

1 **Synergistic Catalysis Enables Chemoselective Asymmetric**

2 **Carbene N–H Insertion of Functionalized Anilines**

3
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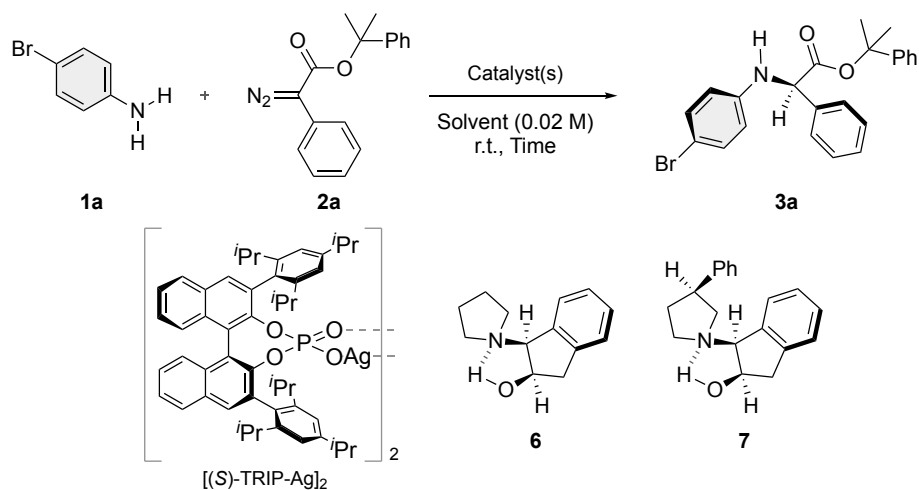
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1 **1. General Information**

2 NMR spectra were recorded on a JEOL ECZ400 spectrometer and a JEOL ECS600
3 spectrometer. Chemical shifts are reported in ppm relative to tetramethylsilane (TMS, δ
4 = 0.00 ppm) as an internal standard in CDCl_3 . Data are reported as follows: chemical shift,
5 multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, and br = broad),
6 integration and coupling constants in Hz. ESI mass spectra were measured on JEOL
7 AccuTOF LC-plus JMS-T100LP. Optical rotations were measured on a JASCO P-1020
8 polarimeter. The enantiomeric ratio (er) was determined by HPLC analysis. HPLC was
9 performed on JASCO HPLC systems consisting of the following: pump, PU-980; detector,
10 UV-970; column DAICEL CHIRALPAK IC-3, CHIRALPAK IG-3, CHIRALPAK IBN-
11 3; mobile phase, *n*-hexane/IPA. Melting points were measured with a SIBATA NEL-270
12 melting point apparatus. Analytical thin layer chromatography was performed on
13 Kieselgel 60F₂₅₄, 0.25 mm thickness plates. Column chromatography was performed with
14 silica gel 60 N (spherical, neutral 63-210 mesh). Reactions were conducted in dry solvent.
15 Other reagents were purified by the standard methods.

1 **2. Additional Studies**

2 **Supplementary Table 1. Examination of catalysts and solvents.**

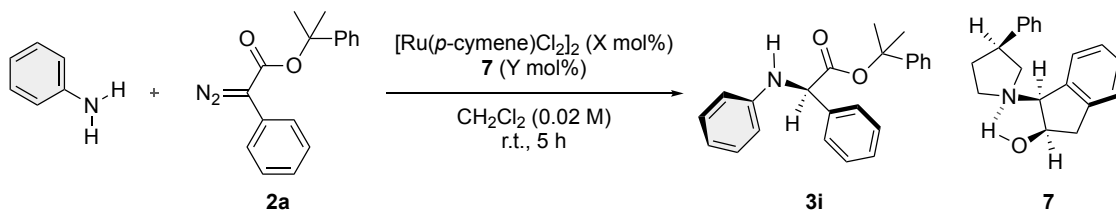


3

Entry	Catalyst(s) (mol%)	Solvent	Time (h)	Yield (%)	e.r.
1	$[(S)\text{-TRIP-Ag}]_2$ (2)	toluene	5	63	44:56
2	$\text{Cu}(\text{OTf})_2$ (2) & 6 (2)	toluene	5	64	50:50
3	$\text{Rh}_2(\text{NHCO}^i\text{Bu})_4$ (2) & 6 (2)	toluene	24	27	84:16
4	Cp_2HfCl_2 (2) & 6 (2)	toluene	5	0	-
5	$\text{RuCl}(p\text{-cymene})[(S,S)\text{-Ts-dpen}]$ (2) & 6 (2)	toluene	24	trace	82:18
6	$[\text{Ru}(p\text{-cymene})\text{Cl}_2]_2$ (2), AgSbF_6 (2) & 6 (2)	toluene	24	47	81:19
7	$\text{Cp}^*\text{RuCl}(\text{cod})$ (2) & 6 (2)	toluene	24	47	56:44
8	$\text{Cp}^*\text{RuCl}(\text{PPh}_3)_2$ (2) & 6 (2)	toluene	5	15	79:21
9	$[\text{Ru}(p\text{-cymene})\text{Cl}_2]_2$ (2) & 6 (2)	PhCl	5	94	93:7
10	$[\text{Ru}(p\text{-cymene})\text{Cl}_2]_2$ (2) & 6 (2)	CH_2Cl_2	5	91	94:6
11	$[\text{Ru}(p\text{-cymene})\text{Cl}_2]_2$ (2) & 7 (5)	CH_2Cl_2	5	99	97:3

4

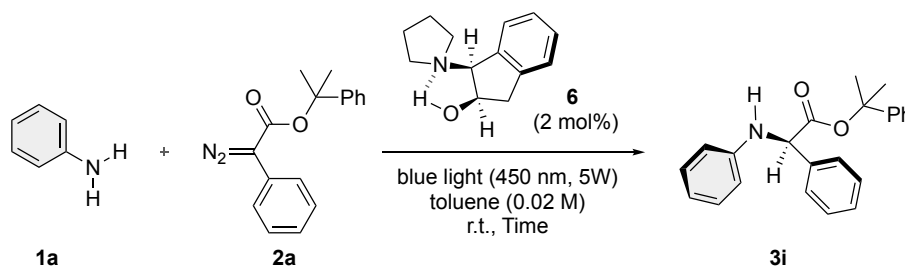
1 **Supplementary Table 2.** Optimization of the ratio of metal catalyst to organocatalyst.



Entry	X	Y	Yield (%)	e.r.
1	2	2	90	73:27
2	5	5	90	93:7
3	3	4	92	90:10
4	5	2	94	78:22

3

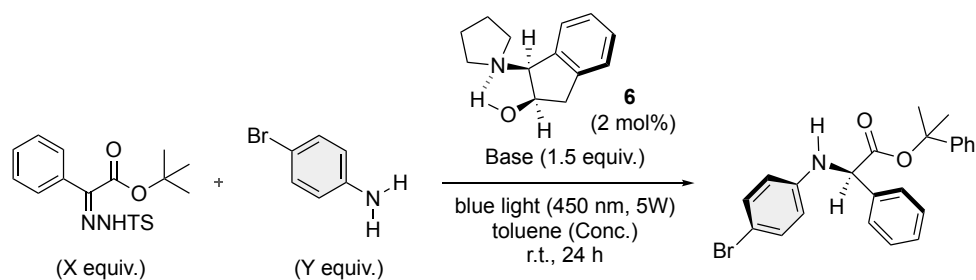
4 **Supplementary Table 3.** Almost no time dependence of enantioselectivity.



Entry	Time	Yield (%)	e.r.
1	15 min	35	88:12
2	30 min	55	88:12
3	1	60	87:13
4	2	49	90:10
5	5	45	90:10

6

1 **Supplementary Table 4.** Investigation of base identity and substrate ratio using *N*-
 2 tosylhydrazone.

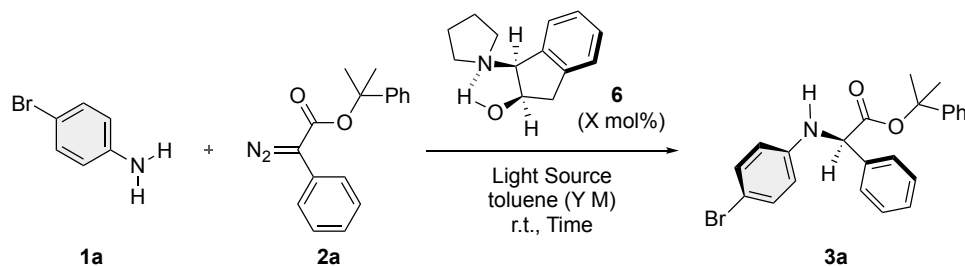


3
 4

Entry	X (equiv.)	Y (equiv.)	Base	Conc. (M)	Yield (%)	e.r.
1	1	3	Cs ₂ CO ₃	0.02	<60	58:42
2	1	3	K ₂ CO ₃	0.02	<52	71:29
3	1	3	NaO ^t Bu	0.02	<49	53:47
4	1	4	Et ₃ N	0.02	59	50:50
5	1	1	K ₂ CO ₃	0.02	25	59:41
6	1.5	1	K ₂ CO ₃	0.02	43	63:37
7	1	4	K ₂ CO ₃	0.02	57	64:36
8	1	4	K ₂ CO ₃	0.02	35	67:33
9	1	4	K ₂ CO ₃	0.02	21	53:47
10	1	4	K ₂ CO ₃	0.05	43	61:39
11	1	4	K ₂ CO ₃	0.10	77	56:44

5
 6

1 **Supplementary Table 5.** Examination of light sources.



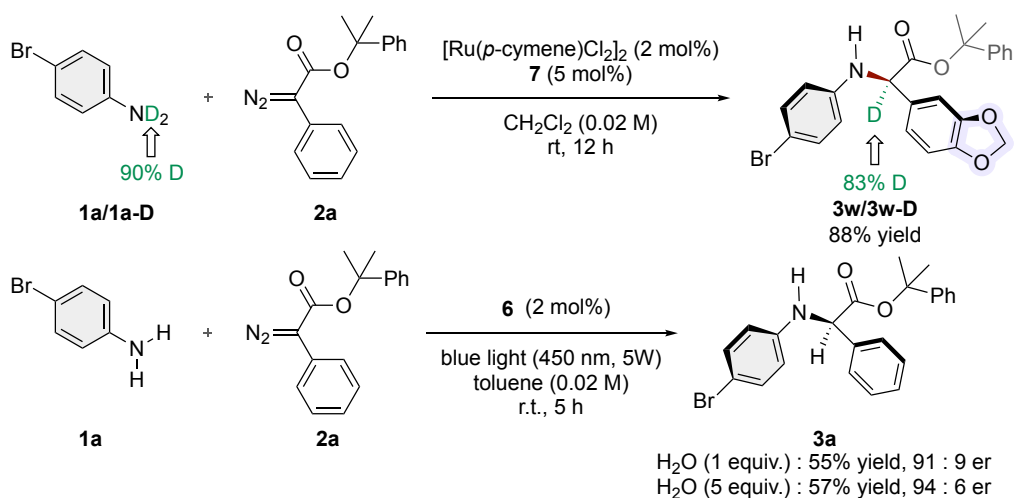
2

Entry	Light Source	X (mol %)	Y (M)	Time	Yield (%)	e.r.
1	450 nm, 5 W×1	10	0.02	5	56	92:8
2	450 nm, 5 W×1	2	0.05	5	62	93:7
3	450 nm, 5 W×1	2	0.10	5	71	90:10
4	450 nm, 5 W×1	2	0.20	5	80	86:14
5	520 nm, 5 W×1	2	0.02	48	48	94:6
6	365 nm, 2 W×4	2	0.02	24	31	92:8
7	450 nm, 30 W×1	2	0.02	1.5	52	92:8

3

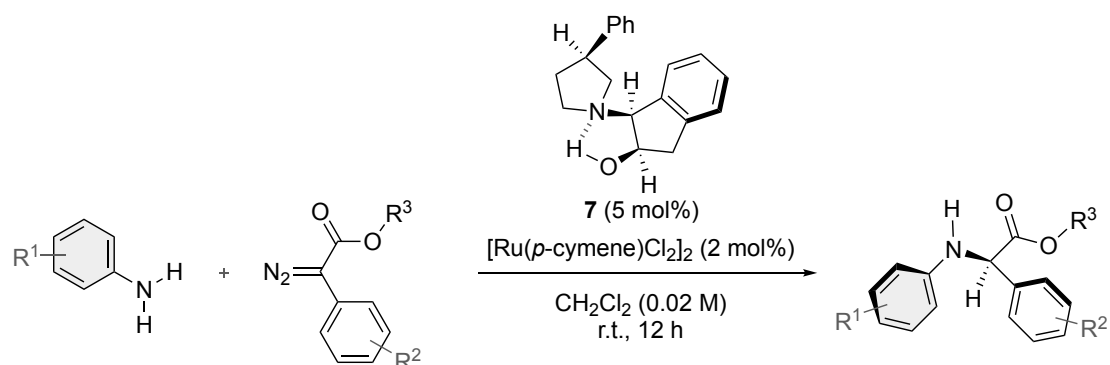
4 **Supplementary Figure 1.** Mechanistic experiments using deuterium labelling and water addition.

5



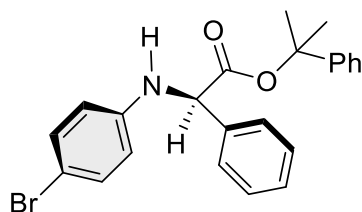
6

1 **3. General Procedure for Ru-Catalyzed Asymmetric N–H Insertion**



4 A pre-dried 30-mL pear-shaped flask was charged with $[\text{Ru}(p\text{-cymene})\text{Cl}_2]_2$ (2.4 mg,
5 0.004 mmol), chiral catalyst (**7**, 2.8 mg, 0.01 mmol), and aniline derivative (0.6 mmol).
6 After adding CH_2Cl_2 (3 mL), the mixture was stirred at room temperature under an argon
7 atmosphere for 5 min. A solution of diazoester derivative (**2**, 0.2 mmol) in CH_2Cl_2 (7 mL)
8 was then added in one portion. The resulting mixture was stirred at room temperature for
9 12 h. The solvent was removed under reduced pressure, and the crude residue was purified
10 by flash column chromatography on silica gel ($n\text{-hexane}/\text{EtOAc} = 15:1$) to afford the
11 corresponding products.

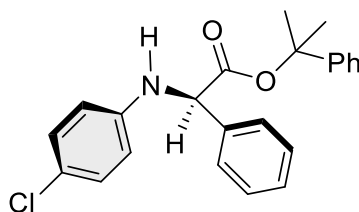
12 2-phenylpropan-2-yl (*R*)-2-((4-bromophenyl)amino)-2-phenylacetate (**3a**)



1 White solid (80.6 mg, 95% yield, 96 : 4 e.r.): m.p. 95-97 °C ;TLC Rf = 0.48 (n-
2 hexane/EtOAc, 6/1); ¹H NMR (400 MHz, CDCl₃) δ 7.44-7.46 (m, 2H), 7.34-7.39 (m, 3H),
3 7.14-7.17 (m, 5H), 6.94-6.97 (m, 2H), 6.36-6.40 (m, 2H), 4.97-5.02 (m, 2H), 1.78 (s, 3H),
4 1.60 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 169.8, 144.9, 144.7, 137.5, 132.0 (2C), 128.9
5 (2C), 128.4, 128.3 (2C), 127.4, 127.3 (2C), 124.1 (2C), 115.0 (2C), 109.6, 83.7, 61.1,
6 29.3, 27.6; IR (ATR) ν 3879, 3404, 3061, 3030, 2980, 2358, 2309, 2108, 1733, 1595
7 cm⁻¹; HRMS (ESI-TOF) [M + Na]⁺ calcd for C₂₃H₂₂BrNNaO₂⁺ m/z 446.0726, found
8 446.0731. [α]_D²⁵ -92.2 (c 1.0, CHCl₃). The enantiomeric ratio was determined by
9 analytical chiral HPLC. Retention time: 7.2 min (major isomer), 14.2 min (minor isomer),
10 IBN-3 column, 95/5 *n*-hexane/IPA, 1.0 mL/min, 254 nm.

11

12 2-phenylpropan-2-yl (*R*)-2-((4-chlorophenyl)amino)-2-phenylacetate (**3b**)



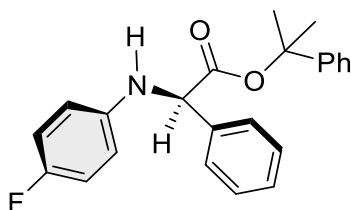
13

14 Colorless amorphous (63.8 mg, 84% yield, 95 : 5 e.r.); TLC Rf = 0.44 (n-hexane/EtOAc,
15 6/1); ¹H NMR (400 MHz, CDCl₃) δ 7.43-7.46 (m, 2H), 7.32-7.39 (m, 3H), 7.13-7.18 (m,
16 3H), 7.00-7.04 (m, 2H), 6.94-6.97 (m, 2H), 6.40-6.44 (m, 2H), 4.99 (s, 2H), 1.78 (s, 3H),
17 1.60 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 169.9, 144.8, 144.5, 137.6, 129.1 (2C), 128.9

1 (2C), 128.5, 128.3 (2C), 127.5 (2C) , 127.4, 124.1 (2C), 122.5, 114.6 (2C), 83.7, 61.2,
2 29.4, 27.6; IR (ATR) ν 4020, 3405, 3062, 3030, 2981, 2935, 2351, 2319, 1734, 1601
3 cm^{-1} ; HRMS (ESI-TOF) $[\text{M} + \text{Na}]^+$ calcd for $\text{C}_{23}\text{H}_{22}\text{ClNNaO}_2^+$ m/z 402.1231, found
4 402.1239. $[\alpha]_D^{25}$ -107.3 (c 1.0, CHCl_3). The enantiomeric ratio was determined by
5 analytical chiral HPLC. Retention time: 5.7 min (major isomer), 9.6 min (minor isomer),
6 IBN-3 column, 90/10 *n*-hexane/IPA, 1.0 mL/min, 254 nm.

7

8 2-phenylpropan-2-yl (*R*)-2-((4-fluorophenyl)amino)-2-phenylacetate (**3c**)



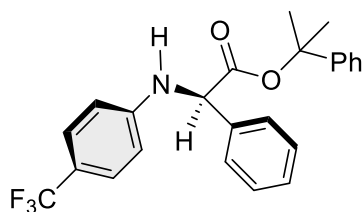
9

10 Pink solid (44.3 mg, 61% yield, 94 : 6 e.r.); m.p. 83-85 °C; TLC R_f = 0.32 (*n*-
11 hexane/EtOAc, 10/1); ^1H NMR (600 MHz, CDCl_3) δ 7.45-7.49 (m, 2H), 7.33-7.40 (m,
12 3H), 7.15-7.20 (m, 3H), 6.95-6.99 (m, 2H), 6.78-6.83 (m, 2H), 6.43-6.47 (m, 2H), 4.98
13 (s, 1H), 4.85 (br s, 1H), 1.78 (s, 3H), 1.61 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.1,
14 156.0 (d, J = 235.1 Hz), 144.8, 142.4, 137.9, 128.9 (2C), 128.4, 128.3 (2C), 127.5 (2C),
15 127.3, 124.1 (2C), 115.74 (d, J = 23.1 Hz, 2C), 114.3 (d, J = 6.7 Hz, 2C), 83.6, 61.8, 29.3,
16 27.6; ^{19}F NMR (376 MHz, CDCl_3) δ -127.5 (m); IR (ATR) ν 3409, 3084, 3062, 3032,
17 2982, 2930, 2343, 2251, 1733, 1614 cm^{-1} ; HRMS (ESI-TOF) $[\text{M} + \text{Na}]^+$ calcd for

1 $C_{23}H_{22}FNNaO_2^+$ m/z 386.1527, found 386.1532. $[\alpha]^{25}_D$ -59.8 (c 1.0, $CHCl_3$). The
2 enantiomeric ratio was determined by analytical chiral HPLC. Retention time: 7.1 min
3 (major isomer), 13.2 min (minor isomer), IBN-3 column, 97/3 *n*-hexane/IPA, 1.0 mL/min,
4 254 nm.

5

6 2-phenylpropan-2-yl (*R*)-2-phenyl-2-((4-(trifluoromethyl)phenyl)amino)acetate (**3d**)



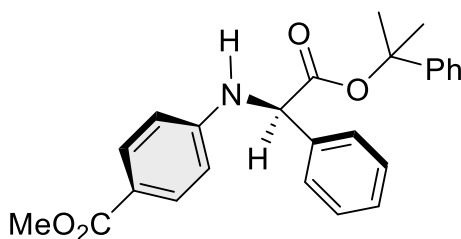
7

8 White solid (78.6 mg, 95% yield, 96 : 4 e.r.); m.p. 109-111 °C; TLC R_f = 0.44 (*n*-
9 hexane/EtOAc, 6/1); 1H NMR (400 MHz, $CDCl_3$) δ 7.15-7.48 (m, 10H), 6.95-6.98 (m,
10 2H), 6.51 (d, J = 8.2 Hz, 2H), 5.34 (d, J = 5.0 Hz, 1H), 5.06 (d, J = 5.5 Hz, 1H), 1.81 (s,
11 3H), 1.62 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.4, 148.2, 144.5, 137.1, 128.9 (2C),
12 128.4, 128.2 (2C), 127.3, 127.3 (2C), 126.5 (q, J = 2.9 Hz, 2C), 124.8 (q, J = 277 Hz),
13 124.0 (2C), 119.3 (q, J = 32.5 Hz), 112.5 (2C), 83.9, 60.5, 29.2, 27.4; ^{19}F NMR (376 MHz,
14 $CDCl_3$) δ -62.4 ; IR (ATR) ν 3399, 3062, 3032, 2982, 2933, 2330, 1896, 1732, 1616, 1586
15 cm^{-1} ; HRMS (ESI-TOF) $[M + Na]^+$ calcd for $C_{24}H_{22}F_3NNaO_2^+$ m/z 436.1495, found
16 436.1496. $[\alpha]^{25}_D$ -99.0 (c 1.0, $CHCl_3$). The enantiomeric ratio was determined by

1 analytical chiral HPLC. Retention time: 5.2 min (major isomer), 8.9 min (minor isomer),
2 IBN-3 column, 90/10 *n*-hexane/IPA, 1.0 mL/min, 254 nm.

