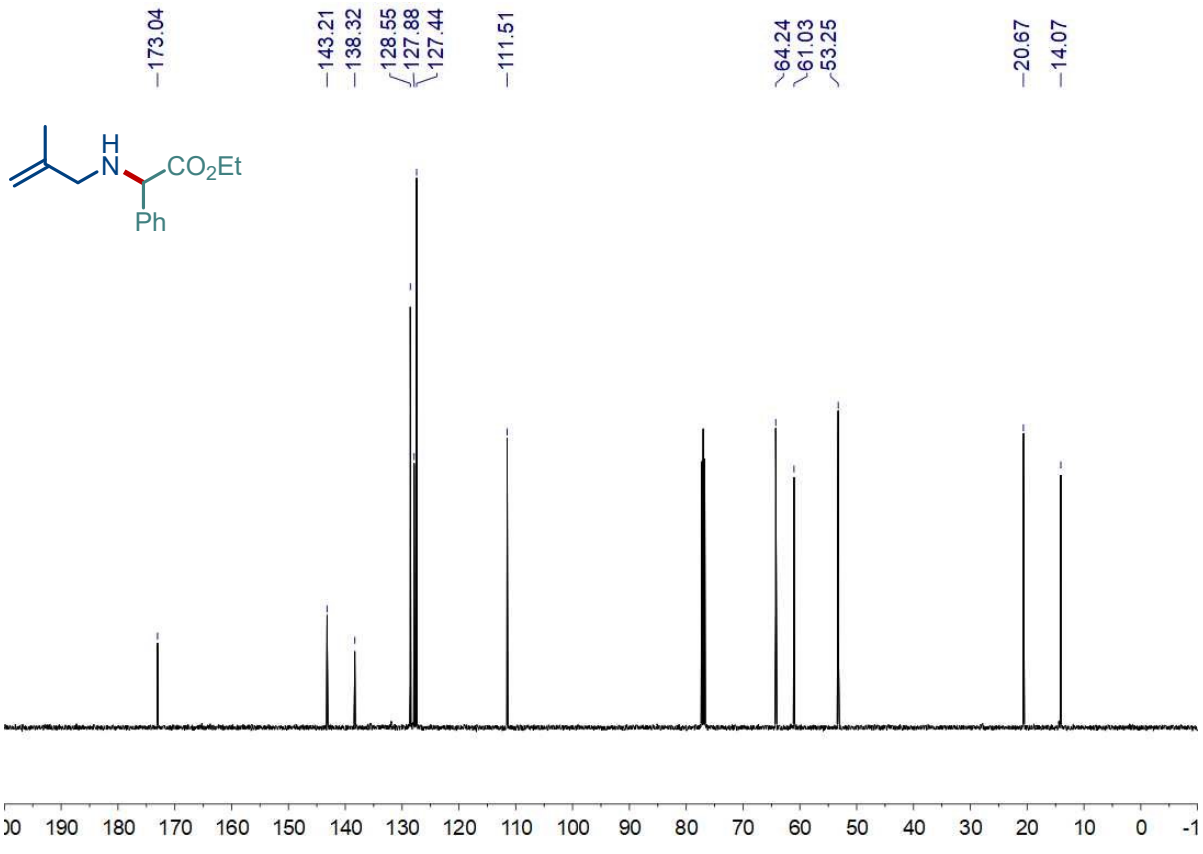
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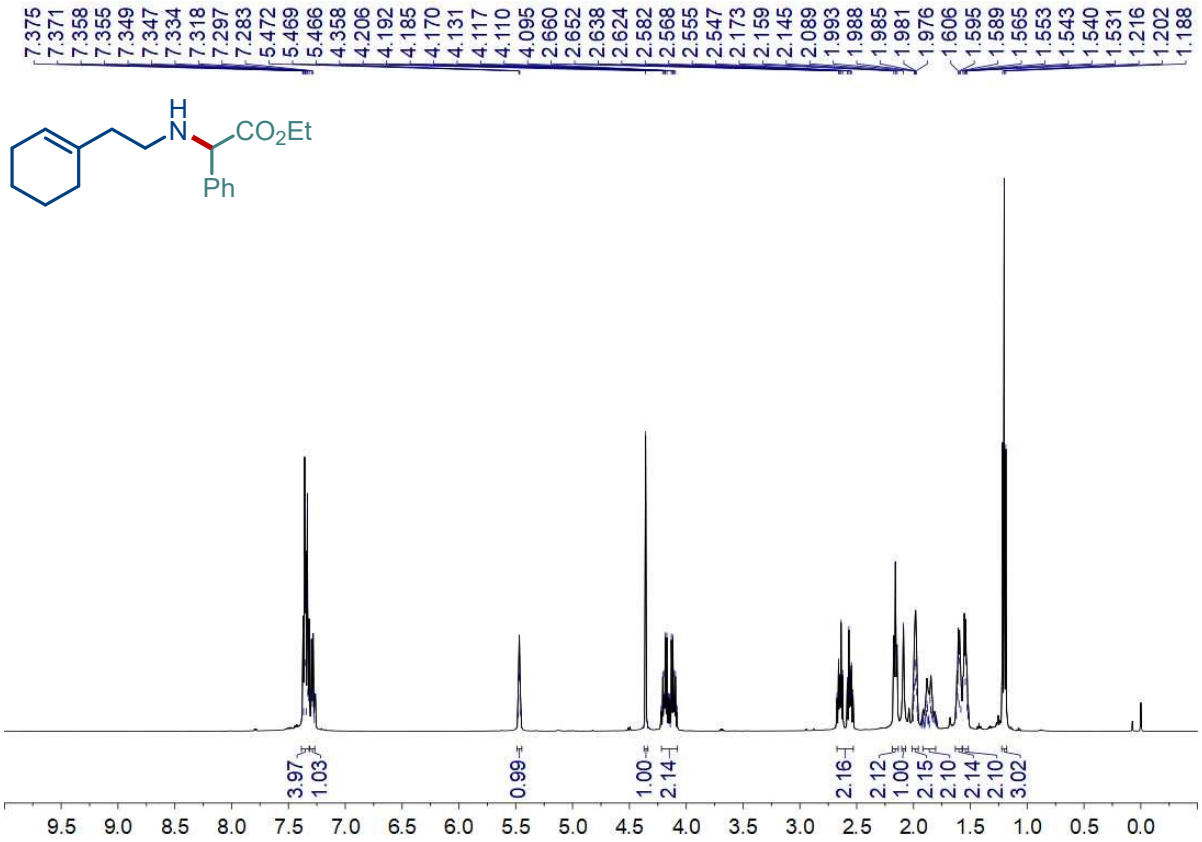
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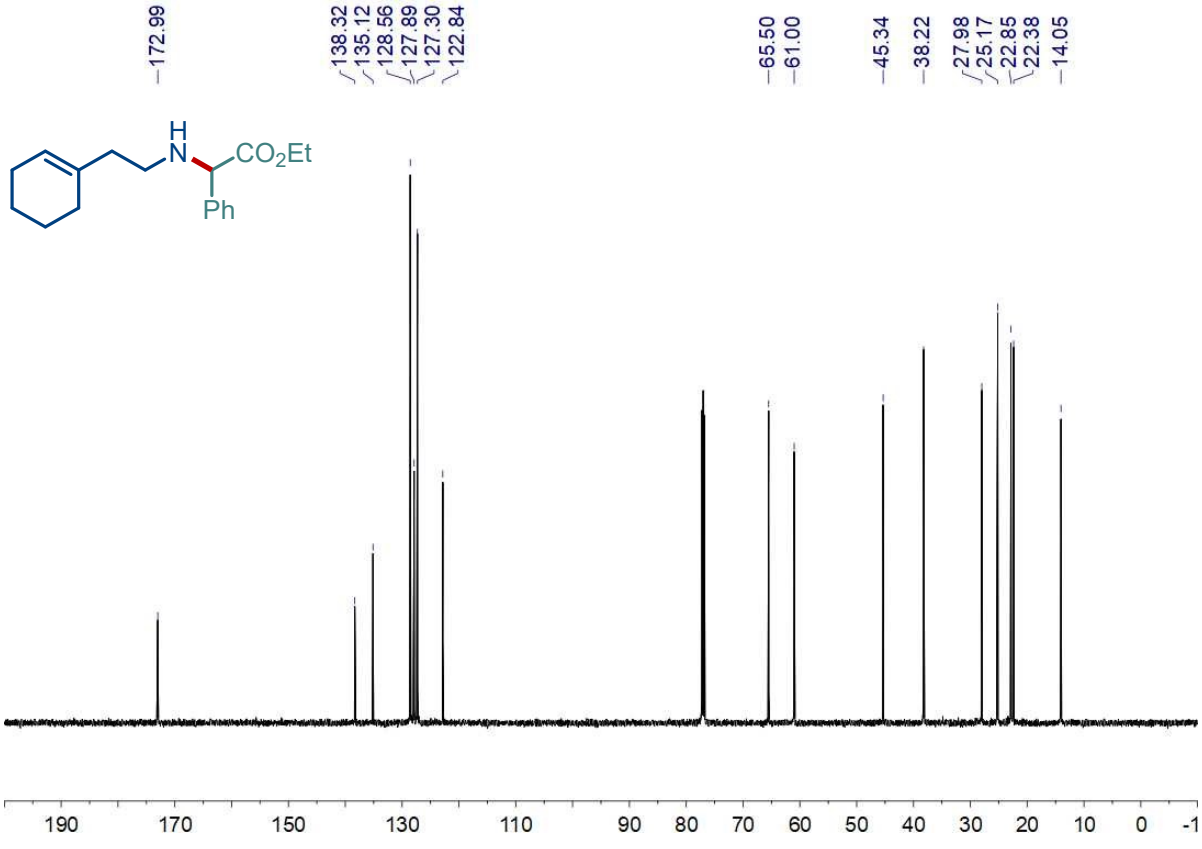
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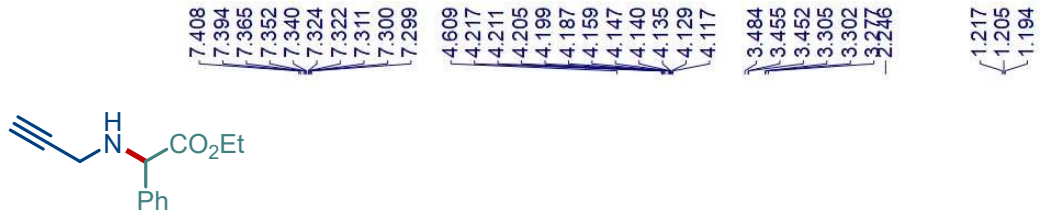
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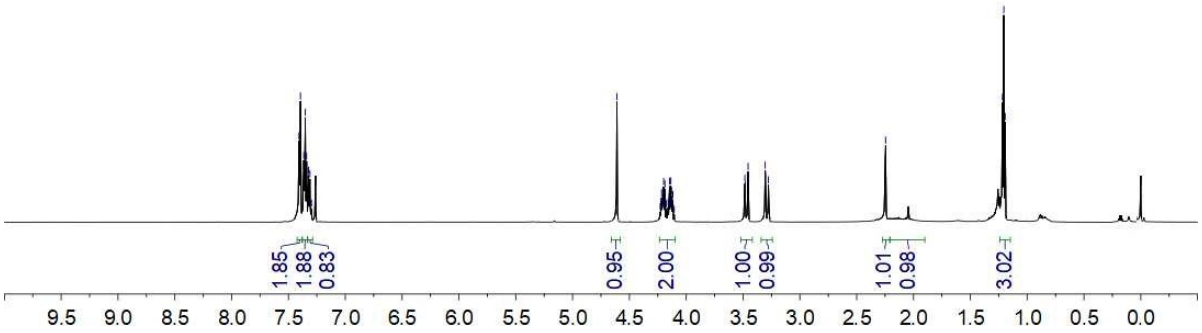
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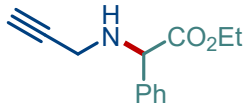
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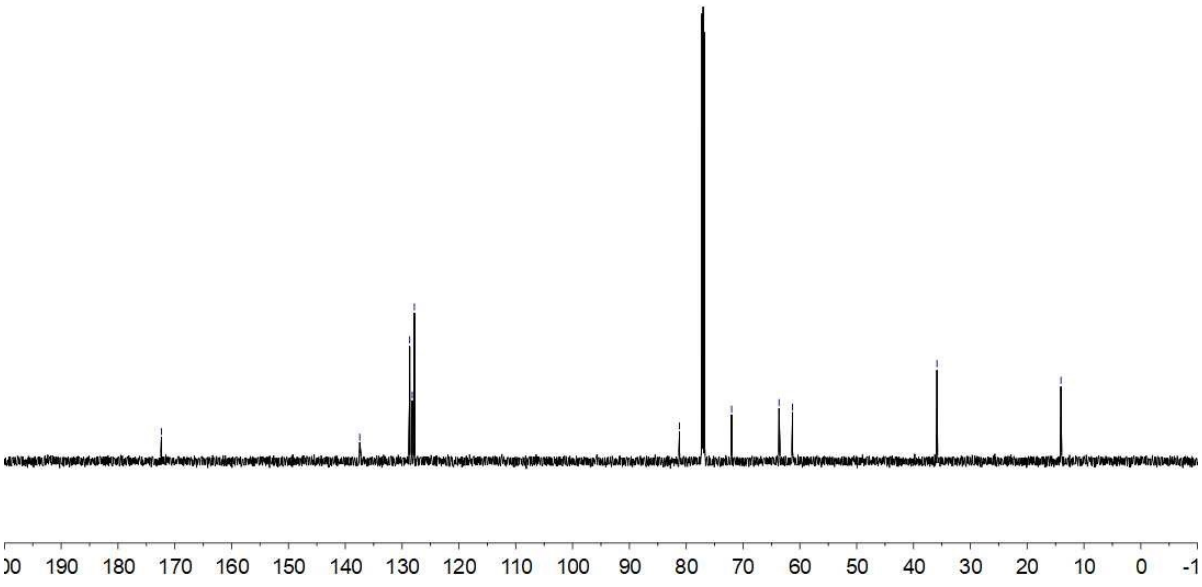
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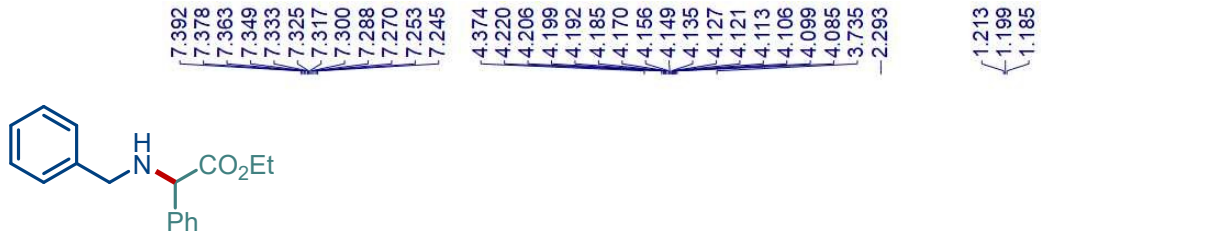
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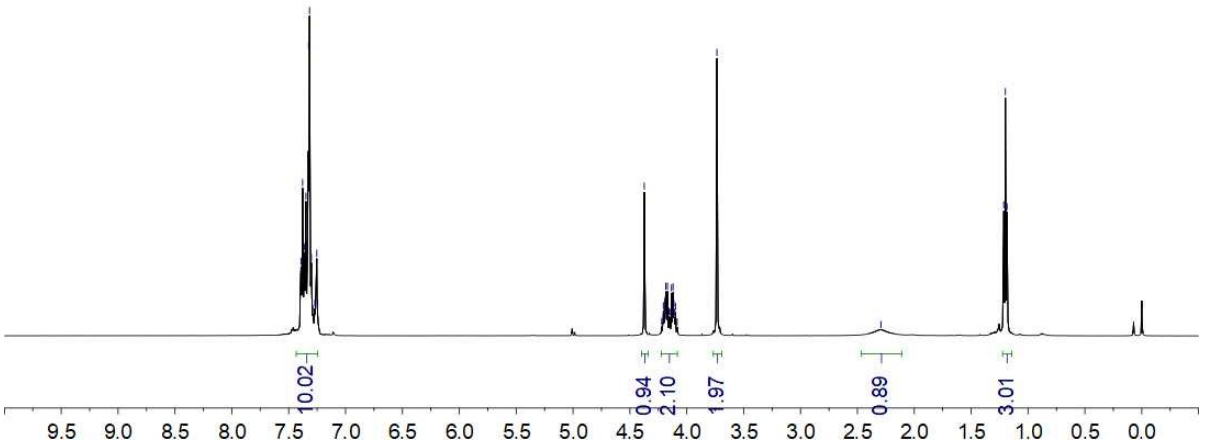
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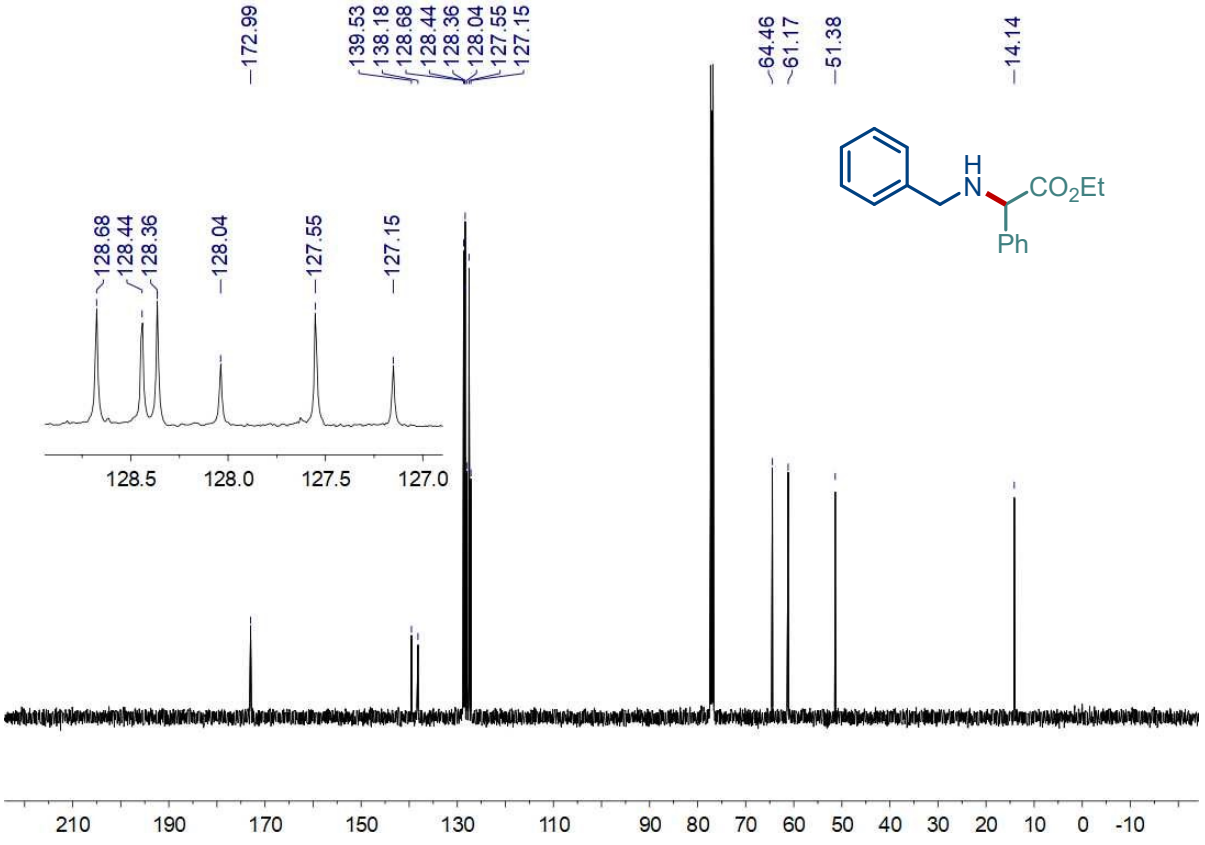
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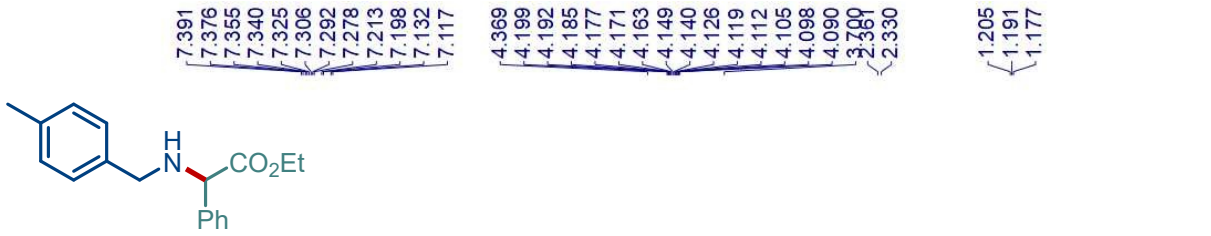
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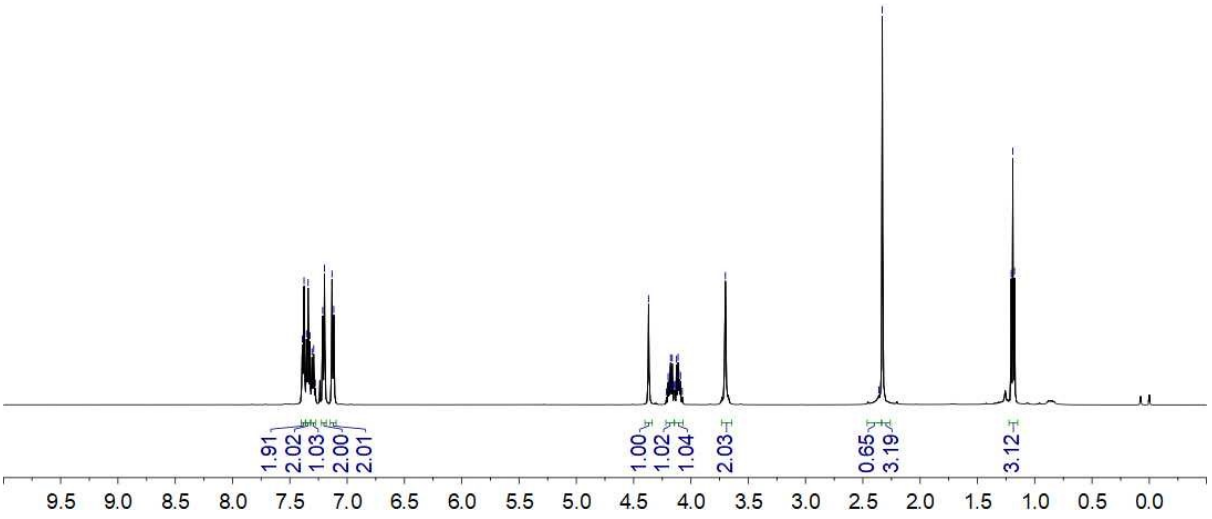
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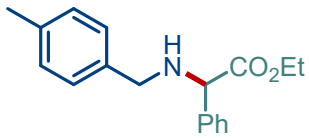
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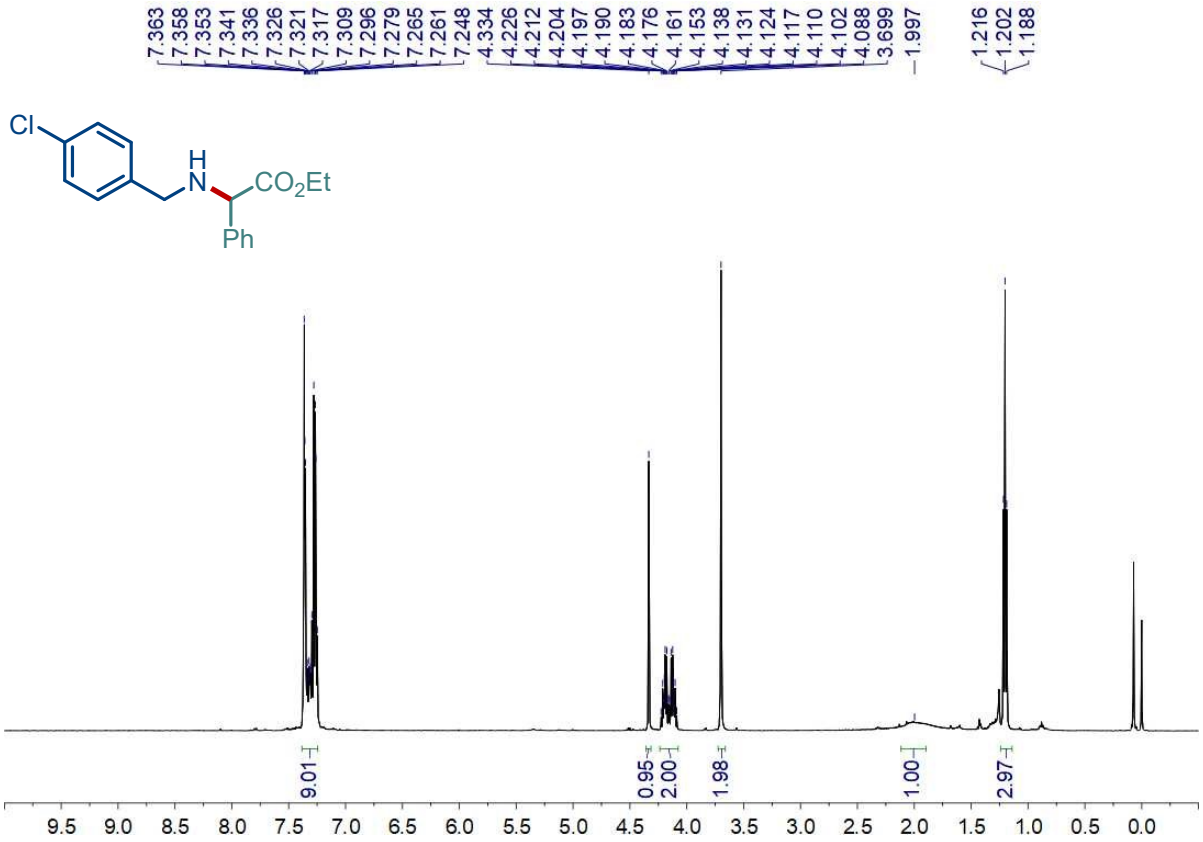
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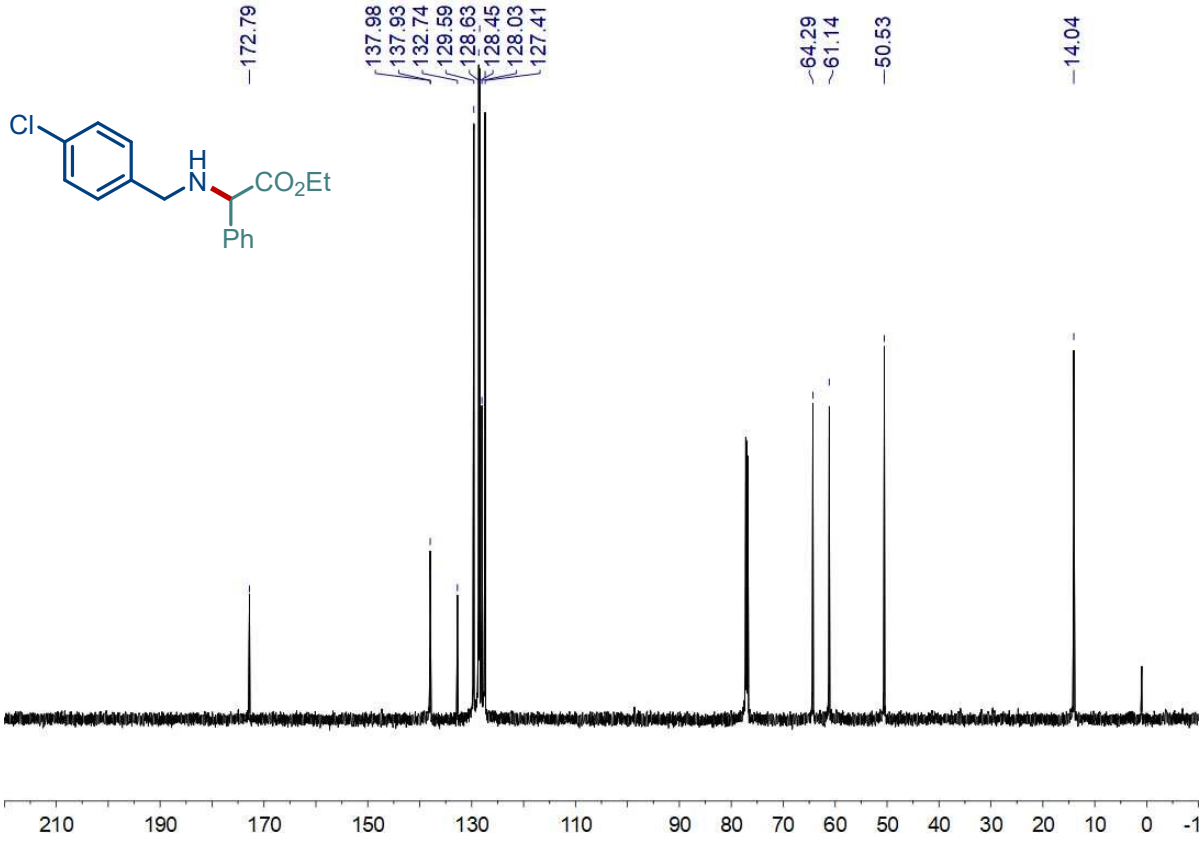
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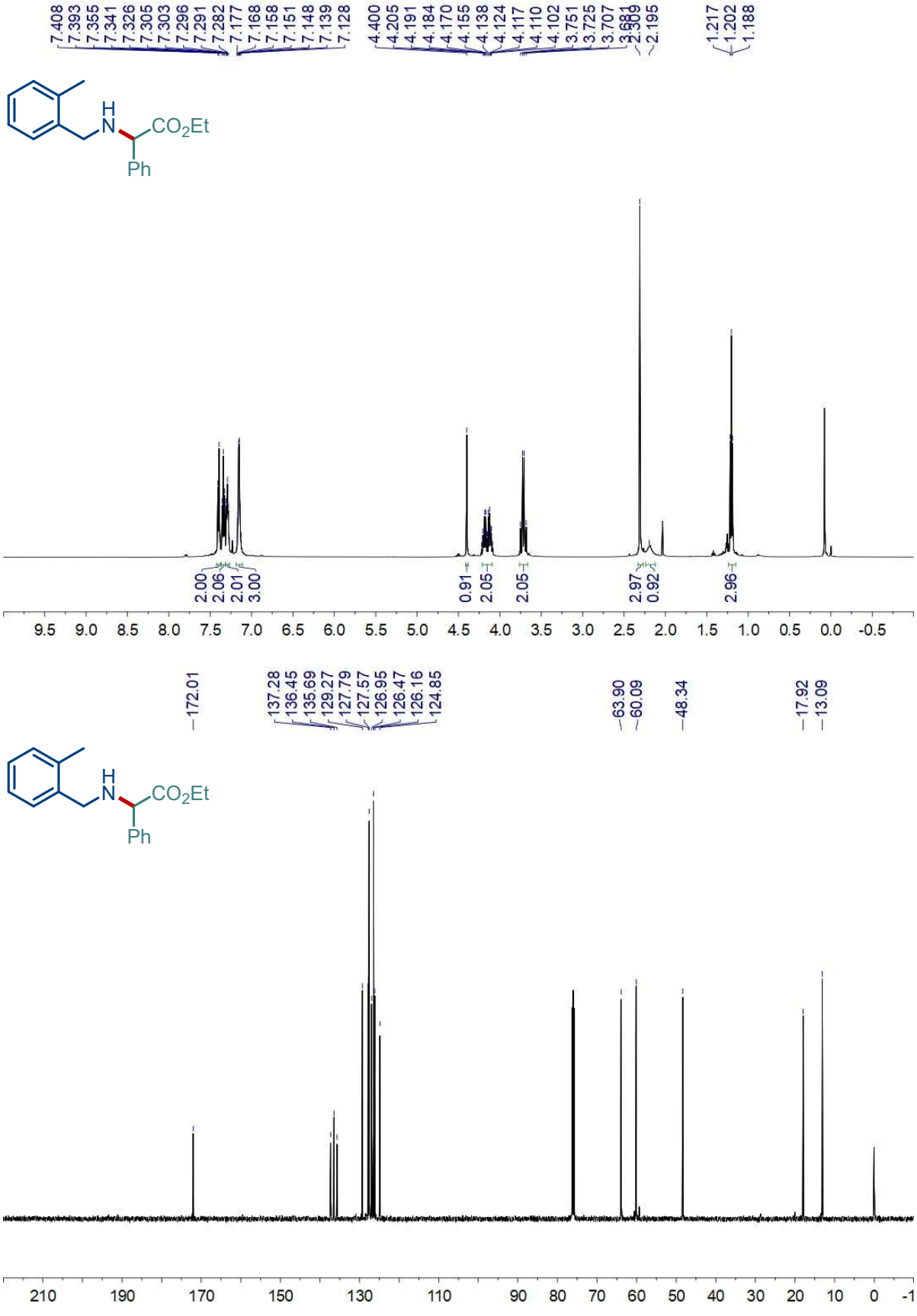