3

4 methyl (*R*)-4-((2-oxo-1-phenyl-2-((2-phenylpropan-2-yl)oxy)ethyl)amino)benzoate (**3e**)

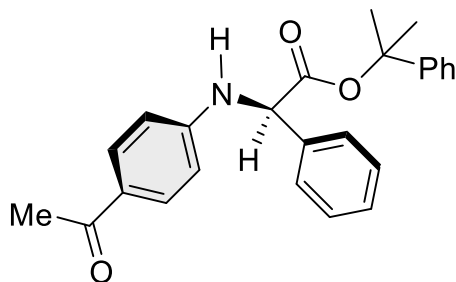


5

6 Colorless amorphous (76.7 mg, 95% yield, 96 : 4 e.r.); TLC R_f = 0.24 (*n*-hexane/EtOAc,
7 6/1); ¹H NMR (400 MHz, CDCl₃) δ 7.78 (d, *J* = 8.7 Hz, 2H), 7.45-7.47 (m, 2H), 7.35-
8 7.41 (m, 3H), 7.14-7.19 (m, 3H), 6.95-6.97 (m, 2H), 6.47 (d, *J* = 8.7 Hz, 2H), 5.44 (d, *J*
9 = 5.5 Hz, 1H), 5.09 (d, *J* = 5.5 Hz, 1H), 3.80 (s, 3H), 1.80 (s, 3H), 1.61 (s, 3H); ¹³C NMR
10 (100 MHz, CDCl₃) δ 169.5, 167.3, 149.6, 144.6, 137.2, 131.5 (2C), 129.0 (2C), 128.5,
11 128.3 (2C), 127.4 (3C), 124.1 (2C), 119.1, 112.4 (2C), 84.0, 60.5, 51.6, 29.3, 27.5; IR
12 (ATR) ν 3388, 3063, 2982, 2948, 2362, 1735, 1707, 1606, 1525, 1496 cm⁻¹; HRMS (ESI-
13 TOF) [M + Na]⁺ calcd for C₂₅H₂₅NNaO₄⁺ *m/z* 426.1676, found 426.1678. [α]_D²⁵ -113.2
14 (c 1.0, CHCl₃). The enantiomeric ratio was determined by analytical chiral HPLC.
15 Retention time: 12.6 min (major isomer), 14.8 min (minor isomer), IBN-3 column, 90/10
16 *n*-hexane/IPA, 1.0 mL/min, 254 nm.

1

2 2-phenylpropan-2-yl (*R*)-2-((4-acetylphenyl)amino)-2-phenylacetate (**3f**)



3

4 Colorless amorphous (72.8 mg, 94% yield, 97 : 3 e.r.); TLC R_f = 0.16 (n-hexane/EtOAc,

5 6/1); ¹H NMR (400 MHz, CDCl₃) δ 7.73 (d, *J* = 8.7 Hz, 2H), 7.45-7.47 (m, 2H), 7.35-

6 7.41 (m, 3H), 7.14-7.19 (m, 3H), 6.94-6.97 (m, 2H), 6.48 (d, *J* = 8.7 Hz, 2H), 5.53 (d, *J*

7 = 5.0 Hz, 1H), 5.10 (d, *J* = 6.0 Hz, 1H), 2.44 (s, 3H), 1.81 (s, 3H), 1.61 (s, 3H); ¹³C NMR

8 (100 MHz, CDCl₃) δ 196.5, 169.4, 149.8, 144.6, 137.1, 130.7 (2C), 129.0 (2C), 128.6,

9 128.3 (2C), 127.4, 127.4 (2C), 127.3, 124.1 (2C), 112.4 (2C), 84.1, 60.4, 29.4, 27.5, 26.1;

10 IR (ATR) ν 3388, 3060, 2982, 2361, 2329, 1735, 1663, 1598, 1525, 1495 cm⁻¹; HRMS

11 (ESI-TOF) [M + Na]⁺ calcd for C₂₅H₂₅NNaO₃⁺ m/z 410.1727, found 410.1728. [α]_D²⁵ –

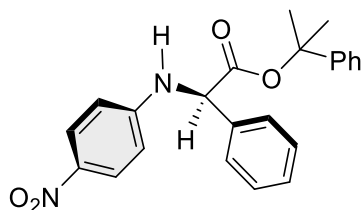
12 121.8 (c 1.0, CHCl₃). The enantiomeric ratio was determined by analytical chiral HPLC.

13 Retention time: 16.3 min (major isomer), 19.6 min (minor isomer), IG-3 column, 90/10

14 *n*-hexane/IPA, 1.0 mL/min, 254 nm.

15

16 2-phenylpropan-2-yl (*R*)-2-((4-nitrophenyl)amino)-2-phenylacetate (**3g**)



1

2 Yellow amorphous (58.6 mg, 75% yield, 96 : 4 e.r.); TLC R_f = 0.32 (n-hexane/EtOAc,

3 6/1); ¹H NMR (400 MHz, CDCl₃) δ 7.96-8.00 (m, 2H), 7.38-7.45 (m, 5H), 7.14-7.20 (m,

4 3H), 6.94-6.97 (m, 2H), 6.42-6.46 (m, 2H), 5.82 (d, *J* = 5.0 Hz, 1H), 5.10 (d, *J* = 5.5 Hz,

5 1H), 1.81 (s, 3H), 1.61 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 169.0, 150.9, 144.4, 138.7,

6 136.4, 129.2 (2C), 128.9, 128.4 (2C), 127.5, 127.3 (2C), 126.3 (2C), 124.1 (2C), 112.2

7 (2C), 84.4, 60.4, 29.4, 27.4; IR (ATR) ν 3382, 3063, 3029, 2982, 2932, 2360, 2353, 2330,

8 1733, 1599 cm⁻¹; HRMS (ESI-TOF) [M + Na]⁺ calcd for C₂₃H₂₂N₂NaO₄⁺ m/z 413.1472,

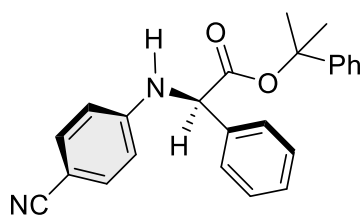
9 found 413.1475. [α]_D²⁵ -131.0 (c 1.0, CHCl₃). The enantiomeric ratio was determined by

10 analytical chiral HPLC. Retention time: 14.5 min (major isomer), 24.1 min (minor

11 isomer), IBN-3 column, 85/15 *n*-hexane/IPA, 1.0 mL/min, 254 nm.

12

13 2-phenylpropan-2-yl (R)-2-((4-cyanophenyl)amino)-2-phenylacetate (**3h**)

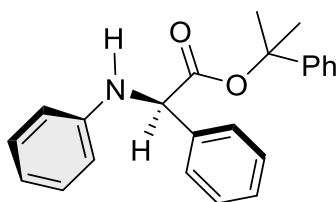


14

1 Colorless amorphous (62.2 mg, 84% yield, 76 : 24 e.r.): TLC Rf = 0.41 (n-hexane/EtOAc,
2 4/1); ¹H NMR (400 MHz, CDCl₃) δ 7.31-7.45 (m, 7H), 7.14-7.21 (m, 3H), 6.93-6.96 (m,
3 2H), 6.45-6.47 (m, 2H), 5.55 (d, *J* = 4.8 Hz, 1H), 5.05 (d, *J* = 4.8 Hz, 1H), 1.80 (s, 3H),
4 1.60 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 169.2, 149.0, 144.5, 136.7, 133.7 (2C), 129.1
5 (2C), 128.8, 128.3 (2C), 127.5, 127.3 (2C), 124.1 (2C), 120.3, 113.2 (2C), 99.6, 84.2,
6 60.3, 29.4, 27.5; IR (ATR) ν 3385, 2981, 2214, 1736, 1607, 1523, 1496, 1452, 1385, 1367
7 cm⁻¹; HRMS (ESI-TOF) [M + Na]⁺ calcd for C₂₄H₂₂N₂NaO₂⁺ m/z 393.1573, found
8 393.1579. [α]_D²⁵ -44.6 (c 0.56, CHCl₃). The enantiomeric ratio was determined by
9 analytical chiral HPLC. Retention time: 14.1 min (major isomer), 23.9 min (minor
10 isomer), IBN-3 column, 85/15 *n*-hexane/IPA, 1.0 mL/min, 254 nm.

11

12 2-phenylpropan-2-yl (*R*)-2-phenyl-2-(phenylamino)acetate (**3i**)



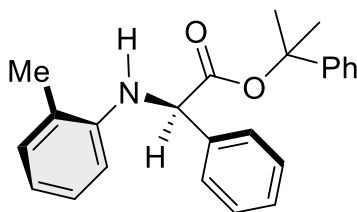
13

14 White solid (53.2 mg, 77% yield, 97 : 3 e.r.); m.p. 105-107 °C; TLC Rf = 0.36 (n-
15 hexane/EtOAc, 8/1); ¹H NMR (400 MHz, CDCl₃) δ 7.43-7.46 (m, 2H), 7.34-7.40 (m, 3H),
16 7.14-7.19 (m, 5H), 6.94-6.98 (m, 2H), 6.36-6.40 (m, 2H), 4.98-5.02 (m, 2H), 1.79 (s, 3H),
17 1.60 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 170.1, 146.1, 144.9, 138.1, 129.3 (2C), 128.9

1 (2C), 128.3 (3C), 127.5 (2C), 127.3, 124.1 (2C), 117.9, 113.5 (2C), 83.5, 61.2, 29.3, 27.7;
2 IR (ATR) ν 3409, 3063, 3028, 2981, 2933, 2359, 1733, 1595, 1496, 1450 cm^{-1} ; HRMS
3 (ESI-TOF) $[\text{M} + \text{Na}]^+$ calcd for $\text{C}_{23}\text{H}_{23}\text{NNaO}_2^+$ m/z 368.1621, found 368.1620; $[\alpha]_D^{25} -$
4 26.7 (c 1.0, CHCl_3). The enantiomeric ratio was determined by analytical chiral HPLC.
5 Retention time: 8.4 min (major isomer), 11.1 min (minor isomer), IBN-3 column, 97/3 *n*-
6 hexane/IPA, 1.0 mL/min, 254 nm.

7

8 2-phenylpropan-2-yl (R)-2-phenyl-2-(*o*-tolylamino)acetate (**3j**)



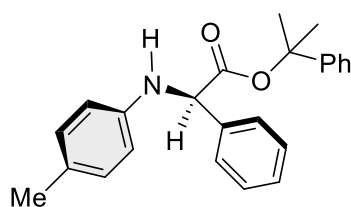
9

10 Yellow solid (54.6 mg, 76% yield, 97 : 3 e.r.); TLC R_f = 0.52 (*n*-hexane/EtOAc, 6/1); ^1H
11 NMR (400 MHz, CDCl_3) δ 7.48-7.52 (m, 2H), 7.33-7.41 (m, 3H), 7.14-7.19 (m, 3H),
12 7.03 (d, J = 7.2 Hz, 1H), 6.92-6.99 (m, 3H), 6.61 (t, J = 7.2 Hz, 1H), 6.34 (d, J = 8.0 Hz,
13 1H), 5.09 (d, J = 5.2 Hz, 1H), 4.92 (d, J = 5.2 Hz, 1H), 2.21 (s, 3H), 1.80 (s, 3H), 1.61 (s,
14 3H); ^{13}C NMR (150 MHz, CDCl_3) δ 170.1, 144.7, 143.9, 138.0, 130.1, 128.7 (2C), 128.2
15 (2C), 128.1, 127.3 (2C), 127.1, 126.9, 123.9 (2C), 122.3, 117.3, 110.6, 83.4, 61.0, 29.4,
16 27.3, 17.4; IR (ATR) ν 3828, 3425, 3060, 3030, 2980, 2931, 2358, 2329, 2319, 2108
17 cm^{-1} ; HRMS (ESI-TOF) $[\text{M} + \text{Na}]^+$ calcd for $\text{C}_{24}\text{H}_{25}\text{NNaO}_2^+$ m/z 382.1778, found

1 382.1770. $[\alpha]_{\text{D}}^{25}$ -61.5 (c 0.47, CHCl_3). The enantiomeric ratio was determined by
2 analytical chiral HPLC. Retention time: 7.2 min (minor isomer), 16.5 min (major isomer),
3 IBN-3 column, 99/1 *n*-hexane/IPA, 1.0 mL/min, 254 nm.

4

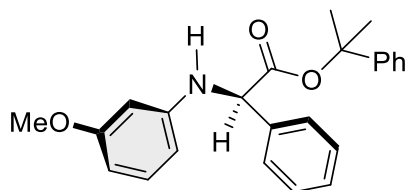
5 2-phenylpropan-2-yl (*R*)-2-phenyl-2-(*p*-tolylamino)acetate (**3k**)



7 Colorless oil (51.0 mg, 71% yield, 93 : 7 e.r.); TLC R_f = 0.32 (*n*-hexane/EtOAc, 10/1);
8 ^1H NMR (400 MHz, CDCl_3) δ 7.46-7.49 (m, 2H), 7.30-7.38 (m, 3H), 7.13-7.18 (m, 3H),
9 6.96-6.99 (m, 2H), 6.90 (d, J = 8.2 Hz, 2H), 6.43-6.46 (m, 2H), 5.02 (s, 1H), 4.80 (s, 1H),
10 2.18 (s, 3H), 1.78 (s, 3H), 1.61 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.2, 144.9,
11 143.8, 138.2, 129.8 (2C), 128.8 (2C), 128.3 (2C), 128.2, 127.5 (2C), 127.2, 127.0, 124.1
12 (2C), 113.6 (2C), 83.4, 61.5, 29.3, 27.7, 20.5; IR (ATR) ν 3412, 3019, 2987, 2974, 2340,
13 2361, 1735, 1617, 1522, 1494 cm^{-1} ; HRMS (ESI-TOF) $[\text{M} + \text{Na}]^+$ calcd for
14 $\text{C}_{24}\text{H}_{25}\text{NNaO}_2^+$ m/z 382.1778, found 382.1776. $[\alpha]_{\text{D}}^{25}$ -84.5 (c 1.0, CHCl_3). The
15 enantiomeric ratio was determined by analytical chiral HPLC. Retention time: 15.2 min
16 (major isomer), 18.1 min (minor isomer), IG-3 column, 95/5 *n*-hexane/IPA, 1.0 mL/min,
17 254 nm.

1

2 2-phenylpropan-2-yl (*R*)-2-((3-methoxyphenyl)amino)-2-phenylacetate (**3l**)



3

4 Colorless oil (72.8 mg, 97% yield, 92 : 8 e.r.); TLC R_f = 0.20 (n-hexane/EtOAc, 6/1); ¹H

5 NMR (600 MHz, CDCl₃) δ 7.47-7.49 (m, 2H), 7.32-7.39 (m, 3H), 7.15-7.19 (m, 3H),

6 6.96-7.02 (m, 3H), 6.24 (dd, *J* = 8.1, 2.1 Hz, 1H), 6.15 (dd, *J* = 7.8, 2.4 Hz, 1H), 6.07 (t,

7 *J* = 2.4 Hz, 1H), 5.03 (d, *J* = 6.0 Hz, 1H), 4.98 (d, *J* = 6.0 Hz, 1H), 3.69 (s, 3H), 1.78 (s,

8 3H), 1.61 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 170.1, 160.7, 147.4, 144.9, 138.1, 130.0,

9 128.9 (2C), 128.3 (3C), 127.5 (2C) , 127.3, 124.1 (2C) ,106.5, 103.1, 99.5, 83.5, 61.2,

10 55.1, 29.3, 27.6; IR (ATR) ν 3839, 3791, 3735, 3648, 3404, 2979, 2359, 2328, 1736, 1614

11 cm⁻¹; HRMS (ESI-TOF) [M + Na]⁺ calcd for C₂₄H₂₅NNaO₃⁺ m/z 398.1727, found

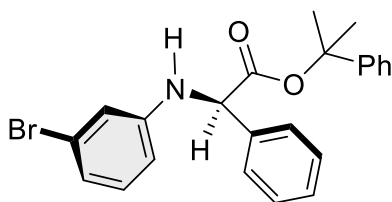
12 398.1731. [α]_D²⁵ -83.1 (c 1.0, CHCl₃). The enantiomeric ratio was determined by

13 analytical chiral HPLC. Retention time: 9.6 min (major isomer), 14.9 min (minor isomer),

14 IBN-3 column, 95/5 *n*-hexane/IPA, 1.0 mL/min, 254 nm.

15

16 2-phenylpropan-2-yl (*R*)-2-((3-bromophenyl)amino)-2-phenylacetate (**3m**)



1

2 Colorless oil (80.6 mg, 95% yield, 96 : 4 e.r.); TLC Rf = 0.33 (n-hexane/EtOAc, 6/1); ^1H

3 NMR (400 MHz, CDCl_3) δ 7.45-7.46 (m, 2H), 7.33-7.40 (m, 3H), 7.14-7.19 (m, 3H),

4 6.96-6.98 (m, 2H), 7.06 (d, $J = 7.3$ Hz, 1H) 6.97-6.99 (m, 3H), 6.92 (t, $J = 16.0$ Hz, 1H),

5 6.76-6.78 (m, 1H), 6.66 (t, $J = 3.7$ Hz, 1H) 6.41 (dd, $J = 8.2$ Hz, 2.3 Hz, 1H), 4.99-5.04

6 (m, 2H), 1.78 (s, 3H), 1.61 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 169.8, 147.3, 144.7,

7 137.4, 129.0 (2C), 130.6, 128.5, 128.3 (2C), 127.4 (2C), 127.3, 124.1 (2C), 123.2, 120.7,

8 116.1, 112.1, 83.8, 61.0, 29.3, 27.6; IR (ATR) ν 3785, 3566, 3399, 3063, 3029, 2981,

9 2930, 2367, 2327, 1733 cm^{-1} ; HRMS (ESI-TOF) $[\text{M} + \text{Na}]^+$ calcd for $\text{C}_{23}\text{H}_{22}\text{BrNNaO}_2^+$

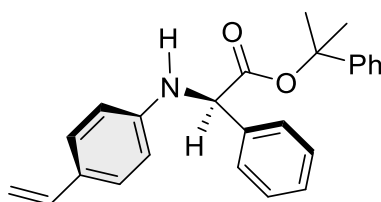
10 m/z 446.0726, found 446.0727. $[\alpha]_D^{25} -83.9$ (c 1.0, CHCl_3). The enantiomeric ratio was

11 determined by analytical chiral HPLC. Retention time: 5.7 min (major isomer), 11.0 min

12 (minor isomer), IBN-3 column, 90/10 n-hexane/IPA, 1.0 mL/min, 254 nm.

13

14 2-phenylpropan-2-yl (*R*)-2-(4-vinylphenyl)amino)acetate (**3n**)

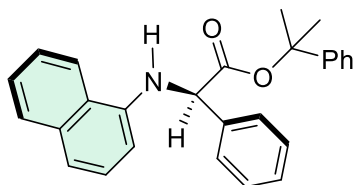


15

1 White solid (50.5 mg, 68% yield, 93 : 7 e.r.); m.p. 50-52 °C; TLC R_f = 0.32 (n-
2 hexane/EtOAc, 10/1); ¹H NMR (600 MHz, CDCl₃) δ 7.46-7.49 (m, 2H), 7.32-7.40 (m,
3 3H), 7.14-7.19 (m, 5H), 6.95-6.99 (m, 2H), 6.55 (dd, *J* = 17.1 Hz, 11.1 Hz, 1H), 6.45-
4 6.49 (m, 2H), 5.47 (dd, *J* = 17.7 Hz, 0.90 Hz, 1H), 5.03-5.07 (m, 2H), 4.98 (dd, *J* = 10.8
5 Hz, 1.2 Hz, 1H), 1.79 (s, 3H), 1.62 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 170.0, 145.7,
6 144.8, 137.9, 136.6, 128.9 (2C), 128.3 (3C), 127.7, 127.5 (2C), 127.4 (2C), 127.3, 124.1
7 (2C), 113.4 (2C), 109.8, 83.6, 61.1, 29.3, 27.6; IR (ATR) ν 3409, 3087, 3060, 3030, 2980,
8 2930, 2368, 2330, 2248, 2017 cm⁻¹; HRMS (ESI-TOF) [M + Na]⁺ calcd for
9 C₂₅H₂₅NNaO₂⁺ m/z 394.1778, found 394.1777. [α]_D²⁵ -98.1 (c 1.0, CHCl₃). The
10 enantiomeric ratio was determined by analytical chiral HPLC. Retention time: 6.8 min
11 (major isomer), 12.1 min (minor isomer), IBN-3 column, 95/5 *n*-hexane/IPA, 1.0 mL/min,
12 254 nm.

13

14 2-phenylpropan-2-yl (*R*)-2-(naphthalen-1-ylamino)-2-phenylacetate (**3o**)



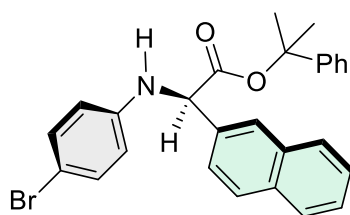
15

16 Colorless amorphous (70.4 mg, 89% yield, 95 : 5 e.r.); TLC R_f = 0.48 (n-hexane/EtOAc,
17 6/1); ¹H NMR (400 MHz, CDCl₃) δ 7.94-7.98 (m, 1H), 7.73-7.78 (m, 1H), 7.57

1 (d, $J = 6.4$ Hz, 2H), 7.34-7.46 (m, 5H), 7.14-7.21 (m, 5H), 6.96-7.02 (m, 2H), 6.33 (dd, J
2 = 6.6, 2.8 Hz, 1H), 5.82 (d, $J = 4.8$ Hz, 1H), 5.22 (d, $J = 4.8$ Hz, 1H), 1.83 (s, 3H), 1.64
3 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.3, 144.9, 141.1, 137.9, 134.4, 128.9 (2C),
4 128.7, 128.4 (3C), 127.5 (2C), 127.4, 126.5, 125.9, 125.0, 124.1 (2C), 123.4, 120.2,
5 117.8, 105.6, 83.7, 61.3, 29.6, 27.5; IR (ATR) ν 3430, 3060, 2980, 1733, 1582, 1526,
6 1478, 1450, 1408, 1384 cm^{-1} ; HRMS (ESI-TOF) $[\text{M} + \text{Na}]^+$ calcd for $\text{C}_{27}\text{H}_{25}\text{NNaO}_2^+$ m/z
7 418.1778, found 418.1785. $[\alpha]_D^{25} +7.9$ (c 1.0, CHCl_3). The enantiomeric ratio was
8 determined by analytical chiral HPLC. Retention time: 9.6 min (major isomer), 12.8 min
9 (minor isomer), IBN-3 column, 97/3 *n*-hexane/IPA, 1.0 mL/min, 254 nm.

10

11 2-phenylpropan-2-yl (*R*)-2-((4-bromophenyl)amino)-2-(naphthalen-2-yl)acetate (**3p**)



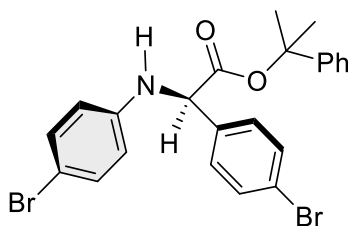
12

13 White solid (94.9 mg, quant., 76 : 24 e.r.); m.p. 106-108 °C; TLC $R_f = 0.38$ (*n*-
14 hexane/EtOAc, 8/1); ^1H NMR (400 MHz, CDCl_3) δ 7.79-7.91 (m, 4H), 7.57 (dd, $J = 8.7$
15 Hz, 1.4 Hz, 2H), 7.48-7.52 (m, 2H), 7.12-7.15 (m, 2H), 7.06 (t, $J = 15.1$ Hz, 2H), 6.93 (d,
16 $J = 7.8$ Hz, 2H), 6.40-6.42 (m, 2H), 5.11-5.15 (m, 2H), 1.78 (s, 3H), 1.59 (s, 3H); ^{13}C
17 NMR (100 MHz, CDCl_3) δ 169.8, 145.0, 144.7, 135.0, 133.5, 133.4, 132.0 (2C), 128.8,

1 127.9, 128.3 (2C), 128.2, 127.4, 126.6, 126.5, 126.4, 125.2, 124.2 (2C), 115.1 (2C), 109.7,
2 83.9, 61.2, 29.2, 27.7; IR (ATR) ν 3410, 3062, 3018, 2980, 2360, 2302, 1734, 1597, 1496,
3 1448 cm^{-1} ; HRMS (ESI-TOF) $[\text{M} + \text{Na}]^+$ calcd for $\text{C}_{27}\text{H}_{24}\text{BrNNaO}_2^+$ m/z 496.0883,
4 found 496.0903. $[\alpha]_D^{25} -70.8$ (c 1.0, CHCl_3). The enantiomeric ratio was determined by
5 analytical chiral HPLC. Retention time: 10.8 min (major isomer), 17.5 min (minor
6 isomer), IBN-3 column, 95/5 *n*-hexane/IPA, 1.0 mL/min, 254 nm.

7

8 2-phenylpropan-2-yl (*R*)-2-(4-bromophenyl)-2-((4-bromophenyl)amino)acetate (**3q**)



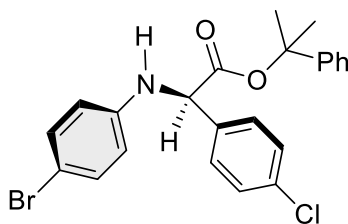
9

10 Colorless amorphous (95.6 mg, 95% yield, 95 : 5 e.r.); TLC R_f = 0.44 (*n*-hexane/EtOAc,
11 6/1); ^1H NMR (600 MHz, CDCl_3) δ 7.50-7.53 (m, 2H), 7.33-7.36 (m, 2H), 7.15-7.22 (m,
12 5H), 6.98-7.01 (m, 2H), 6.33-6.36 (m, 2H), 5.00 (d, J = 3.0 Hz, 1H), 4.94 (d, J = 3.0 Hz,
13 1H), 1.79 (s, 3H), 1.63 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 169.3, 144.6, 144.5, 136.2,
14 134.3, 132.0 (2C), 129.1 (2C), 128.8 (2C), 128.4 (2C), 127.5, 124.1 (2C), 115.0 (2C),
15 109.8, 84.1, 60.5, 29.1, 27.6; IR (ATR) ν 3399, 2981, 2312, 1732, 1596, 1497, 1448, 1404,
16 1385, 1367 cm^{-1} ; HRMS (ESI-TOF) $[\text{M} + \text{Na}]^+$ calcd for $\text{C}_{23}\text{H}_{21}\text{Br}_2\text{NNaO}_2^+$ m/z
17 523.9831, found 523.9830. $[\alpha]_D^{25} -100.1$ (c 1.0, CHCl_3). The enantiomeric ratio was

1 determined by analytical chiral HPLC. Retention time: 9.0 min (major isomer), 16.7 min
2 (minor isomer), IBN-3 column, 95/5 *n*-hexane/IPA, 1.0 mL/min, 254 nm.

3

4 2-phenylpropan-2-yl (*R*)-2-((4-bromophenyl)amino)-2-(4-chlorophenyl)acetate (**3r**)



5

6 Colorless amorphous (55.1 mg, 60% yield, 94 : 6 e.r.); TLC R_f = 0.44 (*n*-hexane/EtOAc,

7 6/1); ¹H NMR (400 MHz, CDCl₃) δ 7.34-7.41 (m, 4H), 7.14-7.22 (m, 5H), 6.98-7.00 (m,

8 2H), 6.32-6.36 (m, 2H), 5.01 (d, *J* = 5.0 Hz, 1H), 4.95 (d, *J* = 5.0 Hz, 1H), 1.79 (s, 3H),

9 1.62 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 169.2, 144.6, 144.5, 136.8, 132.1 (4C), 129.1

10 (2C), 128.4 (2C), 127.5, 124.1 (2C), 122.4, 115.1 (2C), 109.9, 84.1, 60.5, 29.2, 27.7; IR

11 (ATR) ν 3398, 2981, 2352, 2310, 1733, 1597, 1496, 1448, 1408, 1385 cm⁻¹; HRMS (ESI-

12 TOF) [M + Na]⁺ calcd for C₂₃H₂₁BrClINaO₂⁺ *m/z* 480.0336, found 480.0337. [α]_D²⁵ –

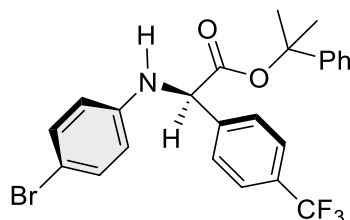
13 109.7 (c 1.0, CHCl₃). The enantiomeric ratio was determined by analytical chiral HPLC.

14 Retention time: 8.3 min (major isomer), 15.0 min (minor isomer), IBN-3 column, 95/5 *n*-

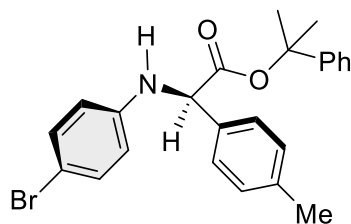
15 hexane/IPA, 1.0 mL/min, 254 nm.

16

1 2-phenylpropan-2-yl (*R*)-2-((4-bromophenyl)amino)-2-(4-
2 (trifluoromethyl)phenyl)acetate (**3s**)



4 Colorless amorphous (73.9 mg, 75% yield, 95 : 5 e.r.); TLC R_f = 0.48 (n-hexane/EtOAc,
5 6/1); ¹H NMR (400 MHz, CDCl₃) δ 7.62 (d, *J* = 8.2 Hz, 1H), 7.57 (d, *J* = 8.2 Hz, 1H),
6 7.14-7.22 (m, 5H), 6.94-6.96 (m, 2H), 6.32-6.35 (m, 2H), 5.06 (dd, *J* = 11.4 Hz, 5.0 Hz,
7 2H), 1.80 (s, 3H), 1.62 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 168.8, 144.3, 144.2, 141.7,
8 132.0 (2C), 130.6 (q, *J* = 32.6 Hz), 128.2 (2C), 127.7 (2C), 127.4, 125.8 (q, *J* = 2.9 Hz,
9 2C), 124.0 (q, *J* = 270.2 Hz), 123.9 (2C), 114.9 (2C), 109.9, 84.2, 60.6, 29.0, 27.4; ¹⁹F
10 NMR (376 MHz, CDCl₃) δ -61.1; IR (ATR) ν 3842, 3404, 2982, 2934, 2351, 2319, 1734,
11 1617, 1597, 1497 cm⁻¹; HRMS (ESI-TOF) [M + Na]⁺ calcd for C₂₄H₂₂BrF₃NO₂⁺ m/z
12 492.0781, found 492.0774. [α]_D²⁵ -76.3 (c 1.0, CHCl₃). The enantiomeric ratio was
13 determined by analytical chiral HPLC. Retention time: 8.7 min (major isomer), 15.2 min
14 (minor isomer), IBN-3 column, 95/5 *n*-hexane/IPA, 1.0 mL/min, 254 nm.
15
16 2-phenylpropan-2-yl (*R*)-2-((4-bromophenyl)amino)-2-(*p*-tolyl)acetate (**3t**)



1

2 White solid (85.0 mg, 97% yield, 92 : 8 e.r.); m.p. 82-84 °C ;TLC Rf = 0.32 (n-

3 hexane/EtOAc, 10/1); ¹H NMR (400 MHz, CDCl₃) δ 7.32 (d, *J* = 7.8 Hz, 2H), 7.13-7.20

4 (m, 7H), 6.97-7.00 (m, 2H), 6.35-6.40 (m, 2H), 4.94-4.98 (m, 2H), 2.36 (s, 3H), 1.77 (s,

5 3H), 1.61 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 170.0, 145.0, 144.8, 138.2, 134.5, 132.0

6 (2C), 129.6 (2C), 128.3 (2C), 127.3 (3C), 124.2 (2C) , 115.1 (2C) , 109.5, 83.6, 60.8, 29.3,

7 27.7, 21.3; IR (ATR) ν 3840, 3415, 3014, 2984, 2927, 2871, 2368, 2350, 2328, 1733

8 cm⁻¹; HRMS (ESI-TOF) [M + Na]⁺ calcd for C₂₄H₂₄BrNNaO₂⁺ m/z 460.0883, found

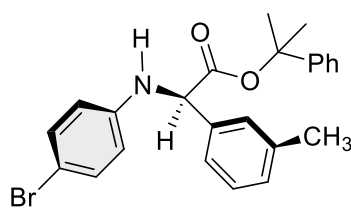
9 460.0885. [α]_D²⁵ -100.7 (c 1.0, CHCl₃). The enantiomeric ratio was determined by

10 analytical chiral HPLC. Retention time: 7.4 min (major isomer), 15.3 min (minor isomer),

11 IBN-3 column, 95/5 *n*-hexane/IPA, 1.0 mL/min, 254 nm.

12

13 2-phenylpropan-2-yl (*R*)-2-((4-bromophenyl)amino)-2-(*m*-tolyl)acetate (**3u**)

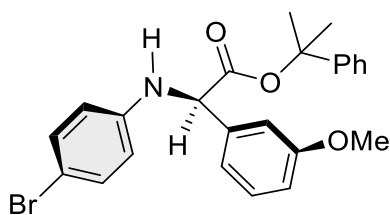


14

1 Colorless oil (65.8 mg, 75% yield, 95 : 5 e.r.); TLC Rf = 0.33 (n-hexane/EtOAc, 6/1); ¹H
2 NMR (400 MHz, CDCl₃) δ 7.22-7.27 (m, 3H), 7.14-7.19 (m, 6H), 6.95-6.98 (m, 2H),
3 6.37-6.41 (m, 2H), 4.93-4.98 (m, 2H), 2.35 (s, 3H), 1.79 (s, 3H), 1.60 (s, 3H); ¹³C NMR
4 (100 MHz, CDCl₃) δ 169.9, 145.0, 144.8, 138.6, 137.4, 132.0 (2C), 129.2, 128.8, 128.3
5 (2C), 127.9, 127.3, 124.7, 124.2 (2C), 115.0 (2C), 109.5, 83.7, 61.1, 29.4, 27.5, 21.6; IR
6 (ATR) ν 3752, 3394, 3025, 2979, 2932, 2370, 2355, 2340, 2330, 1732 cm⁻¹; HRMS (ESI-
7 TOF) [M + Na]⁺ calcd for C₂₄H₂₄BrNNaO₂⁺ m/z 460.0883, found 460.0891. [α]_D²⁵ -76.0
8 (c 1.0, CHCl₃). The enantiomeric ratio was determined by analytical chiral HPLC.
9 Retention time: 6.4 min (major isomer), 11.4 min (minor isomer), IBN-3 column, 95/5 n-
10 hexane/IPA, 1.0 mL/min, 254 nm.

11

12 2-phenylpropan-2-yl (R)-2-((4-bromophenyl)amino)-2-(3-methoxyphenyl)acetate (**3v**)



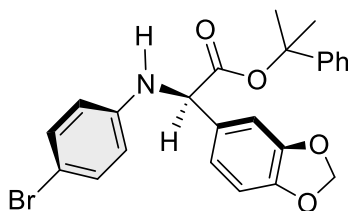
13

14 Colorless oil (80.9 mg, 89% yield, 96 : 4 e.r.); TLC Rf = 0.24 (n-hexane/EtOAc, 6/1); ¹H
15 NMR (400 MHz, CDCl₃) δ 7.29 (t, *J* = 15.6 Hz, 1H), 7.14-7.20 (m, 5H), 7.06 (d, *J* = 7.3
16 Hz, 1H) 6.97-6.99 (m, 3H), 6.87-6.90 (m, 1H), 6.37-6.40 (m, 2H), 5.00 (d, *J* = 5.5 Hz,
17 1H), 4.95 (d, *J* = 5.5 Hz, 1H), 3.77 (s, 3H), 1.79 (s, 3H), 1.61 (s, 3H); ¹³C NMR (100

1 MHz, CDCl₃) δ 169.7, 160.1, 144.9, 144.7, 139.1, 132.0 (2C), 129.9, 128.3 (2C), 127.4,
2 124.2 (2C), 119.9, 115.0 (2C), 114.1, 112.6, 109.6, 83.8, 61.1, 55.4, 29.3, 27.6; IR (ATR)
3 ν 3902, 3839, 3689, 3649, 3542, 3393, 3063, 2980, 2834, 2375 cm⁻¹; HRMS (ESI-TOF)
4 [M + Na]⁺ calcd for C₂₄H₂₄BrNNaO₃⁺ m/z 476.0832, found 476.0833. [α]_D²⁵ -83.1 (c 1.0,
5 CHCl₃). The enantiomeric ratio was determined by analytical chiral HPLC. Retention
6 time: 8.7 min (major isomer), 18.1 min (minor isomer), IBN-3 column, 95/5 *n*-
7 hexane/IPA, 1.0 mL/min, 254 nm.

8

9 2-phenylpropan-2-yl (R)-2-(benzo[d][1,3]dioxol-5-yl)-2-((4-
10 bromophenyl)amino)acetate (**3w**)



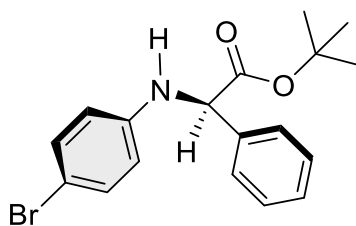
11

12 Colorless amorphous (72.1 mg, 77% yield, 97 : 3 e.r.); TLC R_f = 0.32 (*n*-hexane/EtOAc,
13 10/1); ¹H NMR (400 MHz, CDCl₃) δ 7.15-7.25 (m, 5H), 7.03-7.05 (m, 2H), 6.90-6.96 (m,
14 2H), 6.81 (d, *J* = 7.8 Hz, 2H), 6.36-6.39 (m, 2H), 5.97-5.99 (m, 2H), 4.97 (d, *J* = 5.5 Hz,
15 1H), 4.88 (d, *J* = 5.5 Hz, 1H), 1.79 (s, 3H), 1.64 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ
16 169.8, 148.2, 147.7, 144.8, 132.0 (2C), 131.4, 128.3 (2C), 127.4, 124.2 (2C), 121.1, 115.0
17 (2C), 109.6, 108.6, 107.6, 101.4, 83.8, 60.7, 29.2, 27.7; IR (ATR) ν 3412, 2981, 2360,

1 2351, 2330, 1732, 1396, 1488, 1443, 1385 cm^{-1} ; HRMS (ESI-TOF) $[\text{M} + \text{Na}]^+$ calcd for
2 $\text{C}_{24}\text{H}_{24}\text{BrNNaO}_4^+$ m/z 490.0625, found 490.0629. $[\alpha]^{25}_{\text{D}} -101.7$ (c 1.0, CHCl_3). The
3 enantiomeric ratio was determined by analytical chiral HPLC. Retention time: 10.3 min
4 (major isomer), 26.2 min (minor isomer), IBN-3 column, 95/5 *n*-hexane/IPA, 1.0 mL/min,
5 254 nm.

6

7 *tert*-butyl (*R*)-2-((4-bromophenyl)amino)-2-phenylacetate (**3x**)



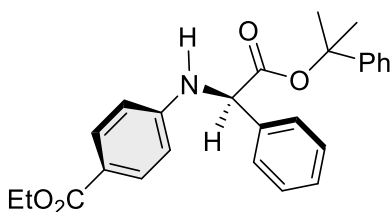
9 White solid (42.0 mg, 58% yield, 95 : 5 e.r.); m.p. 135-137 $^{\circ}\text{C}$; TLC $R_f = 0.32$ (*n*-
10 hexane/EtOAc, 10/1); ^1H NMR (400 MHz, CDCl_3) δ 7.43-7.45 (m, 2H), 7.27-7.36 (m,
11 3H), 7.16-7.19 (m, 2H), 6.39-6.43 (m, 2H), 5.02 (d, $J = 5.2$ Hz, 1H), 4.90 (d, $J = 5.6$ Hz,
12 1H), 1.38 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.6, 145.1, 137.7, 132.0 (2C), 128.8
13 (2C), 128.2, 127.1 (2C), 115.0 (2C), 109.5, 82.7, 61.1, 27.9 (3C); IR (ATR) ν 3737, 3418,
14 3055, 3019, 2980, 2927, 2853, 2370, 2359, 2341 cm^{-1} ; HRMS (ESI-TOF) $[\text{M} + \text{Na}]^+$
15 calcd for $\text{C}_{18}\text{H}_{21}\text{BrNO}_2^+$ m/z 362.0756, found 362.0762. $[\alpha]^{25}_{\text{D}} -67.2$ (c 1.0, CHCl_3). The
16 enantiomeric ratio was determined by analytical chiral HPLC. Retention time: 5.1 min

1 (major isomer), 6.6 min (minor isomer), IBN-3 column, 97/3 *n*-hexane/IPA, 1.0 mL/min,

2 254 nm.

3

4 ethyl (*R*)-4-((2-oxo-1-phenyl-2-((2-phenylpropan-2-yl)oxy)ethyl)amino)benzoate (**3y**)



6 Colorless oil (70.3 mg, 95% yield, 97 : 3 e.r.); TLC R_f = 0.35 (*n*-hexane/EtOAc, 6/1); ¹H

7 NMR (400 MHz, CDCl₃) δ 7.79 (d, *J* = 8.8 Hz, 2H), 7.44-7.47 (m, 2H), 7.35-7.41 (m,

8 3H) 7.14-7.19 (m, 3H), 6.95-6.98 (m, 2H), 6.47 (d, *J* = 8.8 Hz, 2H), 5.40 (d, *J* = 5.6 Hz,

9 1H), 5.09 (d, *J* = 5.6 Hz, 1H), 4.27 (q, *J* = 7.2 Hz, 2H), 1.80 (s, 3H), 1.61 (s, 3H), 1.32 (t,

10 *J* = 6.8 Hz, 3H); ¹³C NMR (400 MHz, CDCl₃) δ 169.4, 166.7, 149.4, 144.5, 137.1, 131.3

11 (2C), 128.9 (2C), 128.4, 128.2 (2C), 127.3 (2C), 124.0 (2C), 119.4, 112.3 (2C) , 83.8,

12 77.2, 60.4, 60.2, 29.2, 27.4, 14.4; IR (ATR) ν 3391, 2980, 1735, 1700, 1606, 1524, 1496,

13 1479, 1450, 1385 cm⁻¹; HRMS (ESI-TOF) [M + Na]⁺ calcd for C₂₆H₂₇NNaO₄⁺ m/z

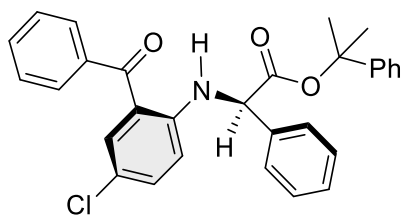
14 440.1832, found 440.1832. [α]_D²⁵ -69.3 (c 0.89, CHCl₃). The enantiomeric ratio was

15 determined by analytical chiral HPLC. Retention time: 12.4 min (major isomer), 15.0 min

16 (minor isomer), IC-3 column, 85/15 *n*-hexane/IPA, 1.0 mL/min, 254 nm.