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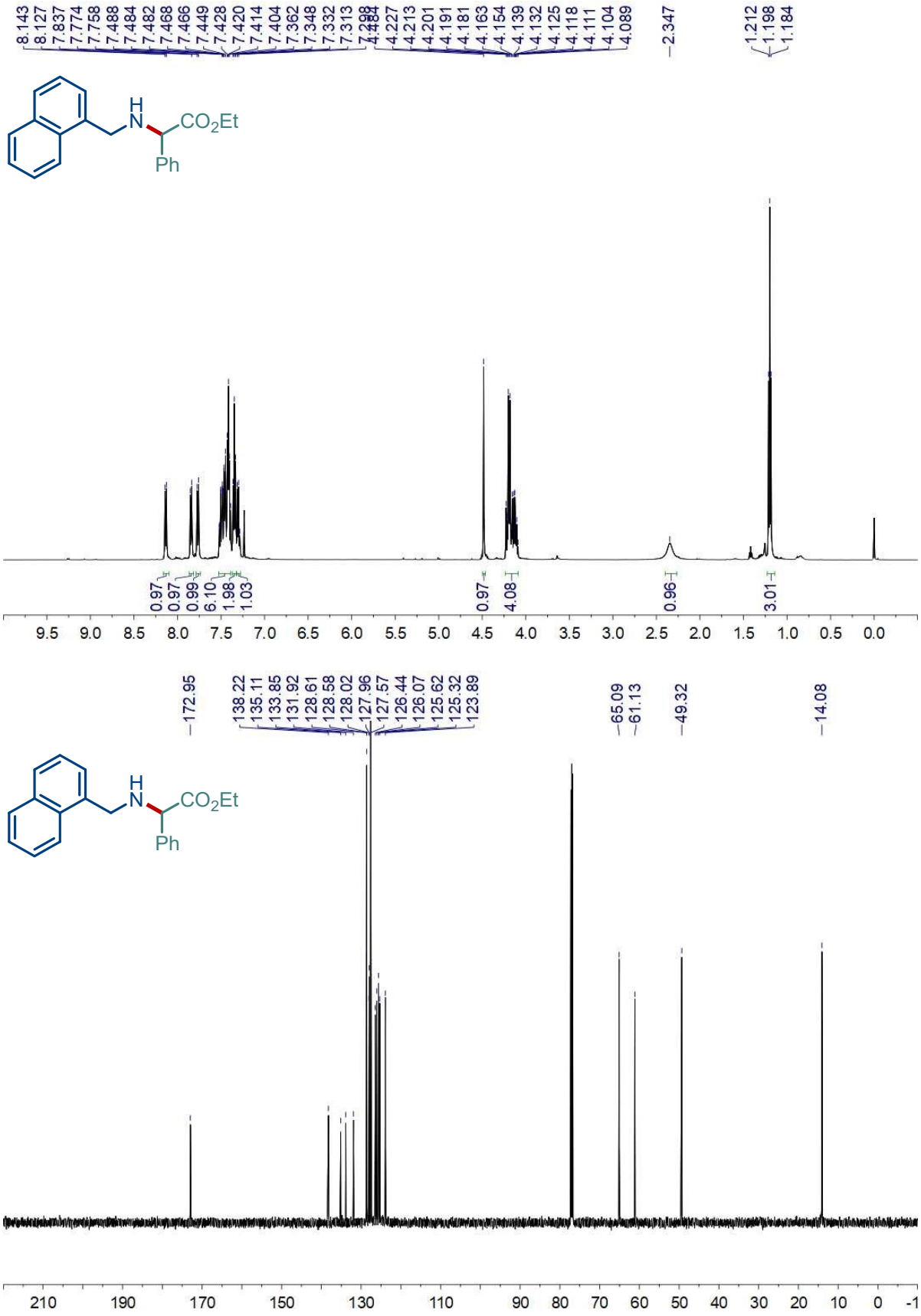
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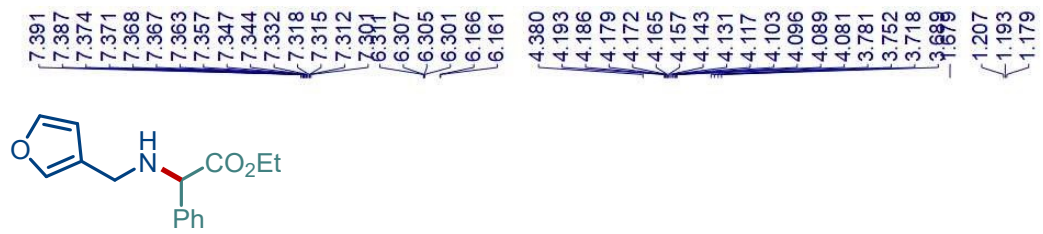
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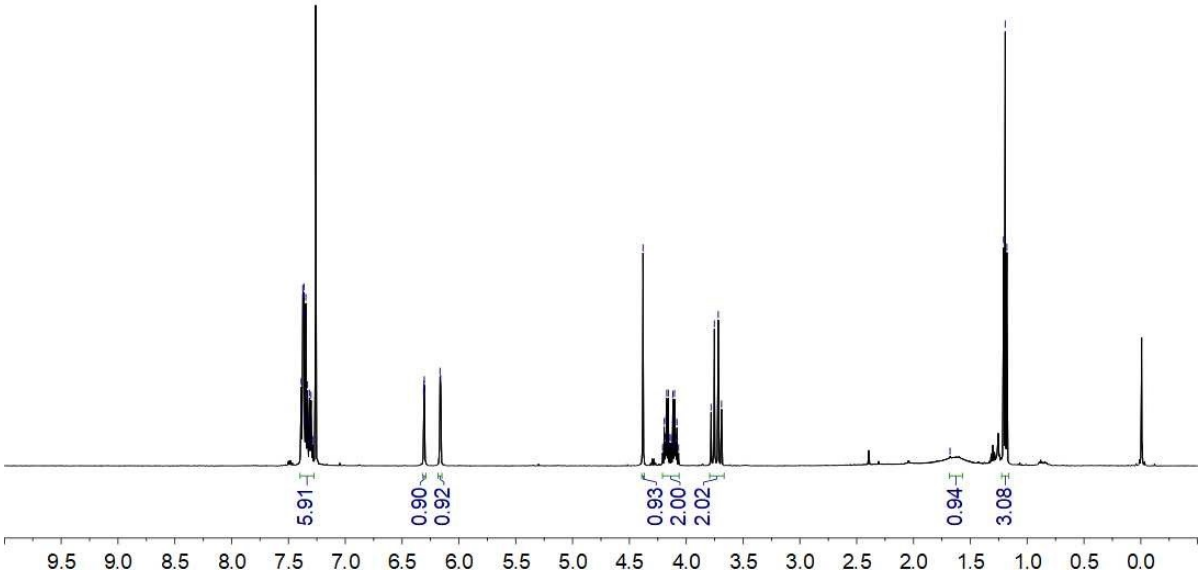
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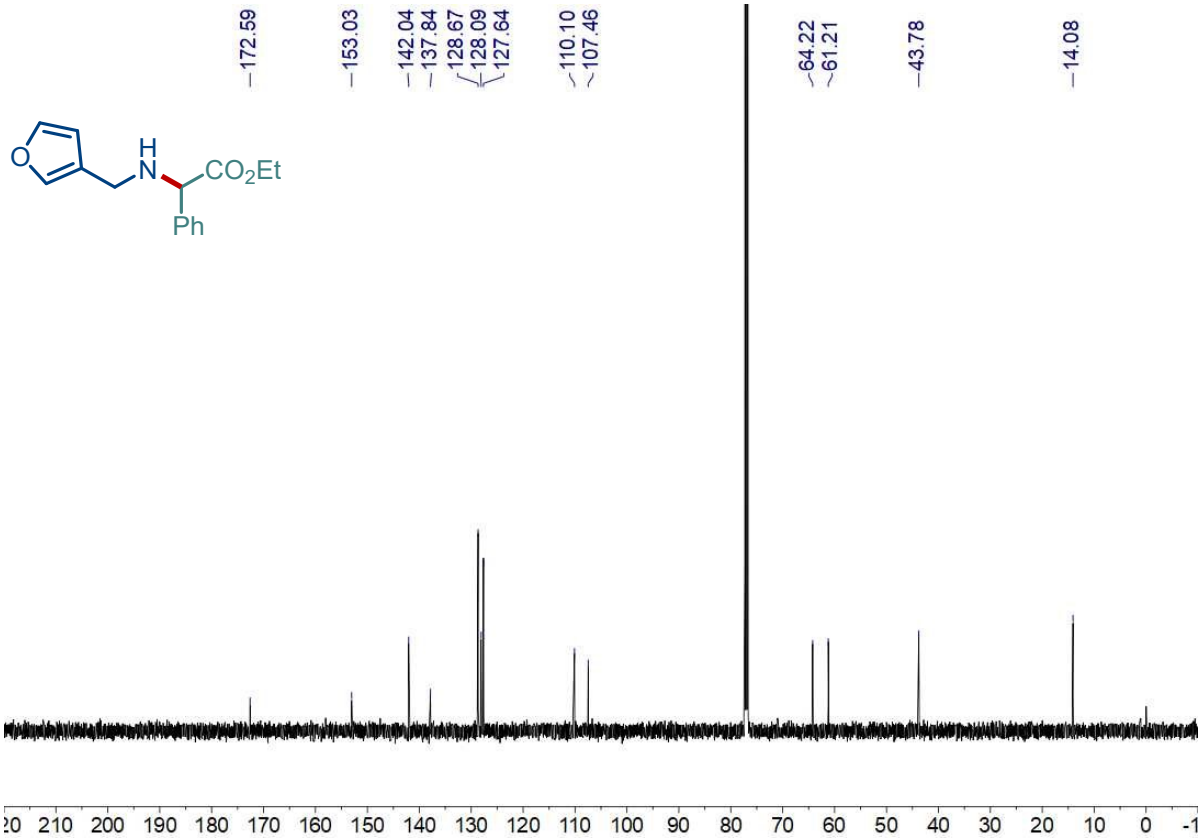
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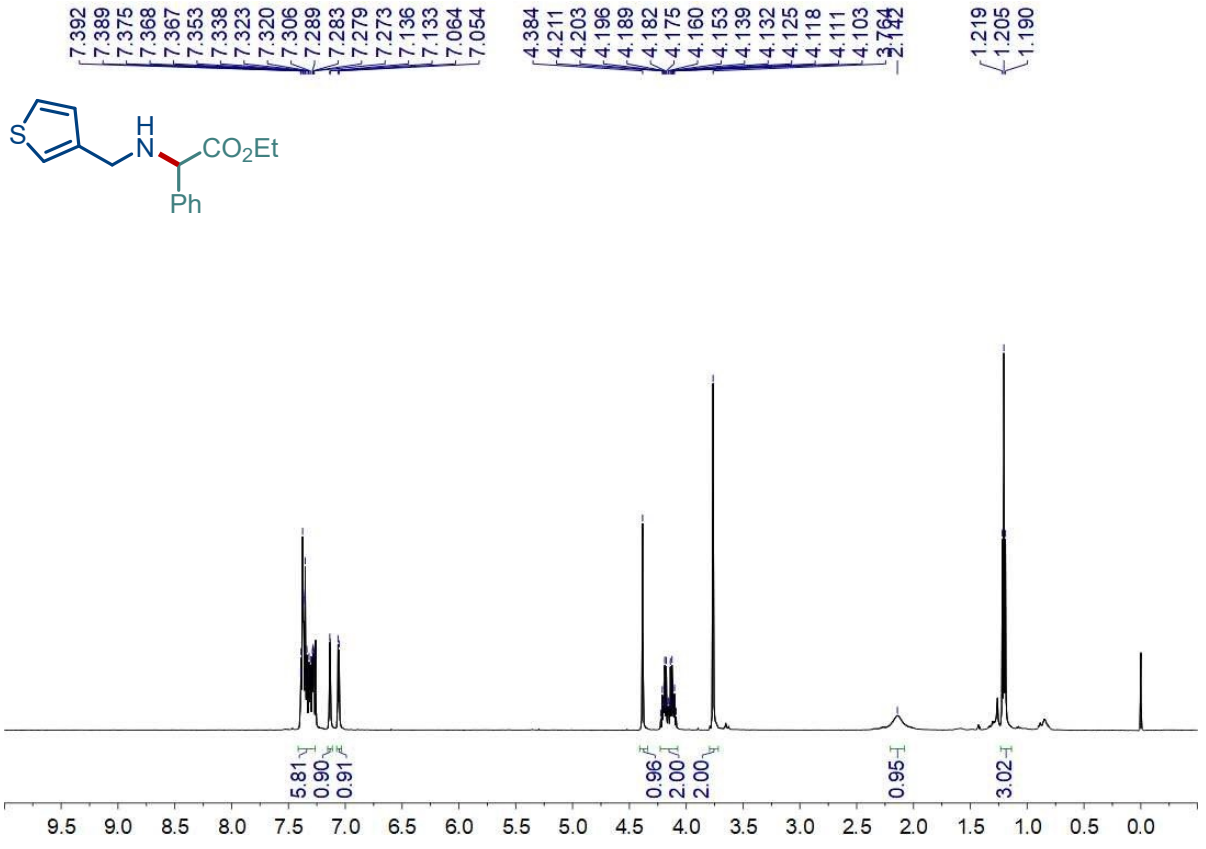
CO2Et
Ph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N
CO2Et
Ph
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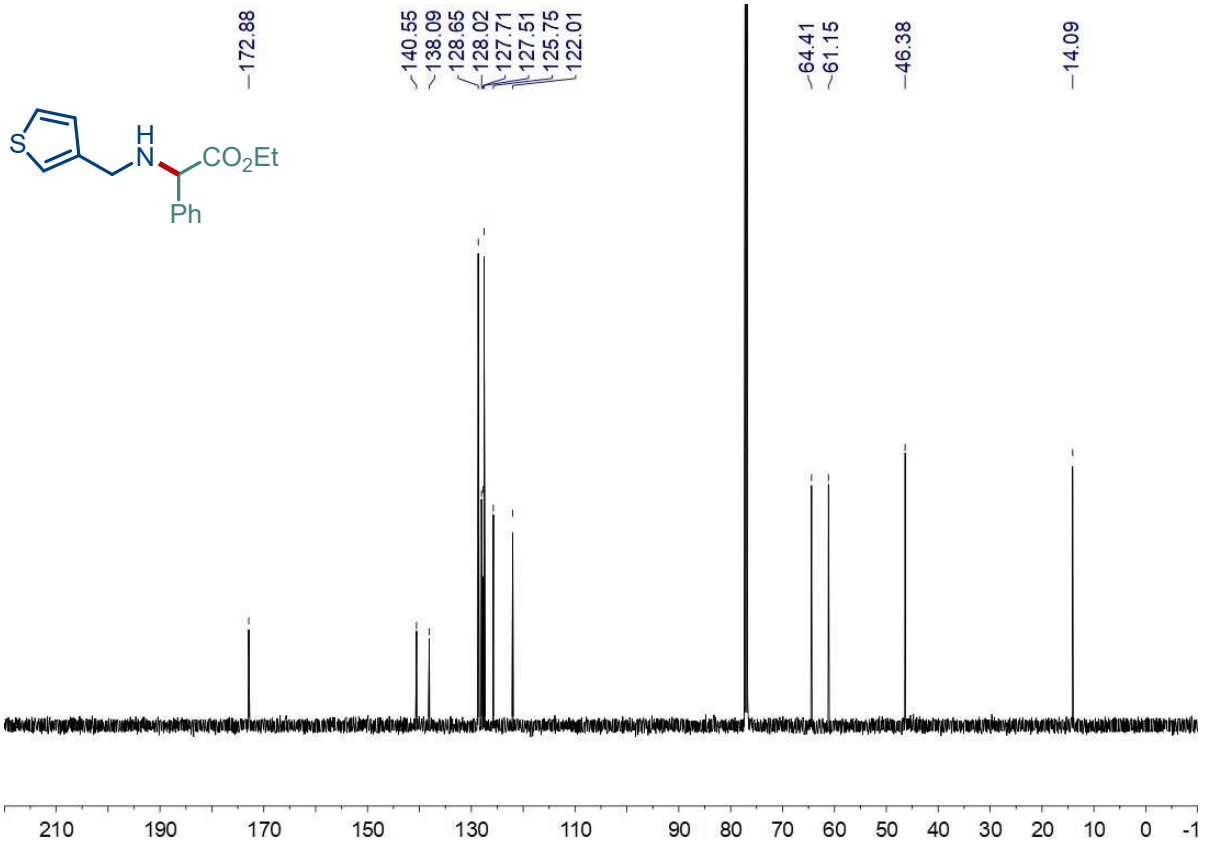
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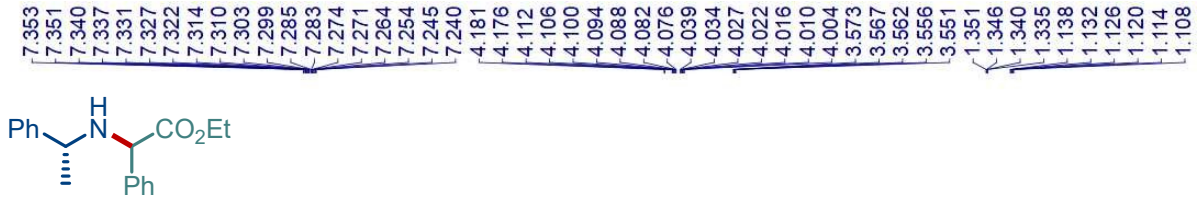
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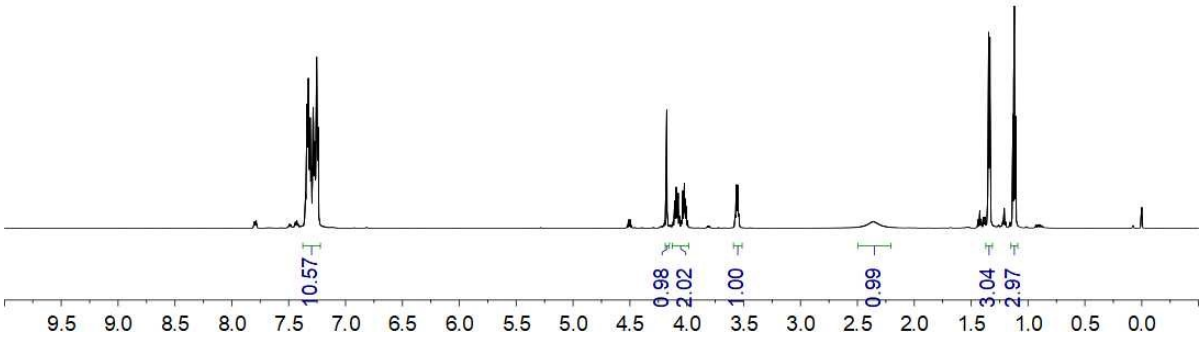
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0.0


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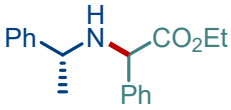
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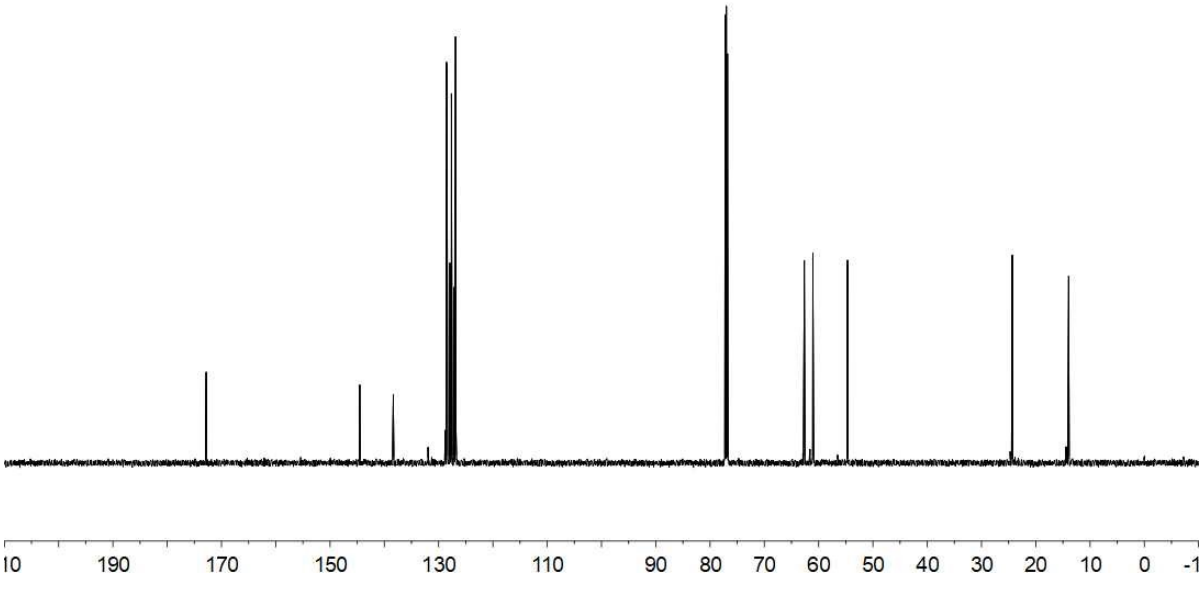
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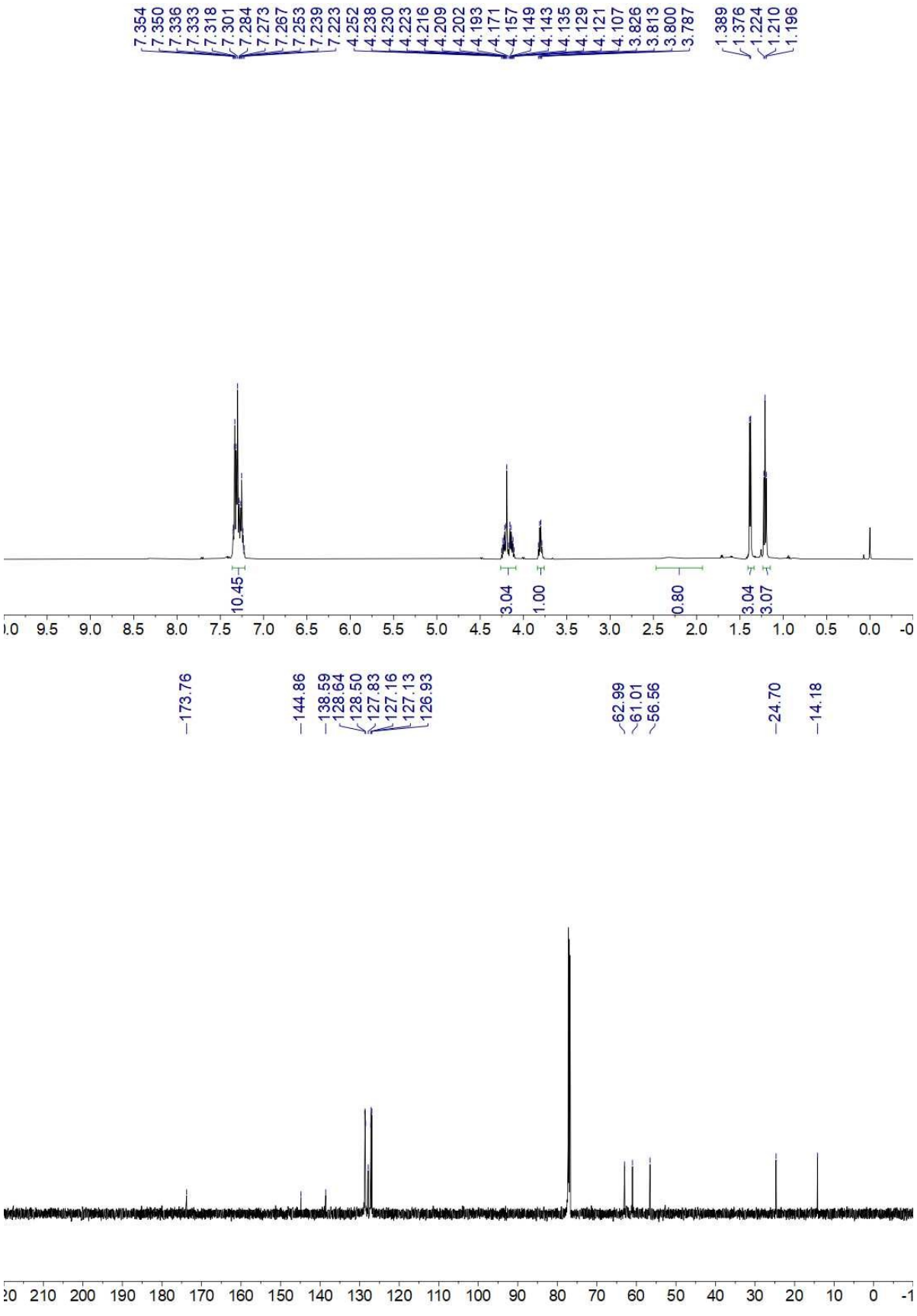
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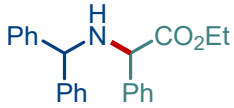
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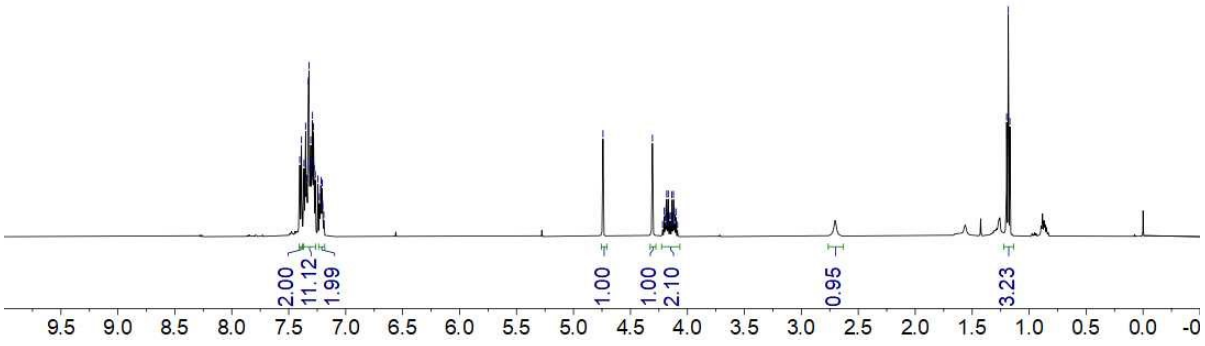
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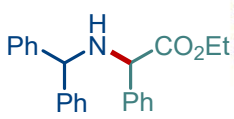
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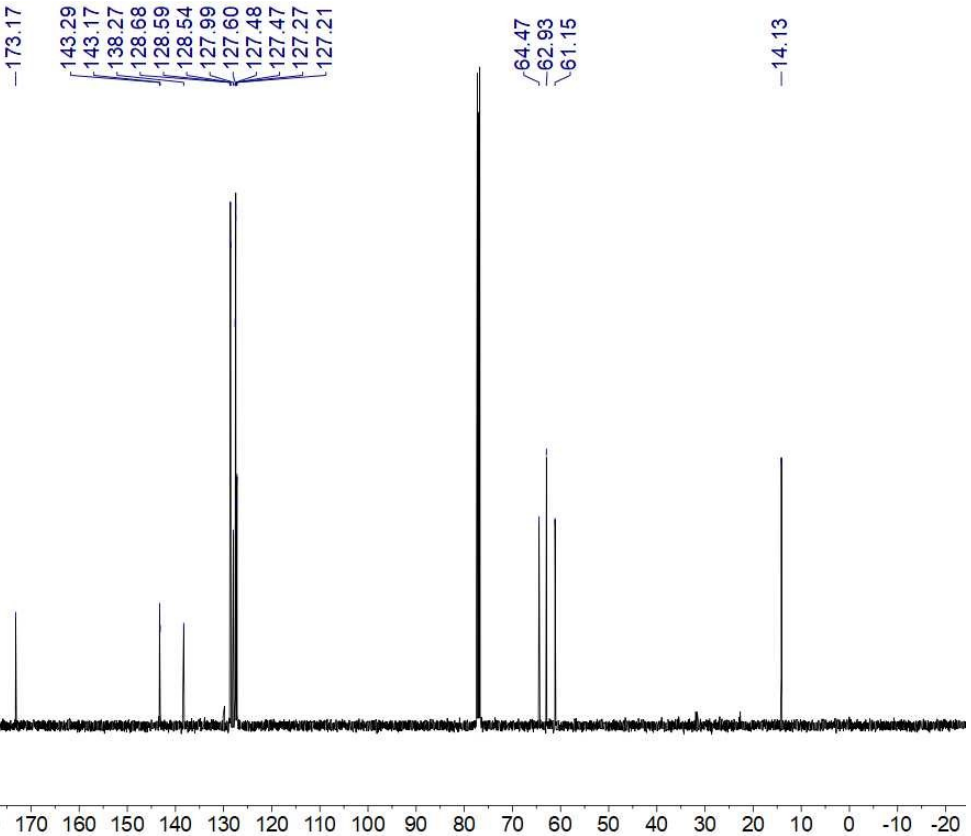
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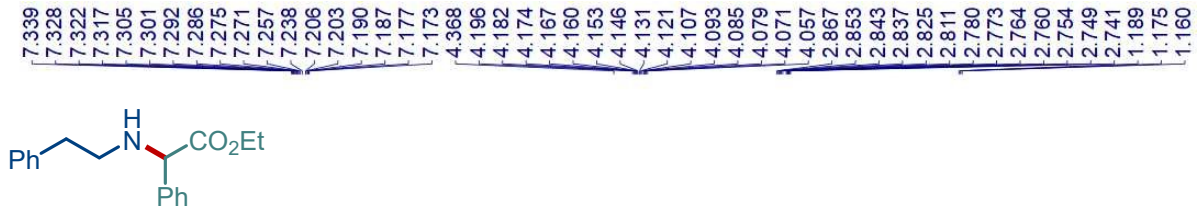
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CO2Et
Ph
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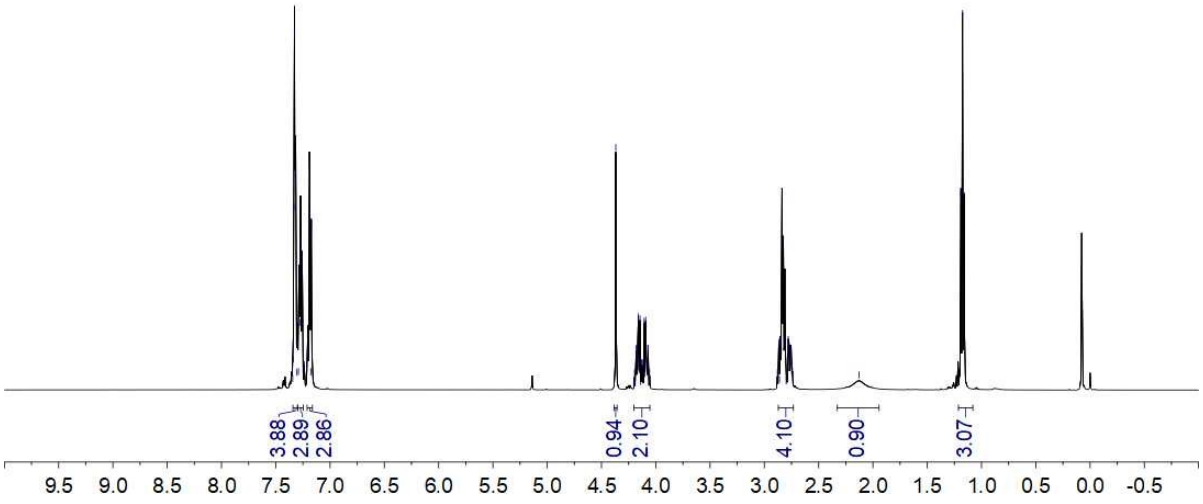
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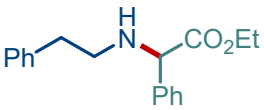
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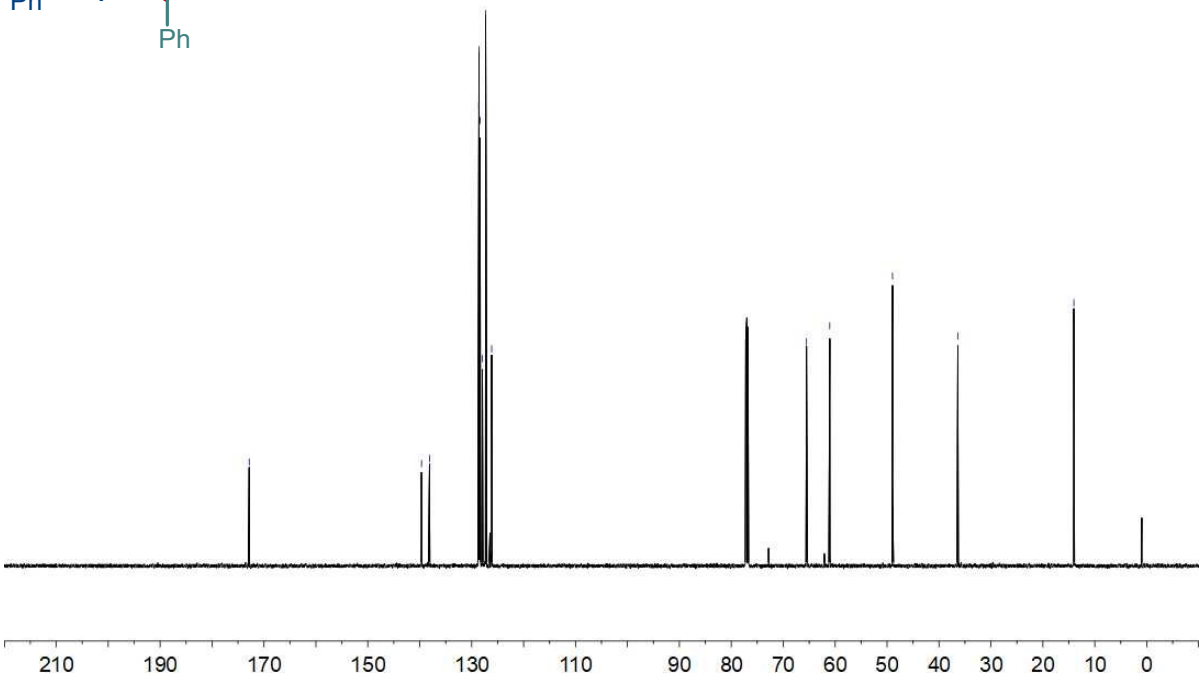
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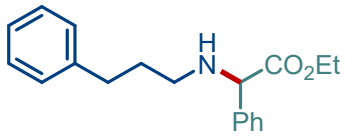
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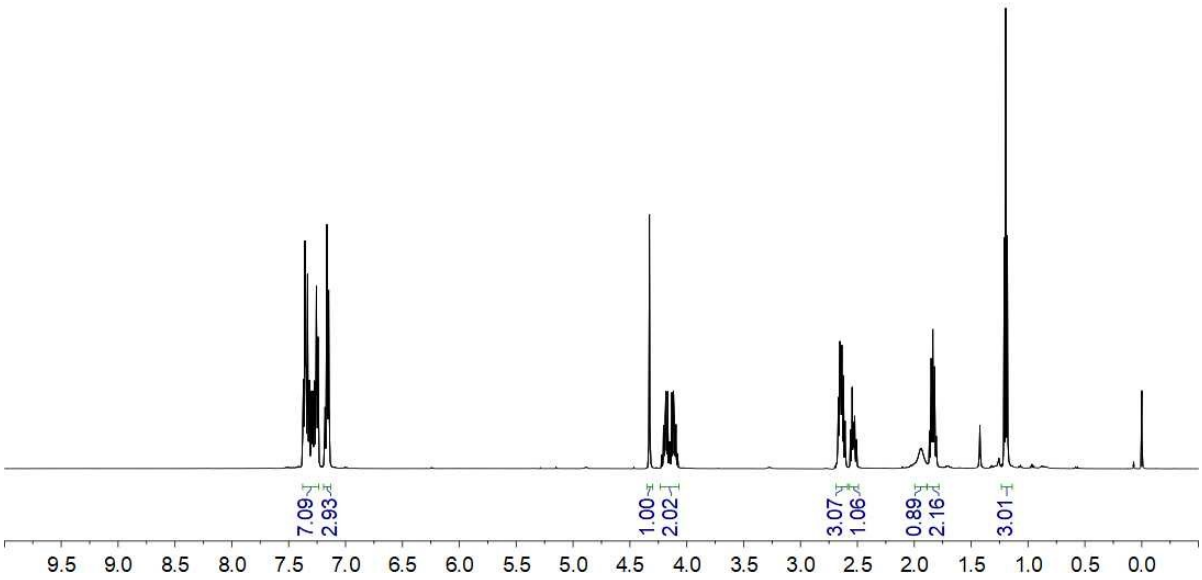
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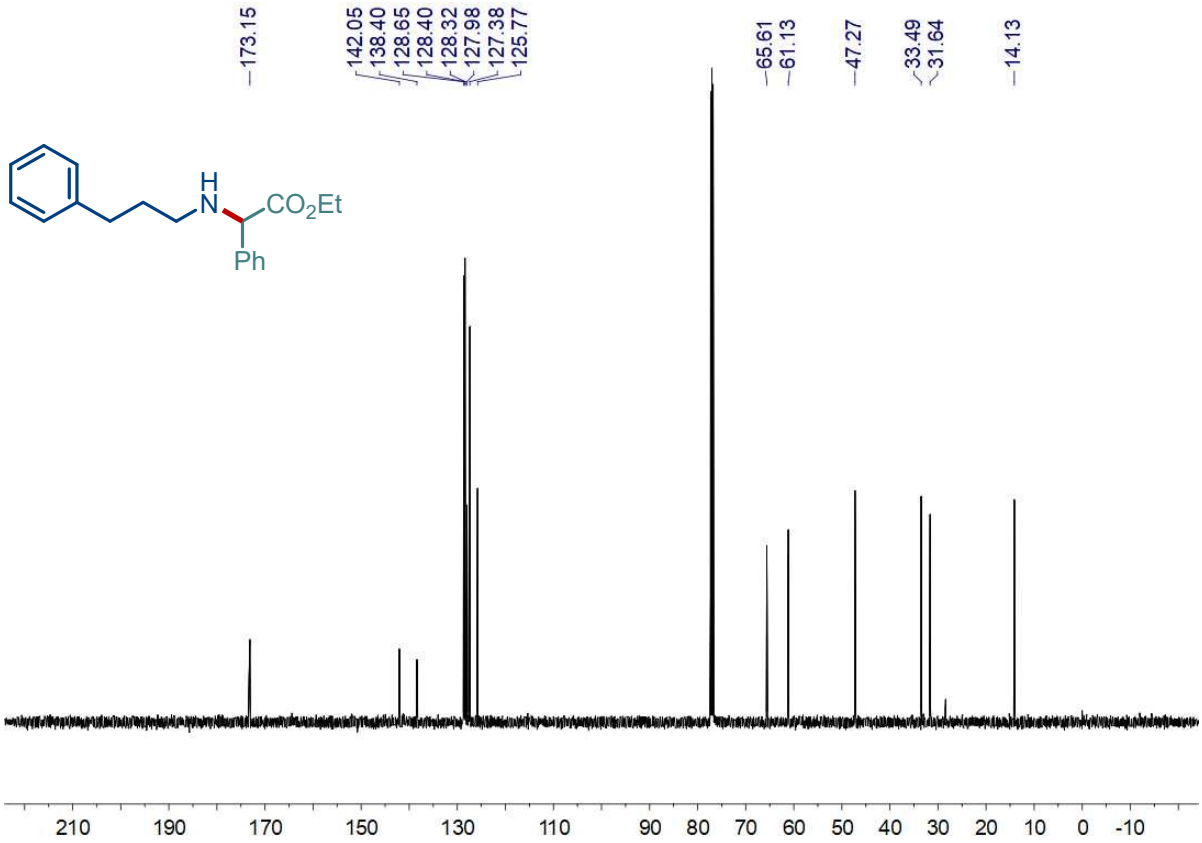
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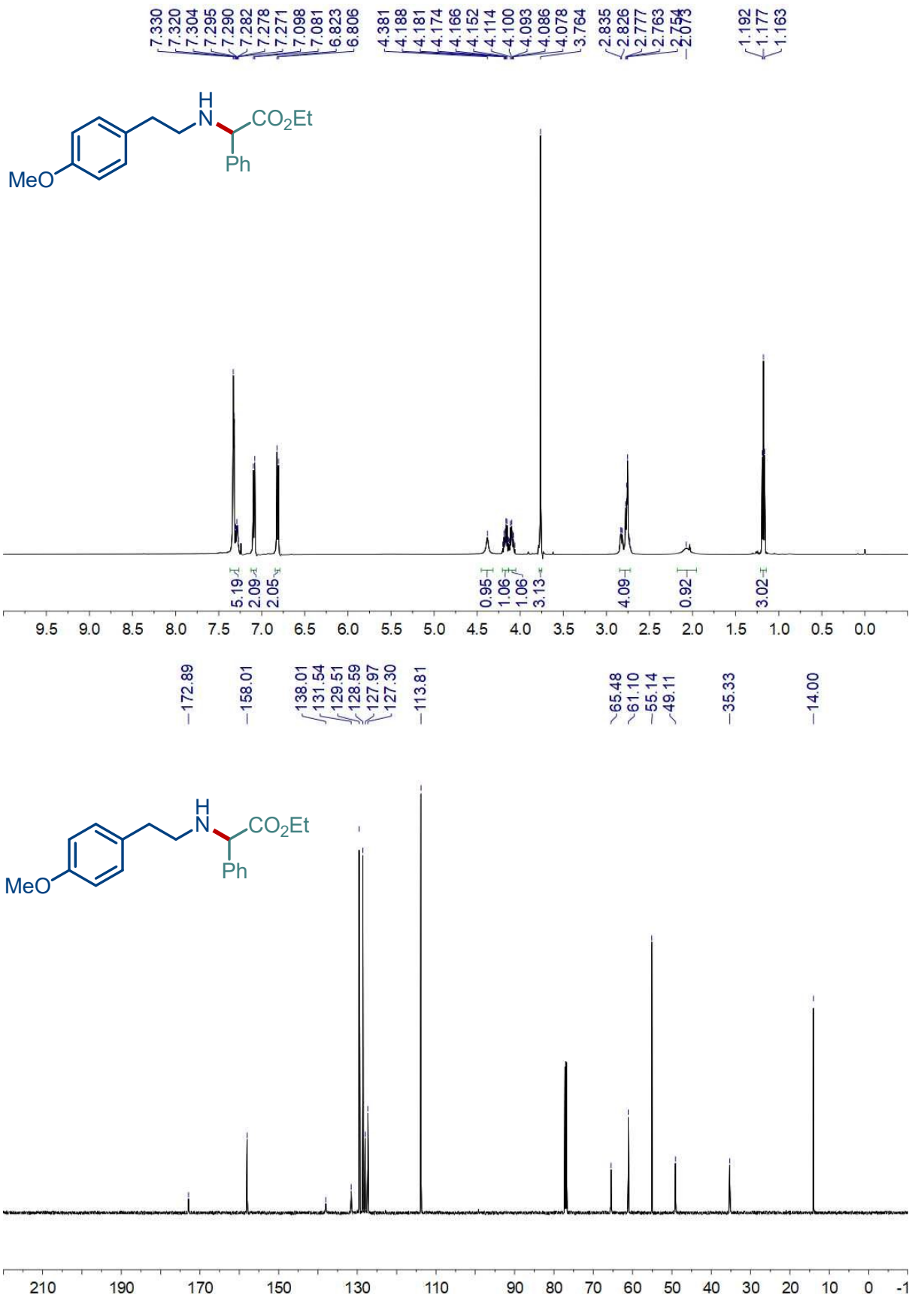
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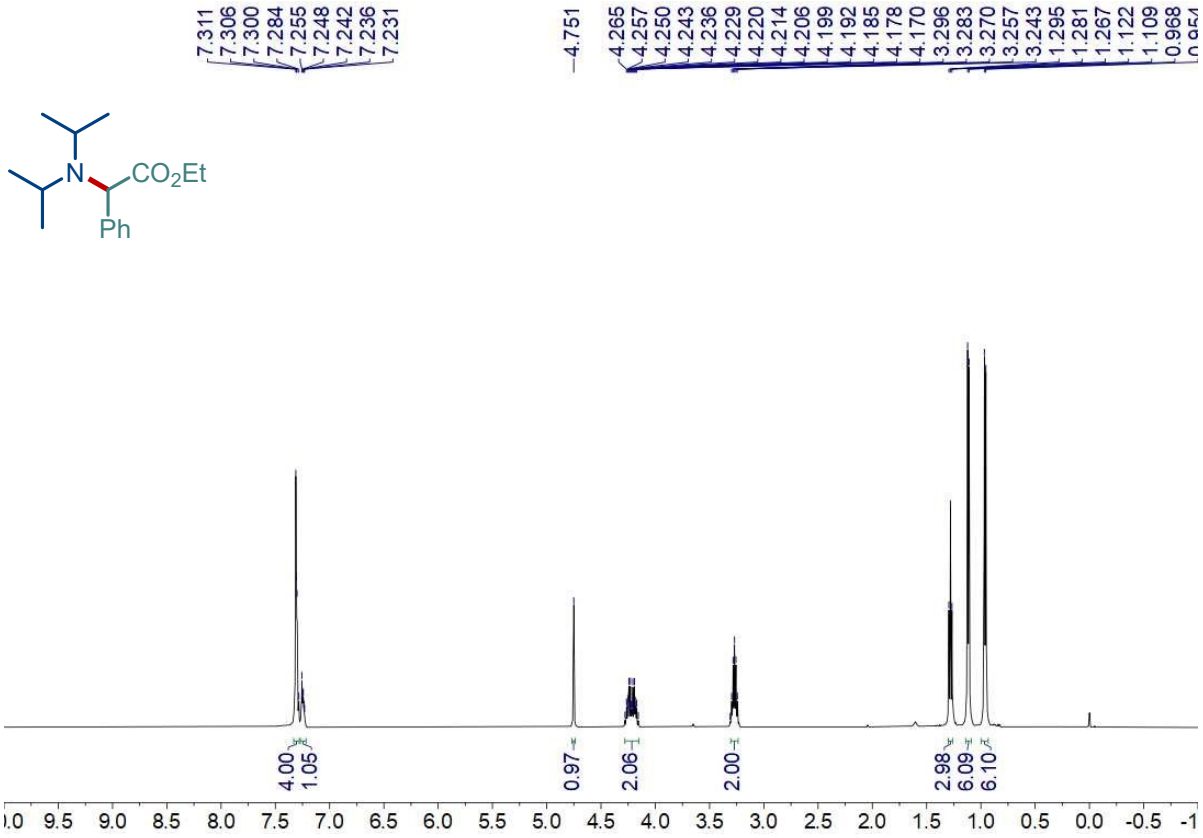
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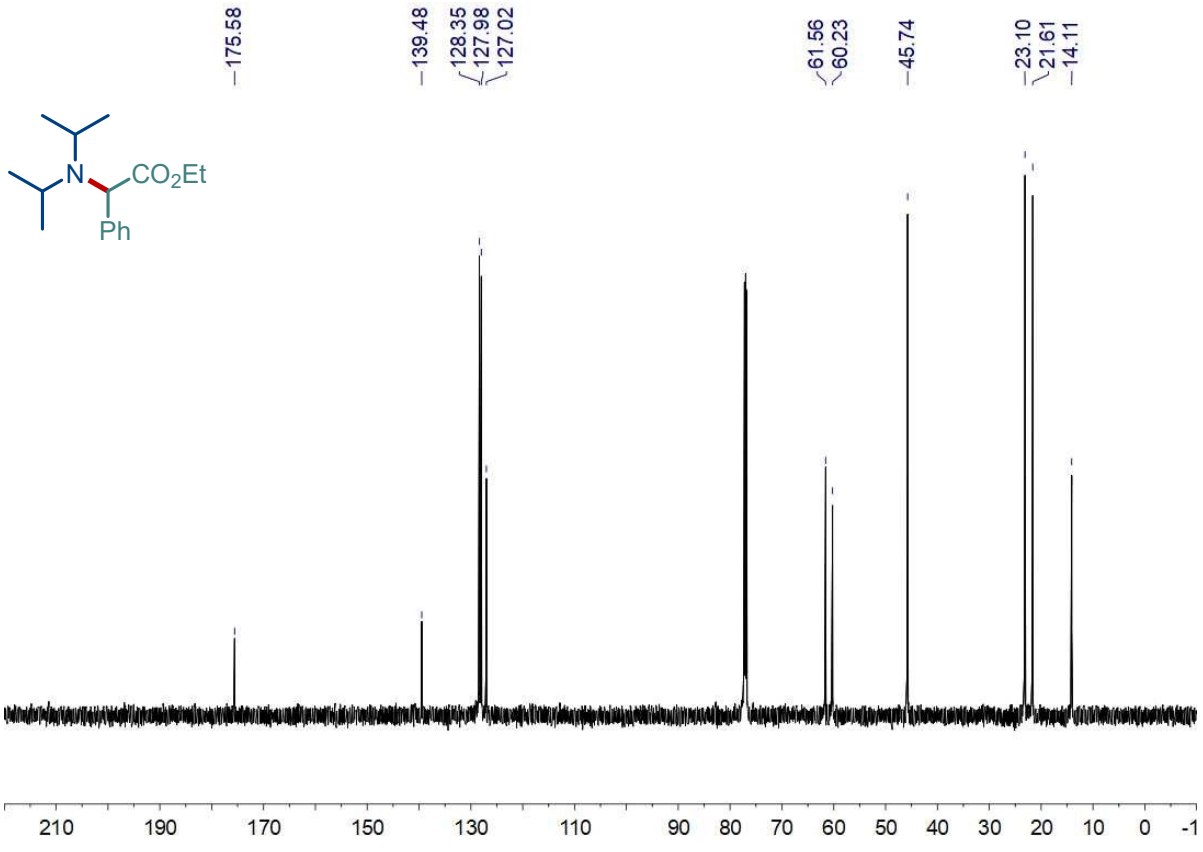
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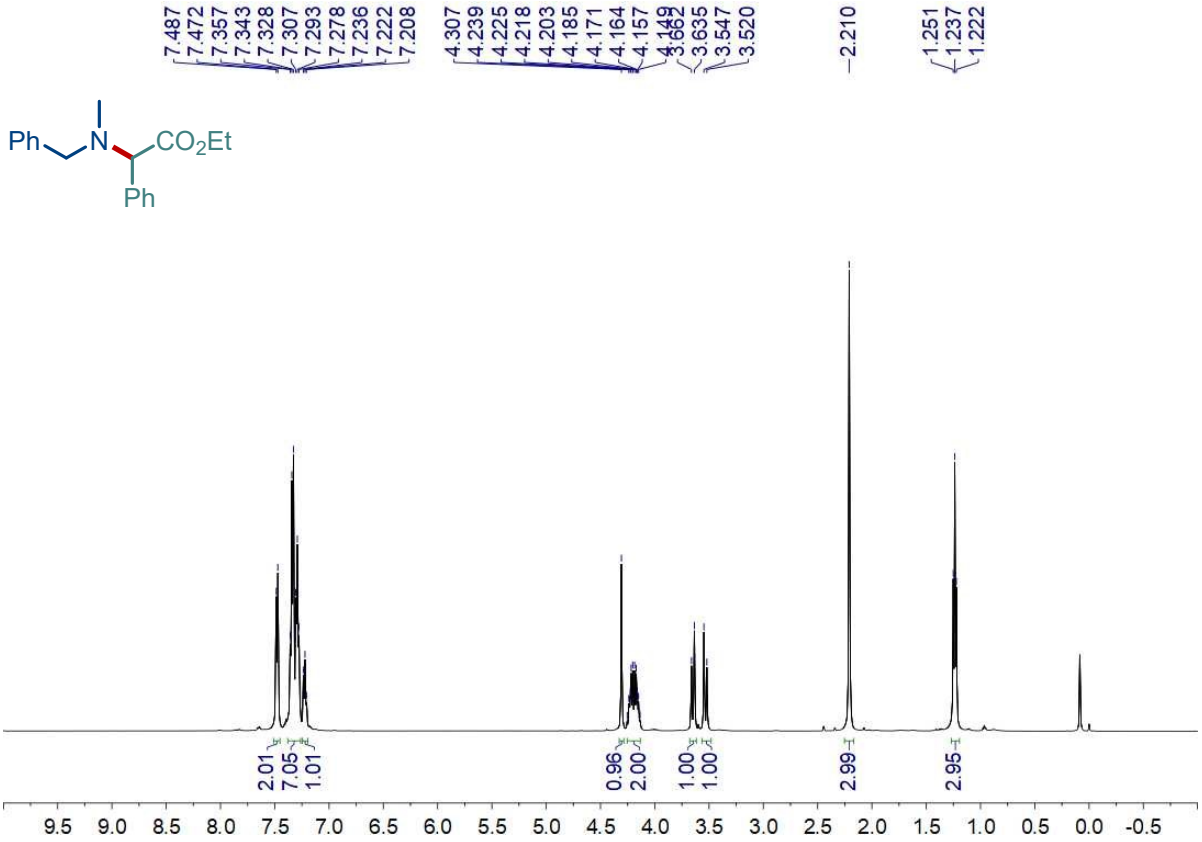
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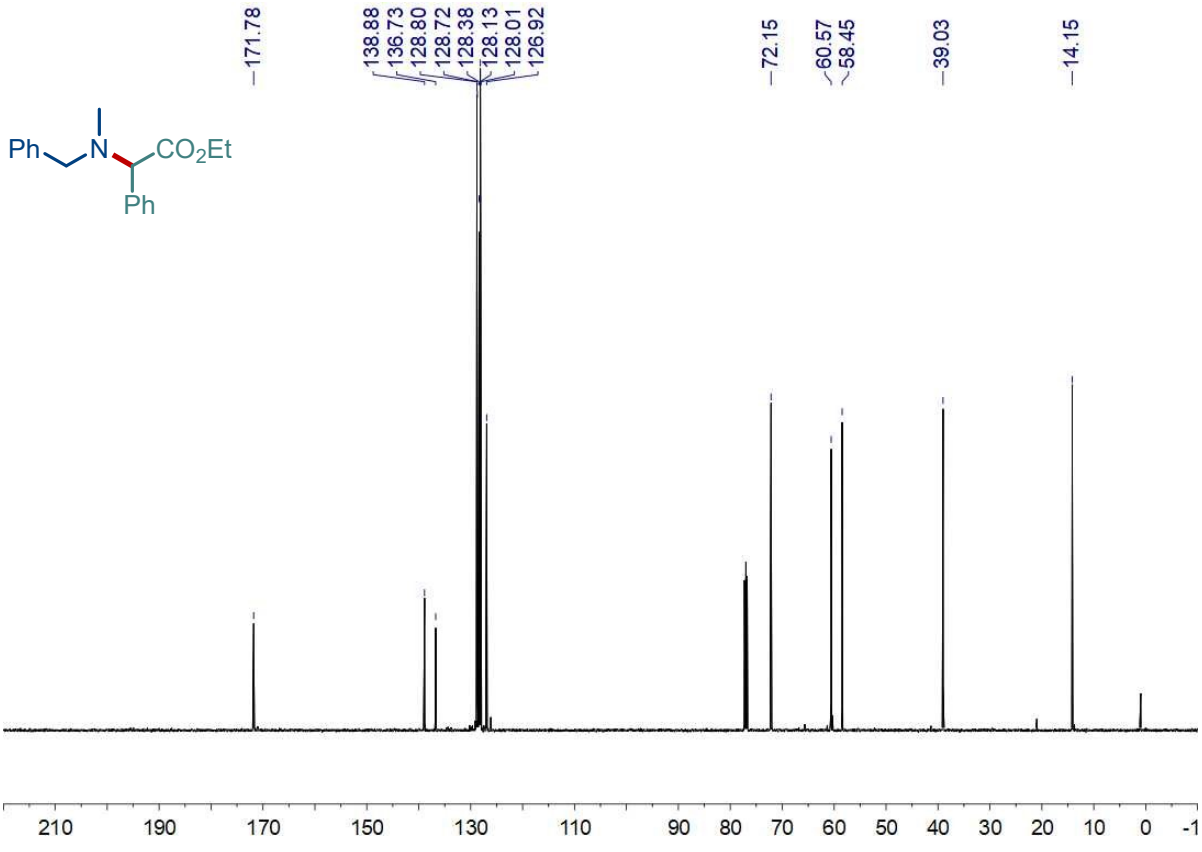
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N
CO2Et
Ph
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -1


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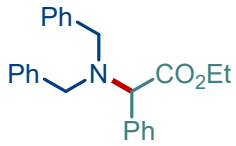
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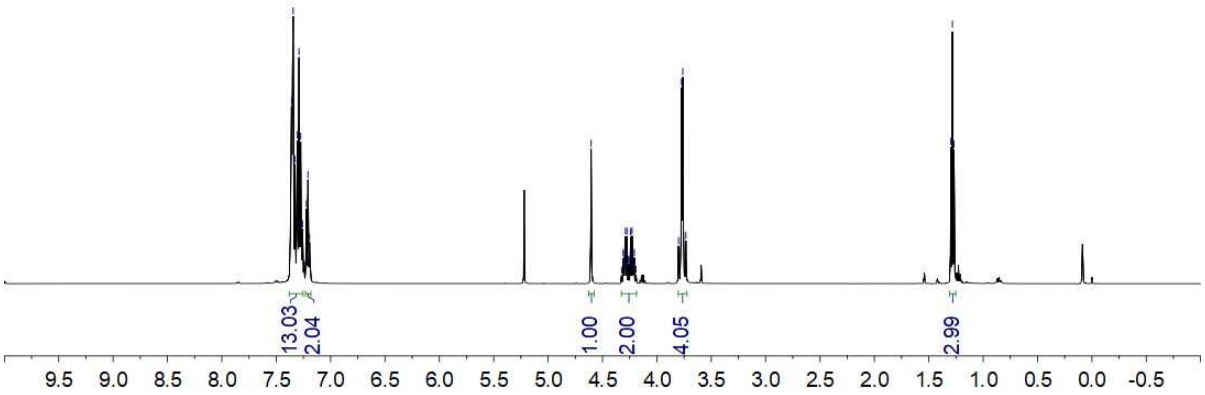