17

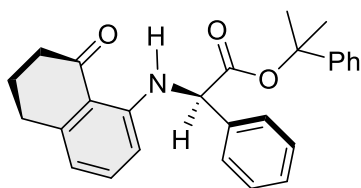
1 2-phenylpropan-2-yl (R)-2-((2-benzoyl-4-chlorophenyl)amino)-2-phenylacetate (**3z**)



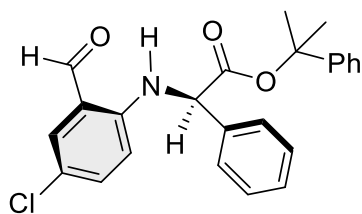
3 Yellow solid (96.8 mg, quant., 84 : 16 e.r.); m.p. 92-95 °C; TLC R_f = 0.42 (n-
4 hexane/EtOAc, 10/1); ¹H NMR (400 MHz, CDCl₃) δ 9.44 (d, *J* = 5.6 Hz, 1H), 7.63 (m,
5 2H), 7.36-7.56 (m, 10H), 7.13-7.19 (m, 4H), 6.97-7.02 (m, 2H), 6.48 (d, *J* = 8.8 Hz, 1H),
6 5.15 (d, *J* = 6.0 Hz, 1H), 1.80 (s, 3H), 1.67 (s, 3H); ¹³C NMR (400 MHz, CDCl₃) δ 197.9,
7 168.6, 147.7, 144.7, 139.4, 136.9, 134.4, 134.0, 131.4, 129.2 (2C), 129.0 (2C), 128.5,
8 128.2 (2C), 128.1 (2C), 127.3 (2C), 127.1, 124.1 (2C), 119.5, 119.2, 114.1, 83.7, 61.0,
9 29.2, 27.4; IR (ATR) ν₂₉₅₆, 2925, 2868, 2854, 2336, 1744, 1712, 1633, 1562, 1508 cm⁻¹;
10 HRMS (ESI-TOF) [M + Na]⁺ calcd for C₃₀H₂₆ClNNaO₃⁺ m/z 506.1493, found 506.1502.
11 [α]_D²⁵ +52.1 (c 0.4, CHCl₃). The enantiomeric ratio was determined by analytical chiral
12 HPLC. Retention time: 8.0 min (major isomer), 11.5 min (minor isomer), IBN-3 column,
13 97/3 *n*-hexane/IPA, 1.0 mL/min, 254 nm.

14

15 2-phenylpropan-2-yl (R)-2-((8-oxo-5,6,7,8-tetrahydronaphthalen-2-yl)amino)-2-
16 phenylacetate (**3aa**)



1
 2 Off-white amorphous (72.8 mg, 88% yield, 90 : 10 er); TLC R_f = 0.26 (n-hexane/EtOAc,
 3 2/1); ¹H NMR (400 MHz, CDCl₃) δ 7.82 (d, *J* = 8.4 Hz, 1H), 7.43-7.47 (m, 2H), 7.36-
 4 7.42 (m, 3H), 7.12-7.19 (m, 3H), 6.96-6.98 (m, 2H), 6.41 (dd, *J* = 8.4 Hz, 2.4 Hz, 1H),
 5 6.24 (d, *J* = 1.6 Hz, 1H), 5.47 (d, *J* = 5.2 Hz, 1H), 5.1 (d, *J* = 5.6 Hz, 1H), 2.75 (dd, *J* =
 6 5.6 Hz, 4.4 Hz, 2H), 2.51 (dd, *J* = 6.7, 6.7 Hz, 2H), 2.01 (m, 2H), 1.80 (s, 3H), 1.62 (s,
 7 3H); ¹³C NMR (400 MHz, CDCl₃) δ 196.8, 169.3, 149.8, 146.7, 144.5, 137.1, 129.5, 128.9
 8 (2C), 128.5, 128.2 (2C), 127.3, 127.2 (2C), 124.0 (2C), 123.5, 111.9, 110.9, 83.9, 60.3,
 9 38.7, 30.1, 29.2, 27.4, 23.3; IR (ATR) ν 3385, 2925, 1736, 1663, 1596, 1518, 1494, 1453,
 10 1435, 1353 cm⁻¹; HRMS (ESI-TOF) [M + Na]⁺ calcd for C₂₇H₂₇NNaO₃⁺ m/z 436.1883,
 11 found 436.1888. [α]_D²⁵ -48.9 (c 1.15, CHCl₃). The enantiomeric ratio was determined by
 12 analytical chiral HPLC. Retention time: 17.0 min (major isomer), 28.5 min (minor
 13 isomer), IC-3 column, 70/30 *n*-hexane/IPA, 1.0 mL/min, 254 nm.
 14
 15 2-phenylpropan-2-yl (*R*)-2-((4-chloro-2-formylphenyl)amino)-2-phenylacetate (**3ab**)



1

2 Yellow amorphous (77.5 mg, 95% yield, 86 : 14 e.r.); TLC R_f = 0.27 (n-hexane/EtOAc,

3 10/1); ¹H NMR (400 MHz, CDCl₃) δ 9.82 (s, 1H), 9.34 (d, *J* = 5.6 Hz, 1H), 7.45-7.47 (m,

4 3H), 7.34-7.41 (m, 3H), 7.13-7.19 (m, 4H), 6.97-6.99 (m, 2H), 6.39 (d, *J* = 9.2 Hz, 1H),

5 5.13 (d, *J* = 6.0 Hz, 1H), 1.81 (s, 3H), 1.66 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 192.7,

6 168.2, 146.6, 144.5, 139.4, 136.6, 135.4, 135.2, 129.0 (2C), 128.5, 128.1 (2C), 127.2 (2C),

7 127.2, 124.0, 120.4, 119.9, 113.6, 83.8, 60.6, 29.3, 27.3; IR (ATR) ν 3307, 2981, 2927,

8 2359, 1741, 1666, 1606, 1568, 1509, 1468 cm⁻¹; HRMS (ESI-TOF) [M + Na]⁺ calcd for

9 C₂₄H₂₂ClNNaO₃⁺ m/z 430.1180, found 430.1186. [α]_D²⁵ +58.3 (c 0.55, CHCl₃). The

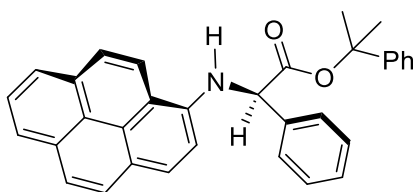
10 enantiomeric ratio was determined by analytical chiral HPLC. Retention time: 11.0 min

11 (major isomer), 14.1 min (minor isomer), IBN-3 column, 97/3 *n*-hexane/IPA, 1.0 mL/min,

12 254 nm.

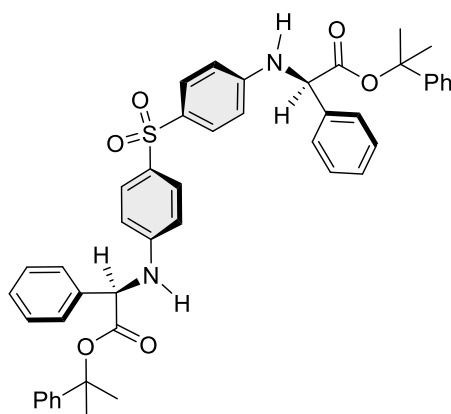
13

14 2-phenylpropan-2-yl (*R*)-2-phenyl-2-(pyren-2-ylamino)acetate (**3ac**)



15

1 Orange solid (74.2 mg, 79% yield, 94 : 6 e.r.); m.p. 118-120 °C; TLC R_f = 0.44 (n-
2 hexane/DCM 2/1); ¹H NMR (400 MHz, CDCl₃) δ 8.12 (d, *J* = 9.2 Hz, 1H), 7.95-8.04 (m,
3 3H), 7.84-7.91 (m, 2H), 7.81 (d, *J* = 8.4 Hz, 1H), 7.73 (d, *J* = 8.8 Hz, 1H), 7.62 (d, *J* =
4 6.4 Hz, 2H), 7.33-7.39 (m, 3H), 7.15-7.21 (m, 3H), 7.03 (d, *J* = 8.4 Hz 1H), 6.99 (dd, *J* =
5 7.6 Hz, 1.6 Hz, 2H), 6.21 (d, *J* = 3.6 Hz, 1H), 5.40 (d, *J* = 3.6 Hz, 1H), 1.87 (s, 3H), 1.65
6 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 170.1, 144.6, 139.8, 137.7, 132.2, 131.6, 128.8
7 (2C), 128.3, 128.2 (2C) , 127.6, 127.4 (2C), 127.3, 126.0, 126.0, 125.9, 125.9, 125.5,
8 124.0 (2C), 123.8, 123.4, 123.3, 123.2, 119.5, 116.7, 109.9, 83.8, 61.2, 29.5, 27.3; IR
9 (ATR) ν 3432, 3034, 2360, 1734, 1624, 1603, 1521, 1489, 1467, 1297 cm⁻¹; HRMS (ESI-
10 TOF) [M + Na]⁺ calcd for C₃₃H₂₇NNaO₂⁺ m/z 492.1934, found 492.1940. [α]_D²⁵ +136.0
11 (c 0.42, CHCl₃). The enantiomeric ratio was determined by analytical chiral HPLC.
12 Retention time: 7.8 min (major isomer), 20.4 min (minor isomer), IC-3 column, 95/5 n-
13 hexane/IPA, 1.0 mL/min, 254 nm.
14
15 bis(2-phenylpropan-2-yl) 2,2'-((sulfonylbis(4,1-phenylene))bis(azanediyl))(2*R*,2'*R*)-
16 bis(2-phenylacetate) (**3ad**)



1

2 White amorphous (64.8 mg, 86% yield (0.1 mmol scale), 93 : 7 dr, 99 : 1 e.r.); TLC Rf =

3 0.22 (n-hexane/EtOAc, 2/1); ¹H NMR (400 MHz, CDCl₃) δ 7.53 (d, *J* = 8.4 Hz, 4H), 7.33-

4 7.43 (m, 10H), 7.12-7.18 (m, 6H), 6.92 (dd, *J* = 7.8 Hz, 1.6 Hz, 4H), 6.42 (d, *J* = 9.2 Hz,

5 4H), 5.45 (d, *J* = 5.2 Hz, 2H), 5.00 (d, *J* = 5.2 Hz, 2H), 1.78 (s, 6H), 1.59 (s, 6H); ¹³C

6 NMR (100 MHz, CDCl₃) δ 169.2 (2C), 148.9 (2C), 144.4 (2C), 136.8 (2C), 130.4 (2C),

7 129.0 (4C), 128.9 (4C), 128.5 (2C), 128.2 (4C) , 127.3 (2C), 127.2 (4C) , 123.9 (4C),

8 112.6 (4C), 83.9 (2C), 60.3 (2C), 29.2 (2C), 27.3 (2C); IR (ATR) ν 3376, 2927, 2364,

9 2354, 1732, 1596, 1514, 1453, 1328, 1298 cm⁻¹; HRMS (ESI-TOF) [M + Na]⁺ calcd for

10 C₄₆H₄₄N₂NaO₆S⁺ m/z 775.2812, found 775.2815. [α]_D²⁵ -74.5 (c 0.35, CHCl₃). The

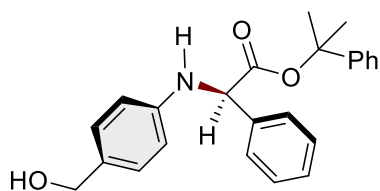
11 enantiomeric ratio was determined by analytical chiral HPLC. Retention time: 24.4 min

12 (minor enantiomer), 29.6 min (meso-diastereomer), 33.1 min (major isomer), IC-3

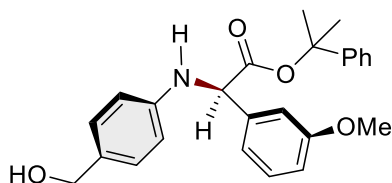
13 column, 70/30 *n*-hexane/IPA, 1.0 mL/min, 254 nm.

14

15 2-phenylpropan-2-yl (*R*)-2-((4-(hydroxymethyl)phenyl)amino)-2-phenylacetate (**9a**)



1
 2 White amorphous (75.0 mg, quant., 93 : 7 e.r.); TLC Rf = 0.19 (n-hexane/EtOAc 2/1); ¹H
 3 NMR (600 MHz, CDCl₃) δ 7.48 (d, *J* = 8.3 Hz, 2H), 7.33-7.39 (m, 3H), 7.15-7.20 (m, 3H),
 4 7.10 (d, *J* = 7.6 Hz, 2H), 6.96-6.99 (m, 2H), 6.50 (d, *J* = 7.6 Hz, 2H), 5.05 (d, *J* = 4.8 Hz,
 5 1H), 5.01 (d, *J* = 4.8 Hz, 1H), 4.49 (s, 2H), 1.79 (s, 3H), 1.62 (s, 3H); ¹³C NMR (100
 6 MHz, CDCl₃) δ 169.9, 145.6, 144.7, 137.8, 130.1, 128.7 (2C), 128.2 (2C), 128.2 (2C),
 7 127.4 (2C), 127.2 (2C), 124.0 (2C), 113.3 (2C), 83.5, 65.3, 61.0, 29.2, 27.5; IR (ATR) ν
 8 3407, 2980, 1734, 1615, 1521, 1496, 1471, 1451, 1385, 1367 cm⁻¹; HRMS (ESI-TOF)
 9 [M + Na]⁺ calcd for C₂₄H₂₅NNaO₃⁺ m/z 398.1727, found 398.1733. [α]_D²⁵ -53.5 (c 0.22,
 10 CHCl₃). The enantiomeric ratio was determined by analytical chiral HPLC. Retention
 11 time: 12.3 min (major isomer), 23.1 min (minor isomer), IC-3 column, 85/15 *n*-
 12 hexane/IPA, 1.0 mL/min, 254 nm.
 13
 14 2-phenylpropan-2-yl (*R*)-2-((4-(hydroxymethyl)phenyl)amino)-2-(3-
 15 methoxyphenyl)acetate (**9b**)

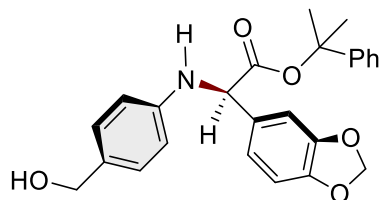


16

1 Yellow amorphous (81.1 mg, quant., 95 : 5 e.r.); TLC Rf = 0.14 (n-hexane/EtOAc 2/1);
2 ¹H NMR (400 MHz, CDCl₃) δ 7.29 (t, *J* = 8.0 Hz, 1H), 7.16-7.20 (m, 3H), 7.07-7.12 (m,
3 3H), 6.97-7.01 (m, 3H), 6.88 (dd, *J* = 8.2, 1.8 Hz, 2H), 6.51 (d, *J* = 8.8 Hz, 2H), 5.01 (s,
4 2H), 4.49 (s, 2H), 3.77 (s, 3H), 1.80 (s, 3H), 1.62 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ
5 169.8, 159.9, 145.6, 144.7, 139.4, 130.1, 129.7, 128.7 (2C), 128.1 (2C), 127.2, 124.0
6 (2C), 119.8, 114.0, 113.3 (2C), 112.5, 83.5, 65.3, 61.0, 55.2, 29.2, 27.5; IR (ATR) ν 3388,
7 2925, 2866, 2364, 1734, 1615, 1600, 1523, 1490, 1463 cm⁻¹; HRMS (ESI-TOF) [M +
8 Na]⁺ calcd for C₂₅H₂₇NNaO₄⁺ m/z 428.1832, found 428.1838. [α]_D²⁵ -26.0 (c 0.52,
9 CHCl₃). The enantiomeric ratio was determined by analytical chiral HPLC. Retention
10 time: 11.3 min (major isomer), 20.6 min (minor isomer), IC-3 column, 80/20 *n*-
11 hexane/IPA, 1.0 mL/min, 254 nm.

12

13 2-phenylpropan-2-yl (*R*)-2-(benzo[*d*][1,3]dioxol-5-yl)-2-((4-
14 (hydroxymethyl)phenyl)amino)acetate (**9c**)



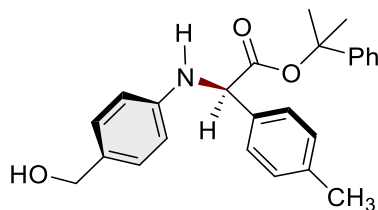
15

16 Colorless amorphous (51.1 mg, 61% yield, 95 : 5 e.r.); TLC Rf = 0.44 (n-hexane/EtOAc
17 2/1); ¹H NMR (400 MHz, CDCl₃) δ 7.21 (d, *J* = 2.0 Hz, 1H), 7.20 (d, *J* = 1.6 Hz, 2H),

1 7.03-7.08 (m, 4H), 6.97 (dd, $J = 8.0, 1.6$ Hz, 1H), 6.96-6.99 (m, 2H), 6.93 (d, $J = 1.6$ Hz,
2 1H), 6.80 (d, $J = 8.0$ Hz, 1H), 6.47 (d, $J = 8.4$ Hz, 1H), 5.98 (d, $J = 1.6$ Hz, 1H), 5.96(d,
3 $J=1.0$ Hz, 1H), 4.93 (s, 2H), 4.30 (s, 2H), 1.78 (s, 3H), 1.64 (s, 3H); ^{13}C NMR (150 MHz,
4 CDCl_3) δ 169.9, 148.0, 147.5, 145.4, 144.7, 131.7, 130.1, 128.7 (2C), 128.1 (2C), 127.2,
5 124.0 (2C), 120.9, 113.3 (2C), 108.4, 107.6, 101.1, 83.5, 65.3, 60.6, 29.0, 27.7; IR (ATR)
6 ν 3413, 2956, 2925, 2855, 2341, 1733, 1614, 1521, 1487, 1444 cm^{-1} ; HRMS (ESI-TOF)
7 $[\text{M} + \text{Na}]^+$ calcd for $\text{C}_{25}\text{H}_{27}\text{NNaO}_3^+$ m/z 442.1625, found 442.1629. $[\alpha]_D^{25} -48.2$ (c 0.51,
8 CHCl_3). The enantiomeric ratio was determined by analytical chiral HPLC. Retention
9 time: 14.0 min (major isomer), 26.5 min (minor isomer), IC-3 column, 80/20 *n*-
10 hexane/IPA, 1.0 mL/min, 254 nm.

11

12 2-phenylpropan-2-yl (*R*)-2-((4-(hydroxymethyl)phenyl)amino)-2-(*p*-tolyl)acetate (**9d**)



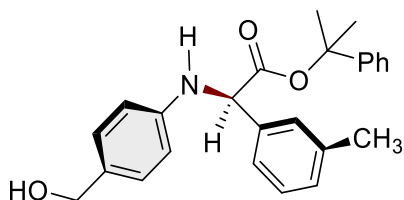
13

14 Colorless amorphous (74.0 mg, 95% yield, 87 : 13 e.r.); TLC $R_f = 0.26$ (*n*-hexane/EtOAc
15 2/1); ^1H NMR (400 MHz, CDCl_3) δ 7.35 (d, $J = 8.0$ Hz, 2H), 7.15-7.20 (m, 5H), 7.10 (d,
16 $J = 8.4$ Hz, 2H), 6.98-7.02 (m, 2H), 6.50 (d, $J = 8.4$ Hz, 2H), 5.02(d, $J = 4.4$ Hz, 1H), 4.96
17 (d, $J = 4.4$ Hz, 1H), 4.49 (s, 2H), 2.37(s, 3H), 1.78 (s, 3H), 1.62 (s, 3H); ^{13}C NMR (100

1 MHz, CDCl₃) δ 170.1, 145.6, 144.8, 137.9, 134.7, 130.0, 129.4 (2C), 128.7 (2C), 128.1
2 (2C), 127.2 (2C), 127.1, 124.0 (2C), 113.3 (2C), 83.3, 65.3, 60.7, 29.1, 27.6, 21.2 ; IR
3 (ATR) ν 3408, 2981, 2927, 2369, 1734, 1616, 1522, 1449, 1384, 1312 cm⁻¹; HRMS (ESI-
4 TOF) [M + Na]⁺ calcd for C₂₅H₂₇NNaO₃⁺ m/z 412.1883, found 412.1882. [α]_D²⁵ -40.2 (c
5 0.34, CHCl₃). The enantiomeric ratio was determined by analytical chiral HPLC.
6 Retention time: 10.2 min (major isomer), 17.7 min (minor isomer), IC-3 column, 80/20
7 *n*-hexane/IPA, 1.0 mL/min, 254 nm.