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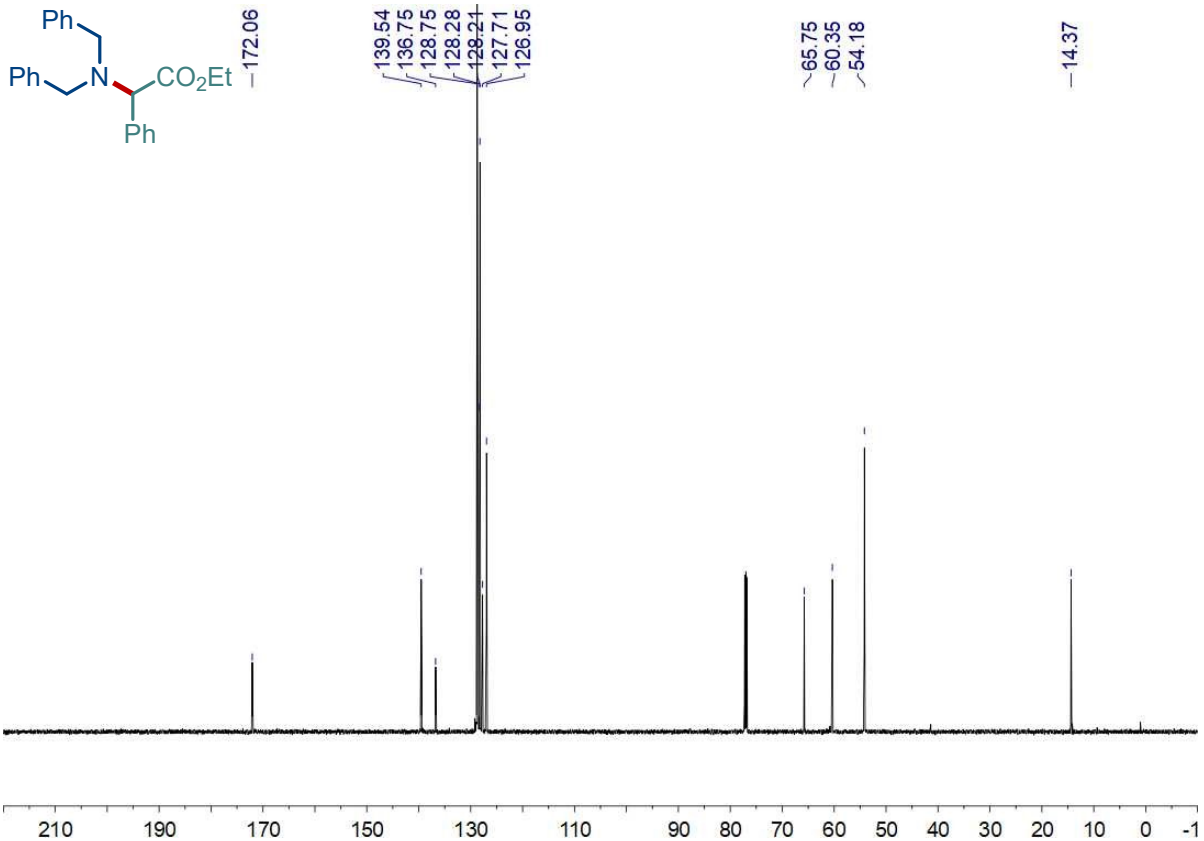
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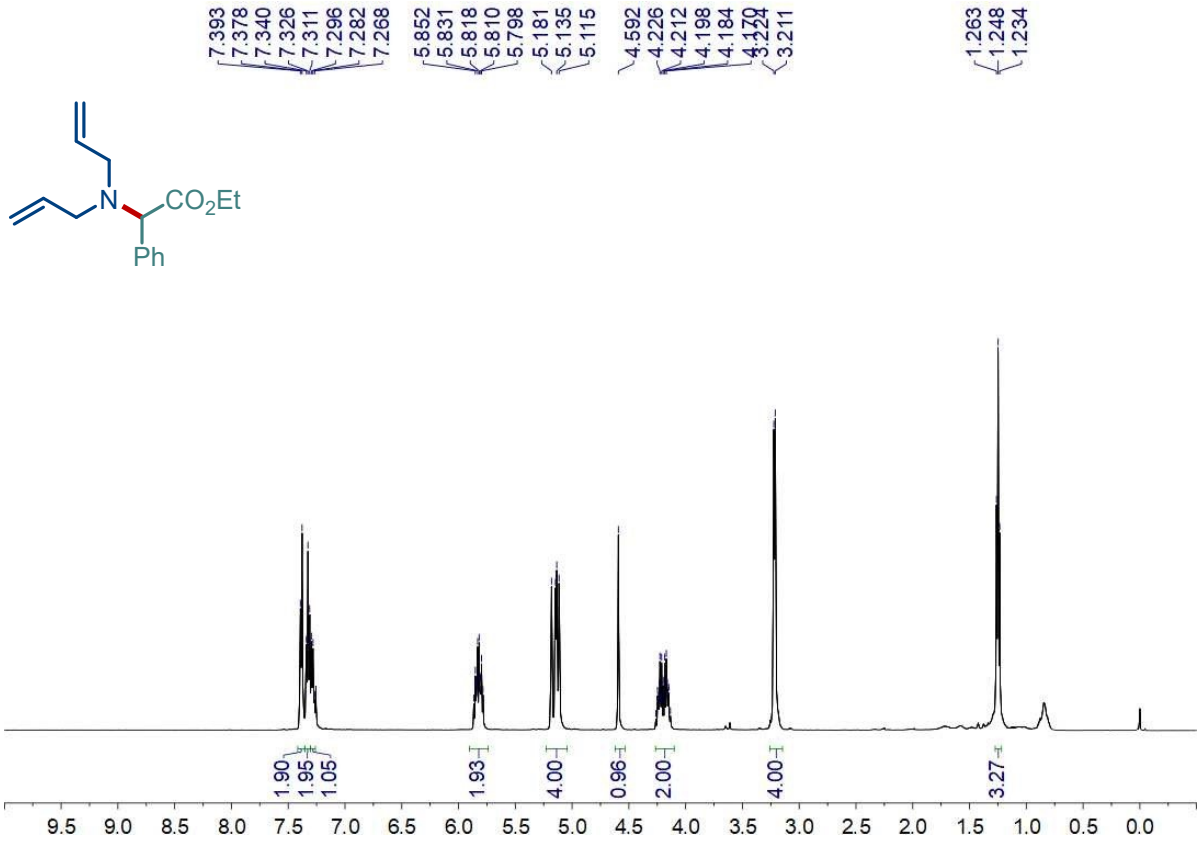
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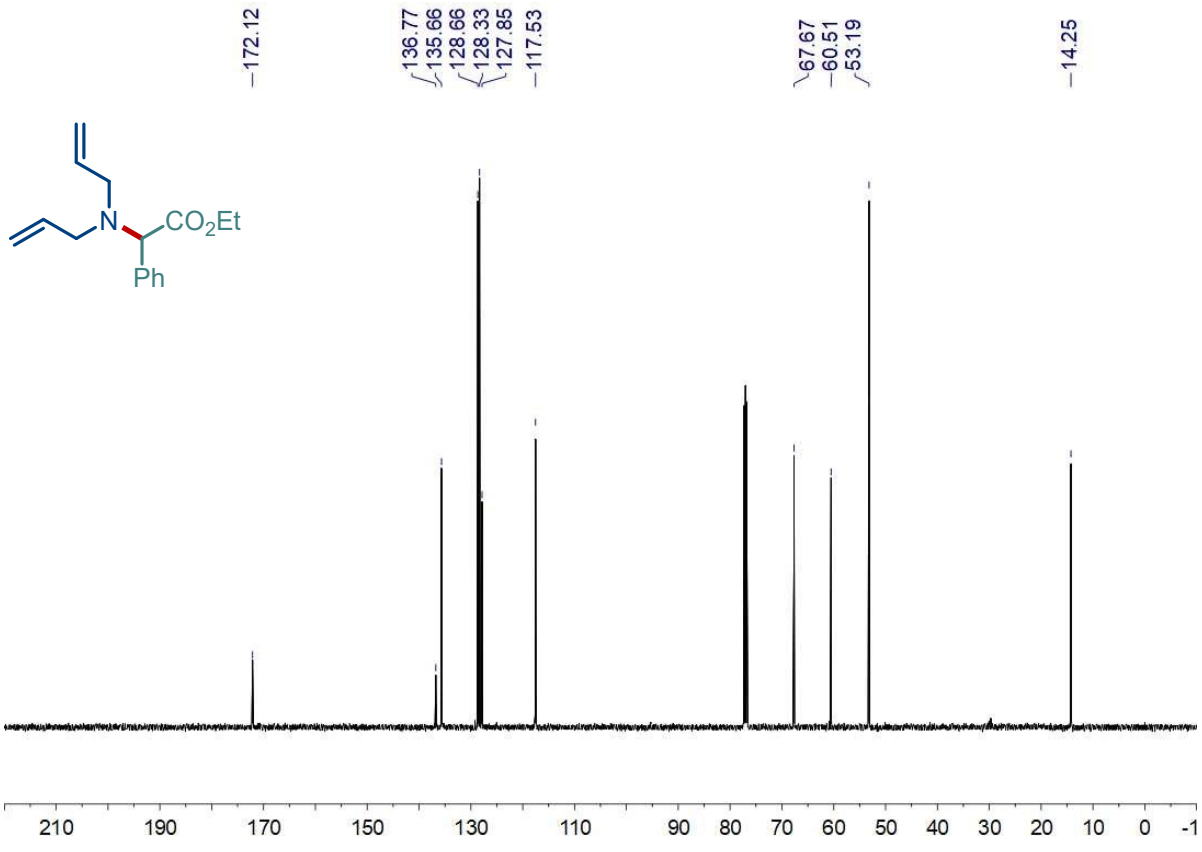
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CO2Et
Ph
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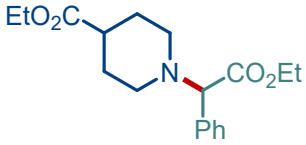
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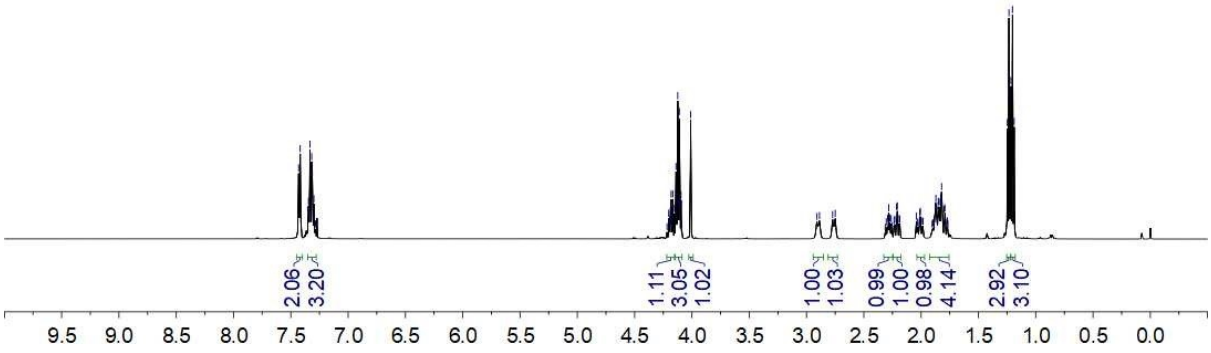
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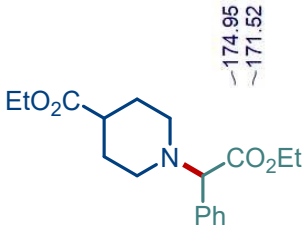
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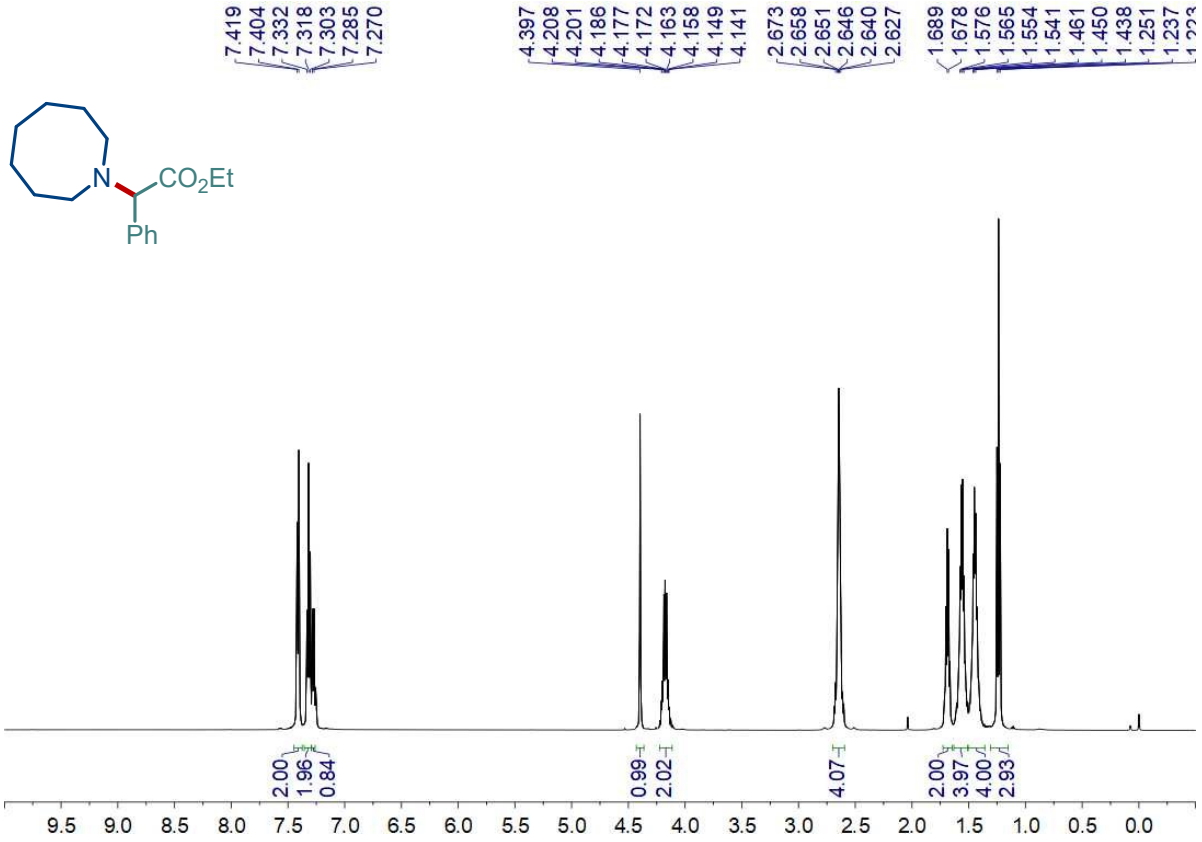
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4.00
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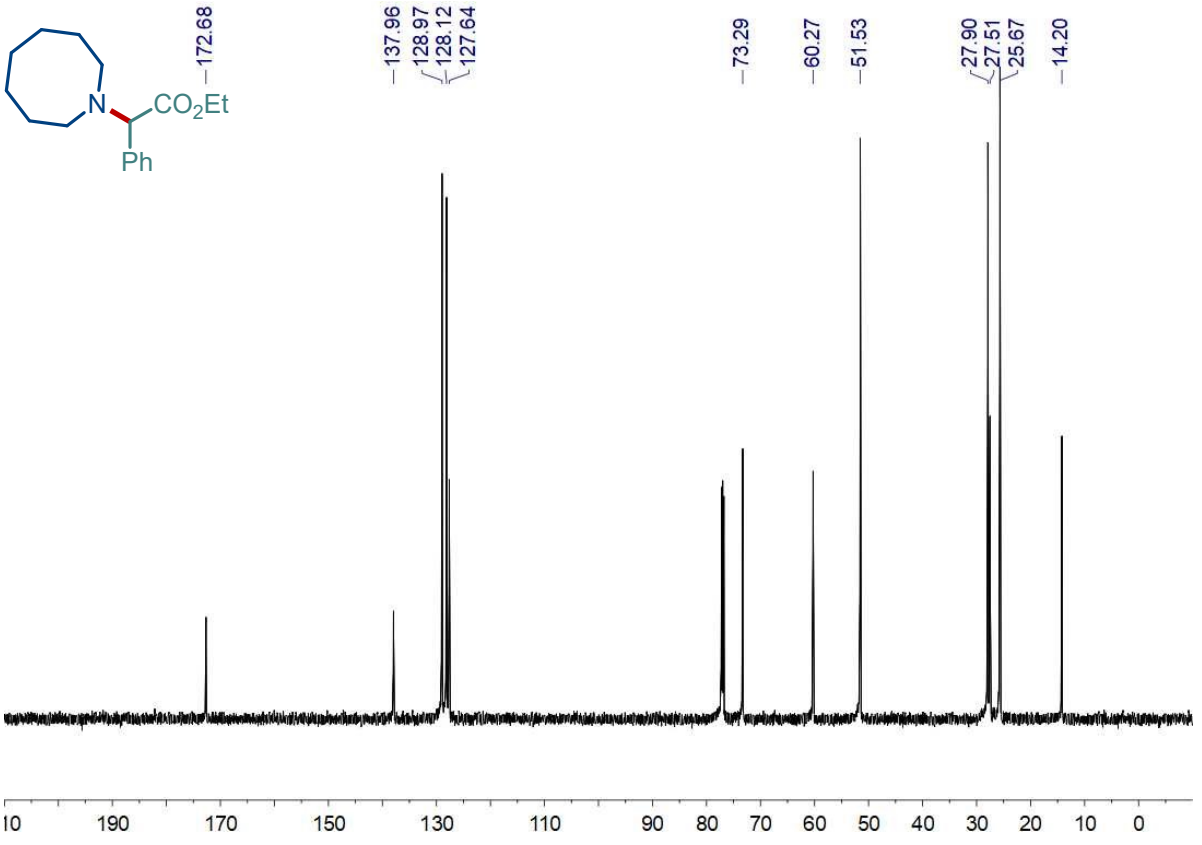
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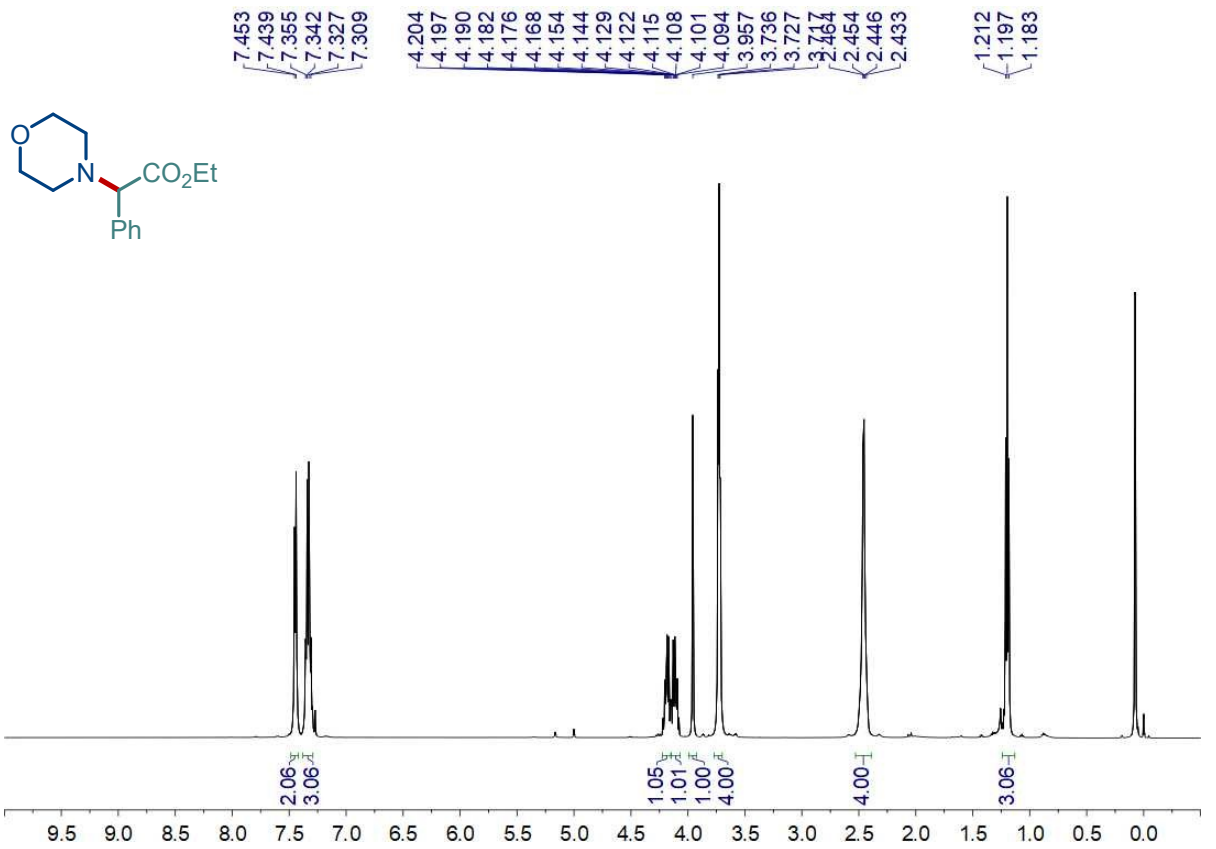
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1.00
4.00
4.00
3.06
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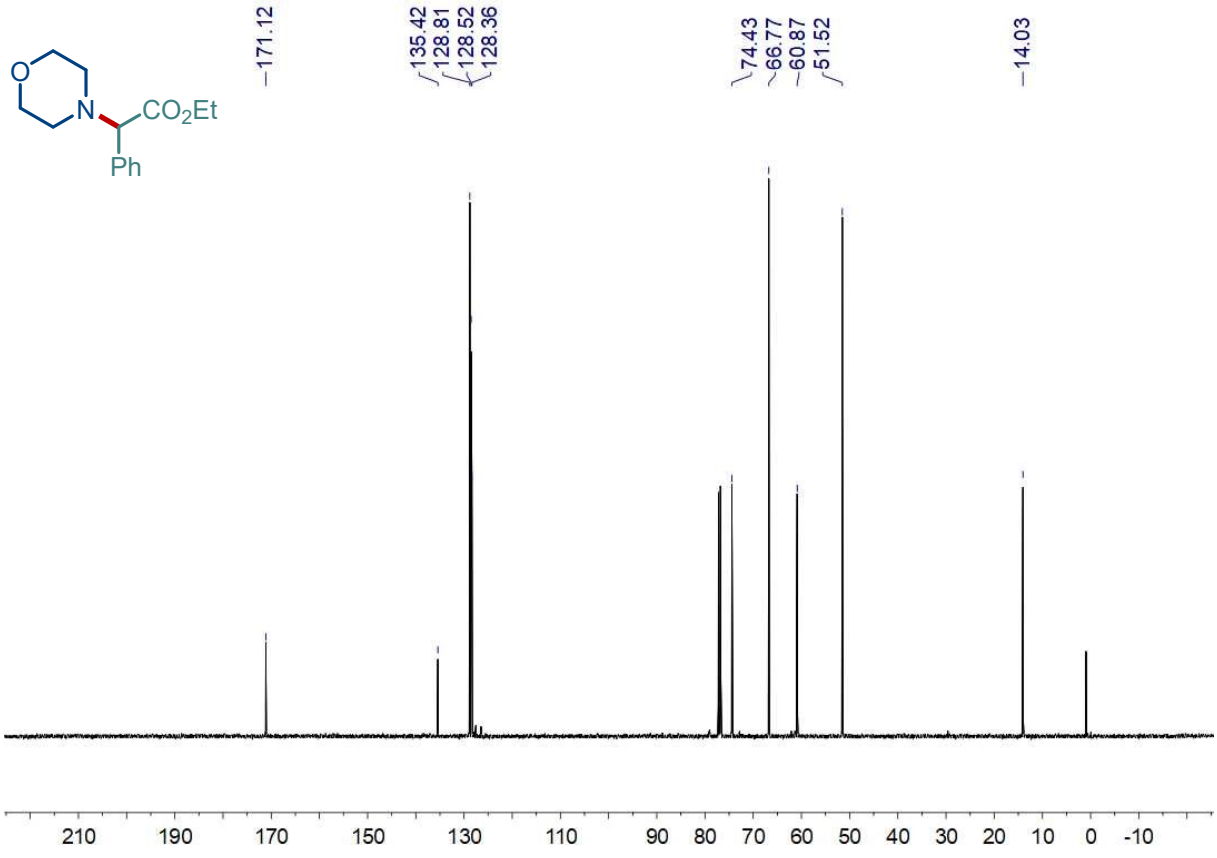
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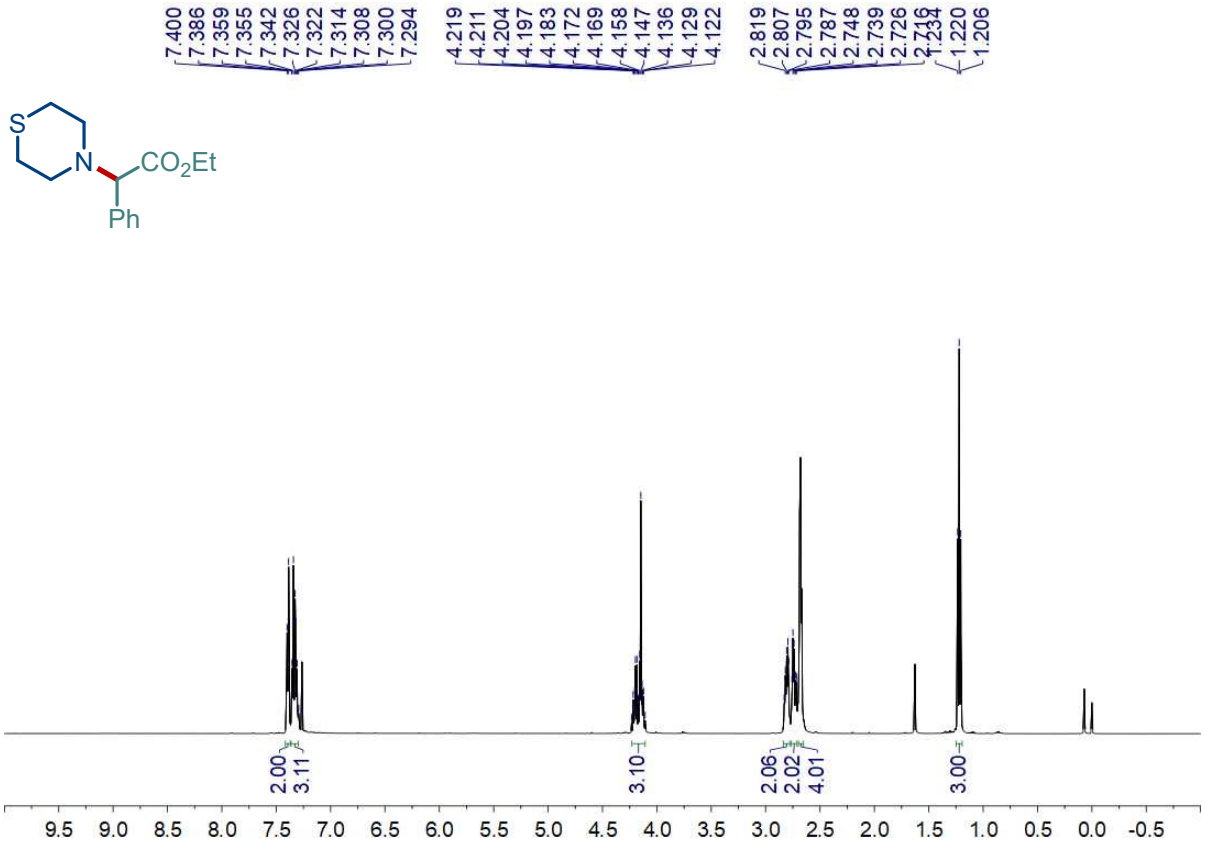
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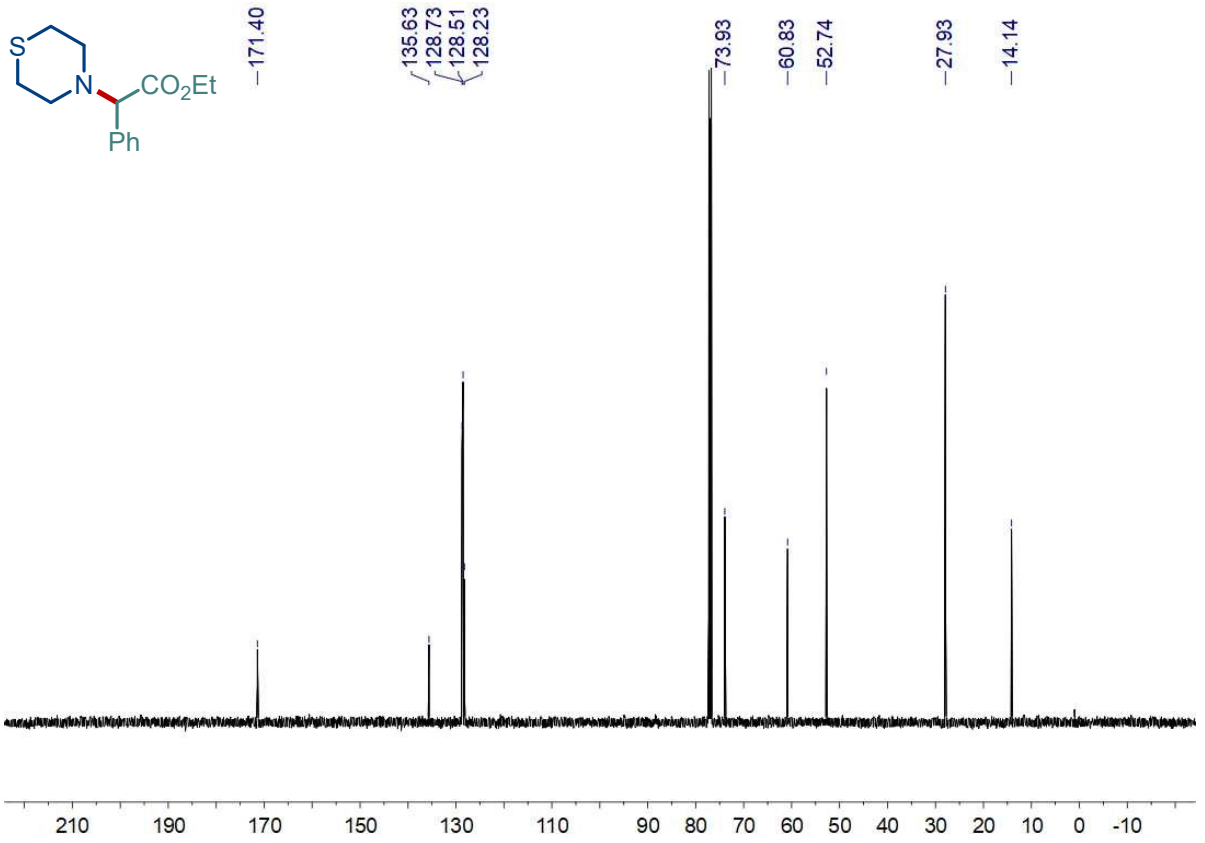
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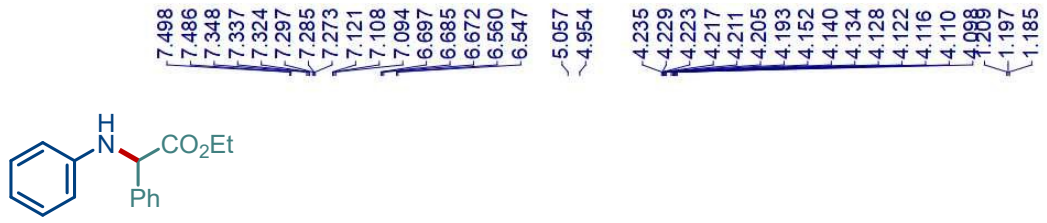
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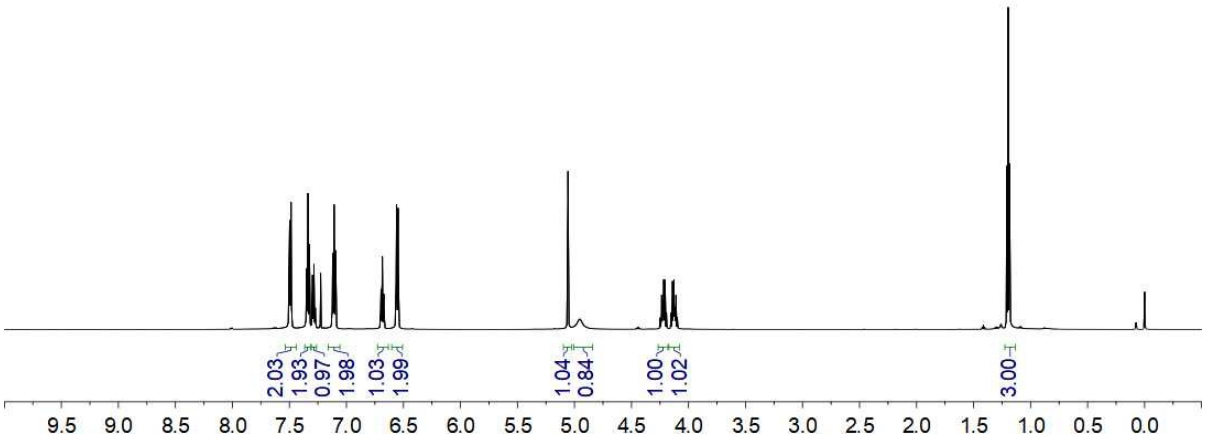
H
N
CO2Et
Ph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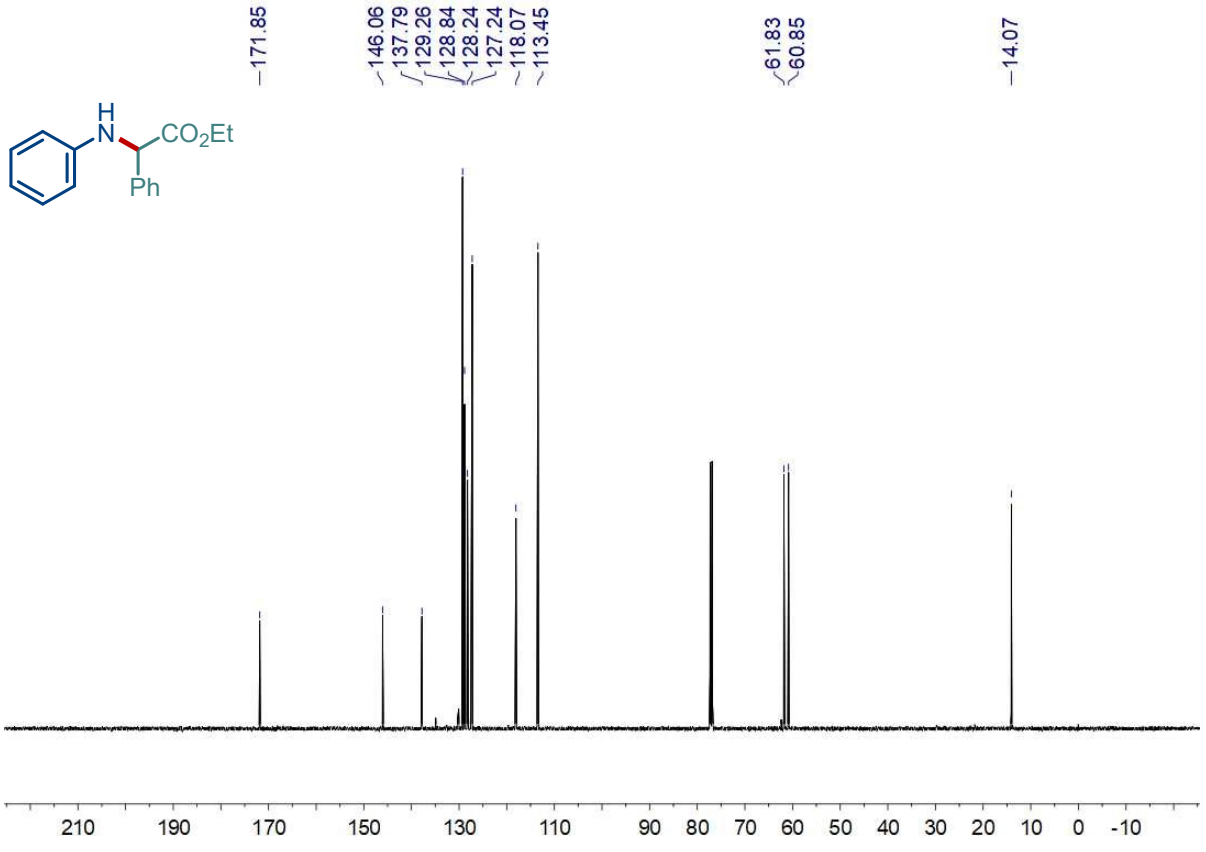
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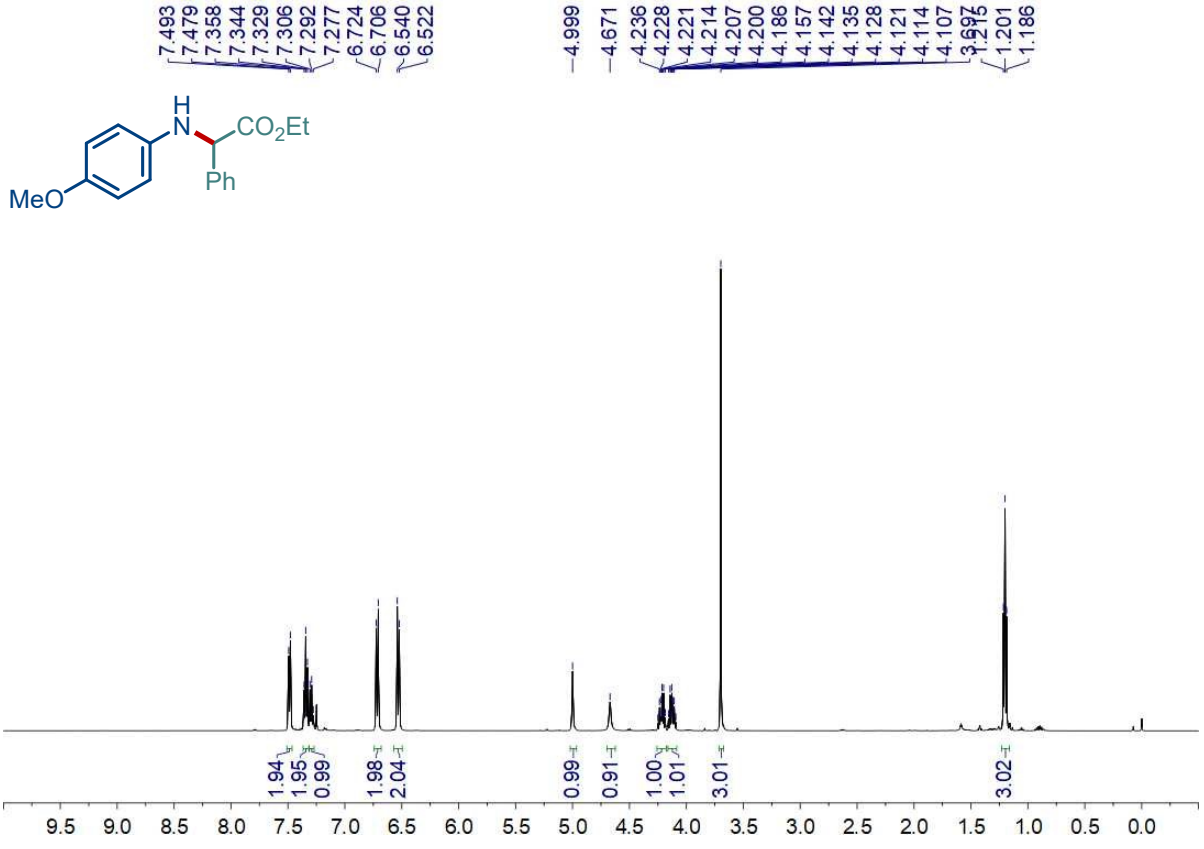
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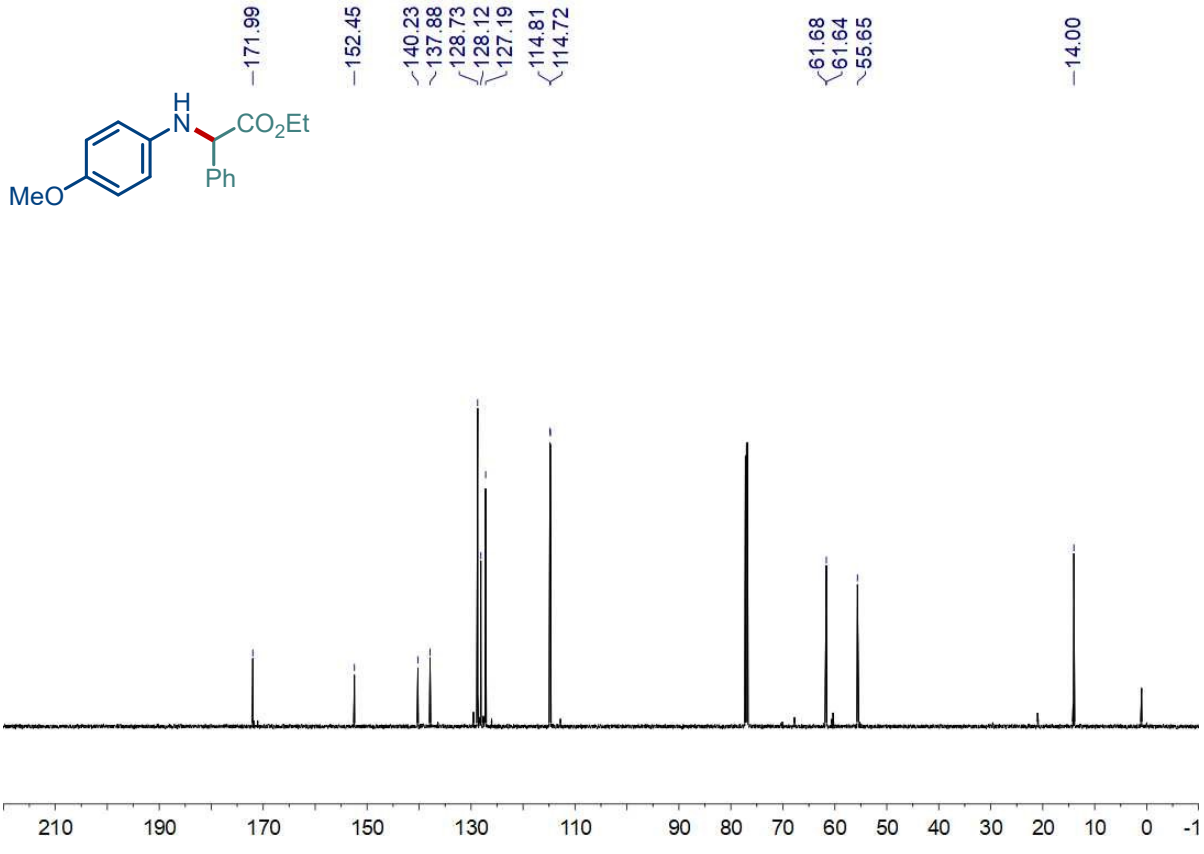
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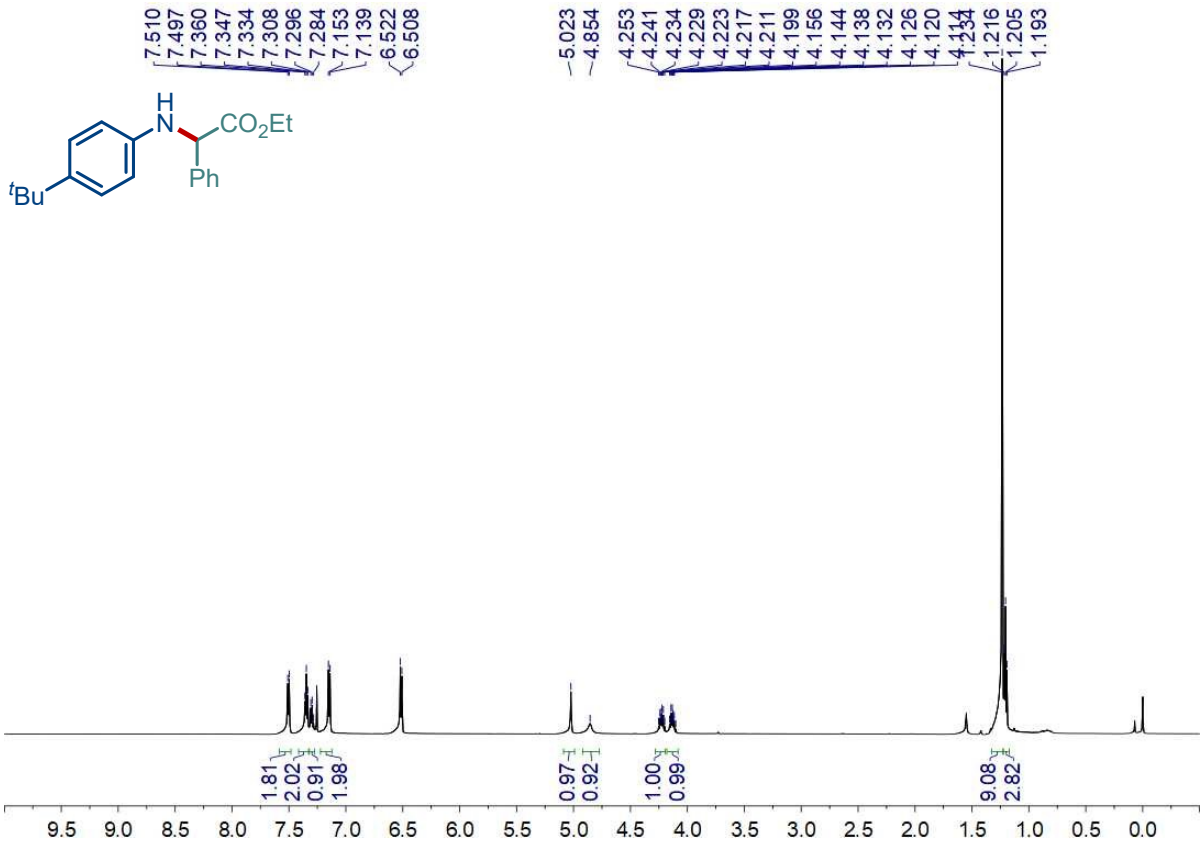
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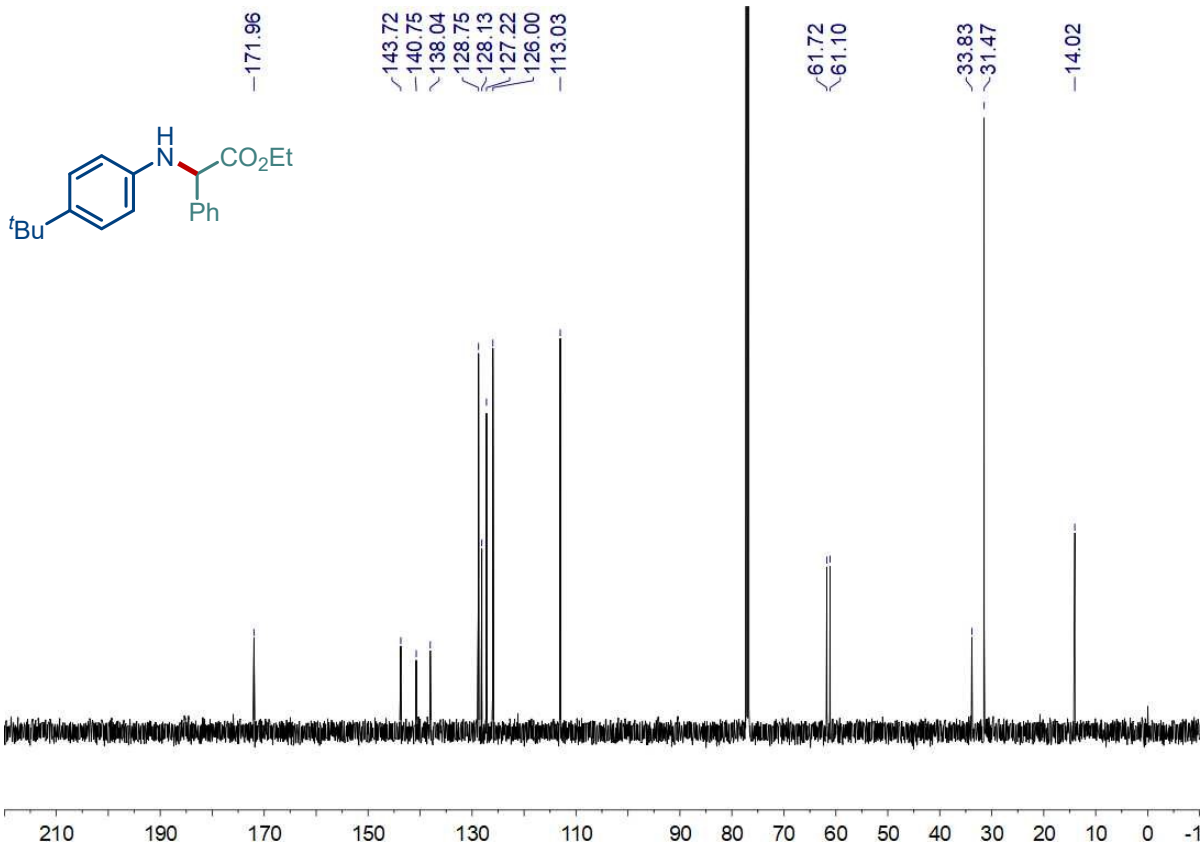
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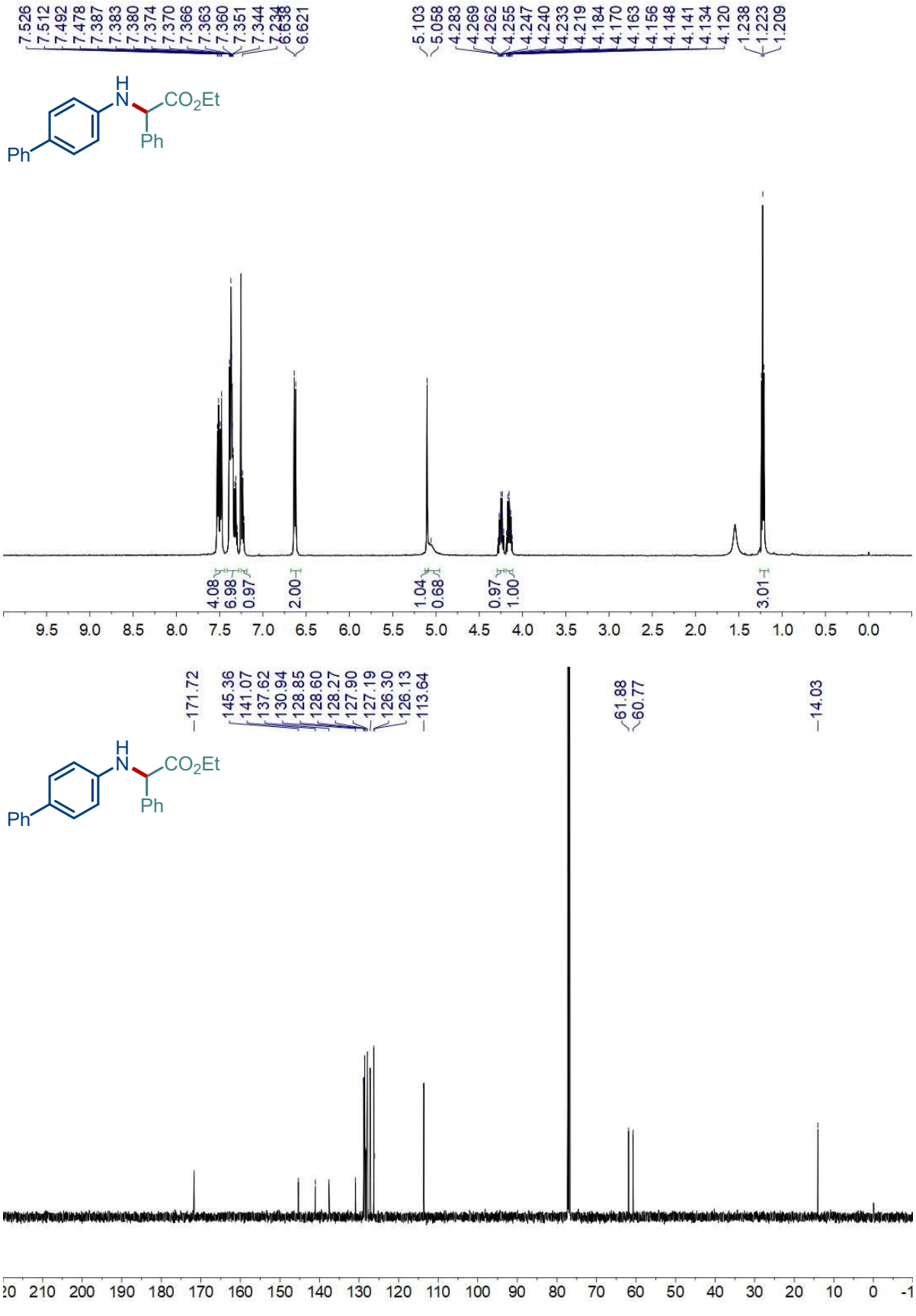
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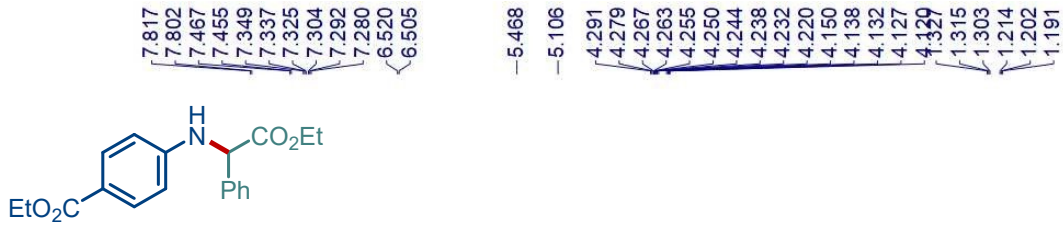
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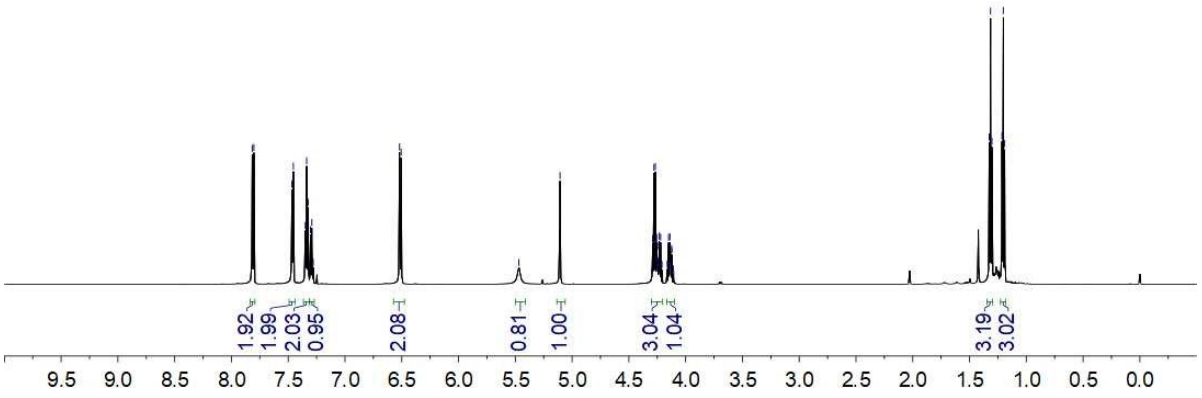
Ph
EtO2C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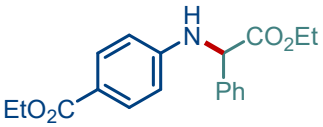
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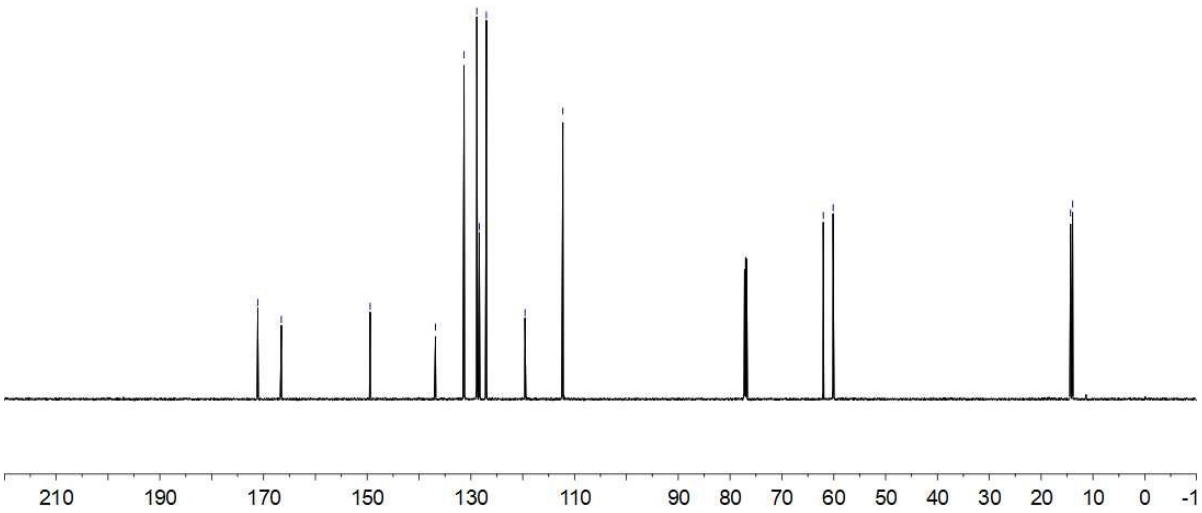
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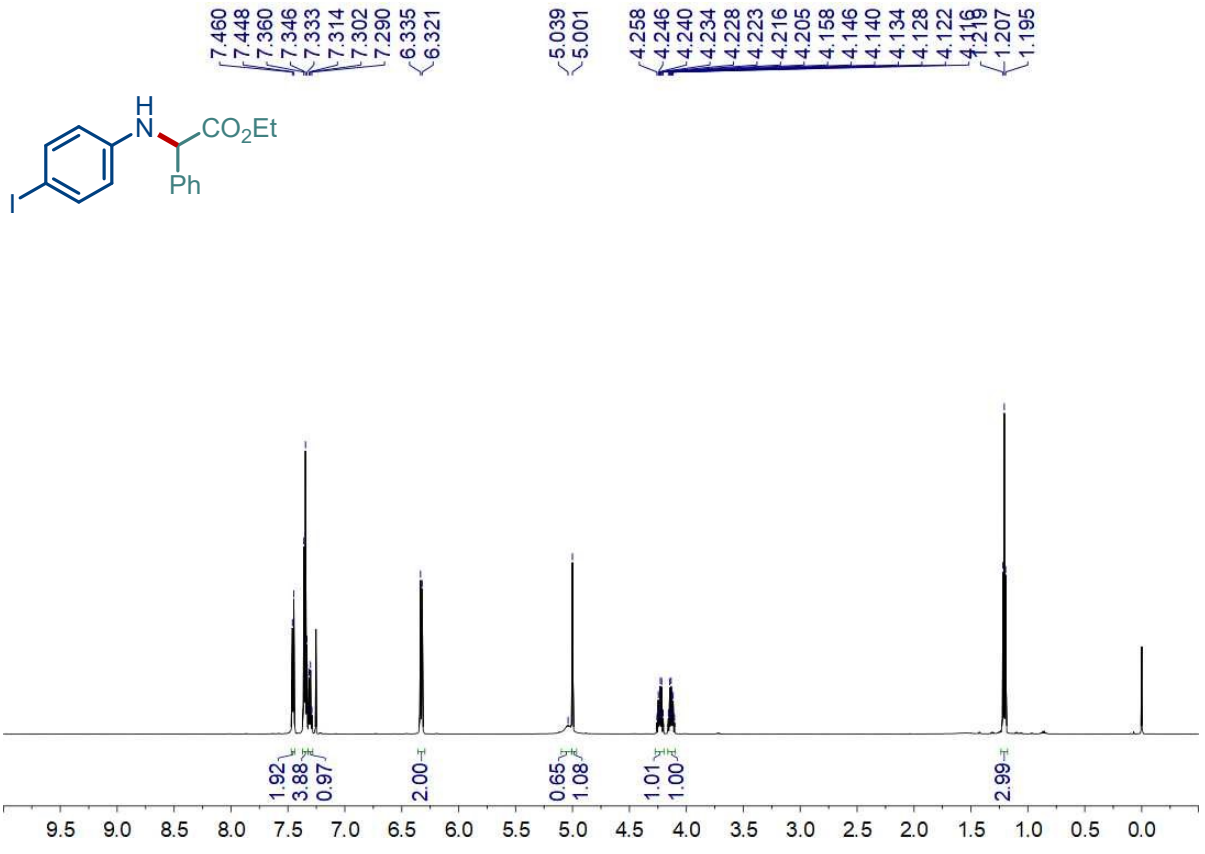
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1.00
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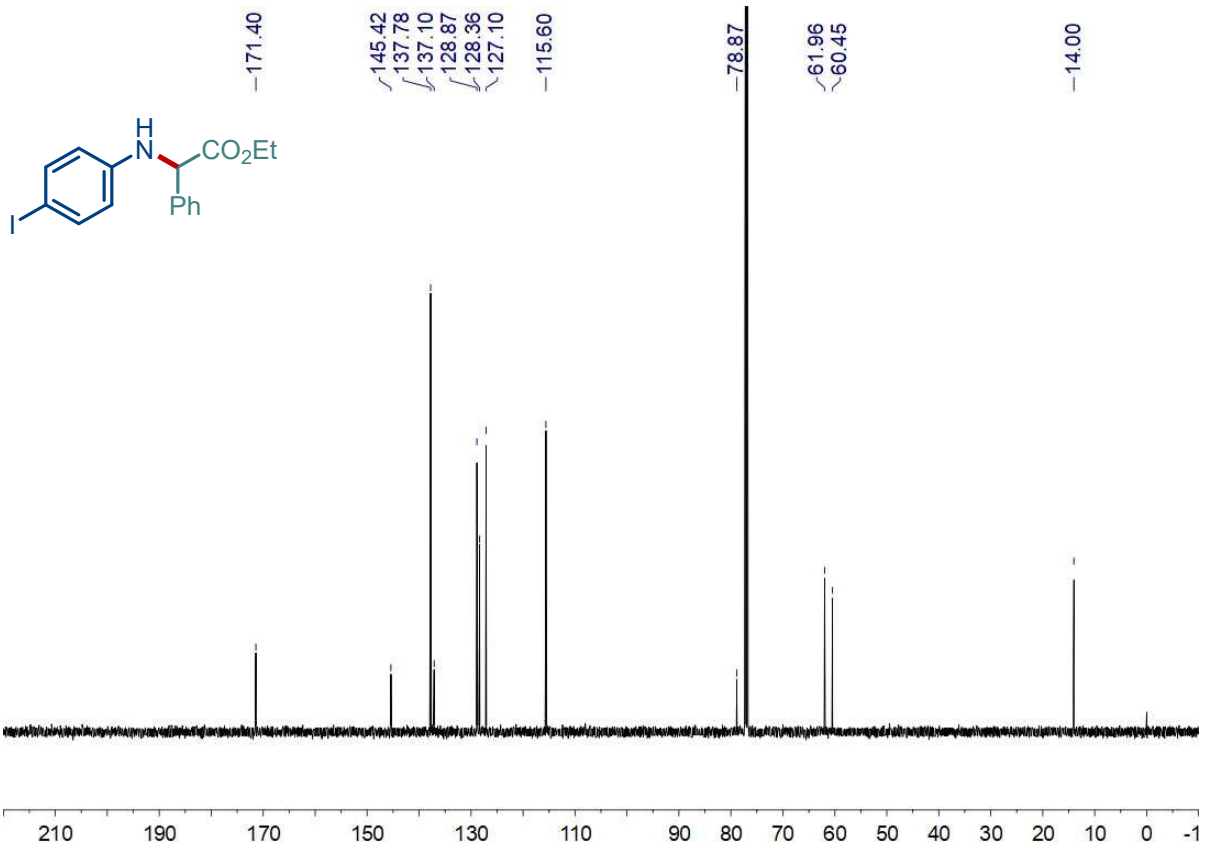
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Ph
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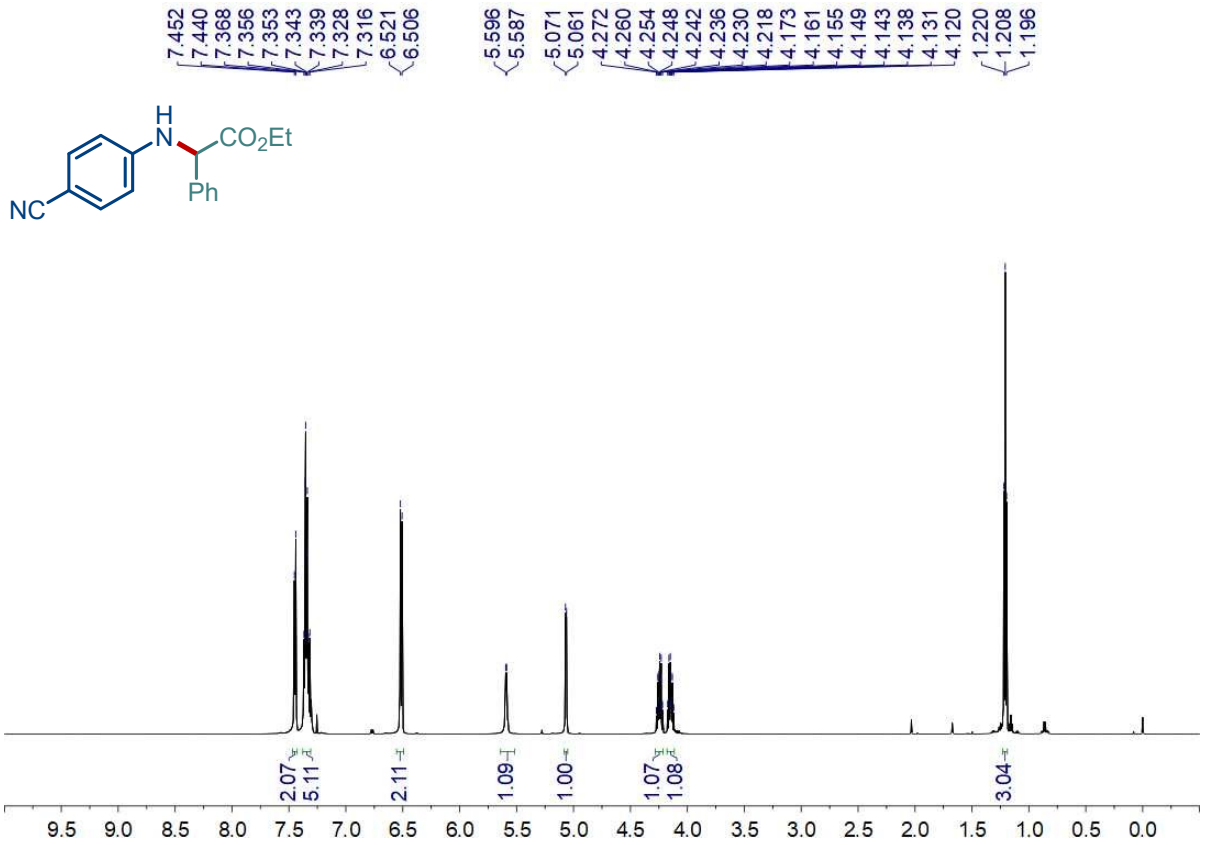
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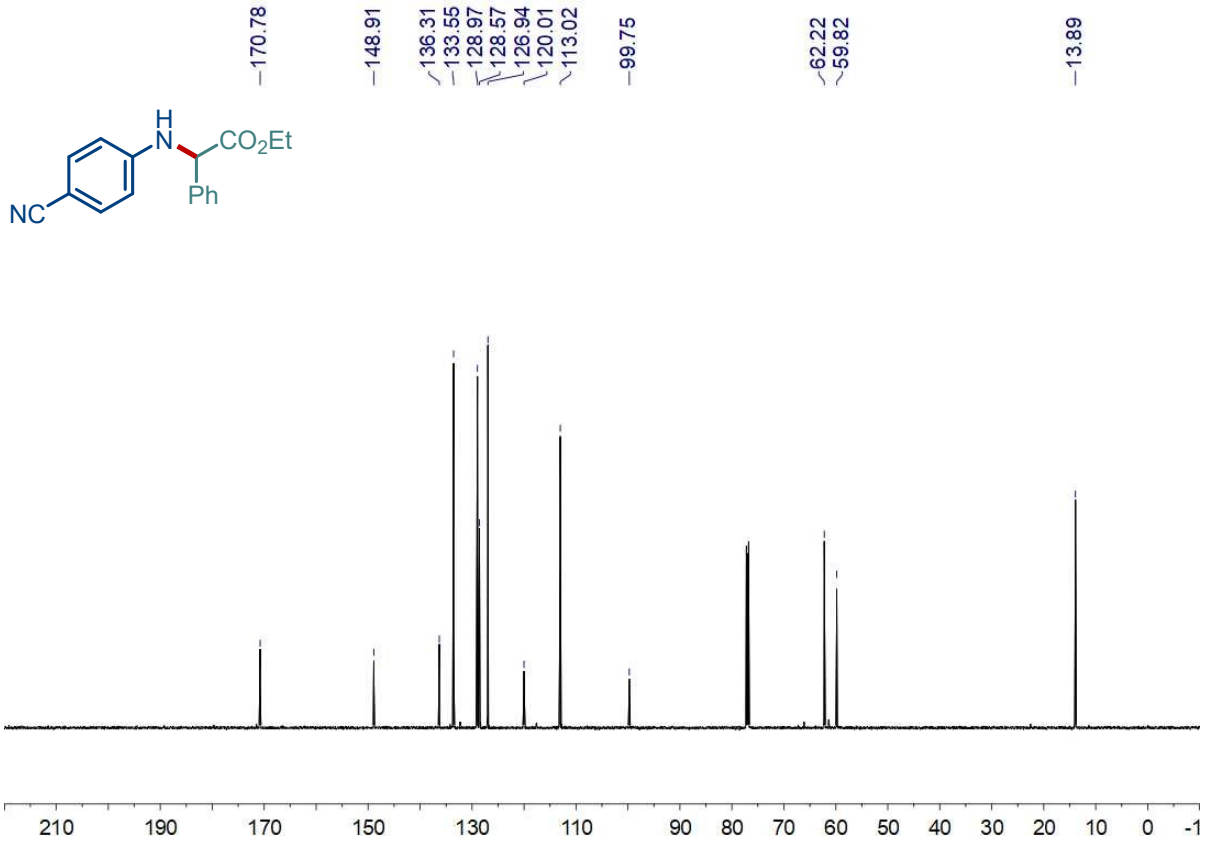