8

9 2-phenylpropan-2-yl (*R*)-2-((4-(hydroxymethyl)phenyl)amino)-2-(*m*-tolyl)acetate (**9e**)



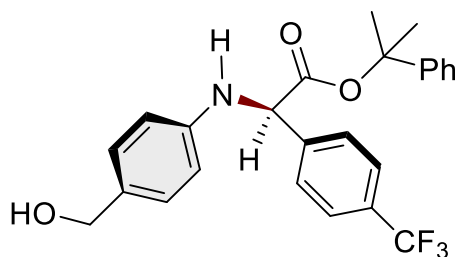
10

11 Colorless amorphous (70.1 mg, 91% yield, 90 : 10 e.r.); TLC R_f = 0.39 (*n*-hexane/EtOAc
12 2/1); ¹H NMR (600 MHz, CDCl₃) δ 7.26-7.30 (m, 2H), 7.25-7.26 (m, 1H, overlapped with
13 residual CHCl₃), 7.14-7.19 (m, 4H), 7.11 (d, *J* = 8.4 Hz, 2H), 6.97 (m, 2H), 6.52 (d, *J* =
14 9.0 Hz, 2H), 5.00(d, *J* = 5.7 Hz, 1H), 4.97 (d, *J* = 5.7 Hz, 1H), 4.50 (s, 2H), 2.353(s, 3H),
15 1.79 (s, 3H), 1.62 (s, 3H); ¹³C NMR (150 MHz, CDCl₃) δ 170.1, 145.7, 144.8, 138.4,
16 137.7, 130.1, 129.0, 128.8 (2C), 128.6, 128.1 (2C), 127.9, 127.2, 124.6, 124.1 (2C), 113.3
17 (2C), 83.4, 65.4, 61.1, 29.2, 27.5, 21.4 ; IR (ATR) ν 3403, 2980, 2921, 1733, 1616, 1522,

1 1496, 1488, 1448, 1297 cm^{-1} ; HRMS (ESI-TOF) $[\text{M} + \text{Na}]^+$ calcd for $\text{C}_{25}\text{H}_{27}\text{NNaO}_3^+$ m/z
2 412.1883, found 412.1888. $[\alpha]_{\text{D}}^{25} -57.0$ (c 0.23, CHCl_3). The enantiomeric ratio was
3 determined by analytical chiral HPLC. Retention time: 9.0 min (major isomer), 15.6 min
4 (minor isomer), IC-3 column, 80/20 *n*-hexane/IPA, 1.0 mL/min, 254 nm.

5

6 2-phenylpropan-2-yl (*R*)-2-((4-(hydroxymethyl)phenyl)amino)-2-(4-
7 (trifluoromethyl)phenyl)acetate (**9f**)

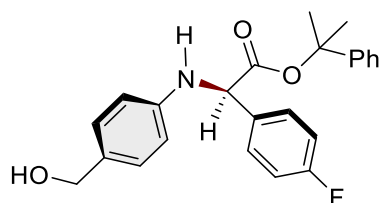


8

9 Yellow solid (75.4 mg, 85% yield, 91 : 9 e.r.); m.p. 83-85 °C; TLC $R_f = 0.32$ (*n*-
10 hexane/EtOAc 2/1); ^1H NMR (400 MHz, CDCl_3) δ 7.64 (dd, $J = 11.0, 9.2\text{Hz}$, 4H), 7.14-
11 7.21 (m, 3H), 7.11 (d, $J = 8.4\text{ Hz}$, 2H), 6.94-6.98 (m, 2H), 6.46 (d, $J = 8.4\text{ Hz}$, 2H), 5.09
12 (m, 2H), 4.50 (s, 2H), 1.80 (s, 3H), 1.63 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 169.0,
13 145.0, 144.3, 142.1, 130.4 (q, $J = 32.0\text{ Hz}$, 2C), 128.7 (2C), 128.2 (2C), 127.7 (2C),
14 127.4, 125.7 (q, $J = 3.8\text{ Hz}$, 2C), 124.0 (q, $J = 279.8\text{ Hz}$), 123.92 (2C), 113.3 (2C), 84.1,
15 65.2, 60.7, 29.0, 27.5; ^{19}F NMR (376 MHz, CDCl_3) δ -62.4; IR (ATR) ν 3403, 2983,
16 2931, 1735, 1616, 1523, 1496, 1472, 1449, 1419 cm^{-1} ; HRMS (ESI-TOF) $[\text{M} + \text{Na}]^+$

1 calcd for $C_{25}H_{24}F_3NNaO_3^+$ m/z 466.1600, found 466.1605. $[\alpha]^{25}_D -61.1$ (c 0.41, $CHCl_3$).
2 The enantiomeric ratio was determined by analytical chiral HPLC. Retention time: 6.8
3 min (major isomer), 10.0 min (minor isomer), IC-3 column, 80/20 *n*-hexane/IPA, 1.0
4 mL/min, 254 nm.

5
6 2-phenylpropan-2-yl (*R*)-2-(4-fluorophenyl)-2-((4-
7 (hydroxymethyl)phenyl)amino)acetate (**9g**)



8
9 Colorless amorphous (63.7 mg, 81% yield, 89 : 11 e.r.); TLC R_f = 0.28 (*n*-hexane/EtOAc
10 2/1); 1H NMR (400 MHz, $CDCl_3$) δ 7.45 (dd, J = 8.4, 5.2 Hz, 2H), 7.17-7.21 (m, 3H),
11 7.04-7.12 (m, 4H), 6.97-7.02 (m, 2H), 6.47 (d, J = 8.4 Hz, 2H), 5.02 (s, 2H), 4.49 (s, 2H),
12 1.79 (s, 3H), 1.62 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.6, 162.6 (d, J = 245.5 Hz),
13 145.3, 144.5, 133.6 (d, J = 3.4 Hz), 130.3, 129.0 (d, J = 8.1 Hz, 2C), 128.7 (2C), 128.2
14 (2C), 127.3, 124.0 (2C), 115.7 (d, J = 21.5 Hz, 2C), 113.3 (2C), 83.7, 65.3, 60.3, 29.11,
15 27.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.9; IR (ATR) ν 3413, 2956, 2926, 2856, 2342,
16 1733, 1615, 1522, 1508, 1469 cm^{-1} ; HRMS (ESI-TOF) $[M + Na]^+$ calcd for
17 $C_{24}H_{24}FNNaO_3^+$ m/z 416.1632, found 416.1629. $[\alpha]^{25}_D -32.6$ (c 0.49, $CHCl_3$). The
18 enantiomeric ratio was determined by analytical chiral HPLC. Retention time: 11.3 min

1 (major isomer), 19.2 min (minor isomer), IC-3 column, 85/15 *n*-hexane/IPA, 1.0 mL/min,

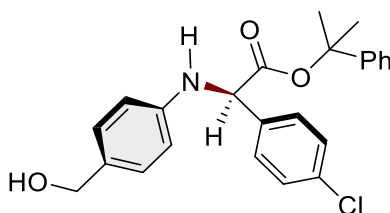
2 254 nm.

3

4 2-phenylpropan-2-yl

(*R*)-2-(4-chlorophenyl)-2-((4-

5 (hydroxymethyl)phenyl)amino)acetate (**9h**)



6

7 Yellow amorphous (46.7 mg, 57% yield, 93 : 7 e.r.); TLC R_f = 0.32 (*n*-hexane/EtOAc

8 2/1); ¹H NMR (400 MHz, CDCl₃) δ 7.43 (d, *J* = 8.4 Hz, 2H), 7.35 (d, 8.4 Hz, 2H), 7.18-

9 7.22 (m, 3H), 7.10 (d, *J* = 8.4 Hz, 2H), 6.99-7.02 (m, 2H), 6.46 (d, *J* = 8.4 Hz, 2H), 5.02

10 (s, 2H), 4.50 (s, 2H), 1.79 (s, 3H), 1.63 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 169.4,

11 145.2, 144.5, 136.5, 134.0, 130.3, 128.9 (2C), 128.7 (2C), 128.7 (2C), 128.2 (2C), 127.3,

12 124.0 (2C), 113.3 (2C), 83.8, 65.3, 60.4, 29.0, 27.6; IR (ATR) ν 3408, 2928, 1736, 1615,

13 1522, 1489, 1308, 1252, 1181, 1367 cm⁻¹; HRMS (ESI-TOF) [M + Na]⁺ calcd for

14 C₂₄H₂₄ClNNaO₃⁺ m/z 432.1337, found 432.1347. [α]_D²⁵ -50.7 (c 0.18, CHCl₃). The

15 enantiomeric ratio was determined by analytical chiral HPLC. Retention time: 17.3 min

16 (major isomer), 30.2 min (minor isomer), IC-3 column, 90/10 *n*-hexane/IPA, 1.0 mL/min,

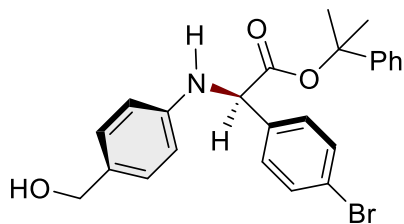
17 254 nm.

1

2 2-phenylpropan-2-yl

(*R*)-2-(4-bromophenyl)-2-((4-

3 (hydroxymethyl)phenyl)amino)acetate (**9i**)



4

5 Colorless amorphous (81.8 mg, 90% yield, 89 : 11 e.r.); TLC R_f = 0.28 (n-hexane/EtOAc

6 2/1); ¹H NMR (400 MHz, CDCl₃) δ 7.50 (d, *J* = 8.4 Hz, 2H), 7.36 (d, *J* = 8.4 Hz, 2H),

7 7.18-7.22 (m, 3H), 7.08 (d, *J* = 8.4 Hz, 2H), 6.98-7.02 (m, 2H), 6.45 (d, *J* = 8.4 Hz, 2H),

8 5.00 (s, 2H), 4.47 (s, 2H), 1.79 (s, 3H), 1.63 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 169.3,

9 145.2, 144.4, 137.0, 131.9 (2C), 130.3, 129.0 (2C), 128.7 (2C), 128.2 (2C), 127.3, 124.0

10 (2C), 122.1, 113.3 (2C), 83.8, 65.2, 60.5, 29.0, 27.5; IR (ATR) ν 3399, 2980, 1732, 1615,

11 1521, 1496, 1485, 1448, 1405, 1385 cm⁻¹; HRMS (ESI-TOF) [M + Na]⁺ calcd for

12 C₂₄H₂₄BrNNaO₃⁺ m/z 476.0832, found 476.0838. [α]_D²⁵ -99.6 (c 0.63, CHCl₃). The

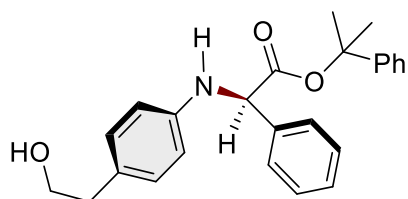
13 enantiomeric ratio was determined by analytical chiral HPLC. Retention time: 9.0 min

14 (major isomer), 14.2 min (minor isomer), IC-3 column, 80/20 *n*-hexane/IPA, 1.0 mL/min,

15 254 nm.

16

17 2-phenylpropan-2-yl (*R*)-2-((4-(2-hydroxyethyl)phenyl)amino)-2-phenylacetate (**9j**)



1

2 Pale yellow amorphous (68.6 mg, 88% yield, 93 : 7 e.r.); TLC Rf = 0.32 (n-hexane/EtOAc

3 2/1); ¹H NMR (400 MHz, CDCl₃) δ 7.48 (dd, *J* = 8.4, 1.6 Hz, 2H), 7.32-7.41 (m, 3H),

4 7.14-7.19 (m, 3H), 6.93-6.99 (m, 4H), 6.48 (d, *J* = 8.4 Hz, 2H), 5.02 (s, 1H), 4.91 (s, 1H),

5 3.74 (t, *J* = 6.4 Hz, 2H), 2.70 (t, *J* = 6.4 Hz, 2H), 1.78 (s, 3H), 1.61 (s, 3H); ¹³C NMR

6 (100 MHz, CDCl₃) δ 170.0, 144.8, 144.6, 138.0, 129.8 (2C), 128.7 (2C), 128.1 (3C),

7 127.4 (2C), 127.2, 127.2, 124.0 (2C), 113.6 (2C), 83.4, 63.9, 61.2, 38.2, 29.1, 27.6; IR

8 (ATR) ν 3367, 2925, 1735, 1616, 1520, 1312, 1257, 1185, 1136, 1105 cm⁻¹; HRMS (ESI-

9 TOF) [M + Na]⁺ calcd for C₂₅H₂₇NNaO₃⁺ m/z 412.1883, found 412.1897. [α]_D²⁵ -58.5 (c

10 0.12, CHCl₃). The enantiomeric ratio was determined by analytical chiral HPLC.

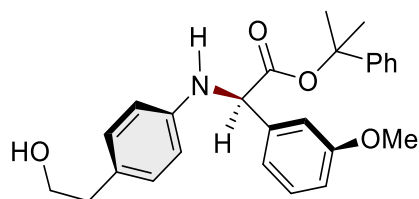
11 Retention time: 8.7 min (major isomer), 12.3 min (minor isomer), IBN-3 column, 85/15

12 *n*-hexane/IPA, 1.0 mL/min, 254 nm.

13

14 2-phenylpropan-2-yl (R)-2-((4-(2-hydroxyethyl)phenyl)amino)-2-(3-

15 methoxyphenyl)acetate (**9k**)



1

2 Colorless amorphous (83.9 mg, quant., 92 : 8 e.r.); TLC Rf = 0.25 (n-hexane/EtOAc 2/1);

3 ^1H NMR (400 MHz, CDCl_3) δ 7.30 (t, $J = 8.0$ Hz, 1H), 7.16-7.20 (m, 3H), 7.09 (d, $J =$

4 7.6 Hz, 1H), 6.98-7.02 (m, 3H), 6.96 (d, $J = 8.4$ Hz, 2H), 6.88 (dd, $J = 8.4, 2.4$ Hz, 1H),

5 6.49 (d, $J = 8.4$ Hz 2H), 4.98 (d, $J = 5.2$ Hz, 1H), 4.89 (d, $J = 5.2$ Hz, 1H), 3.79 (s, 3H),

6 3.75 (q, $J = 6.4$ Hz, 2H), 2.71 (t, $J = 6.4$ Hz, 2H), 1.79 (s, 3H), 1.63 (s, 3H); ^{13}C NMR

7 (150 MHz, CDCl_3) δ 169.9, 159.9, 144.7, 144.6, 139.6, 129.7 (2C), 129.7, 128.1 (2C),

8 127.3, 127.1, 124.0 (2C), 119.8, 113.9, 113.5 (2C), 112.5, 83.4, 63.8, 61.2, 55.2, 38.2,

9 29.1, 27.5; IR (ATR) ν 3411, 2981, 2931, 1733, 1560, 1520, 1489, 1467, 1451, 1436 cm^{-1} ;

10 HRMS (ESI-TOF) $[\text{M} + \text{Na}]^+$ calcd for $\text{C}_{26}\text{H}_{29}\text{NNaO}_4^+$ m/z 442.1989, found 442.1995.

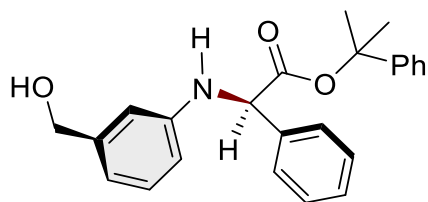
11 $[\alpha]_D^{25} -48.6$ (c 0.49, CHCl_3). The enantiomeric ratio was determined by analytical chiral

12 HPLC. Retention time: 10.1 min (major isomer), 18.6 min (minor isomer), IC-3 column,

13 80/20 *n*-hexane/IPA, 1.0 mL/min, 254 nm.

14

15 2-phenylpropan-2-yl (*R*)-2-((3-(hydroxymethyl)phenyl)amino)-2-phenylacetate (**91**)



1

2 Colorless amorphous (67.6 mg, 90% yield, 89 : 11 e.r.); TLC Rf = 0.32 (n-hexane/EtOAc

3 2/1); ¹H NMR (400 MHz, CDCl₃) δ 7.48 (dd, *J* = 7.6, 1.2 Hz, 2H), 7.31-7.40 (m, 3H),

4 7.14-7.19 (m, 3H), 7.07 (d, *J* = 8.0 Hz, 1H), 6.47-7.00 (m, 2H), 6.64 (d, *J* = 7.6 Hz, 1H),

5 6.54 (s, 1H), 6.44 (dd, *J* = 8.0, 2.0 Hz, 1H), 5.06 (d, *J* = 4.8 Hz, 1H), 4.99 (d, *J* = 4.8 Hz,

6 1H), 4.50 (s, 2H), 1.78 (s, 3H), 1.61 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 169.9, 146.2,

7 144.7, 142.0, 137.8, 129.4, 128.7 (2C), 128.1, 128.1 (2C), 127.3 (2C), 127.1, 124.0 (2C),

8 116.3, 112.5, 111.8, 83.4, 65.4, 61.0, 29.1, 27.5; IR (ATR) ν 3407, 3031, 2980, 2927,

9 1734, 1608, 1592, 1491, 1451, 1385 cm⁻¹; HRMS (ESI-TOF) [M + Na]⁺ calcd for

10 C₂₄H₂₅NNaO₃⁺ m/z 398.1727, found 398.1726. [α]_D²⁵ -52.5 (c 0.44, CHCl₃). The

11 enantiomeric ratio was determined by analytical chiral HPLC. Retention time: 12.5 min

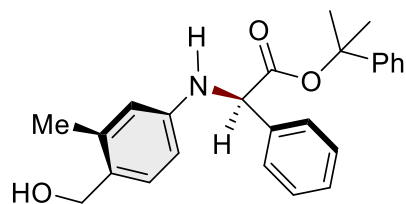
12 (major isomer), 23.6 min (minor isomer), IC-3 column, 85/15 *n*-hexane/IPA, 1.0 mL/min,

13 254 nm.

14

15 2-phenylpropan-2-yl (R)-2-((4-(hydroxymethyl)-3-methylphenyl)amino)-2-

16 phenylacetate (**9m**)



1

2 Pale yellow amorphous (55.3 mg, 71% yield, 96 : 4 e.r.); TLC Rf = 0.36 (n-hexane/EtOAc

3 2/1); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.48 (dd, $J = 8.0, 1.6\text{ Hz}$, 2H), 7.33-7.40 (m, 3H),

4 7.15-7.19 (m, 3H), 7.02 (d, $J = 8.4\text{ Hz}$, 1H), 6.96-7.00 (m, 2H), 6.40 (d, $J = 2.4\text{ Hz}$, 1H),

5 6.31 (dd, $J = 8.0, 2.4\text{ Hz}$, 1H), 5.04 (s, 1H), 4.94 (s, 1H), 4.52 (s, 2H), 2.26 (s, 3H), 1.78

6 (s, 3H), 1.62 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 169.9, 145.8, 144.7, 137.9, 137.9,

7 129.8, 128.7 (2C), 128.2, 128.2 (2C), 127.3 (2C), 127.2, 124.0 (2C), 115.6, 110.3, 83.4,

8 63.6, 61.0, 29.7, 29.2, 27.5, 18.9; IR (ATR) ν 3407, 2925, 2853, 2369, 2351, 1736, 1615,

9 1509, 1453, 1384 cm^{-1} ; HRMS (ESI-TOF) $[\text{M} + \text{Na}]^+$ calcd for $\text{C}_{25}\text{H}_{27}\text{NNaO}_3^+$ m/z

10 412.1883, found 412.1884. $[\alpha]_D^{25} -57.5$ (c 0.08, CHCl_3). The enantiomeric ratio was

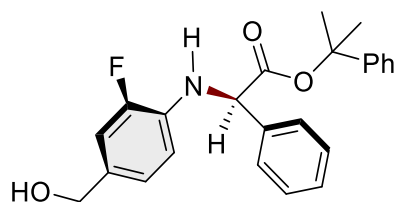
11 determined by analytical chiral HPLC. Retention time: 10.8 min (major isomer), 15.0 min

12 (minor isomer), IBN-3 column, 85/15 *n*-hexane/IPA, 1.0 mL/min, 254 nm.

13

14 2-phenylpropan-2-yl (*R*)-2-((2-fluoro-4-(hydroxymethyl)phenyl)amino)-2-phenylacetate

15 (**9n**)



1

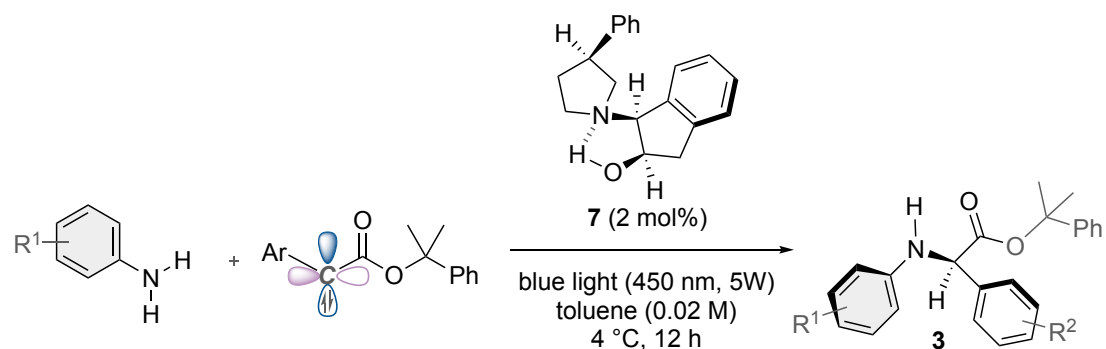
2 Pale yellow amorphous (78.7 mg, quant., yield, 95 : 5 e.r.); TLC Rf = 0.50 (n-
 3 hexane/EtOAc 2/1); ¹H NMR (400 MHz, CDCl₃) δ 7.47 (dd, *J* = 8.0, 1.6 Hz, 2H), 7.34-
 4 7.41 (m, 3H), 7.14-7.19 (m, 3H), 6.95-7.01 (m, 3H), 6.83 (d, *J* = 8.0 Hz, 1H), 6.39 (t, *J* =
 5 8.4 Hz, 1H), 5.24 (s, 2H), 5.06 (d, *J* = 5.6 Hz, 2H), 1.80 (s, 3H), 1.62 (s, 3H); ¹³C NMR
 6 (150 MHz, CDCl₃) δ 169.4, 151.4 (d, *J* = 238.4 Hz), 144.6, 137.3, 133.9 (d, *J* = 11.6 Hz),
 7 130.2 (d, *J* = 5.9 Hz), 128.8 (2C), 128.3, 128.1 (2C), 127.3 (2C), 127.2, 124.0 (2C), 123.3
 8 (d, *J* = 3.0 Hz), 113.8 (d, *J* = 18.8 Hz), 112.8 (d, *J* = 2.9 Hz), 83.6, 64.7, 60.8, 29.3, 27.3;
 9 ¹⁹F NMR (376 MHz, CDCl₃) δ -134.9; IR (ATR) ν 3418, 2929, 2369, 1738, 1632, 1530,
 10 1496, 1455, 1367, 1319 cm⁻¹; HRMS (ESI-TOF) [M + Na]⁺ calcd for C₂₄H₂₄FNNaO₃⁺
 11 m/z 416.1632, found 416.1645. [α]_D²⁵ -59.4 (c 0.39, CHCl₃). The enantiomeric ratio was
 12 determined by analytical chiral HPLC. Retention time: 12.3 min (major isomer), 19.2 min
 13 (minor isomer), IC-3 column, 90/10 *n*-hexane/IPA, 1.0 mL/min, 254 nm.