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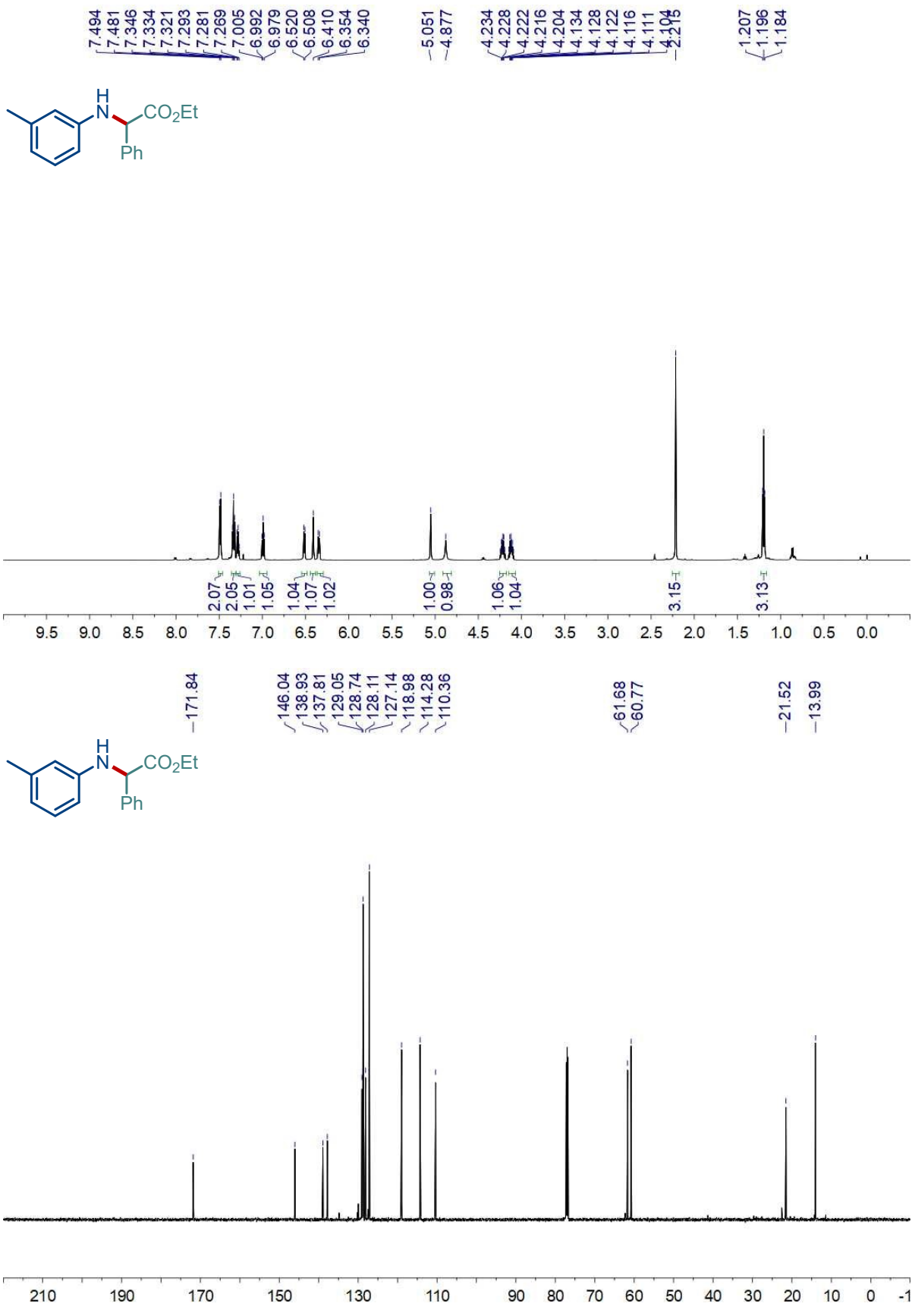
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Ph
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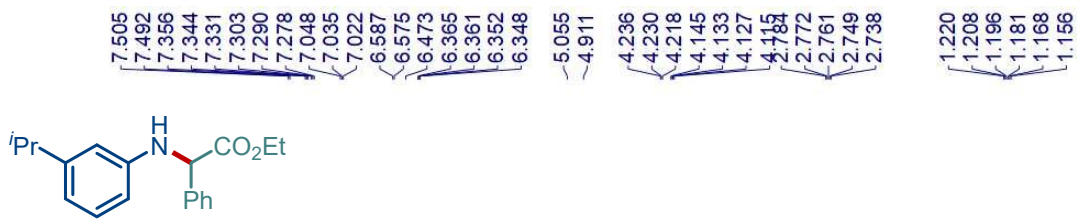
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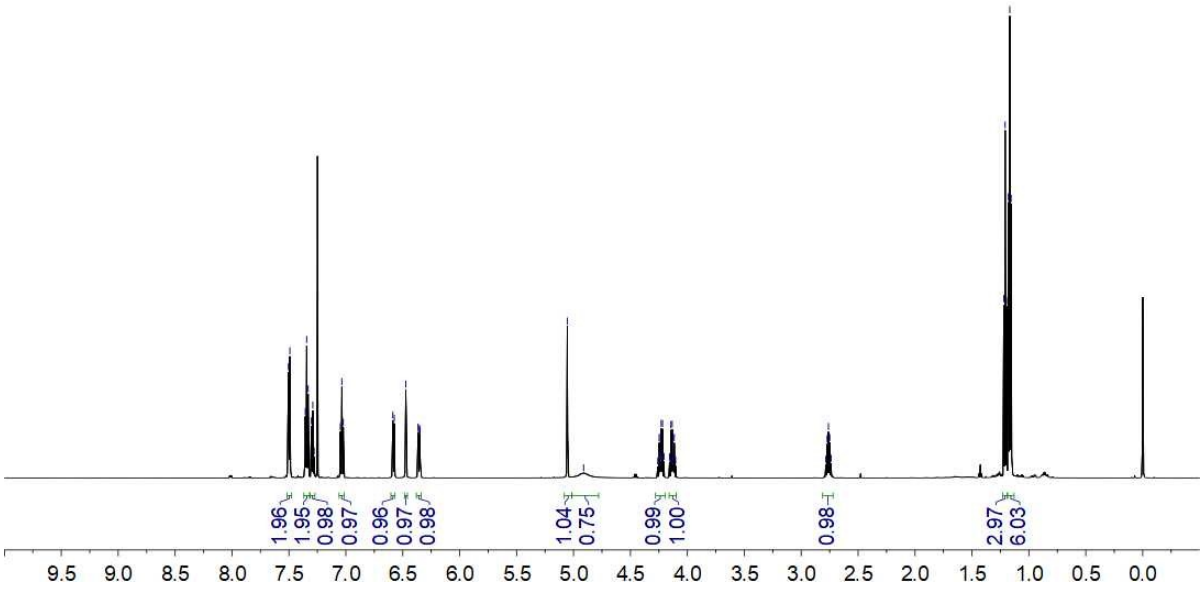
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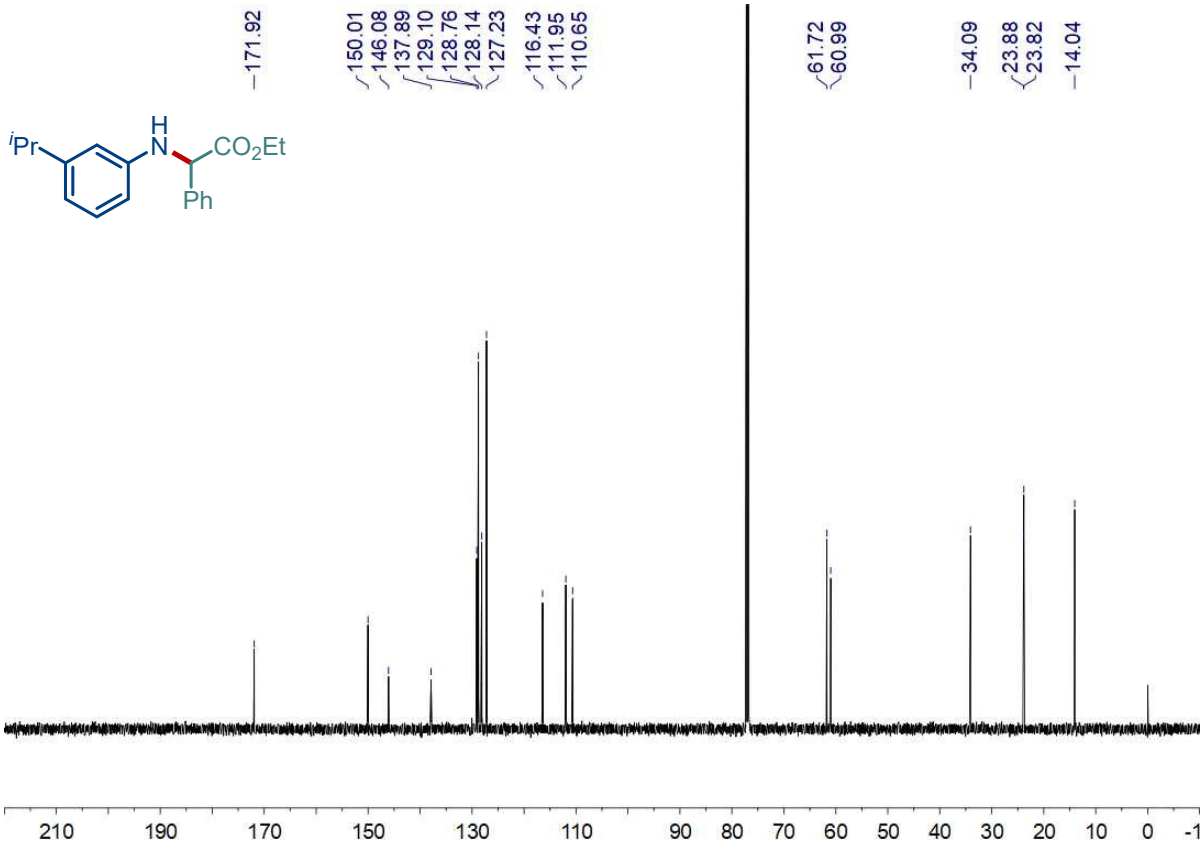
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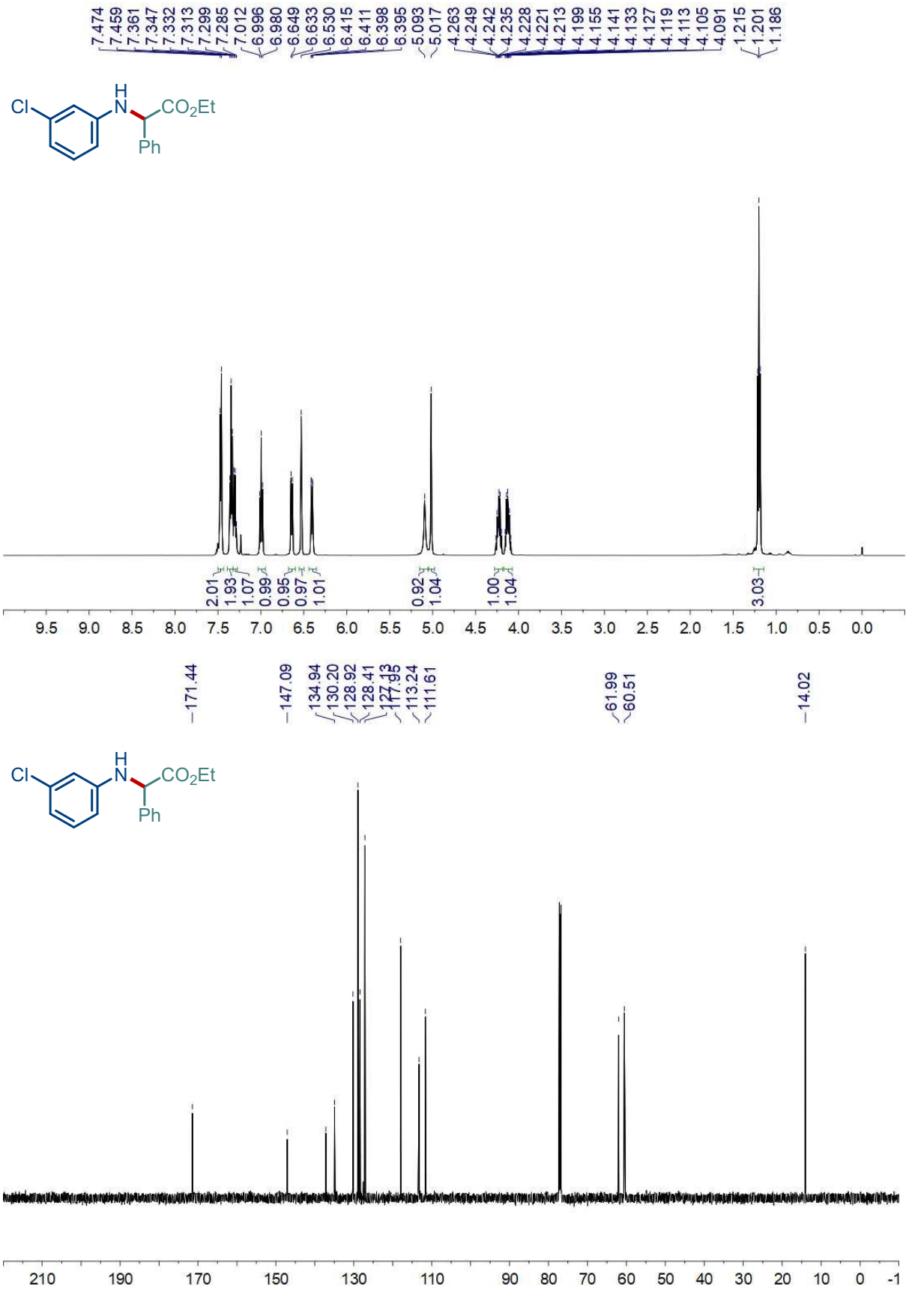
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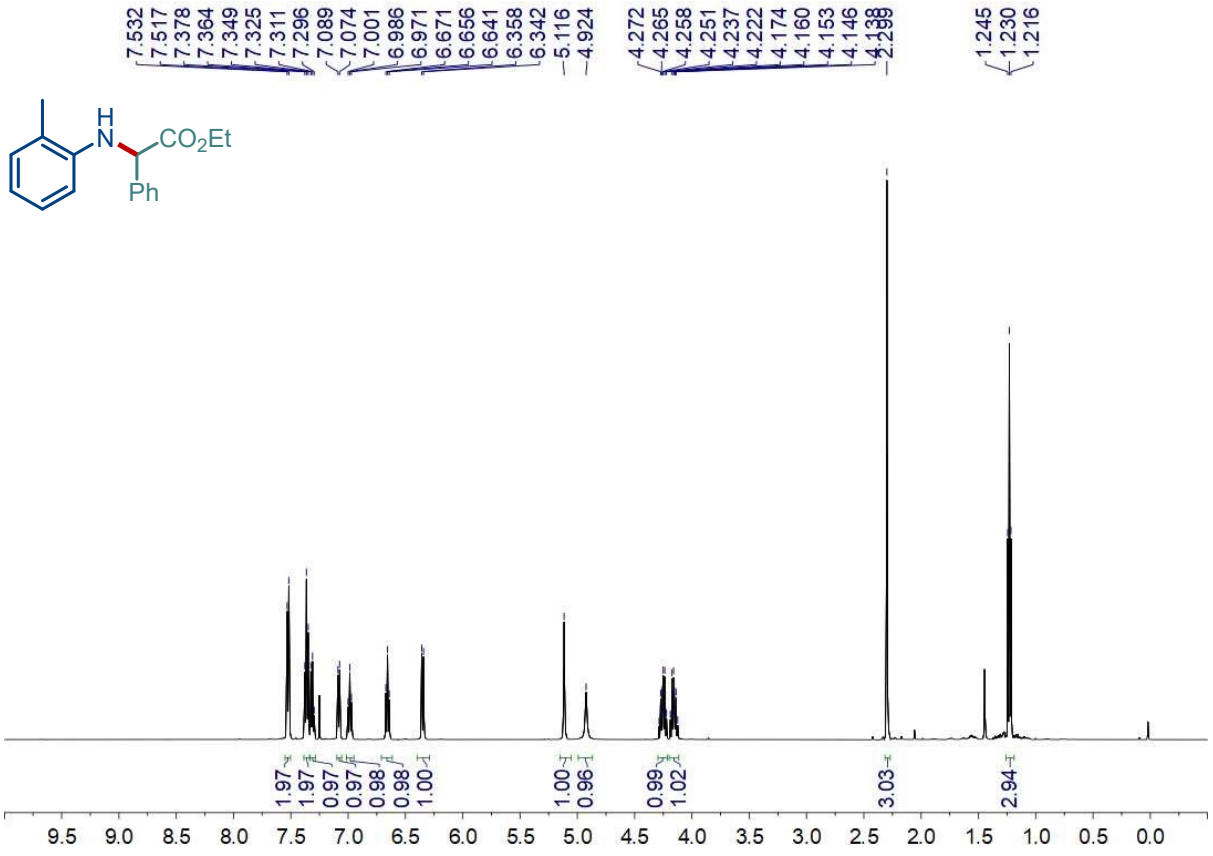
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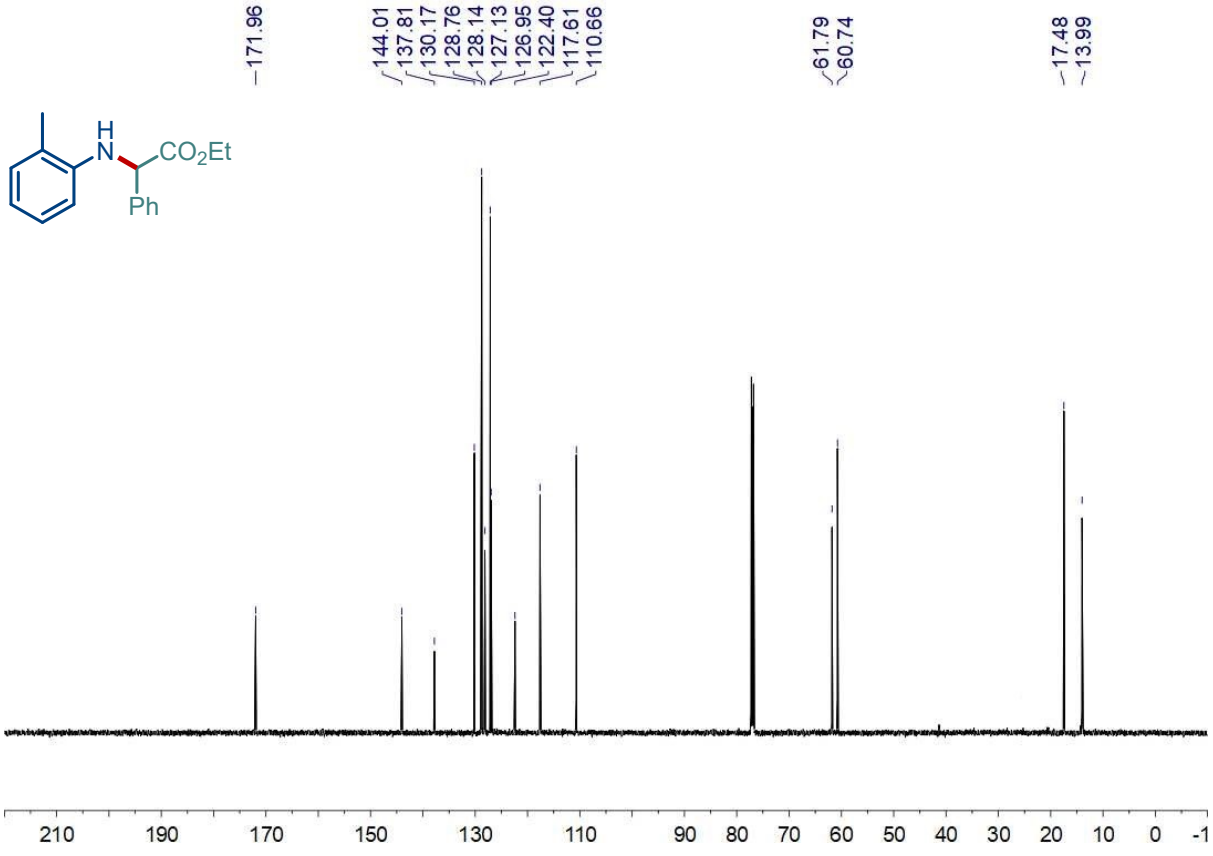
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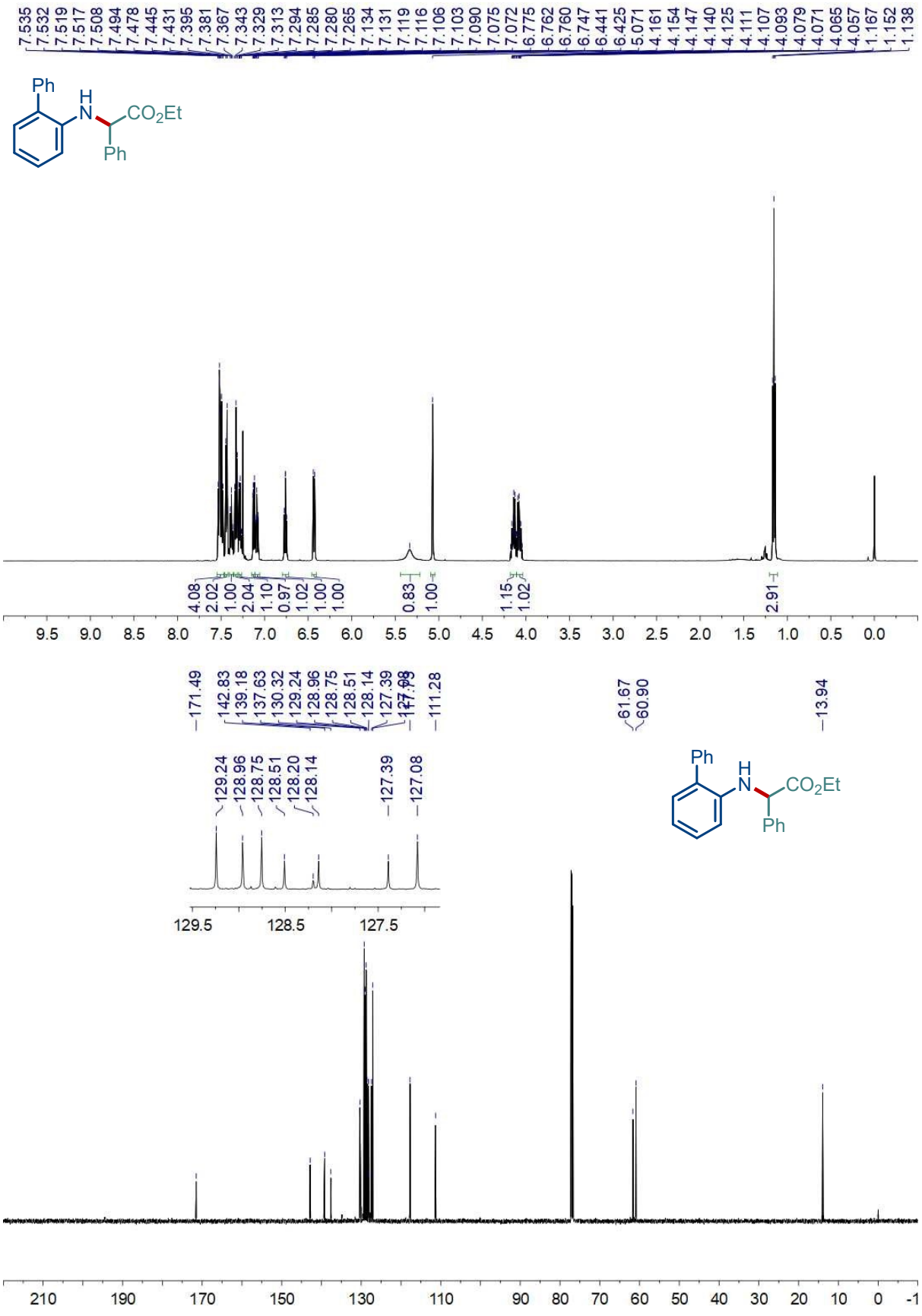
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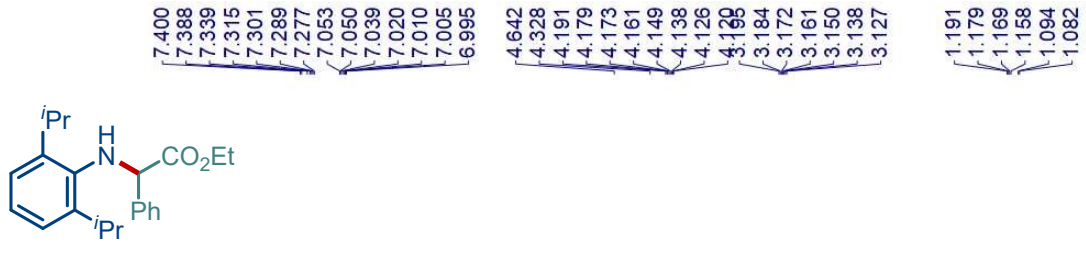
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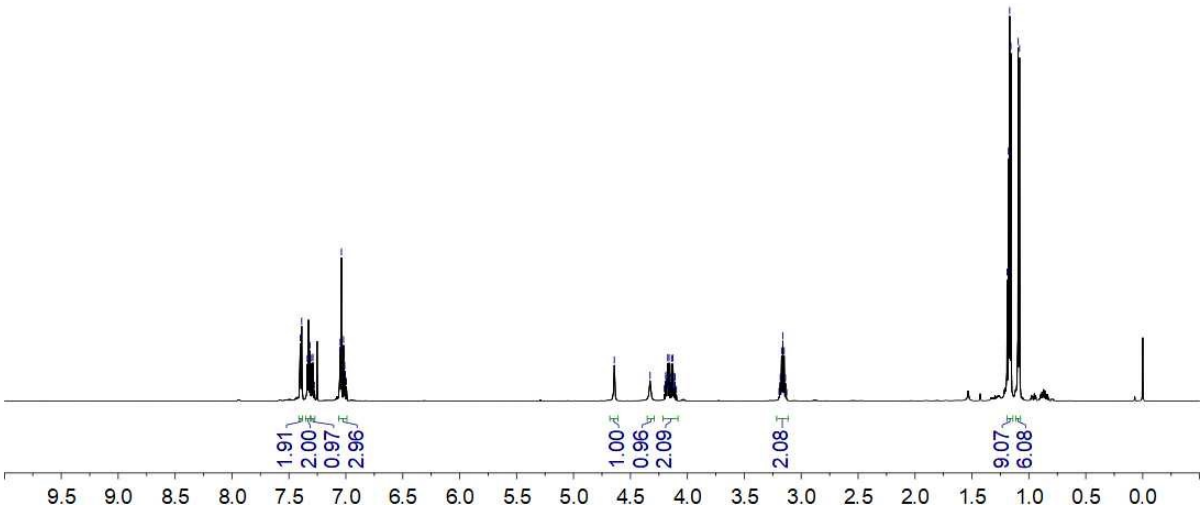
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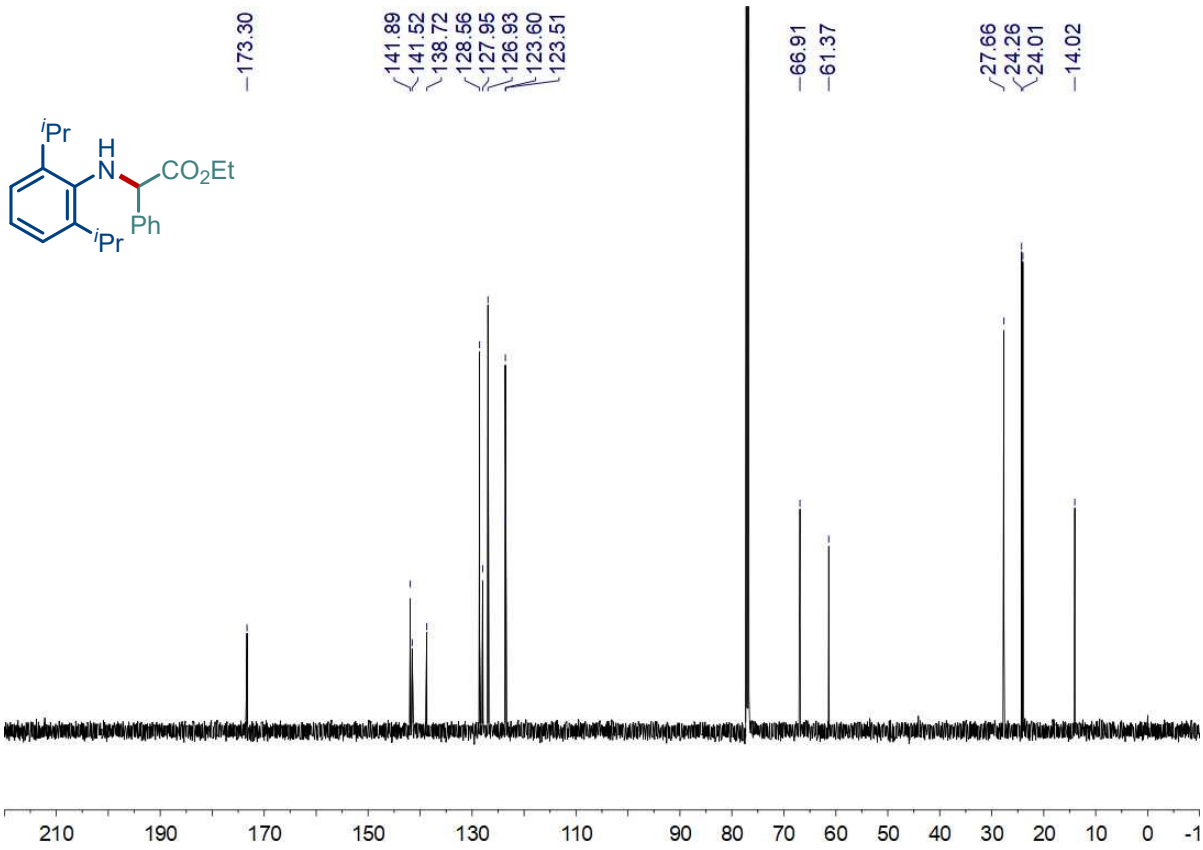
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Ph
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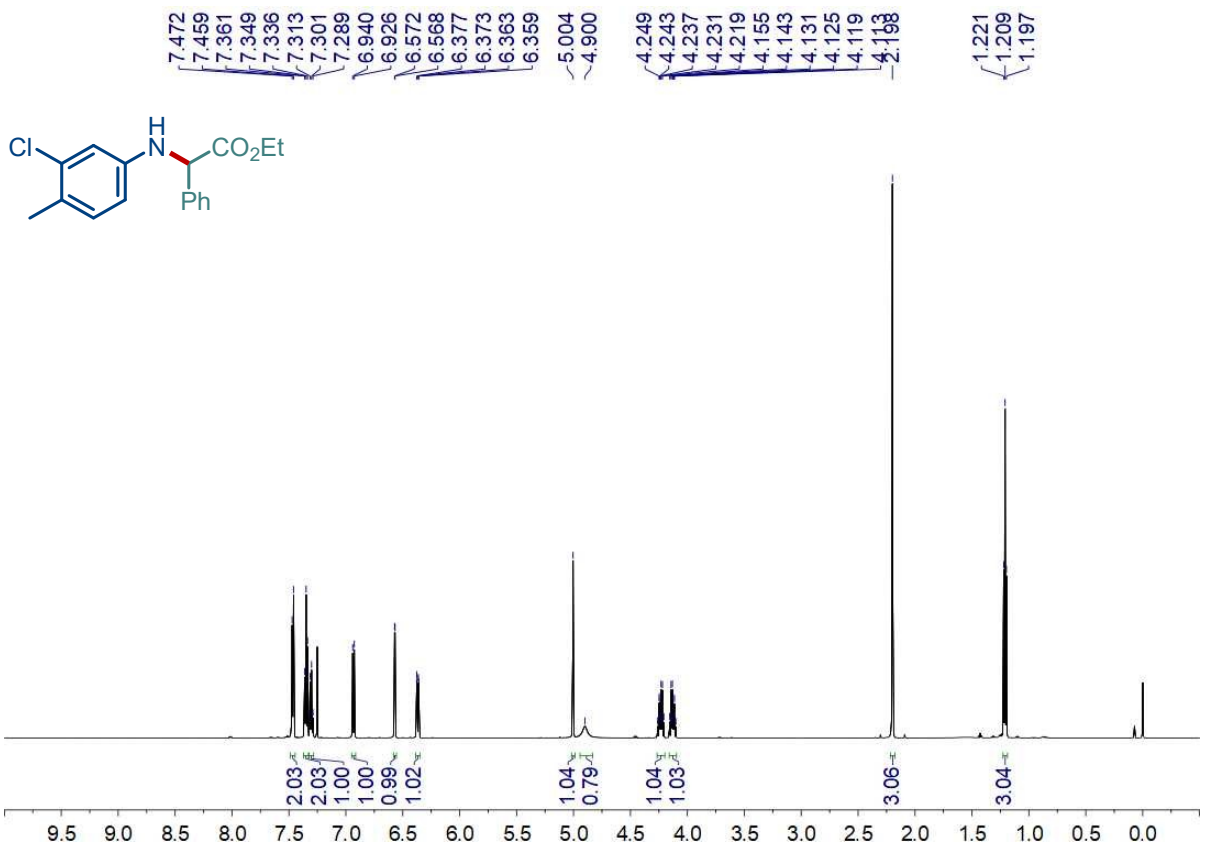
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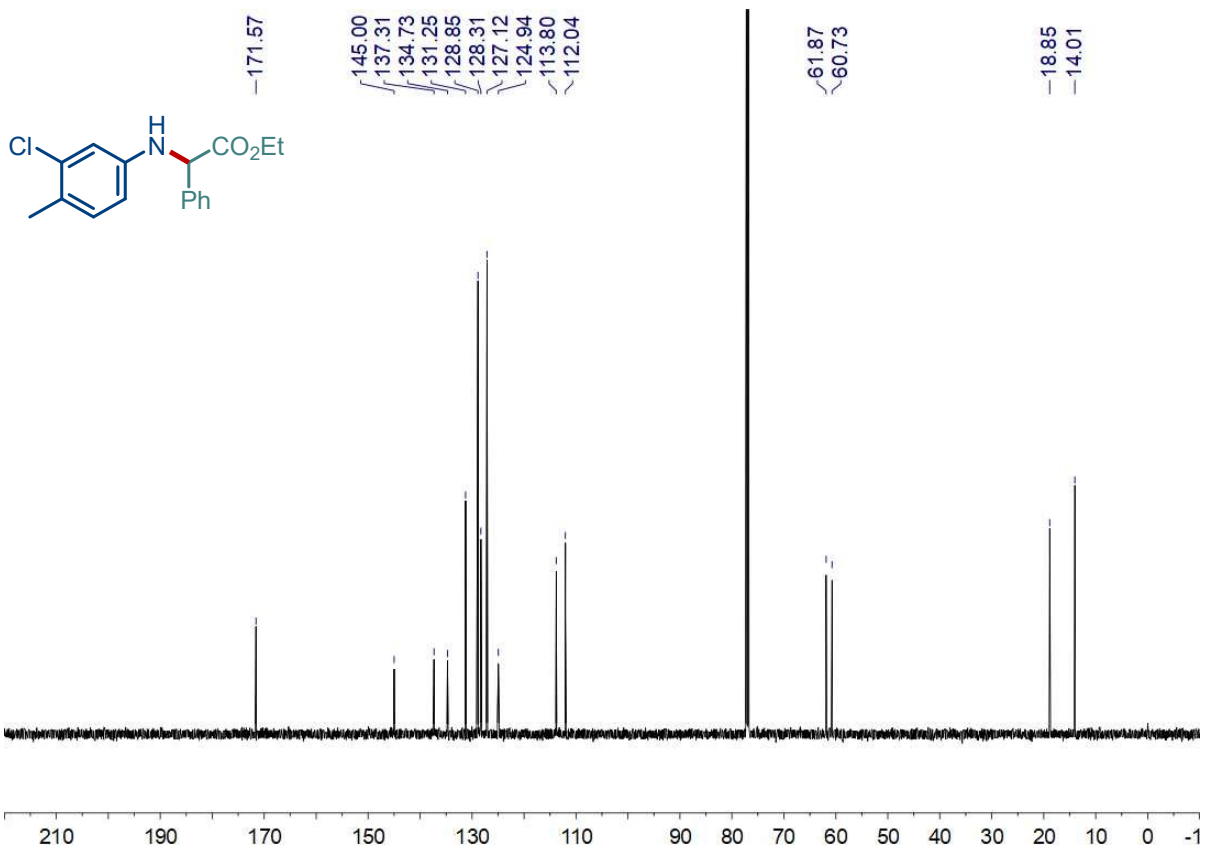
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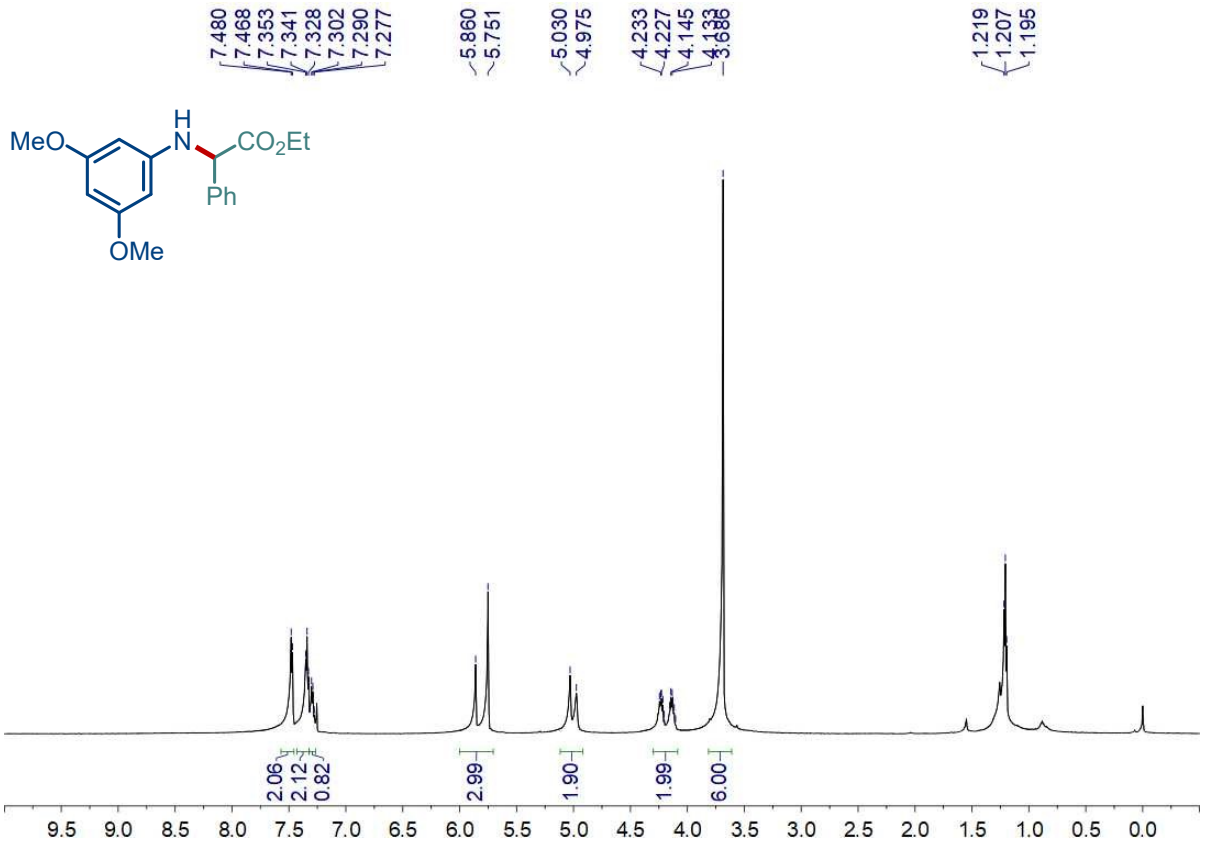
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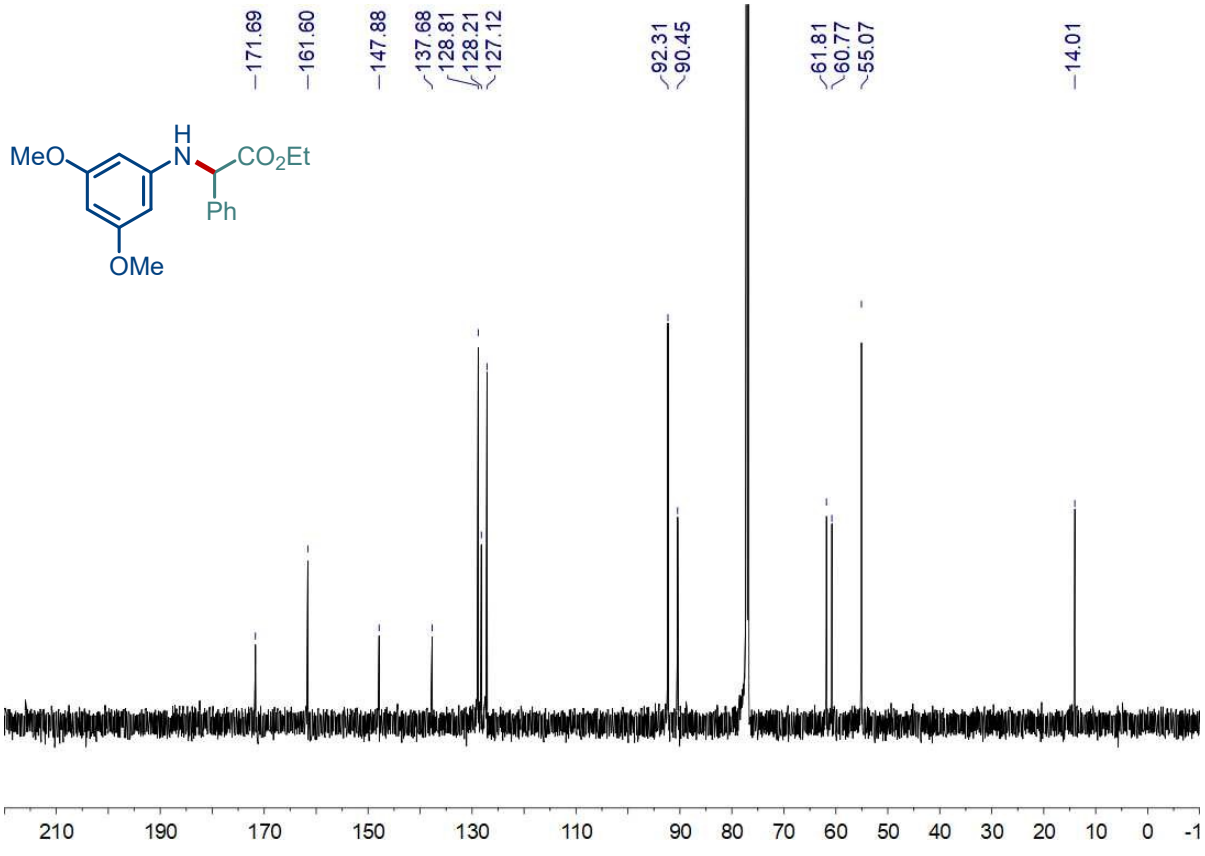