14

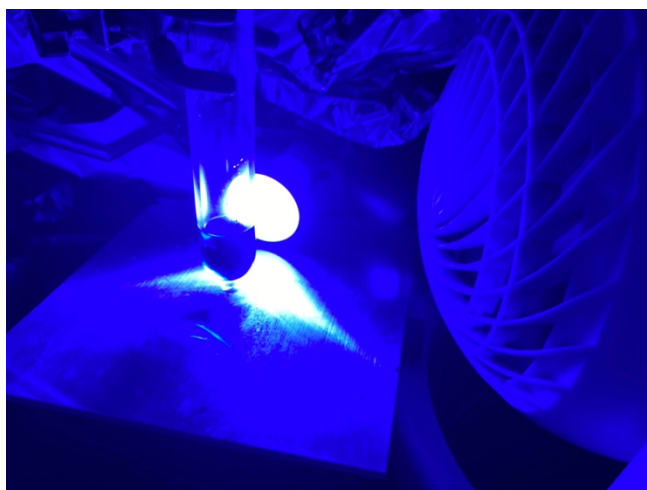
15

16

1 **4. General Procedure for Light-promoted Asymmetric N–H Insertion**

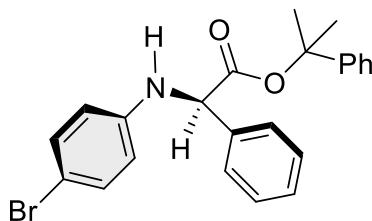


3 A 50-mL Schlenk tube was charged with aniline derivative (1.2 mmol), diazoester
4 derivative (0.2 mmol), chiral catalyst (7, 1.1 mg, 0.004 mmol), and toluene (10.0 mL).
5 The reaction mixture was irradiated with 450 nm light from a 5 W LED at 4 °C for 12 h.
6 The solvent was removed under reduced pressure, and the crude residue was purified by
7 flash column chromatography on silica gel (*n*-hexane/EtOAc = 15:1) to afford the
8 corresponding products.



(in a cold room at 4 °C)

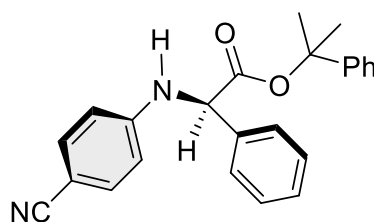
1 2-phenylpropan-2-yl (*R*)-2-((4-bromophenyl)amino)-2-phenylacetate (**3a**)



2
3 White solid (62.8 mg, 74% yield, 95 : 5 e.r.). The spectroscopic and analytical data,
4 including ^1H NMR, ^{13}C NMR, IR, and HRMS, were consistent with those of the product
5 obtained from the ruthenium-catalyzed reaction.

6

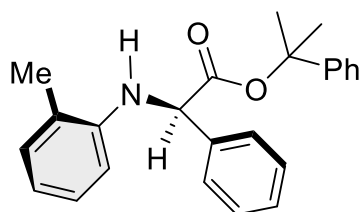
7 2-phenylpropan-2-yl (*R*)-2-((4-cyanophenyl)amino)-2-phenylacetate (**3h**)



8
9 Colorless amorphous (51.9 mg, 70% yield, 91 : 9 e.r.). The spectroscopic and analytical
10 data, including ^1H NMR, ^{13}C NMR, IR, and HRMS, were consistent with those of the
11 product obtained from the ruthenium-catalyzed reaction.

12

13 2-phenylpropan-2-yl (*R*)-2-phenyl-2-(*o*-tolylamino)acetate (**3j**)

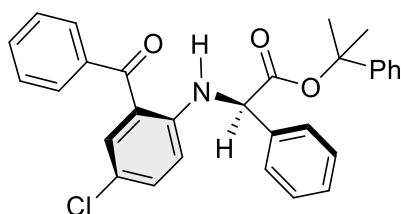


1

2 Yellow solid (48.2 mg, 67% yield, 91 : 9 e.r.). The spectroscopic and analytical data,
 3 including ^1H NMR, ^{13}C NMR, IR, and HRMS, were consistent with those of the product
 4 obtained from the ruthenium-catalyzed reaction.

5

6 ethyl *(R)*-3-benzoyl-4-((2-oxo-1-phenyl-2-((2-phenylpropan-2-
 7 yl)oxy)ethyl)amino)benzoate (**3z**)

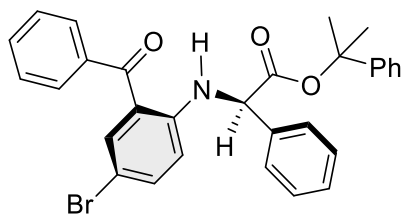


8

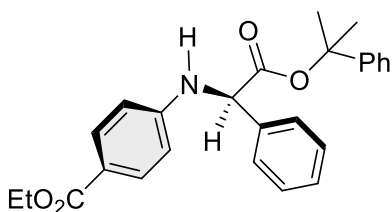
9 Yellow solid (50.3 mg, 52% yield, 88 : 12 e.r.). The spectroscopic and analytical data,
 10 including ^1H NMR, ^{13}C NMR, IR, and HRMS, were consistent with those of the product
 11 obtained from the ruthenium-catalyzed reaction.

12

13 2-phenylpropan-2-yl *(R)*-2-((2-benzoyl-4-bromophenyl)amino)-2-phenylacetate (**3ae**)



1
 2 Yellow amorphous (52.8 mg, 50% yield, 89 : 11 e.r.); TLC Rf = 0.33(n-hexane/EtOAc,
 3 10/1); ¹H NMR (400 MHz, CDCl₃) δ 9.47 (d, *J* = 5.6 Hz, 1H), 7.58-7.65 (m, 3H), 7.43-
 4 7.57 (m, 5H), 7.33-7.43 (m, 3H), 7.30 (dd, *J* = 9.0, 2.2 Hz, 1H), 7.11-7.18 (m, 3H), 6.95-
 5 7.02 (m, 2H), 6.43 (d, *J* = 9.2 Hz, 1H), 5.14 (d, *J* = 5.6 Hz, 1H) 1.80 (s, 3H), 1.66 (s, 3H);
 6 ¹³C NMR (150 MHz, CDCl₃) δ 197.8, 168.5, 148.0, 144.7, 139.4, 137.1, 136.9, 131.4,
 7 129.2 (2C), 128.9 (2C), 128.5, 128.2 (2C), 128.1 (2C), 127.3 (2C), 127.2, 127.1, 124.1
 8 (2C), 119.8, 114.5, 106.2, 83.7, 60.9, 29.2, 27.4 ; IR (ATR) ν 3390, 2979, 2926, 2870,
 9 1717, 1661, 1596, 1518, 1496, 1468 cm⁻¹; HRMS (ESI-TOF) [M + Na]⁺ calcd for
 10 C₃₀H₂₆BrNNaO₃⁺ m/z 550.0988, found 550.1001. [α]_D²⁵ +53.2 (c 0.37, CHCl₃). The
 11 enantiomeric ratio was determined by analytical chiral HPLC. Retention time: 8.9 min
 12 (major isomer), 13.1 min (minor isomer), IBN-3 column, 98/2 *n*-hexane/IPA, 1.0 mL/min,
 13 254 nm.
 14
 15 ethyl (*R*)-4-((2-oxo-1-phenyl-2-((2-phenylpropan-2-yl)oxy)ethyl)amino)benzoate (**3y**)

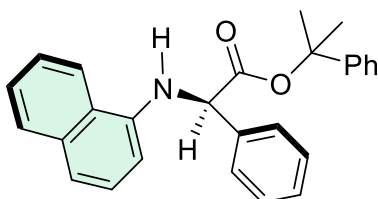


1

2 Colorless oil (70.3 mg, 68% yield, 95 : 5 e.r.). The spectroscopic and analytical data,
 3 including ^1H NMR, ^{13}C NMR, IR, and HRMS, were consistent with those of the product
 4 obtained from the ruthenium-catalyzed reaction.

5

6 2-phenylpropan-2-yl (*R*)-2-(naphthalen-1-ylamino)-2-phenylacetate (**3o**)

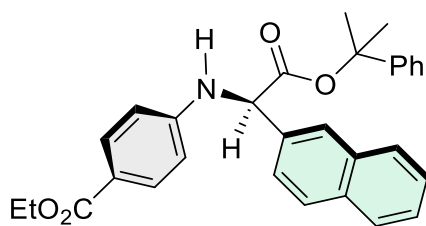


7

8 Colorless amorphous (50.6 mg, 64% yield, 83 : 17 e.r.). The spectroscopic and analytical
 9 data, including ^1H NMR, ^{13}C NMR, IR, and HRMS, were consistent with those of the
 10 product obtained from the ruthenium-catalyzed reaction.

11

12 ethyl (*R*)-4-((1-(naphthalen-2-yl)-2-oxo-2-((2-phenylpropan-2-
 13 yl)oxy)ethyl)amino)benzoate (**3af**)



1

2 Colorless amorphous (66.1 mg, 73% yield, 94 : 6 e.r.); TLC Rf = 0.41 (n-hexane/EtOAc

3 4/1); ¹H NMR (600 MHz, CDCl₃) δ 7.85-7.92 (m, 3H), 7.82 (dd, *J* = 6.0, 3.0 Hz, 1H),

4 7.78 (d, *J* = 9.0 Hz, 2H), 7.58 (d, *J* = 8.4 Hz, 1H), 7.49-7.53 (m, 2H), 7.15 (t, *J* = 7.2 Hz,

5 1H), 7.07 (t, *J* = 7.8 Hz, 2H), 6.94 (d, *J* = 8.4 Hz, 2H), 6.52 (d, *J* = 8.4 Hz, 2H), 5.52 (d,

6 *J* = 4.8 Hz, 1H), 5.25 (d, *J* = 4.8 Hz, 1H), 4.26 (q, *J* = 7.2 Hz, 2H), 1.79 (s, 3H), 1.61 (s,

7 3H), 1.30 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 169.4, 166.6, 149.4, 144.4,

8 134.5, 133.3, 133.2, 131.3 (2C), 128.7, 128.1 (2C), 128.0, 127.7, 127.2, 126.5, 126.4,

9 126.3, 124.9, 124.0 (2C), 119.4, 112.3 (2C), 84.0, 60.5, 60.1, 29.0, 27.5, 14.3; IR (ATR)

10 ν 3391, 2980, 2932, 1734, 1700, 1605, 1578, 1524, 1496, 1478 cm⁻¹; HRMS (ESI-TOF)

11 [M + Na]⁺ calcd for C₃₀H₂₉NNaO₄⁺ m/z 490.1989, found 490.1984. [α]_D²⁵ -94.8 (c 0.57,

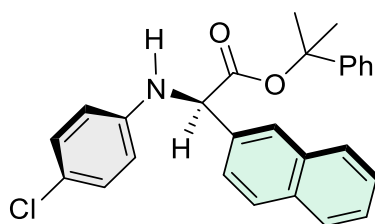
12 CHCl₃). The enantiomeric ratio was determined by analytical chiral HPLC. Retention

13 time: 10.2 min (major isomer), 12.8 min (minor isomer), IC-3 column, 75/25 *n*-

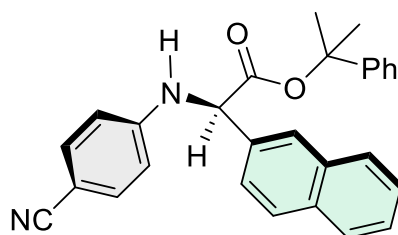
14 hexane/IPA, 1.0 mL/min, 254 nm.

15

16 2-phenylpropan-2-yl (*R*)-2-((4-chlorophenyl)amino)-2-(naphthalen-2-yl)acetate (**3ag**)



1
 2 White solid (62.2mg, 75% yield, 93 : 7 e.r.); m.p. 72-74 °C; TLC R_f = 0.35 (n-
 3 hexane/EtOAc 4/1); ¹H NMR (600 MHz, CDCl₃) δ 7.91 (s, 1H), 7.85-7.89 (m, 2H), 7.81-
 4 7.84 (m, 1H), 7.58 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.49-7.53 (m, 2H), 7.14 (t, *J* = 7.2 Hz, 1H),
 5 7.07 (t, *J* = 7.2 Hz, 1H), 7.02 (d, *J* = 9.0 Hz, 2H), 6.92-6.95 (m, 2H), 6.47 (d, *J* = 8.4 Hz,
 6 2H), 5.15 (d, *J* = 5.4 Hz, 1H), 5.09 (d, *J* = 5.4 Hz, 1H), 1.78 (s, 3H), 1.60 (s, 3H); ¹³C
 7 NMR (150 MHz, CDCl₃) δ 169.7, 144.5, 144.4, 134.9, 133.3, 133.3, 129.0 (2C), 128.7,
 8 128.1 (2C), 128.0, 127.7, 127.2, 126.5, 126.3, 126.3, 125.1, 124.0 (2C), 122.4, 114.5 (2C),
 9 83.8, 61.2, 29.0, 27.6; IR (ATR) ν 3405, 3056, 2980, 1733, 1600, 1448, 1384, 1367, 1323,
 10 1274 cm⁻¹; HRMS (ESI-TOF) [M + Na]⁺ calcd for C₂₇H₂₄ClNNaO₂²⁺ m/z 452.1388,
 11 found 452.1387. [α]_D²⁵ -109.9 (c 0.53, CHCl₃). The enantiomeric ratio was determined
 12 by analytical chiral HPLC. Retention time: 10.8 min (major isomer), 18.2 min (minor
 13 isomer), IBN-3 column, 95/5 *n*-hexane/IPA, 1.0 mL/min, 254 nm.
 14
 15 2-phenylpropan-2-yl (*R*)-2-((4-cyanophenyl)amino)-2-(naphthalen-2-yl)acetate (**3ah**)



1

2 Colorless amorphous (64.8mg, 77% yield, 93 : 7 e.r.); TLC Rf = 0.41 (n-hexane/EtOAc

3 4/1); ¹H NMR (600 MHz, CDCl₃) δ 7.85-7.90 (m, 3H), 7.80-7.83 (m, 1H), 7.55 (d, *J* =

4 8.4 Hz, 1H), 7.50-7.53 (m, 2H), 7.30 (d, *J* = 9.0 Hz, 2H), 7.14 (t, *J* = 7.2 Hz, 1H), 7.05 (t,

5 *J* = 7.2 Hz, 2H), 6.92 (d, *J* = 8.4 Hz, 2H), 6.50 (d, *J* = 9.0 Hz, 2H), 5.65 (s, 1H), 5.20 (d,

6 *J* = 4.8 Hz, 1H), 1.79 (s, 3H), 1.59 (s, 3H); ¹³C NMR (150 MHz, CDCl₃) δ 169.1, 148.8,

7 144.2, 134.0, 133.6 (2C), 133.3, 128.9, 128.1 (2C), 128.0, 127.7, 127.3, 126.5, 126.5,

8 126.4, 124.7, 124.7, 124.0 (2C), 120.1, 113.1 (2C), 99.6, 84.2, 60.3, 29.0, 27.5 ; IR (ATR)

9 ν 3385, 3058, 2982, 2215, 1734, 1574, 1496, 1474, 1448, 1385 cm⁻¹; HRMS (ESI-TOF)

10 [M + Na]⁺ calcd for C₂₈H₂₄N₂NaO₂²⁺ m/z 443.1730, found 443.1746. [α]_D²⁵ -128.0 (c

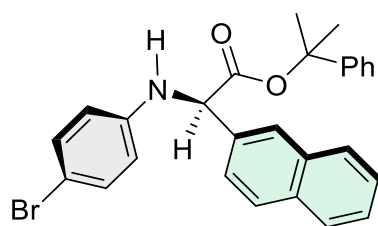
11 0.57, CHCl₃). The enantiomeric ratio was determined by analytical chiral HPLC.

12 Retention time: 14.0 min (major isomer), 19.3 min (minor isomer), IBN-3 column, 80/20

13 *n*-hexane/IPA, 1.0 mL/min, 254 nm.

14

15 2-phenylpropan-2-yl (*R*)-2-((4-bromophenyl)amino)-2-(naphthalen-2-yl)acetate (**3p**)



1

2 White solid (68.2 mg, 72% yield, 95 : 5 e.r.). The spectroscopic and analytical data,

3 including ^1H NMR, ^{13}C NMR, IR, and HRMS, were consistent with those of the product

4 obtained from the ruthenium-catalyzed reaction.

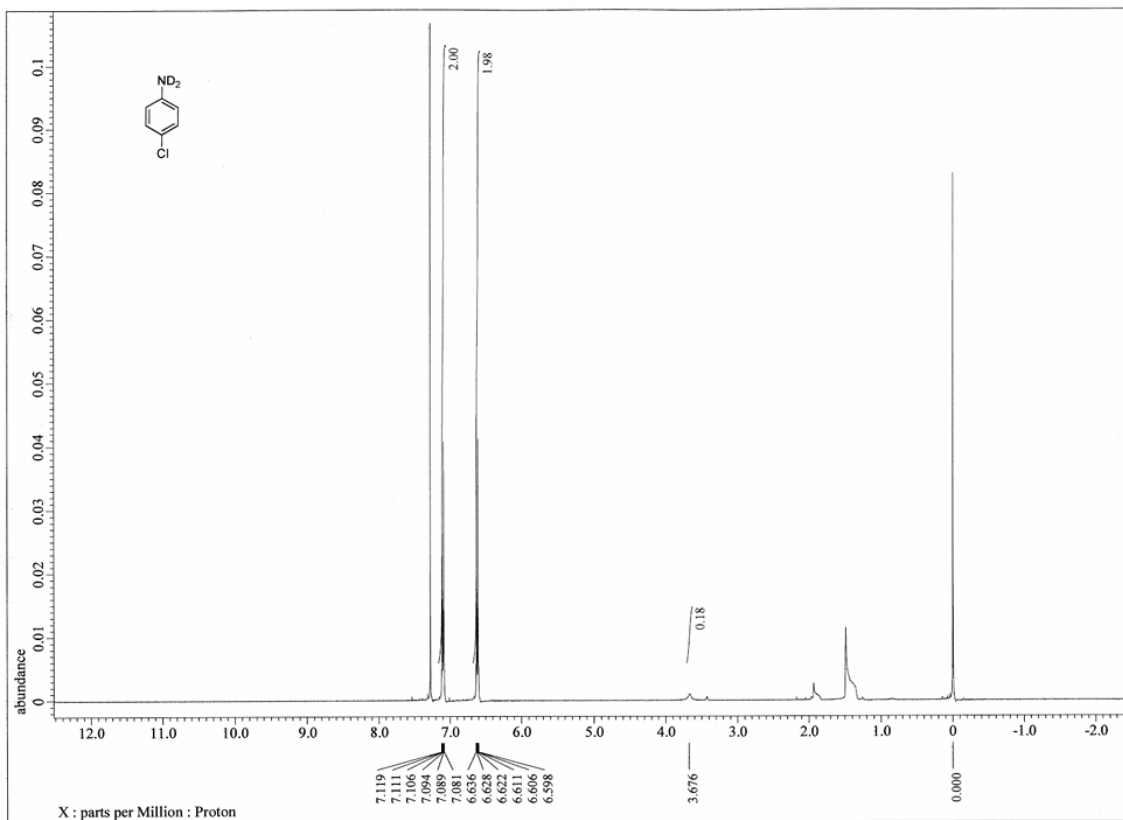
5

6

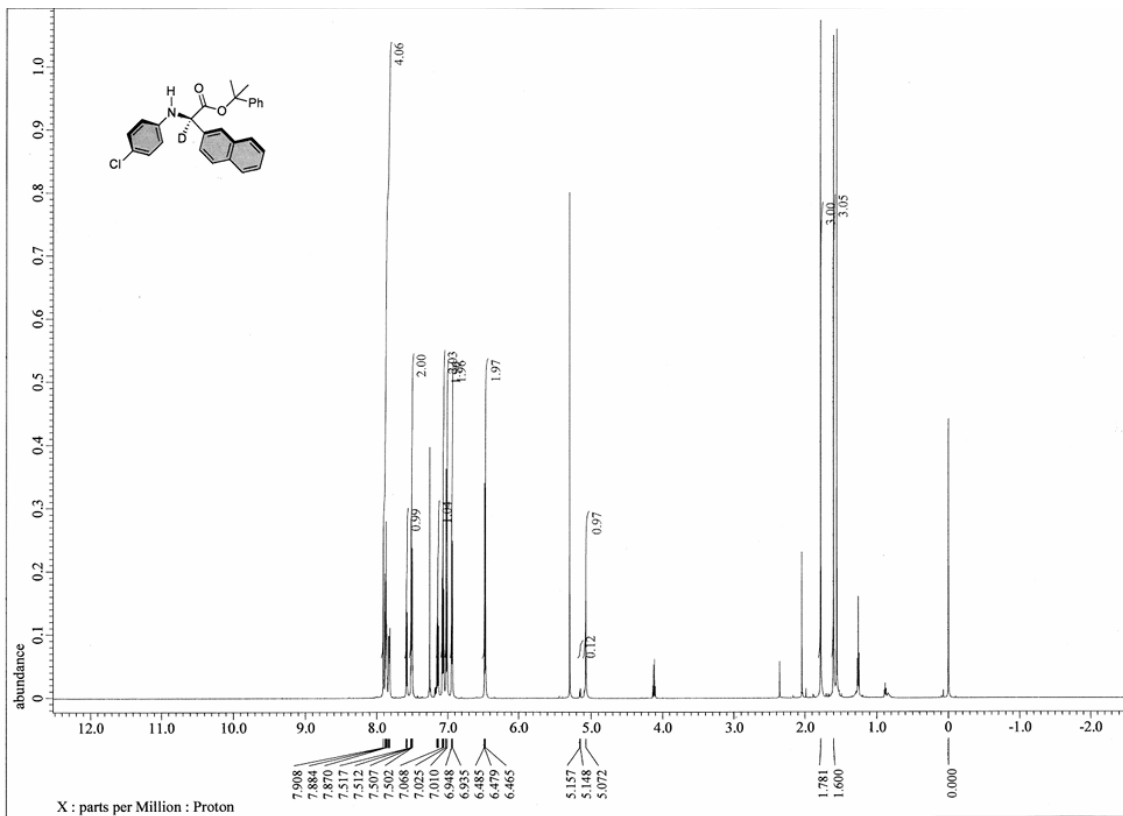
1 **5. Deuterium Labelling Experiment**

2 *N*-deuterium-labeled aniline derivative was synthesized according to the following
3 procedure. In a dried 30-mL eggplant-shaped flask, aniline derivative (0.66 mmol) was
4 dissolved in CD₃OD (1.0 mL, 0.66 M), and the solution was stirred at room temperature
5 for 4 hours. Then the solution was concentrated under vacuum to remove the solvent.
6 CD₃OD (1.0 mL) was added into the flask again and the solution was stirred at room
7 temperature for another 4 hours. After that, the resulting solution was concentrated under
8 vacuum to give the desired product in quantitative yield.