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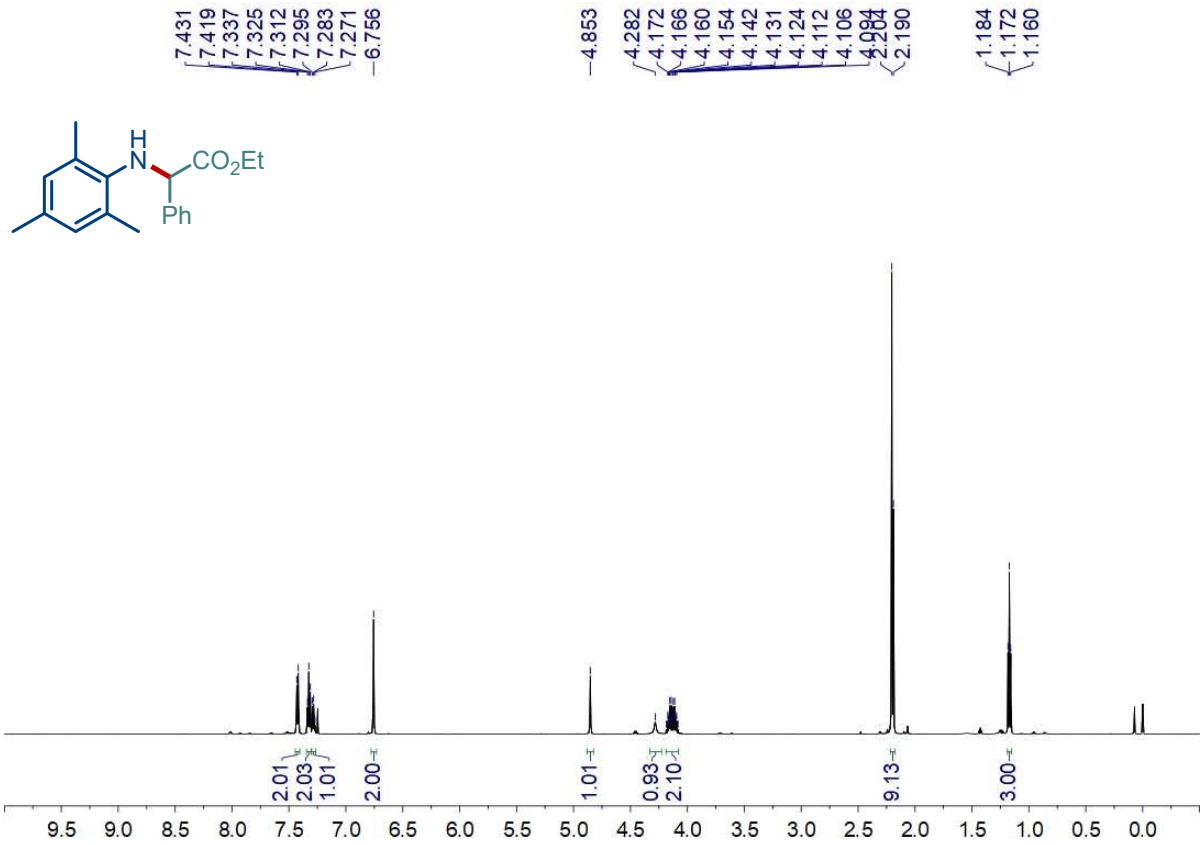
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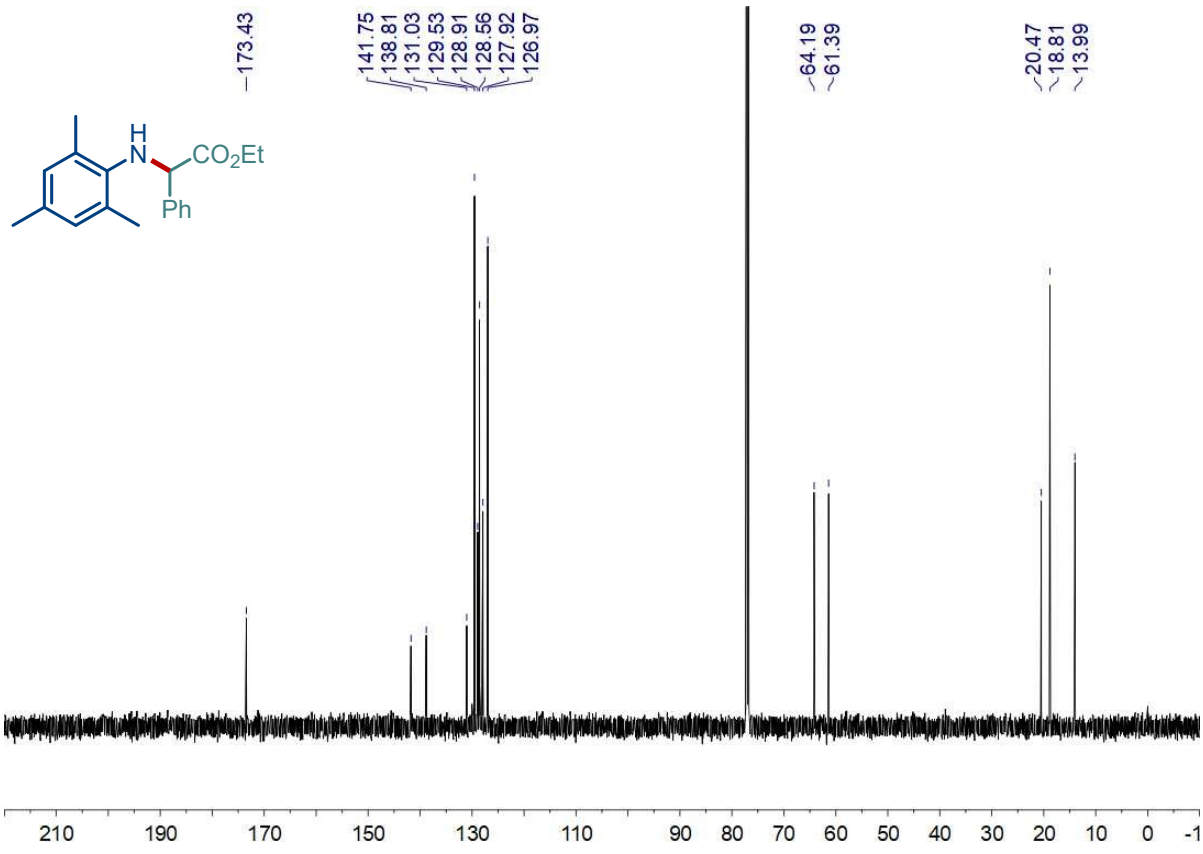
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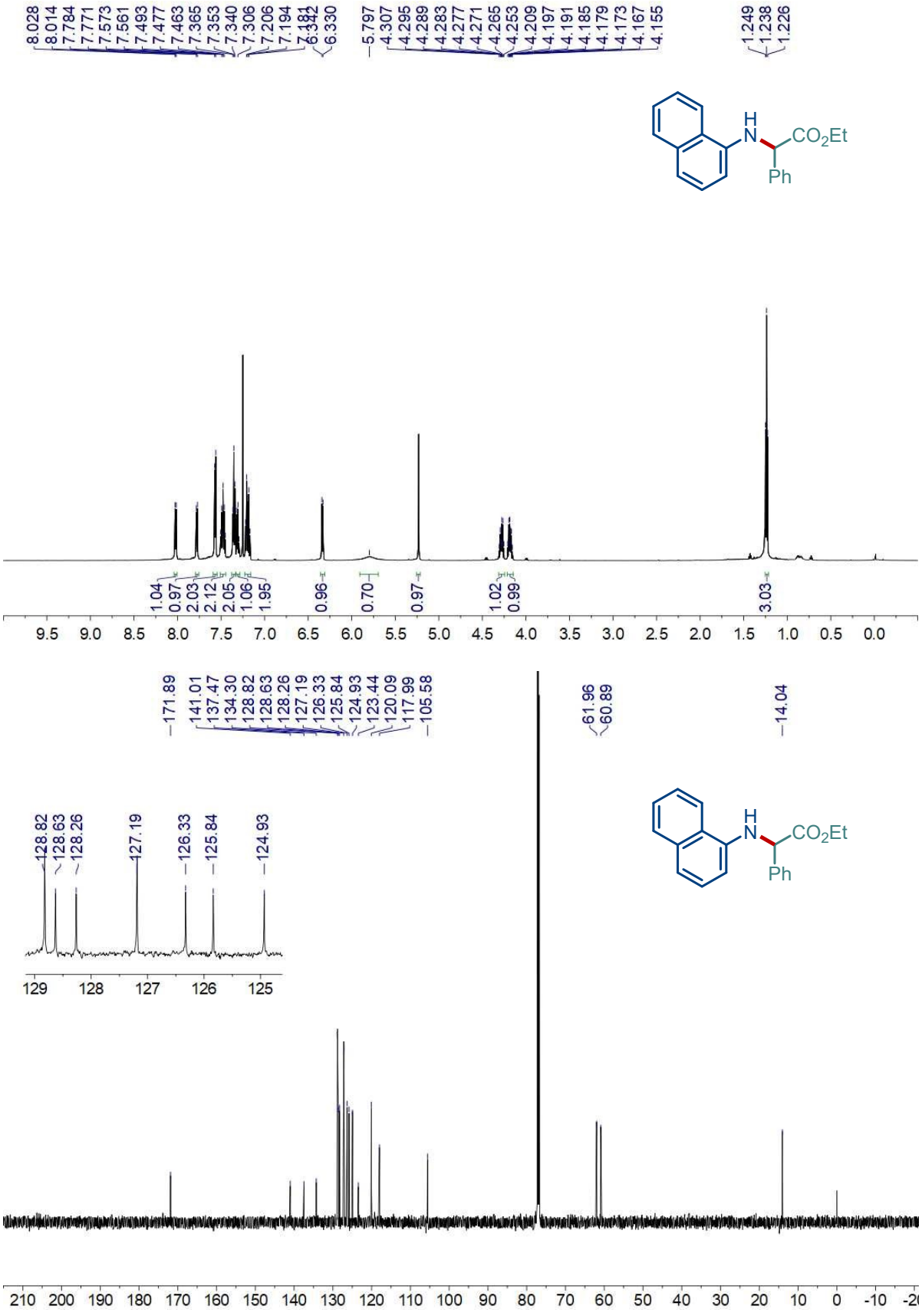
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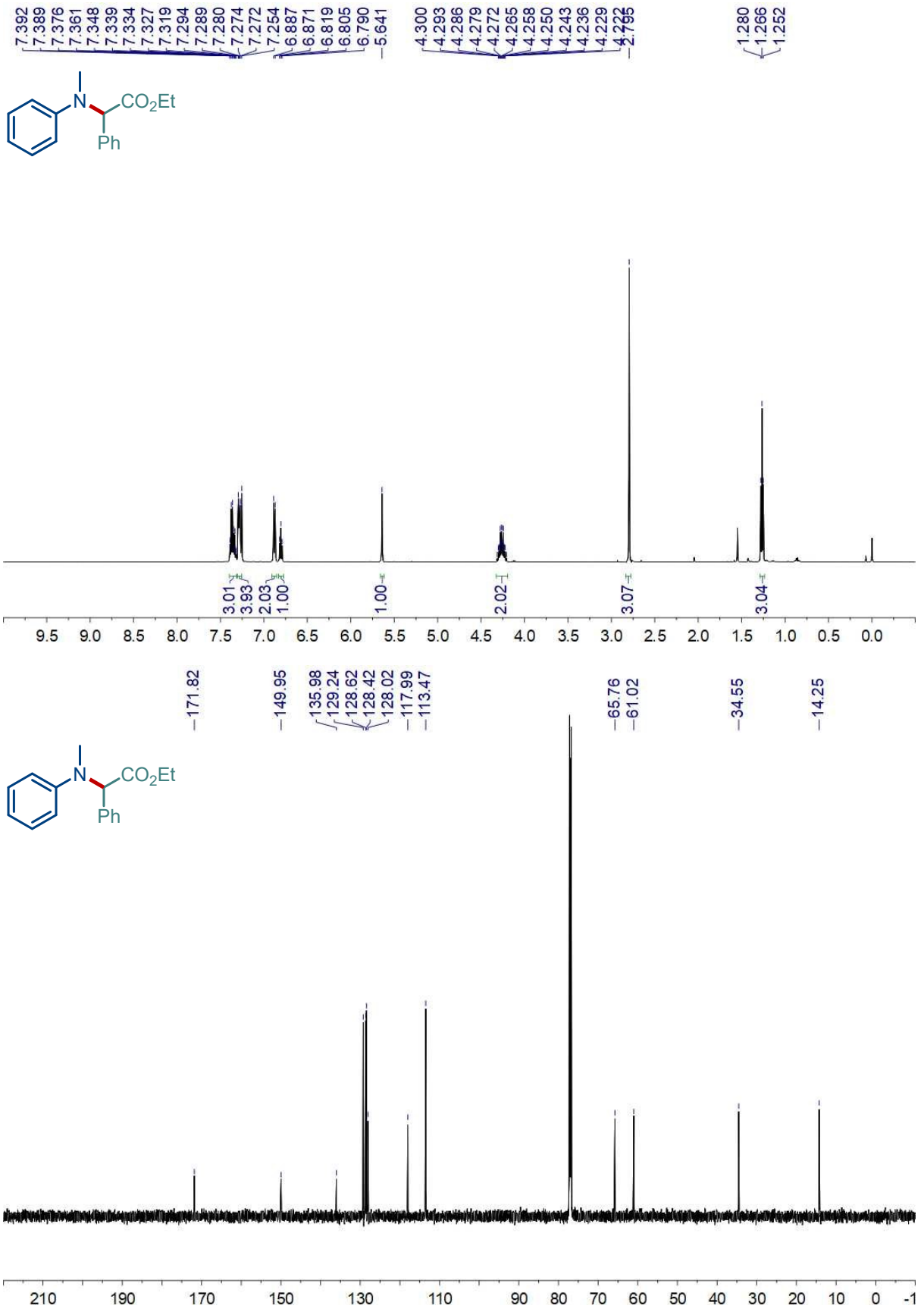
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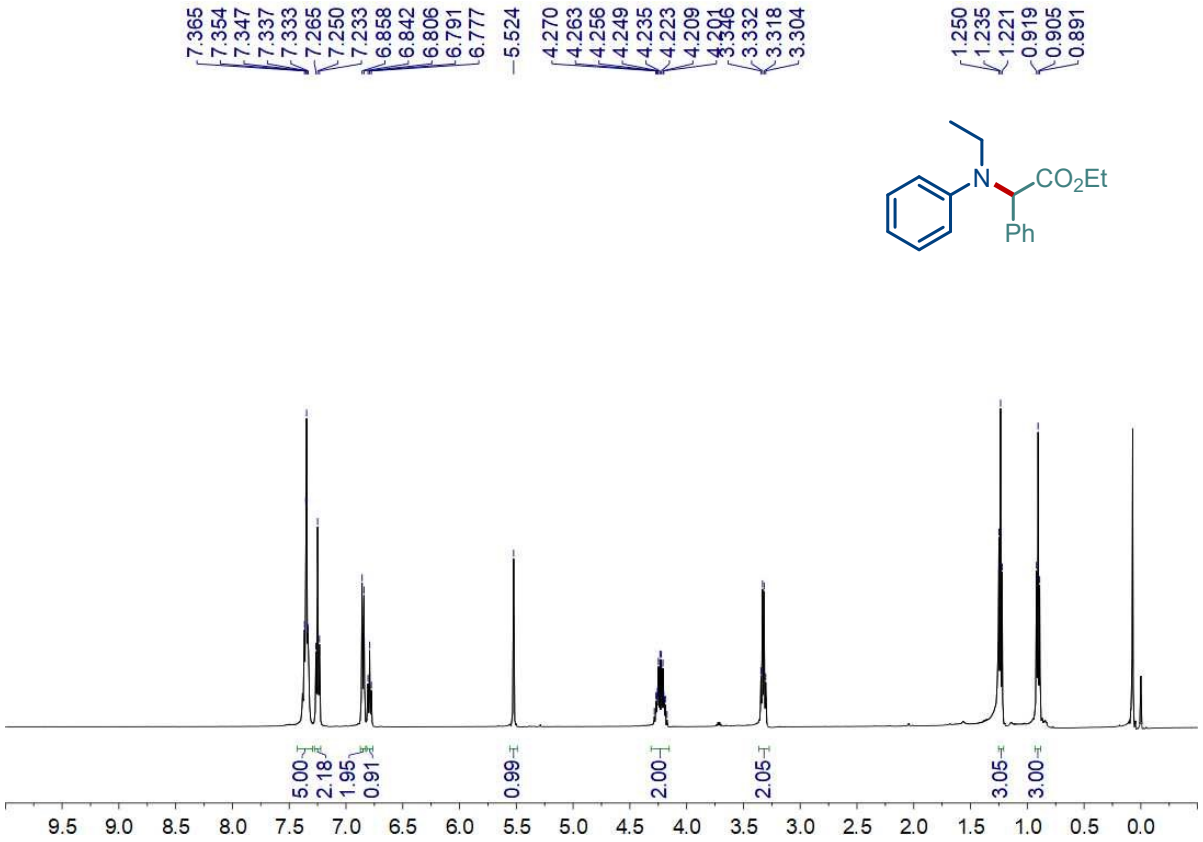
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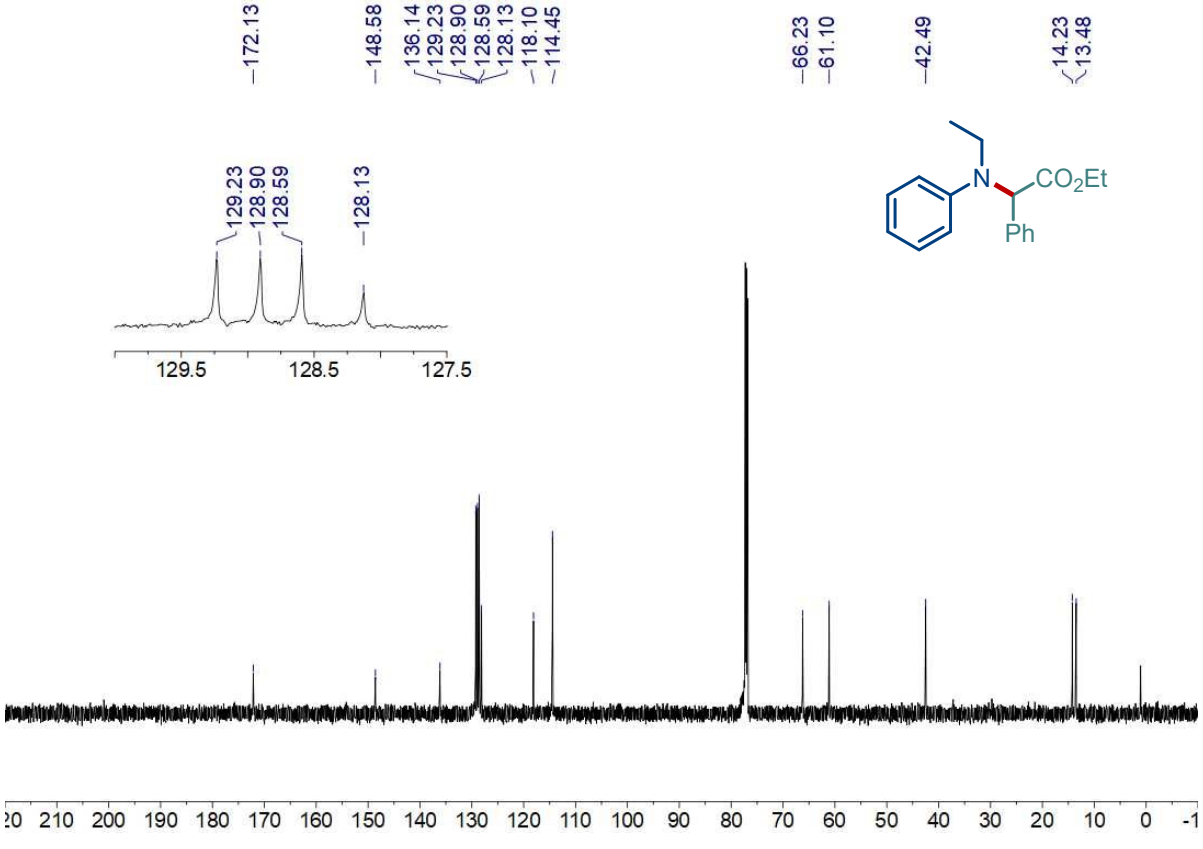
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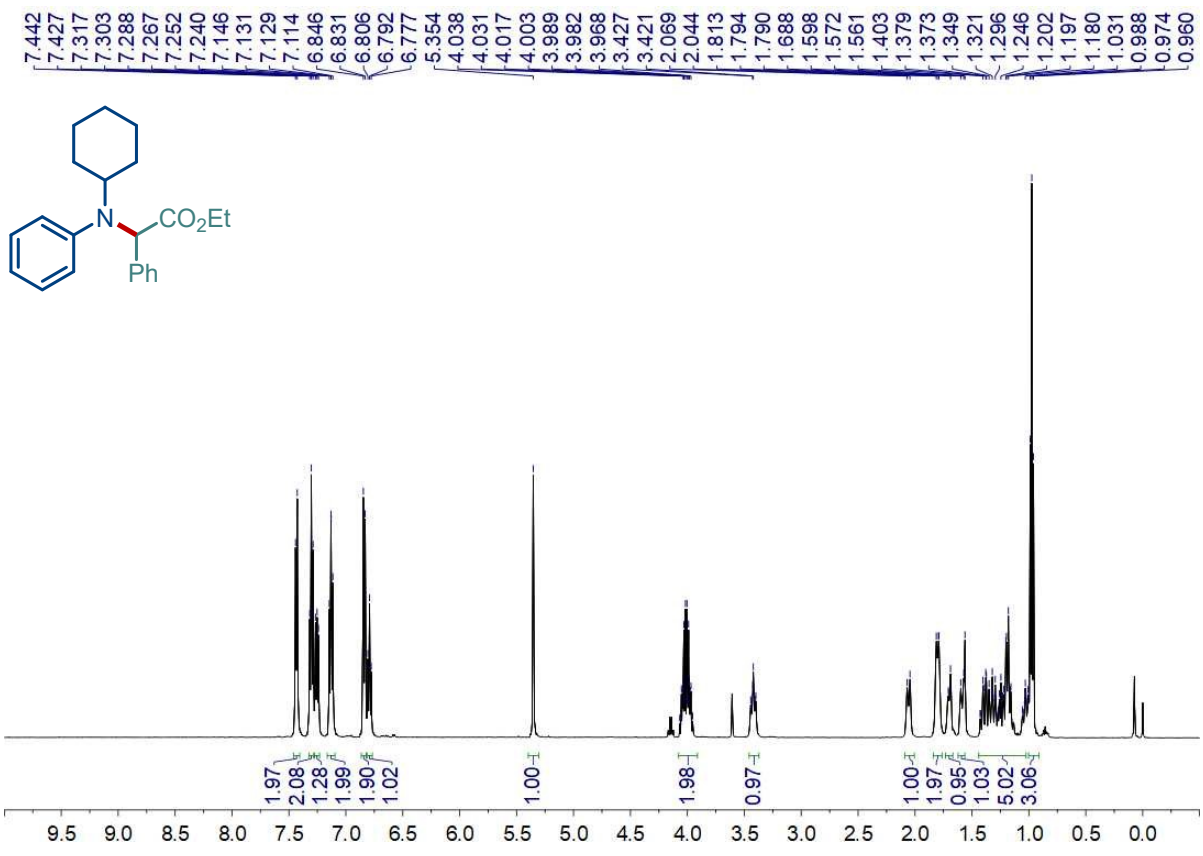
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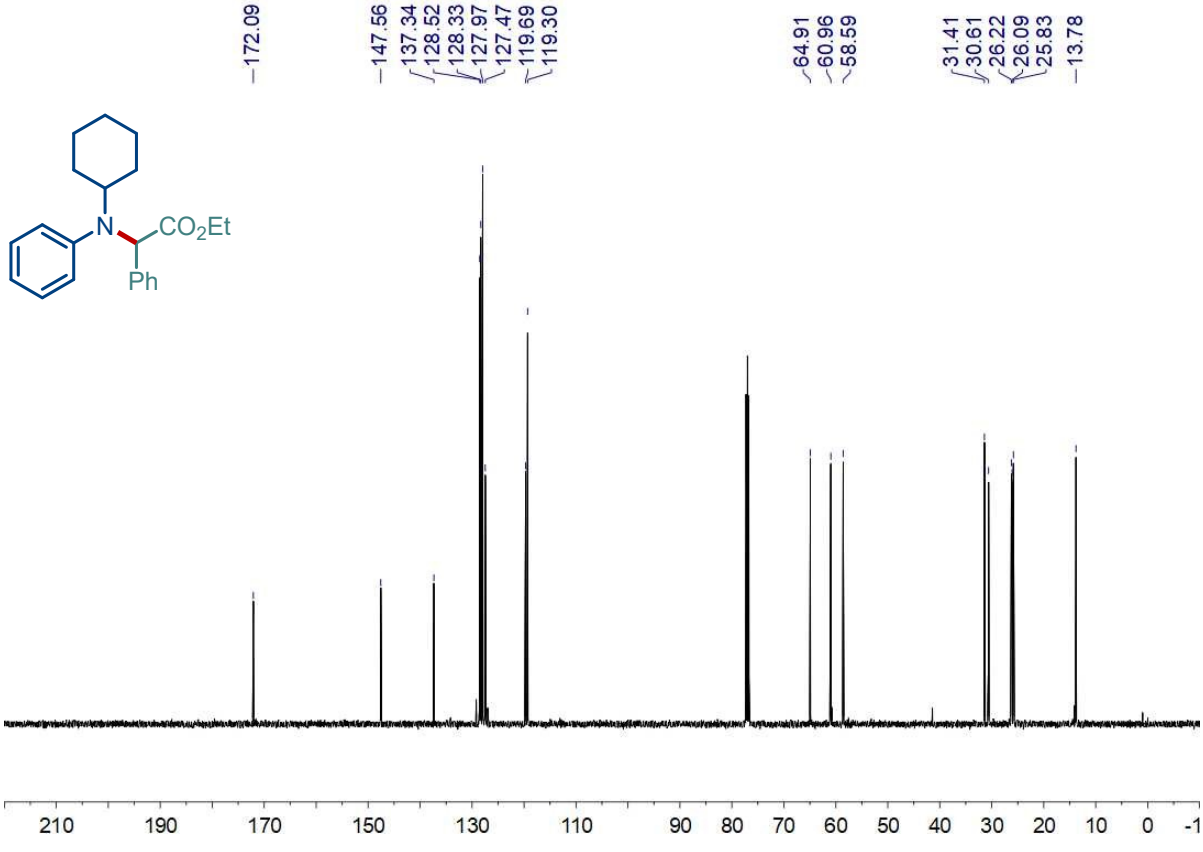
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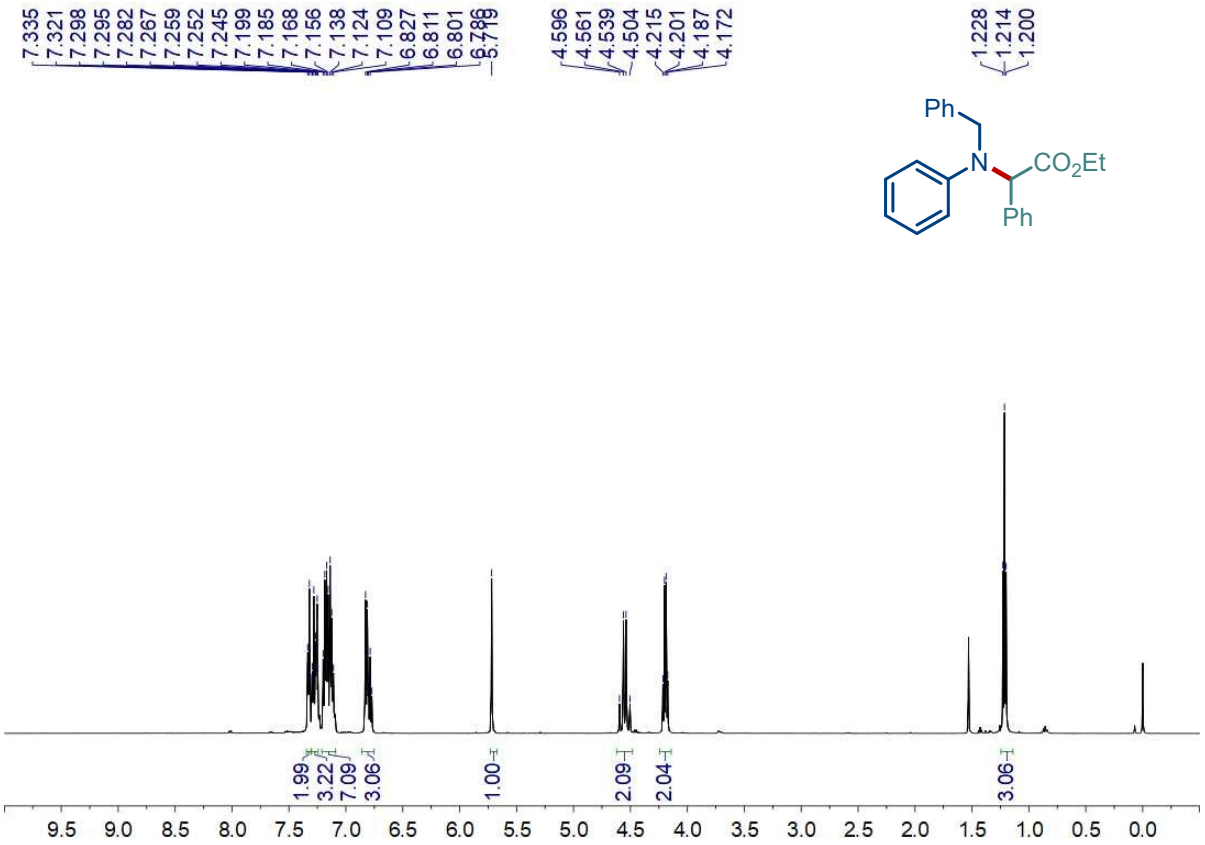
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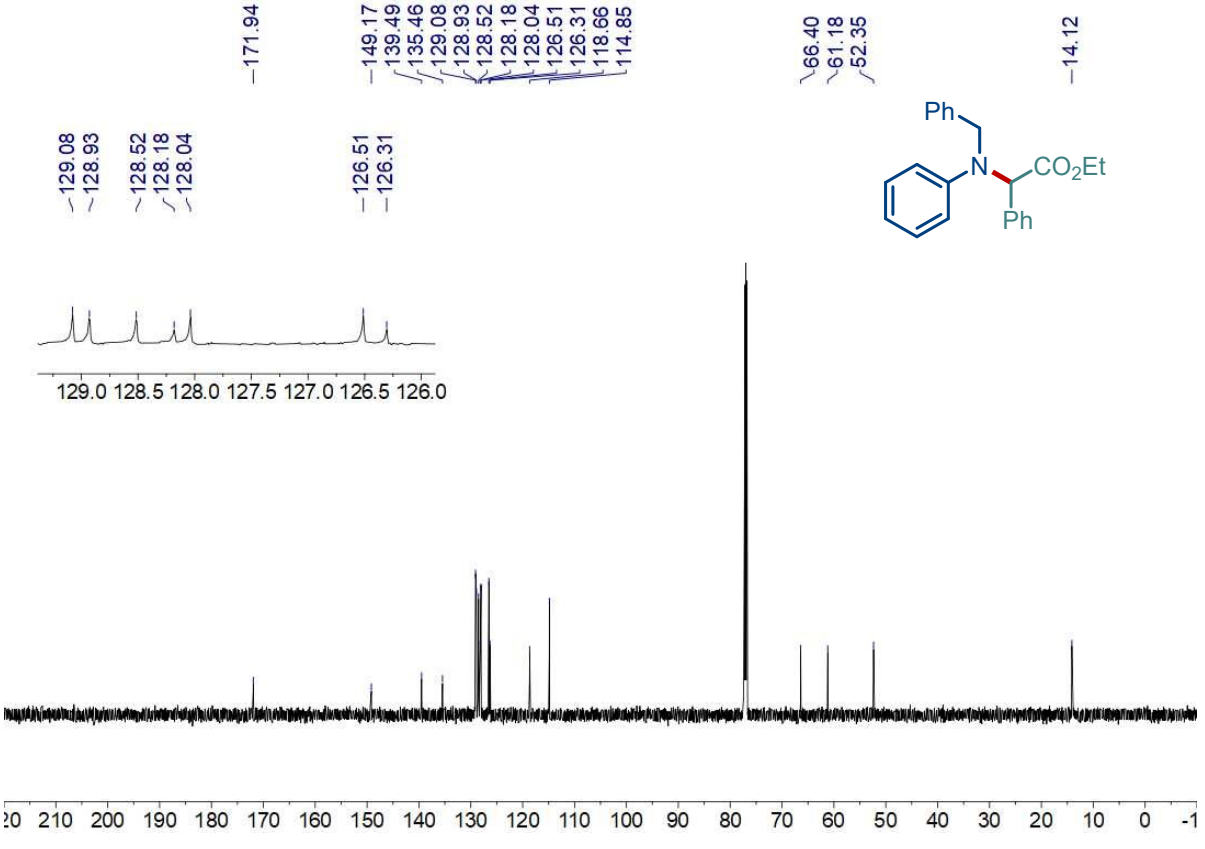
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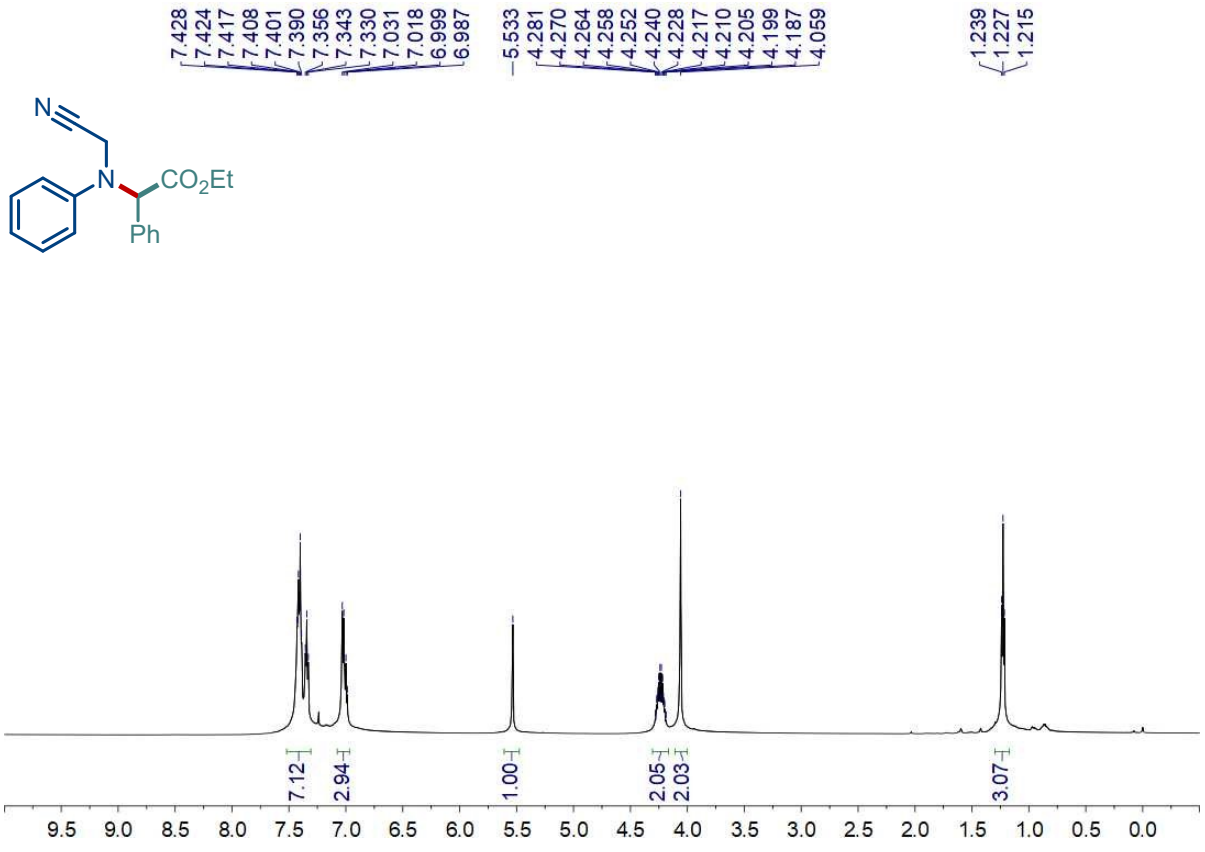
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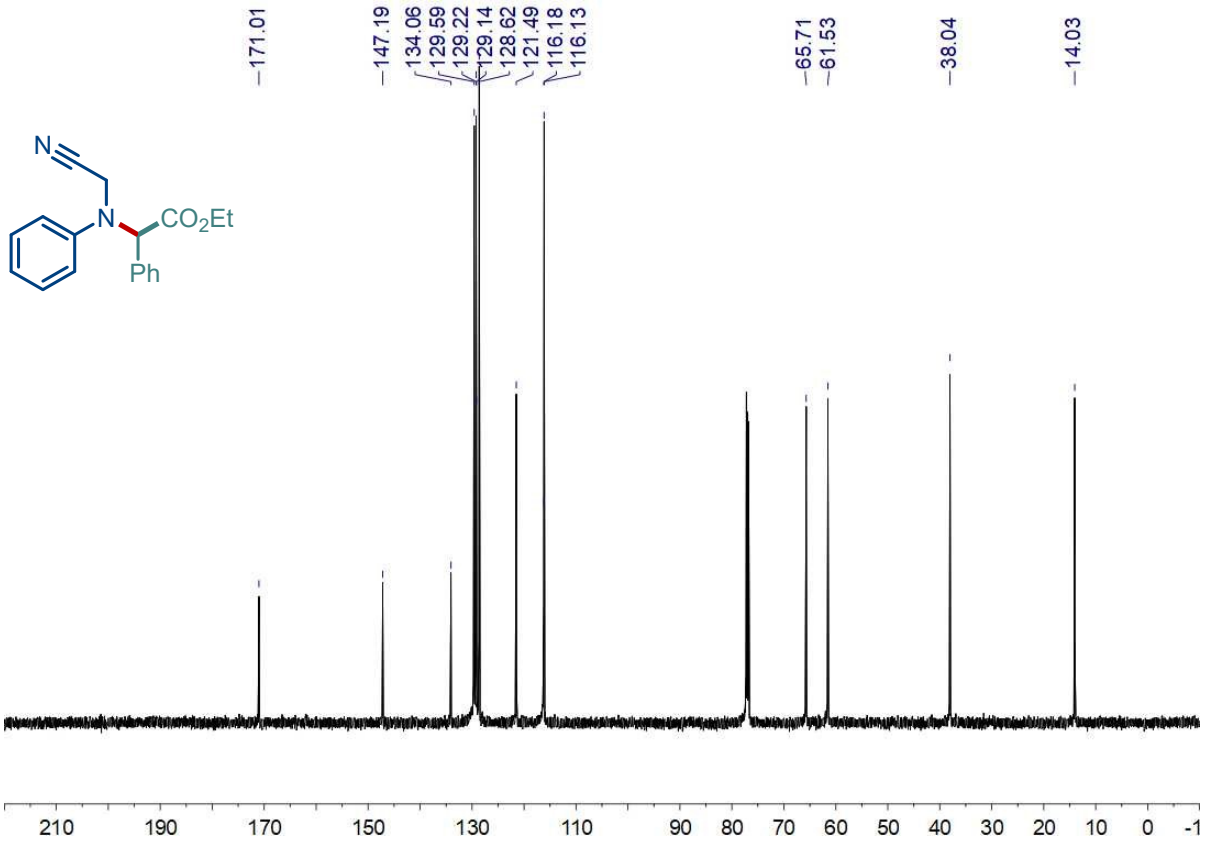
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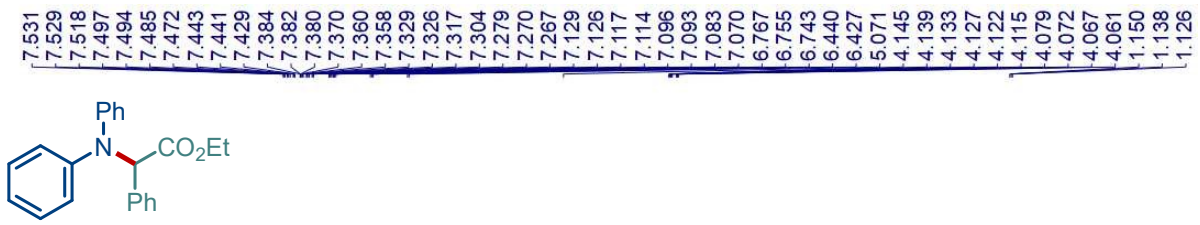
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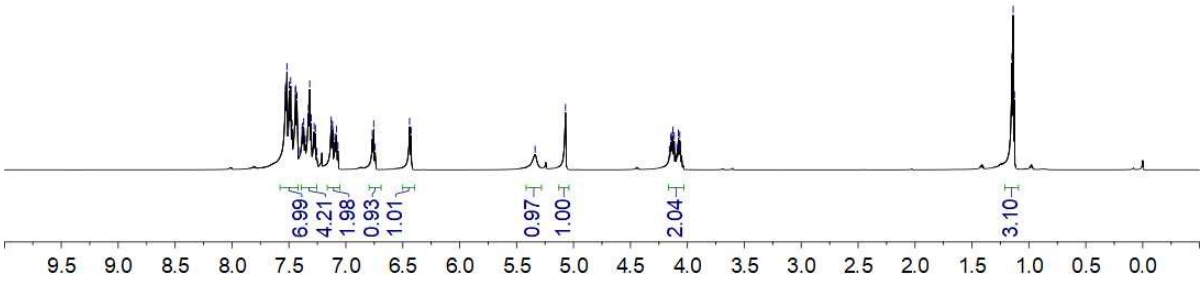
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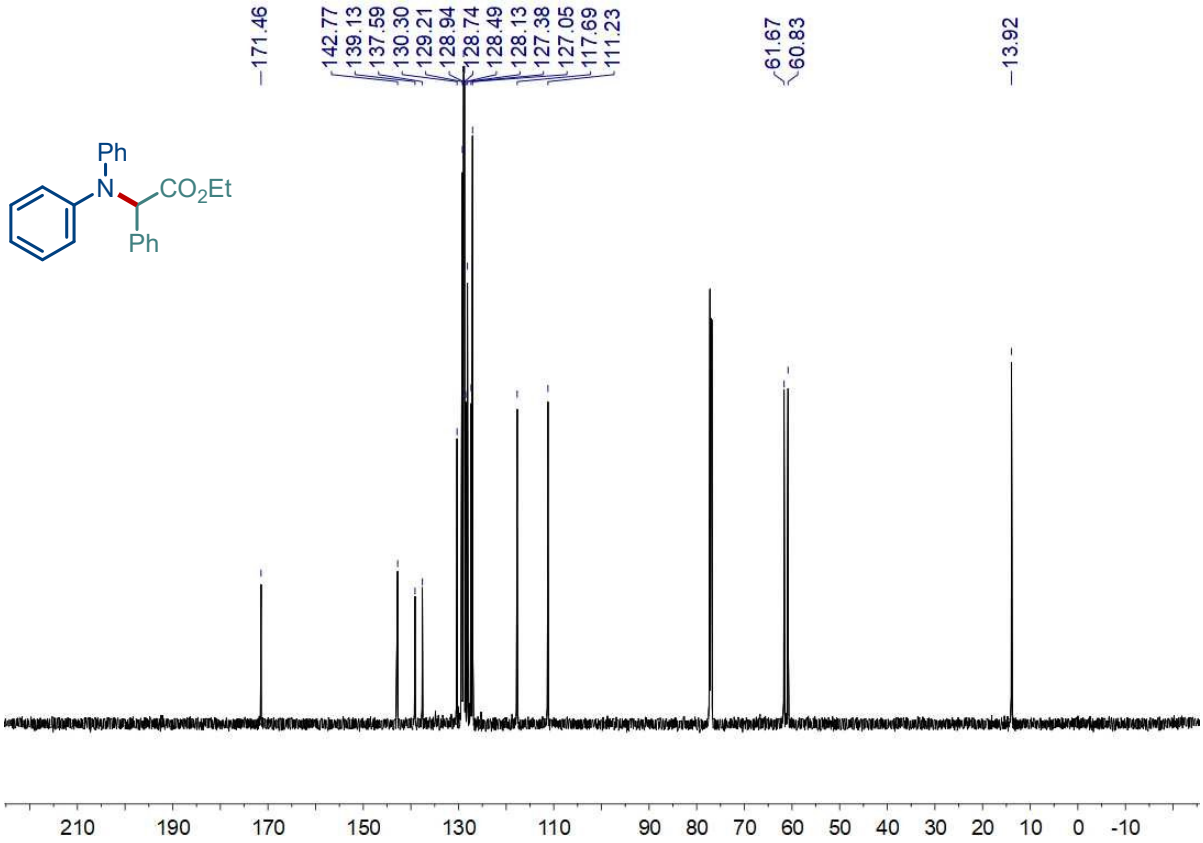
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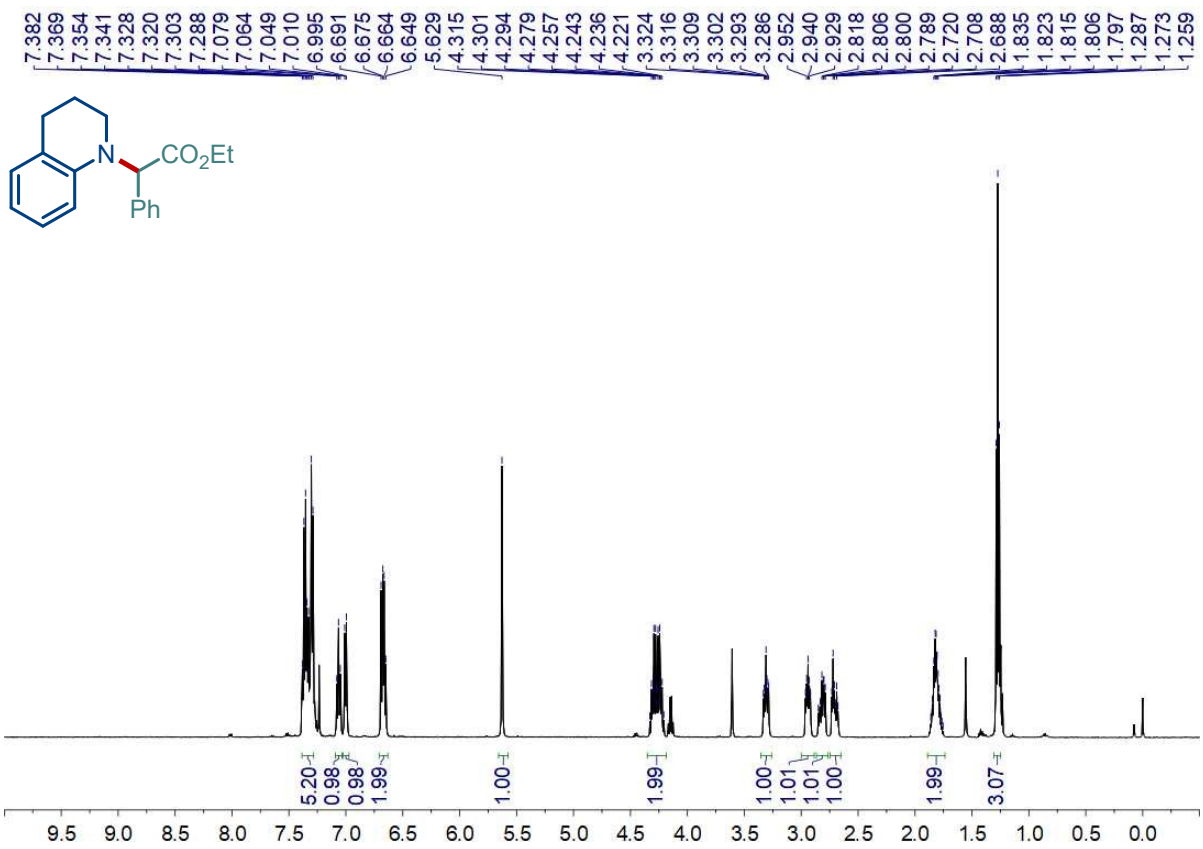