9



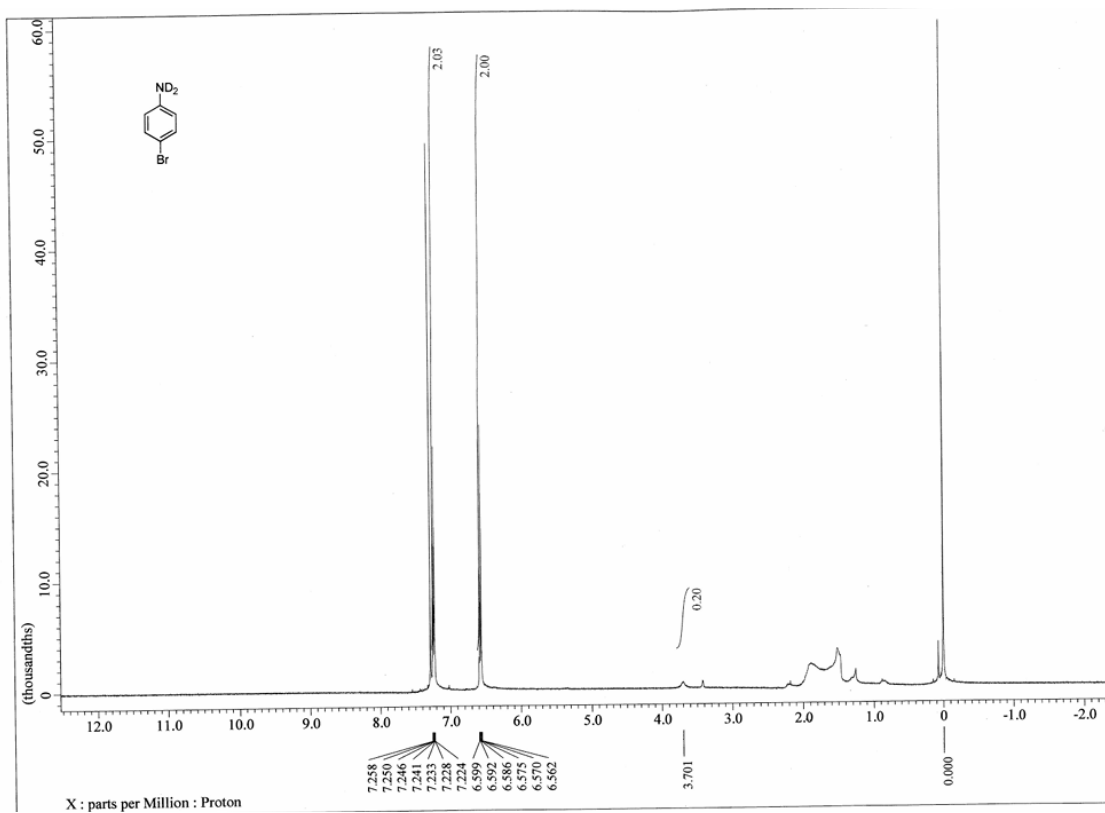
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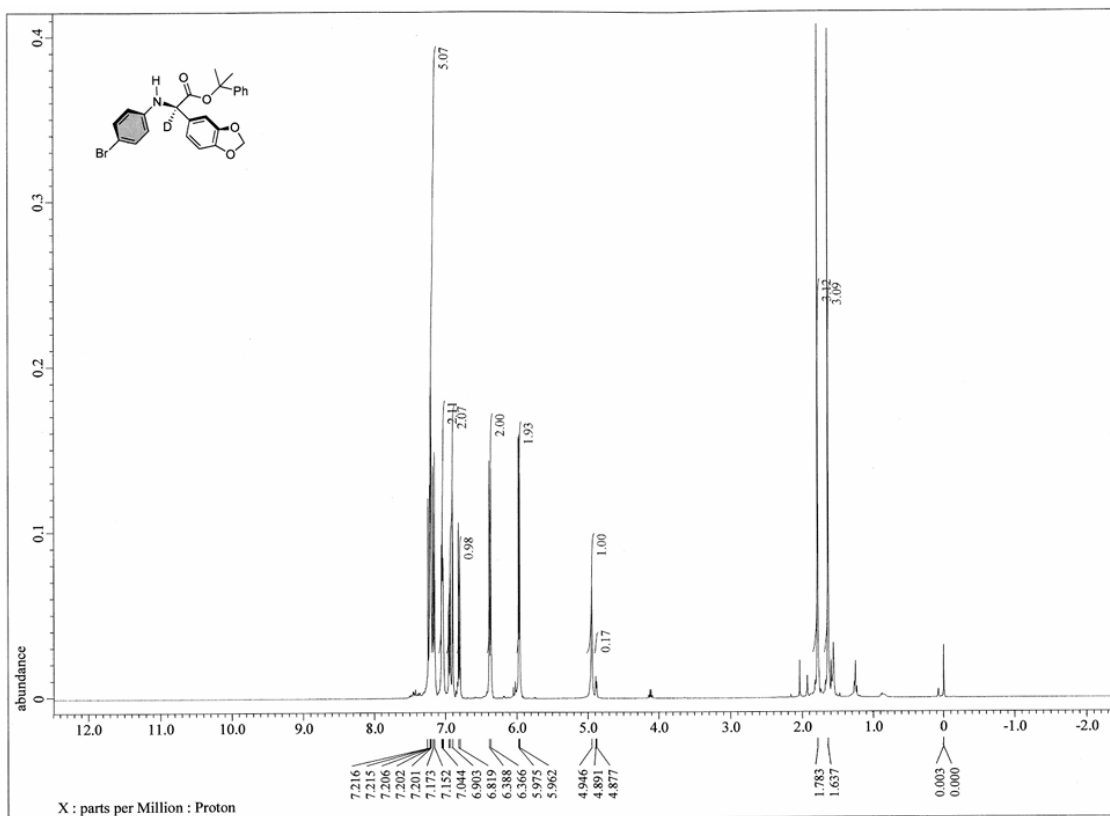
2

3

1



2



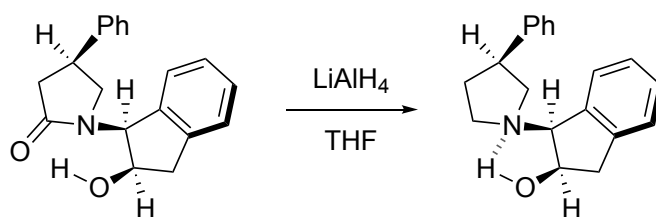
3

1 **6. Synthesis of Catalyst and Substrates**

2 Catalyst **7** was synthesized by reducing the corresponding reported amide precursor¹.

3

4 (1*S*,2*R*)-1-((*S*)-3-phenylpyrrolidin-1-yl)-2,3-dihydro-1*H*-inden-2-ol (**7**)



5

6 LiAlH₄ (113.1 mg, 2.98 mmol, 2.0 equiv.) was added to a solution of (*S*)-1-((1*S*,2*R*)-2-

7 hydroxy-2,3-dihydro-1*H*-inden-1-yl)-4-phenylpyrrolidin-2-one (437.1 mg, 1.49 mmol,

8 1.00 equiv.) in THF (5 mL). The mixture was stirred at 50 °C for 20 h. The reaction

9 mixture was allowed to cool down to room temperature and water (10 mL) and CH₂Cl₂

10 (10 mL) were added. The layers were separated and the aqueous phase was extracted with

11 CH₂Cl₂ (3 × 5 mL). The combined organic layers were dried over MgSO₄, and

12 concentrated. The residue was purified by flash chromatography on silica to afford **7** as a

13 solid (291.4 mg, 70% yield).

14 m.p. 65-67 °C; TLC R_f = 0.25 (n-hexane/EtOAc, 1/1); ¹H NMR (600 MHz, CDCl₃) δ

15 7.36 (d, *J* = 7.2 Hz, 1H), 7.24-7.29 (m, 3H), 7.16-7.23 (m, 5H), 4.44 (dd, *J* = 7.5, 7.5 Hz,

16 1H), 4.30 (d, *J* = 7.8 Hz, 1H), 3.29 (quint, *J* = 8.4 Hz, 1H), 3.19 (dd, *J* = 15.9, 7.5 Hz,

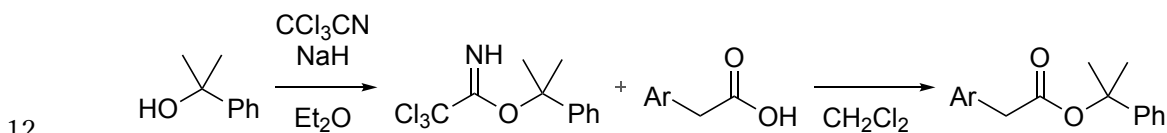
17 1H), 3.05 (t, *J* = 8.1 Hz, 1H), 2.95-3.00 (m, 1H), 2.88 (t, *J* = 8.0 Hz, 1H), 2.75-2.83 (m,

1 2H), 2.23-2.29 (m, 1H), 1.83-1.90 (m, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 144.6, 142.0,
2 138.8, 128.7 (2C), 128.6, 127.3 (2C), 126.8, 126.4, 126.3, 125.6, 70.6, 66.6, 58.7, 50.7,
3 43.2, 40.9, 33.0; IR (ATR) ν 3310, 3063, 3025, 2916, 2819, 1602, 1493, 1479, 1457, 1401
4 cm⁻¹; HRMS (ESI-TOF) [M + H]⁺ calcd for C₁₉H₂₂NO⁺ m/z 280.1696, found 280.1695.
5 [α]_D²⁵ +38.1 (c 1.0, CHCl₃).

6
7 For the preparation of substrates, known compounds were synthesized according to
8 literature procedures^{2,3}, and unknown compounds were synthesized according to the
9 following general procedures.

10

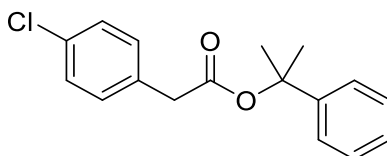
11 **General Procedure A for the Synthesis of Phenylpropan-2-yl 2-Phenylacetates**



13 Sodium hydride (240 mg, 10 mmol) was suspended in anhydrous ether (1.5 mL) and a
14 solution of 2-phenyl-2-propanol (1.36 g, 10 mmol) in ether (1.0 mL) was added dropwise
15 with stirring under an Ar atmosphere. After the solids dissolved, the solution was cooled
16 to 0 °C. Trichloroacetonitrile (1.05 mL, 10.5 mmol) was added dropwise and the reaction
17 mixture was allowed to return to room temperature for 1 hour. The reaction mixture was
18 quenched with MeOH and concentrated to a syrup. The mixture was filtered and the filter

1 cake was washed with pentane (20 mL × 2). The filtrate was concentrated to give the
2 crude imidate that was used for the next step without further purification. The imidate
3 was added to 2-phenylacetic acid (1.2 g, 8.8 mmol) in dry CH₂Cl₂ under Ar at room
4 temperature. The mixture was stirred for 12 h and filtered to remove trichloroacetamide.
5 The filter cake was washed with CH₂Cl₂. The combined organic layer was concentrated.
6 The residue was purified by flash chromatography on silica to afford the product as an
7 oil.

9 2-phenylpropan-2-yl 2-(4-chlorophenyl)acetate (**e1**)

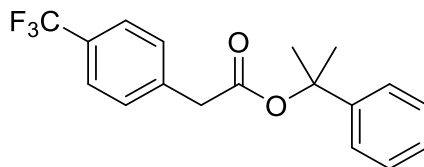


10

11 Prepared according to the General Procedure A using (4-chlorophenyl)acetic acid (341.2
12 mg, 2.0 mmol) and isolated as colorless oil (381.2 mg, 66% yield); TLC R_f = 0.42 (n-
13 hexane/EtOAc, 6/1); ¹H NMR (400 MHz, CDCl₃) δ 7.29-7.19 (m, 9H), 3.55 (s, 2H), 1.74
14 (s, 6H); ¹³C NMR (100 MHz, CDCl₃) δ 169.7, 145.6, 133.0, 132.9, 130.8 (2C), 128.7
15 (2C), 128.3 (2C), 127.2, 124.3 (2C), 82.4, 42.0, 28.6 (2C); IR (ATR) ν 3090, 3062, 3030,
16 2981, 2939, 2368, 2342, 2310, 1733, 1601 cm⁻¹; HRMS (ESI-TOF) [M + Na]⁺ calcd for
17 C₁₇H₁₇ClO₂⁺ m/z 311.0809, found 311.0827.

1

2 2-phenylpropan-2-yl 2-(4-(trifluoromethyl)phenyl)acetate (**e2**)



3

4 Prepared according to the General Procedure A using 4-(trifluoromethyl)benzeneacetic

5 acid (510.4 mg, 2.5 mmol) and isolated as colorless oil (475.4 mg, 59% yield); TLC Rf =

6 0.36 (n-hexane/EtOAc, 8/1); ¹H NMR (400 MHz, CDCl₃) δ 7.58 (d, *J* = 7.8 Hz, 2H), 7.38

7 (d, *J* = 8.2 Hz, 2H), 7.22-7.29 (m, 5H), 3.65 (s, 2H), 1.76 (s, 6H); ¹³C NMR (100 MHz,

8 CDCl₃) δ 169.2, 145.3, 138.2, 129.7 (2C), 129.3 (d, *J* = 31.6 Hz), 128.3 (2C), 127.1, 126.3

9 (d, *J* = 166.8 Hz), 125.5 (q, *J* = 3.8 Hz, 2C), 124.2 (2C), 82.5, 42.3, 28.5 (2C); ¹⁹F NMR

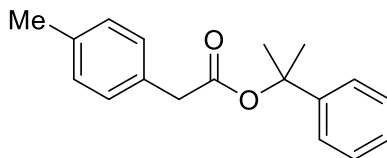
10 (376 MHz, CDCl₃) δ -62.4; IR (ATR) ν 3548, 2983, 2936, 2364, 2351, 2325, 1733, 1619,

11 1585, 1496 cm⁻¹; HRMS (ESI-TOF) [M + Na]⁺ calcd for C₁₈H₁₇F₃NaO₂⁺ m/z 345.1073,

12 found 345.1079.

13

14 2-phenylpropan-2-yl 2-(*p*-tolyl)acetate (**e3**)



15

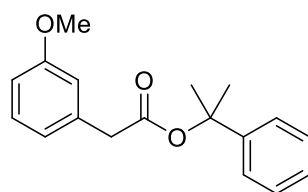
16 Prepared according to the General Procedure A using *p*-tolylacetic acid (300.4 mg, 2.0

17 mmol) and isolated as colorless oil (322.0 mg, 60% yield); TLC Rf = 0.50 (n-

1 hexane/EtOAc, 8/1); ^1H NMR (400 MHz, CDCl_3) δ 7.11-7.28 (m, 9H), 3.54 (s, 2H), 2.33
2 (s, 3H), 1.74 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.4, 145.9, 136.6, 131.4, 129.3
3 (4C), 128.3 (2C), 127.0, 124.3 (2C), 82.0, 42.3, 28.7 (2C), 21.2 ; IR (ATR) ν 3090, 3055,
4 3027, 2979, 2924, 2868, 2368, 2330, 1732, 1604 cm^{-1} ; HRMS (ESI-TOF) $[\text{M} + \text{H}]^+$ calcd
5 for $\text{C}_{18}\text{H}_{21}\text{O}_2^+$ m/z 269.1536, found 269.1543.

6

7 2-phenylpropan-2-yl 2-(3-methoxyphenyl)acetate (**e4**)

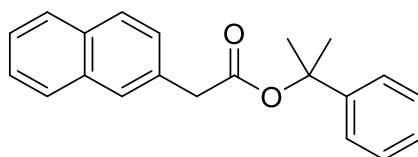


8

9 Prepared according to the General Procedure A using (3-methoxyphenyl)acetic acid
10 (332.3 mg, 2.0 mmol) and isolated as colorless oil (261.6 mg, 46% yield); TLC R_f = 0.27
11 (n-hexane/EtOAc, 8/1); ^1H NMR (400 MHz, CDCl_3) δ 7.29-7.19 (m, 6H), 6.86 (d, J =
12 7.8 Hz, 1H), 6.80-6.82 (m, 2H), 3.78 (s, 3H), 3.56 (s, 2H), 1.75 (s, 6H); ^{13}C NMR (100
13 MHz, CDCl_3) δ 170.0, 159.7, 145.7, 135.8, 129.6, 128.3 (2C) , 127.1, 124.3 (2C) , 121.8,
14 114.8, 112.8, 82.1, 55.3, 42.8, 28.6 (2C); IR (ATR) ν 3060, 2980, 2938, 2835, 2363, 2343,
15 1732, 1601, 1585, 1492 cm^{-1} ; HRMS (ESI-TOF) $[\text{M} + \text{Na}]^+$ calcd for $\text{C}_{18}\text{H}_{20}\text{NaO}_3^+$ m/z
16 307.1305, found 307.1321.

17

1 2-phenylpropan-2-yl 2-(naphthalen-2-yl)acetate (**e5**)

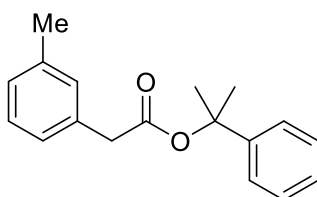


2

3 Prepared according to the General Procedure A using 2-naphthaleneacetic acid (744.8 mg,
4 4.0 mmol) and isolated as white solid (608.8 mg, 50% yield); m.p. 39-41 °C; TLC Rf =
5 0.50 (n-hexane/EtOAc, 8/1); ¹H NMR (400 MHz, CDCl₃) δ 7.77-7.83 (m, 3H), 7.71 (s,
6 1H), 7.40-7.47 (m, 3H), 7.18-7.23 (m, 5H), 3.75 (s, 2H), 1.75 (s, 6H); ¹³C NMR (100 MHz,
7 CDCl₃) δ 170.1, 145.7, 133.6, 132.5, 131.9, 128.3 (2C), 128.2, 128.1, 127.8 (2C), 127.6,
8 127.1, 126.2, 125.8, 124.3 (2C), 82.2, 42.9, 28.7 (2C); IR (ATR) ν 3840, 3056, 3023,
9 2979, 2932, 2367, 2355, 2308, 1731, 1634 cm⁻¹; HRMS (ESI-TOF) [M + Na]⁺ calcd for
10 C₂₁H₂₀NaO₂⁺ m/z 327.1356, found 327.1359.

11

12 2-phenylpropan-2-yl 2-(m-tolyl)acetate (**e6**)

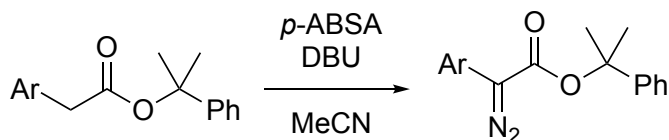


13

14 Prepared according to the General Procedure A using (3-methylphenyl)acetic acid (750.9
15 mg, 5.0 mmol) and isolated as colorless oil (872.2 mg, 65% yield) : TLC Rf = 0.56 (n-
16 hexane/EtOAc, 6/1); ¹H NMR (400 MHz, CDCl₃) δ 7.18-7.28 (m, 6H), 7.07 (d, *J* = 6.9

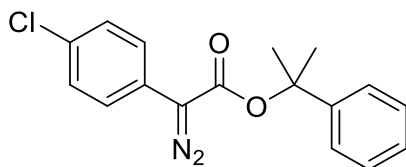
1 Hz, 3H), 3.55 (s, 2H), 2.33 (s, 3H), 1.75 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.1,
2 145.7, 138.0, 134.1, 130.0, 128.3, 128.1 (2C), 127.6, 126.9, 126.3, 124.2 (2C), 81.9, 42.7,
3 28.5 (2C), 21.3; IR (ATR) ν 3841, 3648, 3566, 3062, 3017, 2983, 2941, 2868, 2367, 2352
4 cm^{-1} ; HRMS (ESI-TOF) $[\text{M} + \text{Na}]^+$ calcd for $\text{C}_{18}\text{H}_{20}\text{NaO}_2^+$ m/z 291.1356, found
5 291.1364.
6

1 **General Procedure B for the Synthesis of α -Diazoesters**



4 To a stirred suspension of 2-phenylpropan-2-yl 2-phenylacetate (5.0 mmol, 1 equiv.) and
5 4-acetamidobenzenesulfonyl azide (*p*-ABSA) (2.88 g, 6 mmol, 1.2 equiv.) in CH₃CN (15
6 mL) at 0 °C, DBU (1.05 mL, 7 mmol, 1.4 equiv.) was added under an Ar atmosphere.
7 After stirring for 12 h, the reaction mixture was quenched with saturated NH₄Cl solution
8 and extracted with Et₂O. The organic phase was dried over Na₂SO₄ and evaporated to
9 give the crude product. Purification by column chromatography gave the α -alkyl
10 diazoester as a yellow solid.