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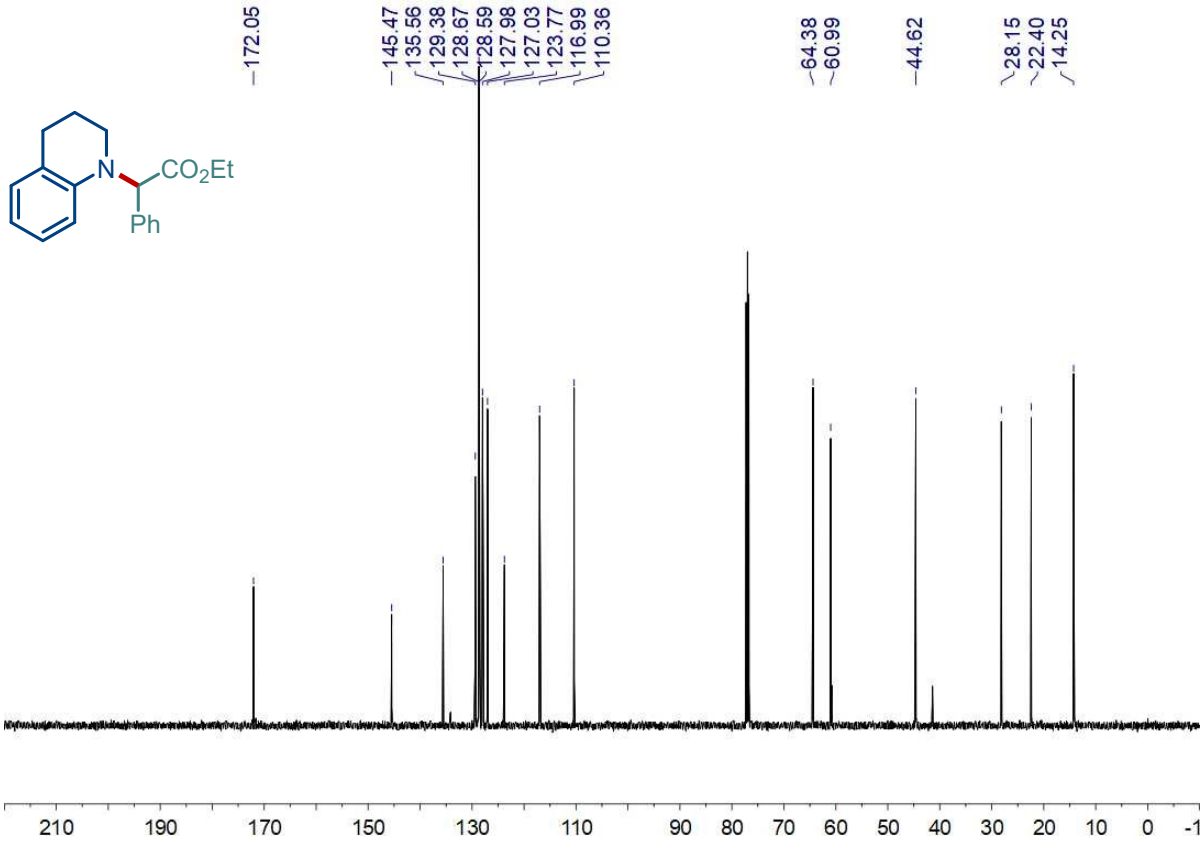
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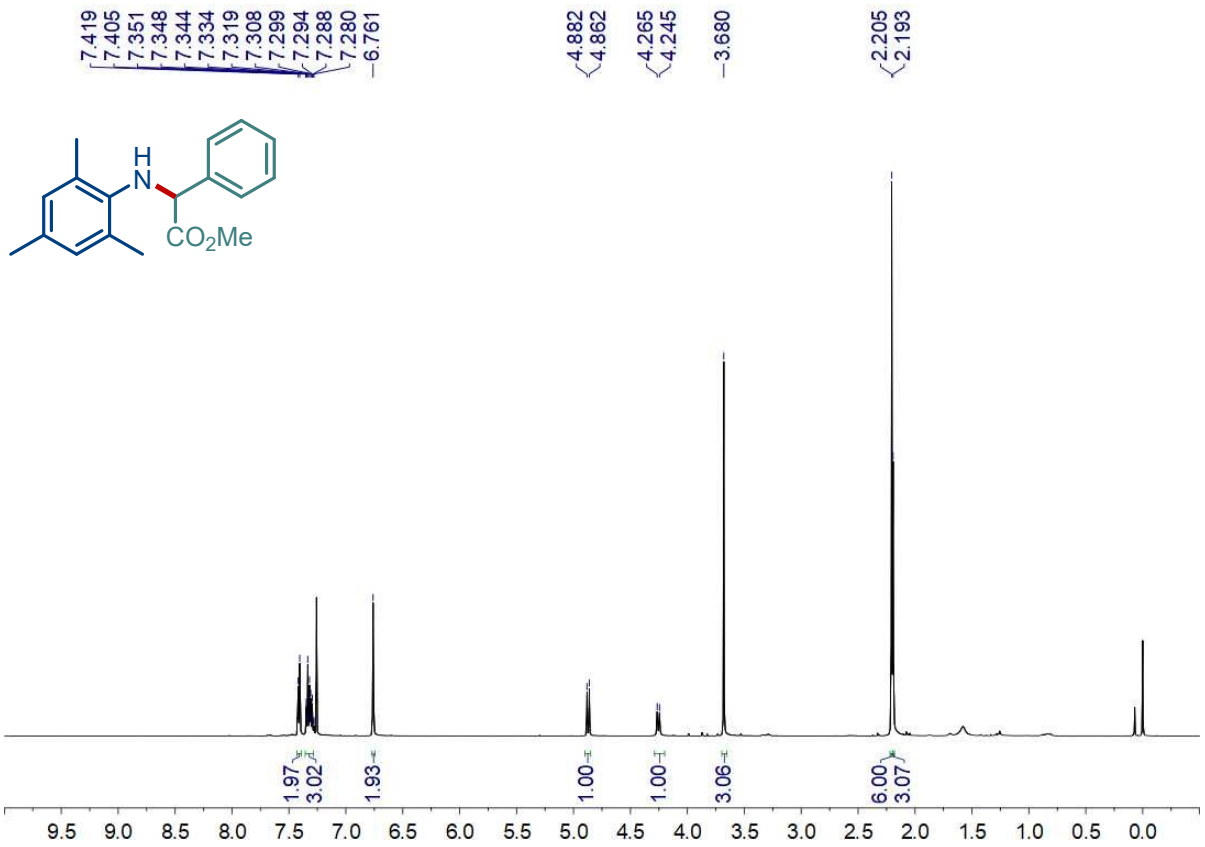
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1.00
1.00
3.06
6.00
3.07
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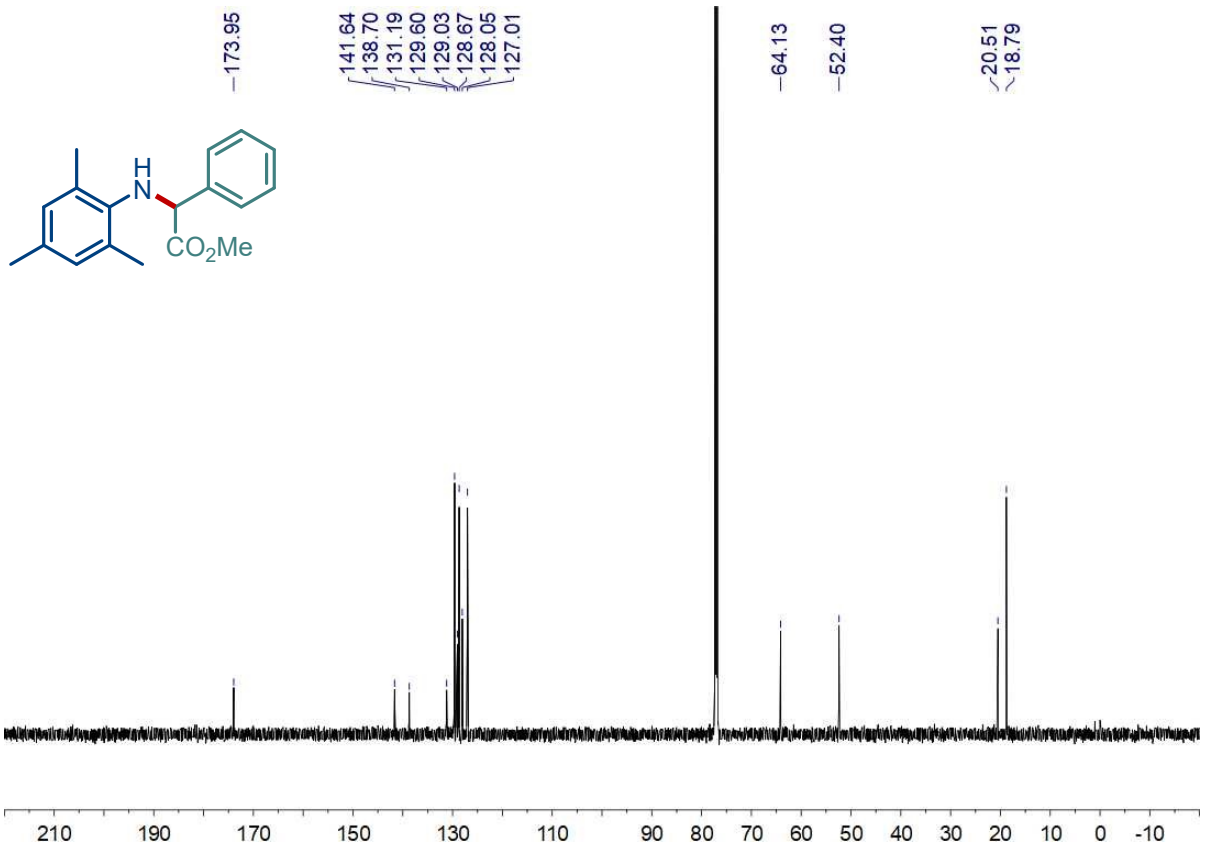
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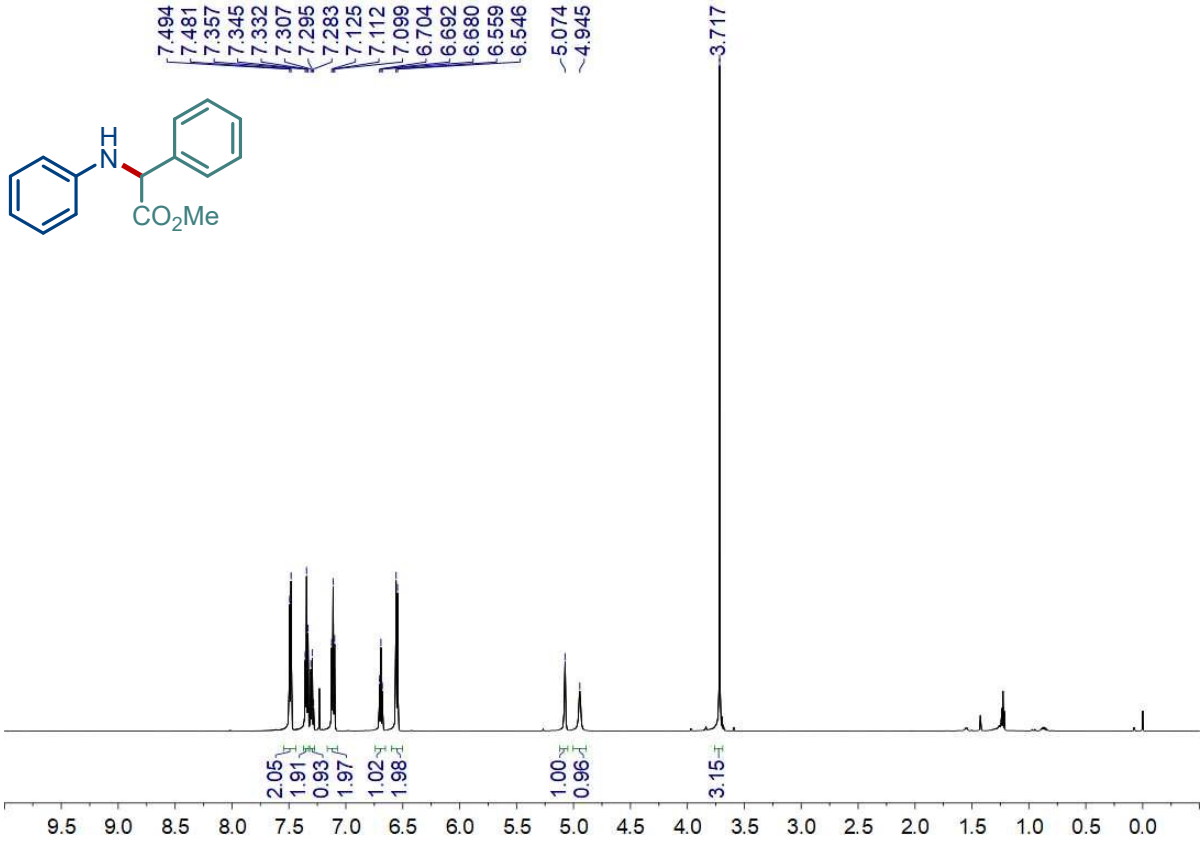
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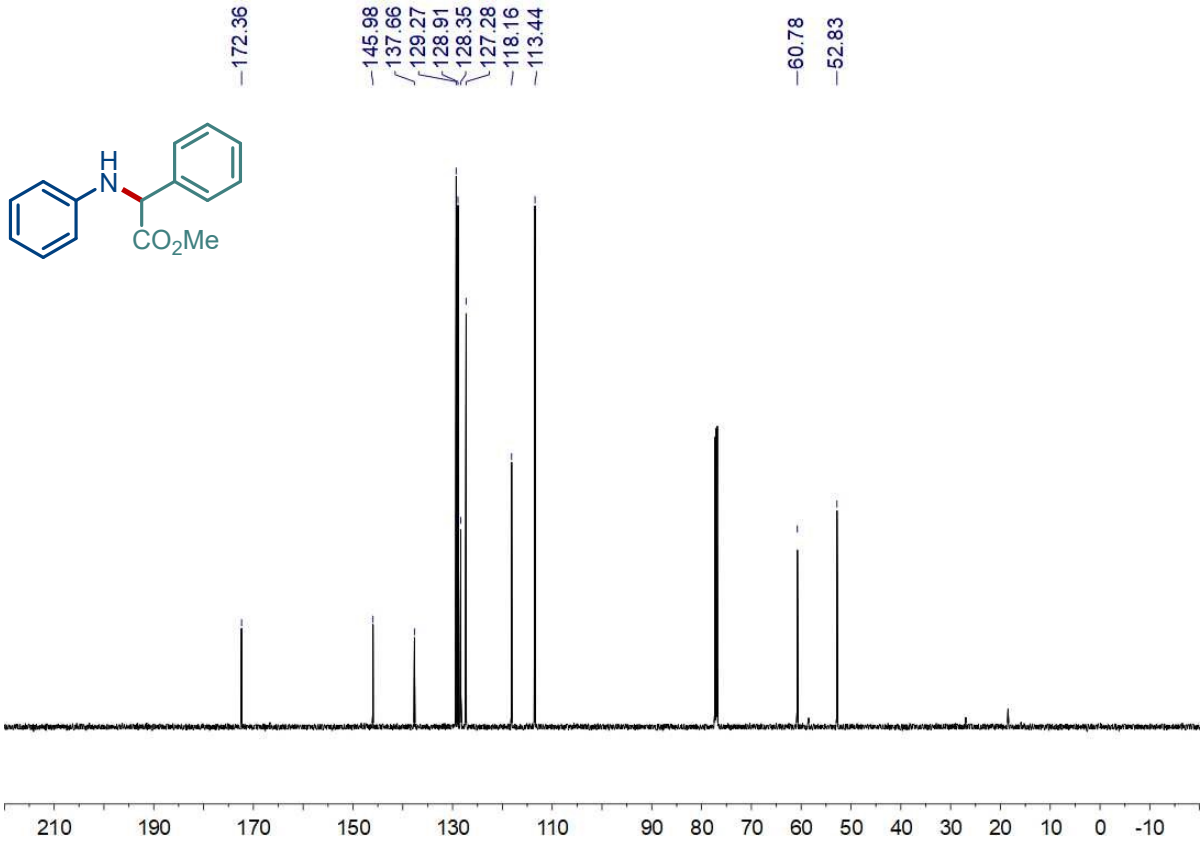
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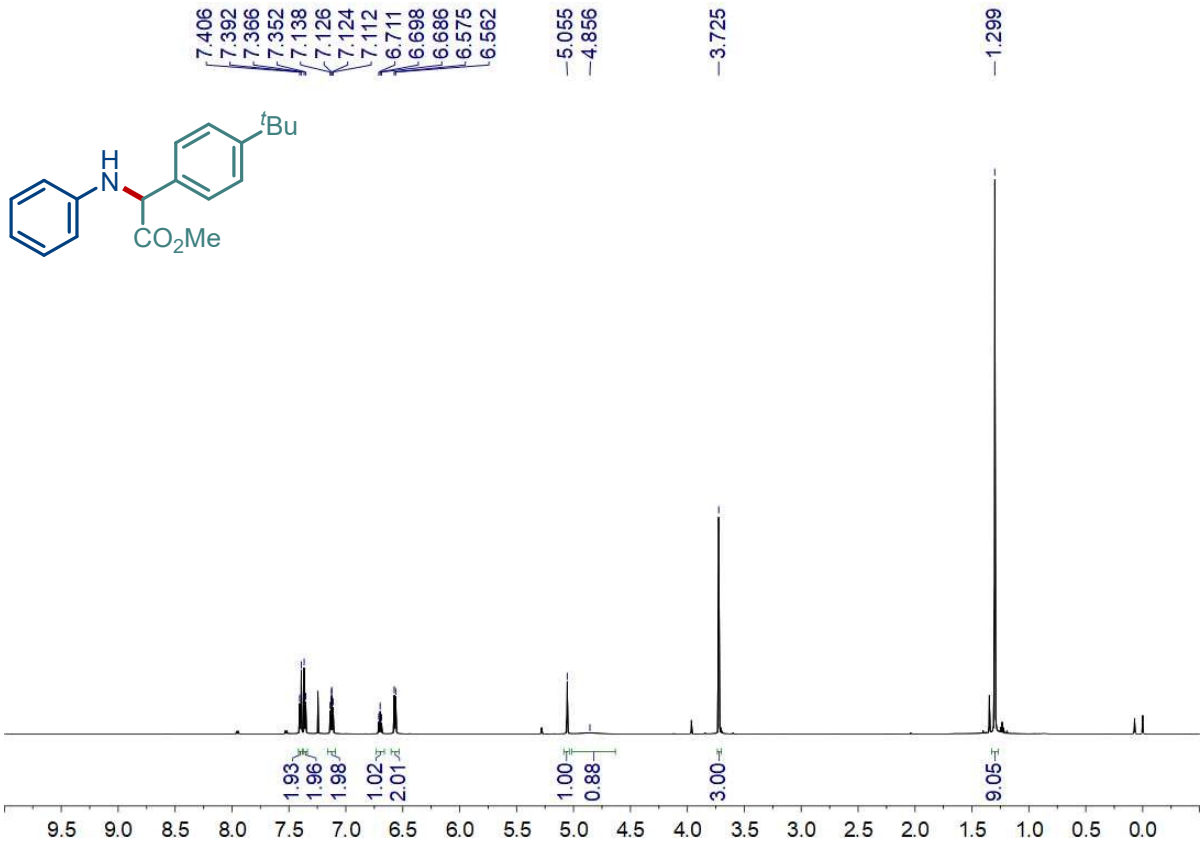
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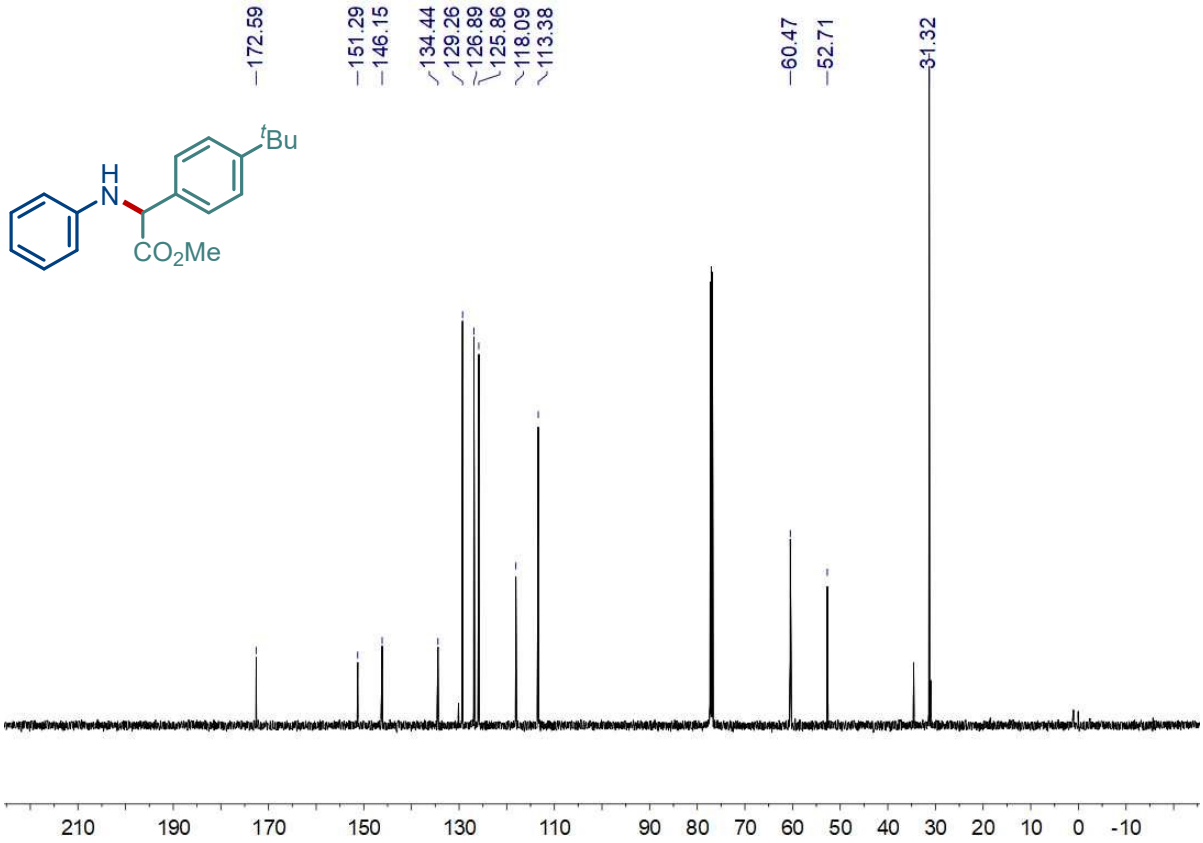
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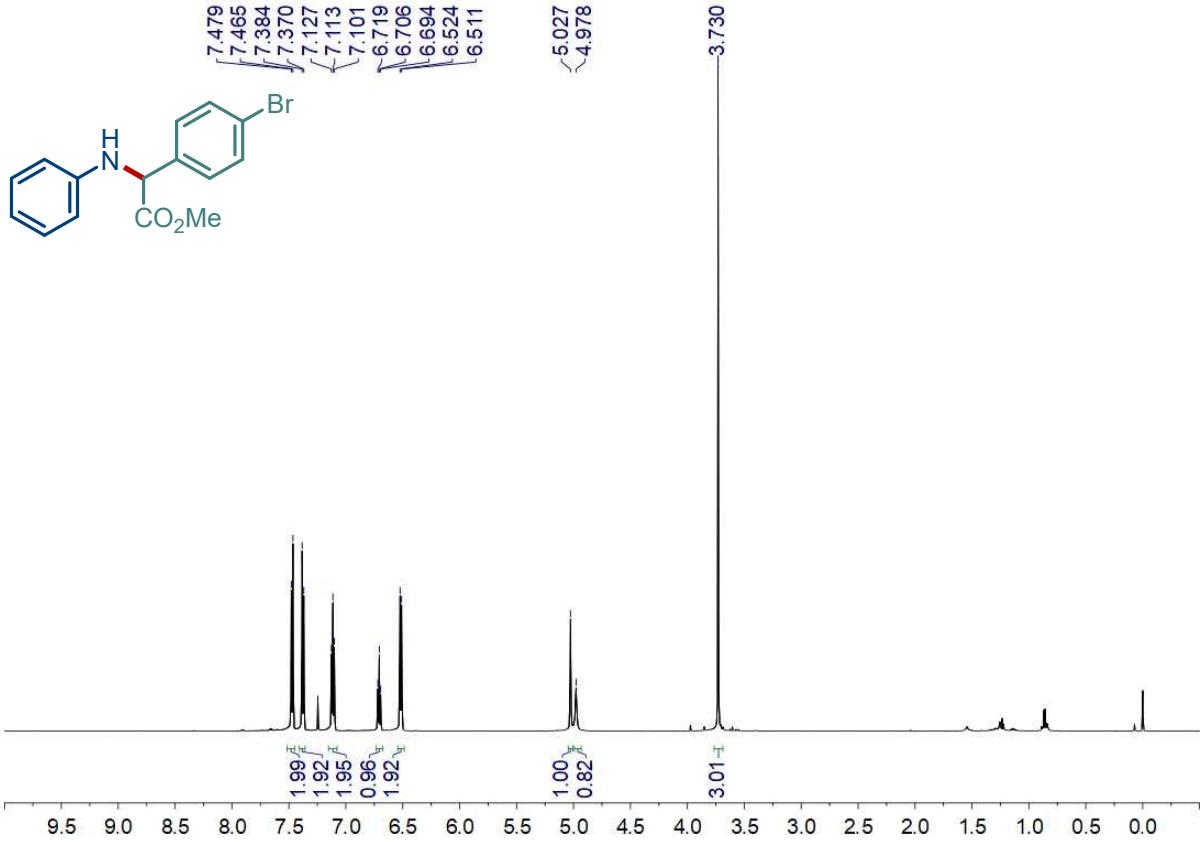
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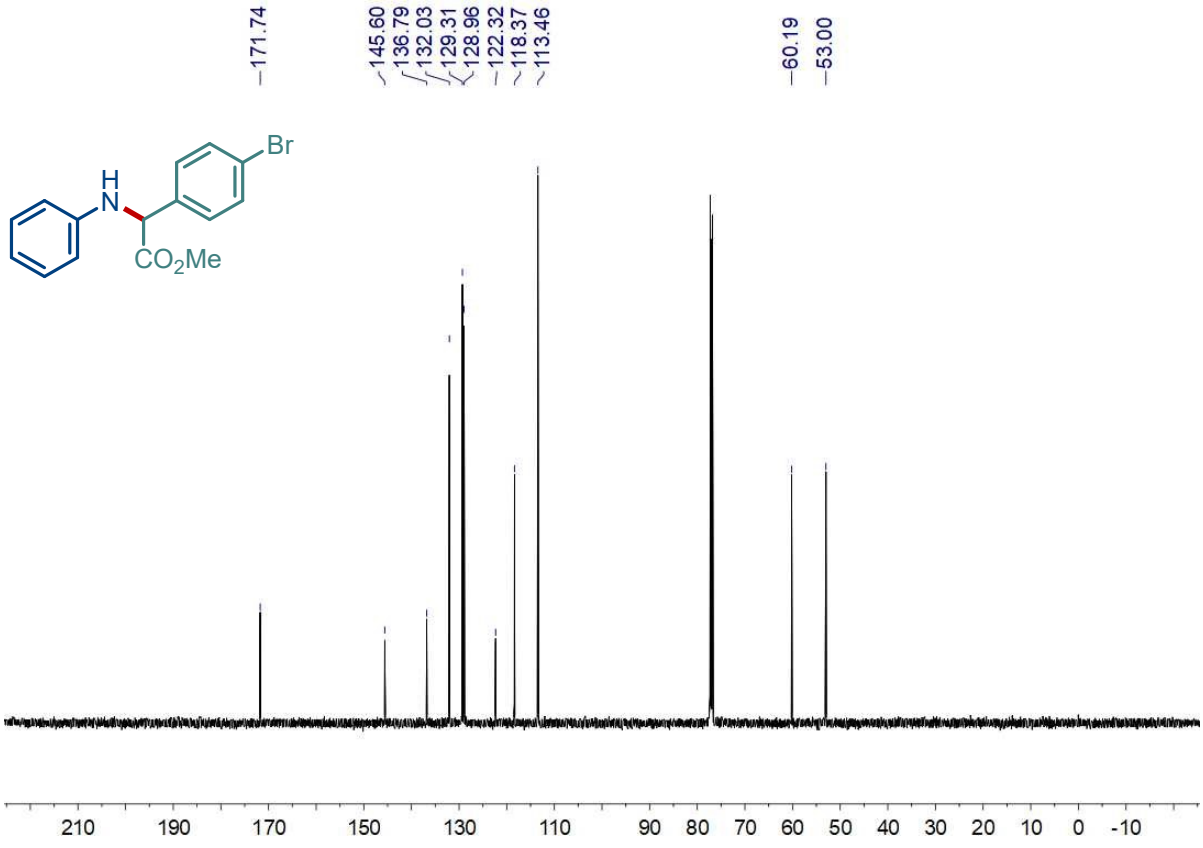
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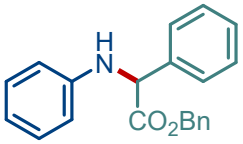
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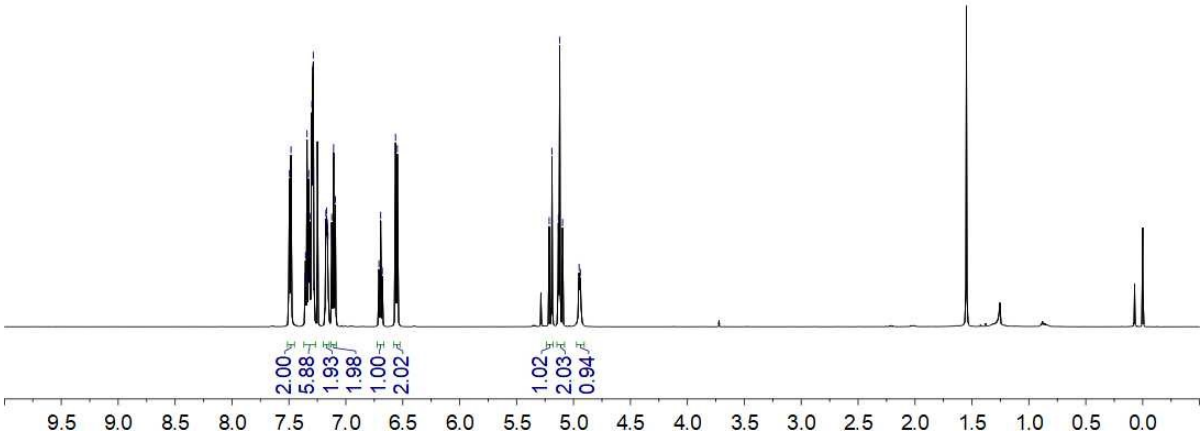
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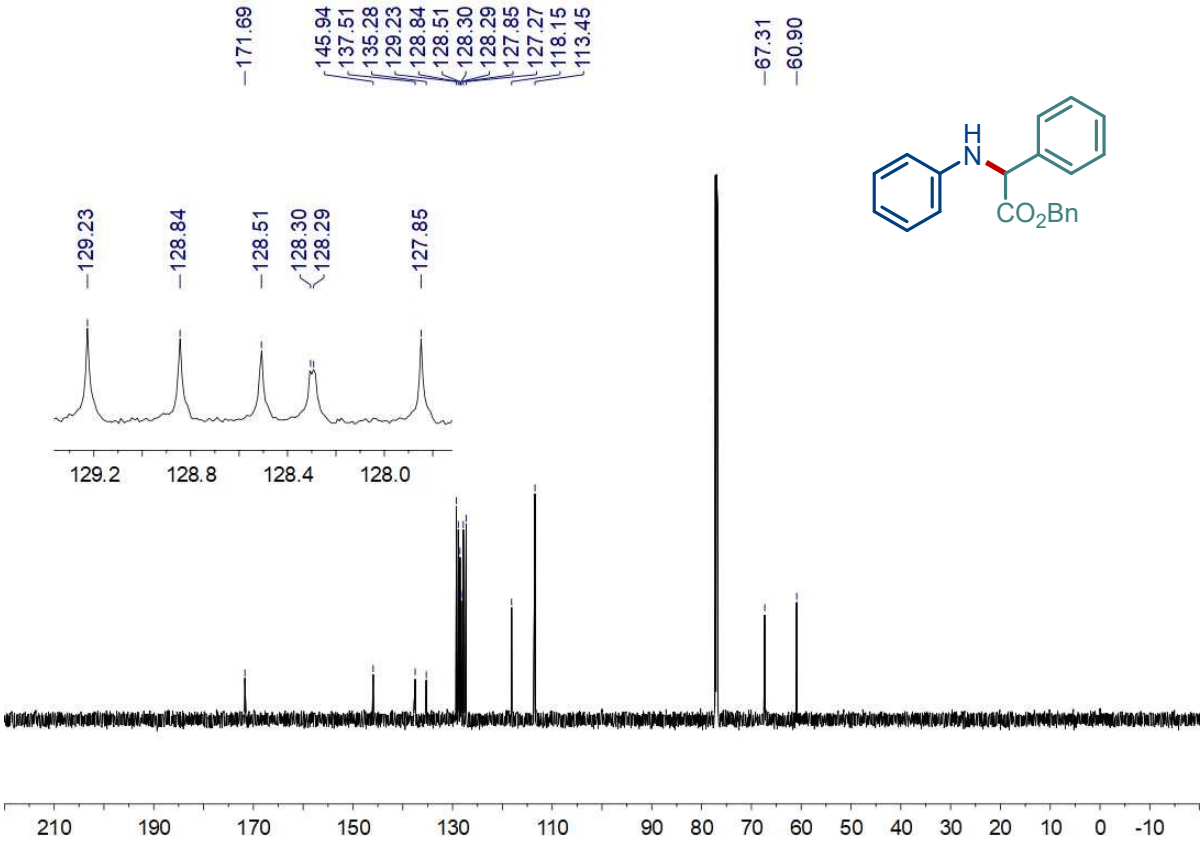
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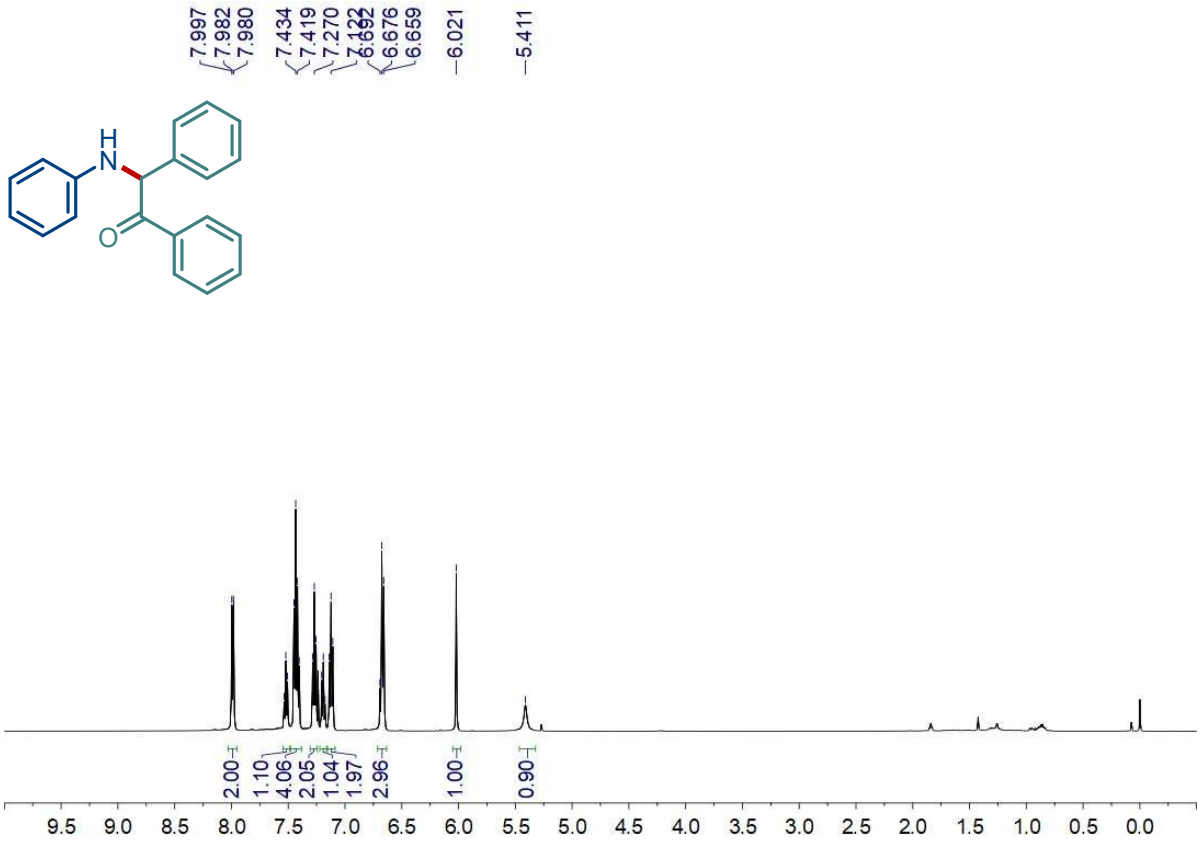
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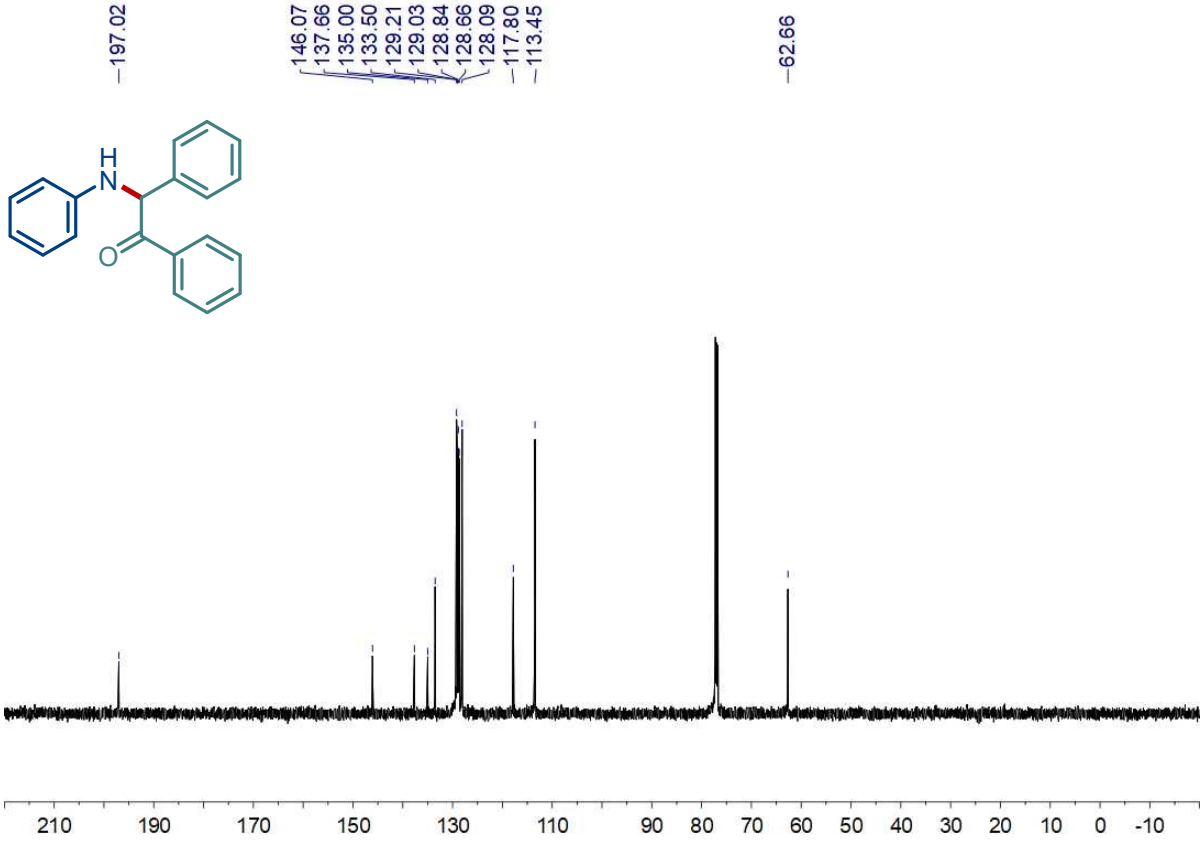
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