11 2-phenylpropan-2-yl 2-(4-chlorophenyl)-2-diazoacetate (**d1**)

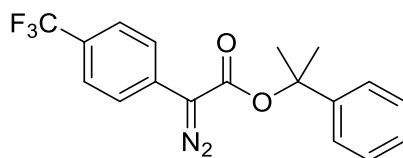


13 Prepared according to the General Procedure B using **e1** (346.5 mg, 1.2 mmol) and
14 isolated as yellow solid (313.5 mg, 83% yield); m.p. 35-37 °C; TLC R_f = 0.64 (n-
15 hexane/EtOAc, 10/1); ¹H NMR (400 MHz, CDCl₃) δ 7.41-7.25 (m, 9H), 1.86 (s, 6H); ¹³C
16 NMR (100 MHz, CDCl₃) δ 163.6, 145.5, 131.3, 129.1 (2C), 128.5 (2C), 127.3 (2C), 125.1

1 (2C), 124.5, 124.3 (2C), 83.4, 29.0 (2C); IR (ATR) ν 3869, 3065, 3019, 2985, 2945, 2366,
2 2307, 2085, 1699, 1495 cm^{-1} ; HRMS (ESI-TOF) $[\text{M} + \text{Na}]^+$ calcd for $\text{C}_{17}\text{H}_{15}\text{ClN}_2\text{NaO}_2^+$
3 m/z 337.0714, found 337.0707.

4

5 2-phenylpropan-2-yl 2-diazo-2-(4-(trifluoromethyl)phenyl)acetate (**d2**)



6

7 Prepared according to the General Procedure B using **e2** (419.0 mg, 1.3 mmol) and

8 isolated as yellow oil (343.2 mg, 76% yield); TLC R_f = 0.50 (n-hexane/EtOAc, 10/1); ^1H

9 NMR (400 MHz, CDCl_3) δ 7.54 (s, 4H), 7.39-7.42 (m, 2H), 7.33-7.37 (m, 2H), 7.24-7.28

10 (m, 1H), 1.87 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 163.1, 145.4, 130.5, 128.6 (3C),

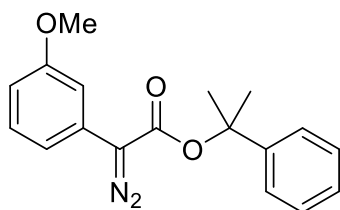
11 127.5, 125.8 (2C), 124.3 (3C), 123.5 (3C), 83.7, 29.0 (2C); ^{19}F NMR (376 MHz, CDCl_3)

12 δ -62.3; IR (ATR) ν 3594, 3063, 2983, 2938, 2363, 2326, 2085, 1703, 1614, 1575 cm^{-1} ;

13 HRMS (ESI-TOF) $[\text{M} + \text{Na}]^+$ calcd for $\text{C}_{18}\text{H}_{15}\text{F}_3\text{N}_2\text{NaO}_2^+$ m/z 371.0978, found 371.0978.

14

15 2-phenylpropan-2-yl 2-diazo-2-(3-methoxyphenyl)acetate (**d4**)



1

2 Prepared according to the General Procedure B using **e4** (233.2 mg, 0.82 mmol) and

3 isolated as yellow oil (182.9 mg, 72% yield); TLC Rf = 0.48 (n-hexane/EtOAc, 6/1); ¹H

4 NMR (400 MHz, CDCl₃) δ 7.39-7.42 (m, 2H), 7.33-7.37 (m, 2H), 7.23-7.28 (m, 2H), 7.11

5 (t, *J* = 4.6 Hz, 1H), 6.96 (dd, *J* = 8.2 Hz, 0.9 Hz, 1H), 6.69 (dd, *J* = 8.0 Hz, 1.8 Hz, 1H),

6 3.77 (s, 3H), 1.87 (s, 6H); ¹³C NMR (100 MHz, CDCl₃) δ 163.8, 160.1, 145.7, 129.9,

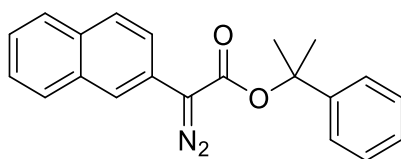
7 128.5 (3C), 127.3 (2C), 124.3 (2C), 116.1, 114.5, 109.7, 83.2, 55.4, 29.1 (2C); IR (ATR)

8 ν 3793, 3061, 2980, 2937, 2836, 2356, 2339, 2316, 2077, 1699 cm⁻¹; HRMS (ESI-TOF)

9 [M + H]⁺ calcd for C₁₈H₁₉N₂O₃⁺ m/z 311.1390, found 311.1405.

10

11 2-phenylpropan-2-yl 2-diazo-2-(naphthalen-2-yl)acetate (**d5**)



12

13 Prepared according to the General Procedure B using **e5** (456.6 mg, 1.5 mmol) and

14 isolated as yellow solid (525.9 mg, 90% yield); m.p. 55-57 °C; TLC Rf = 0.48 (n-

15 hexane/EtOAc, 6/1); ¹H NMR (400 MHz, CDCl₃) δ 8.09 (d, *J* = 1.8 Hz, 2H), 7.73-7.82

16 (m, 3H), 7.35-7.49 (m, 7H), 7.25-7.30 (m, 1H), 1.90 (s, 6H); ¹³C NMR (100 MHz, CDCl₃)

1 δ 164.2, 145.7, 133.7, 131.4, 128.6 (4C), 127.7 (2C), 127.3, 126.6, 125.7, 124.3 (2C) ,
2 123.0, 122.6, 121.9, 83.3, 29.1 (2C); IR (ATR) ν 3741, 3567, 3094, 3058, 3027, 2981,
3 2938, 2336, 2077, 1770 cm^{-1} ; HRMS (ESI-TOF) $[\text{M} + \text{Na}]^+$ calcd for $\text{C}_{21}\text{H}_{18}\text{N}_2\text{NaO}_2^+$
4 m/z 353.1260, found 353.1254.
5

B. Intensity Measurements

1		
2		
3		
4		
5	Diffractionmeter	R-AXIS RAPID
6		
7	Radiation	CuKa ($\lambda = 1.54187 \text{ \AA}$)
8		multi-layer mirror
9	monochromated	
10		
11	Voltage, Current	40kV, 30mA
12		
13	Temperature	-180.0°C
14		
15	Detector Aperture	460.0 x 256.0 mm
16		
17	Data Images	45 exposures
18		
19	w oscillation Range (c=54.0, f=0.0)	80.0 - 260.0°
20		
21	Exposure Rate	2.0 sec./°
22		
23	w oscillation Range (c=54.0, f=90.0)	80.0 - 260.0°
24		
25	Exposure Rate	2.0 sec./°
26		
27	w oscillation Range (c=54.0, f=180.0)	80.0 - 260.0°
28		
29	Exposure Rate	2.0 sec./°
30		
31	w oscillation Range (c=54.0, f=270.0)	80.0 - 260.0°
32		
33	Exposure Rate	2.0 sec./°
34		
35	w oscillation Range (c=0.0, f=0.0)	80.0 - 260.0°
36		

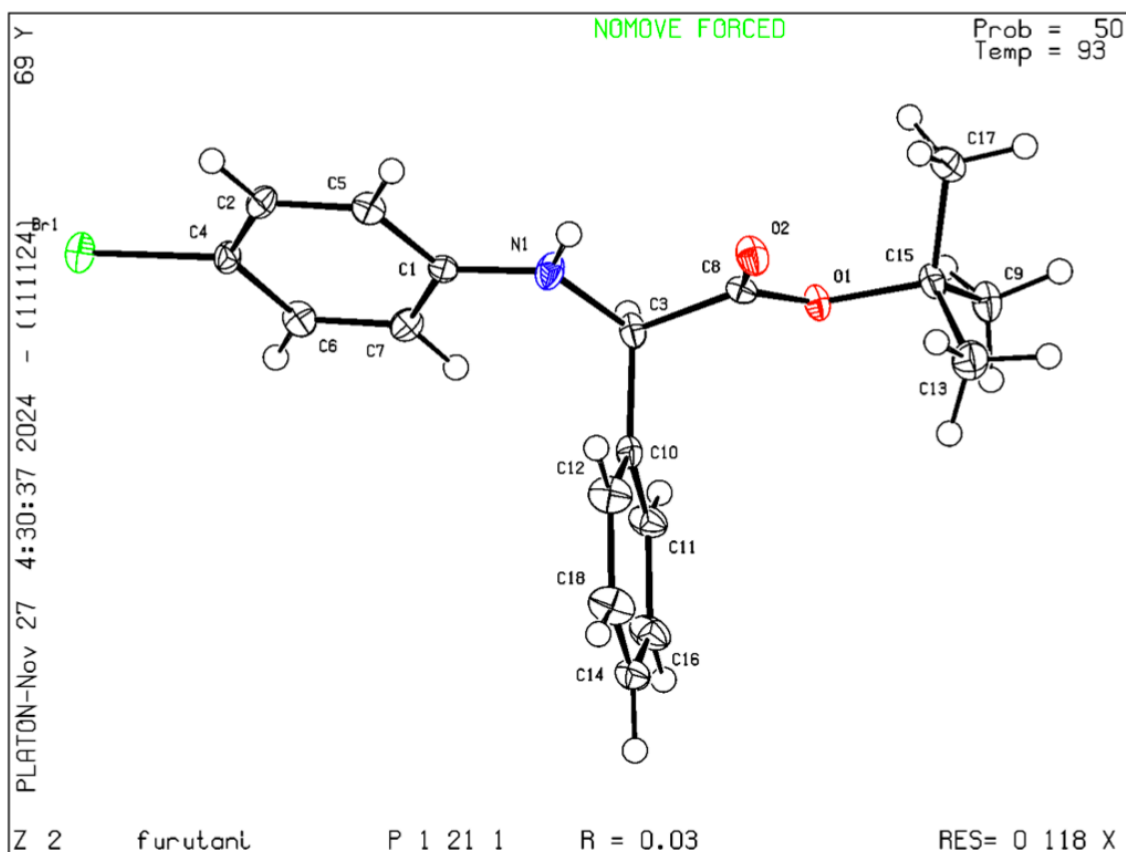
1	Exposure Rate	2.0 sec./ ^o
2		
3	Detector Position	127.40 mm
4		
5	Pixel Size	0.100 mm
6		
7	2 θ max	136.5 ^o
8		
9	No. of Reflections Measured	Total: 9173
10		Unique: 2892 (R _{int} = 0.0745)
11		Friedel pairs: 1305
12		
13	Corrections	Lorentz-polarization
14		Absorption
15		(trans. factors: 0.380 - 0.501)
16		
17		
18		
19		

C. Structure Solution and Refinement

1		
2		
3		
4		
5	Structure Solution	Direct Methods
6		
7	Refinement	Full-matrix least-squares on F^2
8		
9	Function Minimized	$\sum w (F_o^2 - F_c^2)^2$
10		
11	Least Squares Weights	$w = 1 / [s^2(F_o^2) + (0.0155 \cdot P)^2$
12		$+ 0.0000 \cdot P]$
13		where $P = (\text{Max}(F_o^2, 0) +$
14	$2F_c^2)/3$	
15		
16	$2\theta_{\text{max}}$ cutoff	136.5°
17		
18	Anomalous Dispersion	All non-hydrogen atoms
19		
20	No. Observations (All reflections)	2892
21		
22	No. Variables	199
23		
24	Reflection/Parameter Ratio	14.53
25		
26	Residuals: R_1 ($I > 2.00s(I)$)	0.0307
27		
28	Residuals: R (All reflections)	0.0316
29		
30	Residuals: wR_2 (All reflections)	0.0749
31		
32	Goodness of Fit Indicator	1.065
33		
34	Flack Parameter (Friedel pairs = 1305)	0.001(18)
35		

1	Max Shift/Error in Final Cycle	0.000
2		
3	Maximum peak in Final Diff. Map	0.58 e ⁻ /Å ³
4		
5	Minimum peak in Final Diff. Map	-0.33 e ⁻ /Å ³

The ellipsoid contour probability level in the ORTEP is 50%.



ORTEP of **3x**

1 **8. Computational Details**

2 Computational optimizations of the molecular structures were carried out using the hybrid
3 density functional method based on Becke's three-parameter exchange functional and the
4 Lee-Yang-Parr nonlocal correlation functional ((R/U)B3LYP),⁴ with the def2-SVPP basis
5 set for H, C, N, O, Cl, and Ru.⁵ Vibrational frequencies were computed at the same level
6 to verify whether each optimized structure corresponds to an energy minimum on the
7 potential energy surfaces (no imaginary frequency) or a transition state (one imaginary
8 frequency) and to evaluate its zero-point vibrational energy (ZPVE) and thermal
9 corrections. The intrinsic reaction coordinate (IRC) method was used to track minimum-
10 energy paths from transition structures to the corresponding local minima.⁶ Single-point
11 energies were calculated at the (R/U)M08-HX level⁷ using the SDD basis set for Ru, and
12 the 6-311++G** basis set for H, C, N, O, and Cl in dichloromethane or toluene solvent.
13 Non-covalent interactions were visualized using Visual Molecular Dynamics (VMD)
14 software (ver. 1.9.4a57). The source files were created from the corresponding XYZ files
15 using NCIPLLOT (ver. 4.0).⁸ Cylinder representations of transition structures were
16 generated using CYLview Visualization software. Topographic steric maps were
17 calculated by the SambVca 2.1 web tool.⁹ Visualization of molecular orbitals was
18 performed with Avogadro software.¹⁰

1 Supplementary Table 6.

	E((R/U)b3lyp/def2-SVPP) (A.U.)	E((R/U)M08-HX/SDD/6- 311++G**) (A.U.)
CP1	-2498.984114	-2500.30722
TS1	-2498.98365	-2500.30658
CP2 _{Assoc}	-2499.014359	-2500.34976
INT1 _{Diss}	-1094.618876	-1095.48252
[Ru(<i>p</i> -cymene)Cl ₂] ₂	-1404.339237	-1404.803828
CP3	-3134.099884	-3135.95547
TS2	-3134.079488	-3135.95267
CP4	-3134.110854	-3135.98109
CP5	-3134.105342	-3135.96982
TS3	-3134.091706	-3135.94383
CP6	-2499.029364	-2500.35724
6	-635.078184	-635.601471
TS3 _{major}	-3364.97084	-3366.9997
TS3 _{minor}	-3364.97009	-3366.9959
TS_Ru-N _{ylide}	-2613.410768	-2614.83543
Ru-N _{ylide}	-2613.44216	-2614.87919
TS_Ru-O _{ylide}	-2613.404357	-2614.82552
Ru-O _{ylide}	-2613.421173	-2614.84696
S ₀ -2a	-917.363393	-917.34009
*S _n -2a	-917.270839	-917.244803
S _I -2a	-917.301681	-917.294528
T _n -2a	-917.313158	-917.282113
T _I -2a	-917.316704	-917.286037
³ TS4	-917.300404	-917.267942

³ carbene	-807.799899	-807.781315
¹ TS4	-917.30666	-917.282846
¹ carbene	-807.792836	-807.781449
MECP	-807.788979	-807.775631
TS5	-1095.404254	-1095.398537
IN1	-1095.46456	-1095.475713
TS6	-1095.462335	-1095.471084
IN2	-1095.480069	-1095.492823
TS7 _{major_298K}	-1962.105501	-1962.14932
TS7 _{minor_298K}	-1962.104265	-1962.14314
TS11 _{298K}	-2245.921218	-2245.96175
TS10 _{298K}	-1958.30968	-1958.34208
TS9 _{298K}	-1670.688771	-1670.71643
TS8 _{298K}	-1383.066556	-1383.0892
TS7 _{major_195K}	-1962.105501	-1962.14932
TS7 _{minor_195K}	-1962.104265	-1962.14314
TS11 _{195K}	-2245.921218	-2245.96175
TS10 _{195K}	-1958.30968	-1958.34208
TS9 _{195K}	-1670.688771	-1670.71643
TS8 _{195K}	-1383.066556	-1383.0892
aniline ₄	-1150.44373	-1150.46647
7	-866.630444	-866.655726

1	CP1			
2	Zero-point correction=			0.621002 (Hartree/Particle)
3	Thermal correction to Energy=			0.661918
4	Thermal correction to Enthalpy=			0.662862
5	Thermal correction to Gibbs Free Energy=			0.543704
6	Sum of electronic and zero-point Energies=			-2498.363112
7	Sum of electronic and thermal Energies=			-2498.322196
8	Sum of electronic and thermal Enthalpies=			-2498.321252
9	Sum of electronic and thermal Free Energies=			-2498.440410
10	Cartesian Coordinates			
11	Atom	X	Y	Z
12	-----			
13	C	4.07167300	-1.20917300	-1.50536600
14	C	4.07098600	0.05651400	-0.82989500
15	C	3.73830200	0.17731400	0.53454800
16	C	3.18239400	-0.99986900	1.14924600
17	C	3.07996700	-2.22759000	0.45980600
18	C	3.60428500	-2.36602700	-0.87730700
19	H	4.36780000	-1.24404200	-2.55625600
20	H	4.38949200	0.93522500	-1.39159100
21	H	2.79703700	-0.94780000	2.16982800
22	H	2.62811900	-3.08630400	0.95936300
23	Ru	1.84390600	-0.67273400	-0.64061800
24	Cl	0.29212900	-2.33624100	-1.43194400
25	Cl	1.25690100	0.66503600	-2.55373900
26	C	0.50638200	-0.01596100	0.58482200
27	C	0.31686100	1.34196200	1.07637900
28	C	-0.27524000	1.58511900	2.34726400
29	C	0.69095000	2.46321900	0.29320500
30	C	-0.45696400	2.88194800	2.81564500
31	H	-0.56840500	0.74551100	2.98184800
32	C	0.47813000	3.75932400	0.75748200
33	H	1.10327900	2.28984600	-0.70292500
34	C	-0.08463900	3.97478100	2.02003200
35	H	-0.90100700	3.04676300	3.80196000
36	H	0.74144600	4.61006500	0.12290400

1	H	-0.24650700	4.99485900	2.38184500
2	C	-0.25635600	-1.07464500	1.35146700
3	O	0.28825600	-1.70841700	2.23363400
4	O	-1.53375100	-1.15900700	0.99718300
5	C	-2.47517500	-2.15891900	1.57432400
6	C	3.96826100	1.43324900	1.36158600
7	H	3.03233500	1.63165100	1.91342100
8	C	5.07389500	1.16722700	2.40606900
9	H	6.04113200	0.95657700	1.91411500
10	H	5.20704800	2.05136900	3.05466700
11	H	4.83013400	0.30820600	3.05567900
12	C	4.29873300	2.67838400	0.53055500
13	H	3.53372900	2.87420700	-0.23855200
14	H	4.34858900	3.56430800	1.18688800
15	H	5.27945300	2.58414500	0.02925900
16	C	3.52553100	-3.68995900	-1.57908400
17	H	4.01634500	-4.47819500	-0.98000600
18	H	2.46310300	-3.96794100	-1.71105900
19	H	4.00135600	-3.64944300	-2.57208900
20	C	-3.33910700	4.79462800	-1.05090900
21	C	-2.35942500	4.49174400	-2.00519400
22	C	-1.88405000	3.18980900	-2.15939500
23	C	-2.38831600	2.13603500	-1.35851600
24	C	-3.37937900	2.45123300	-0.39797500
25	C	-3.84135400	3.75835700	-0.25247500
26	H	-3.70984200	5.81758600	-0.93603800
27	H	-1.95506100	5.28515500	-2.64371000
28	H	-1.11443500	2.96541600	-2.90402700
29	H	-3.78715300	1.64970800	0.22653800
30	H	-4.61155400	3.97109800	0.49727200
31	N	-1.95036300	0.84643600	-1.53051700
32	H	-1.09066300	0.68096100	-2.05499900
33	H	-2.15617000	0.16009700	-0.81157700
34	C	-1.89076100	-3.57777800	1.47253700
35	H	-1.53243500	-3.77751400	0.45055300
36	H	-1.05111700	-3.71532500	2.16967400

1	H	-2.68606300	-4.30365300	1.71520500
2	C	-2.73006300	-1.76635400	3.03221600
3	H	-3.15640500	-0.75177200	3.10382800
4	H	-3.43096000	-2.47482100	3.50415400
5	H	-1.78553300	-1.80109100	3.59607000
6	C	-3.71189100	-2.04472900	0.67632700
7	C	-3.56055000	-2.15055000	-0.71859100
8	C	-5.00523100	-1.88356800	1.19620900
9	C	-4.66985900	-2.09067600	-1.56453000
10	H	-2.56198100	-2.26445500	-1.14987000
11	C	-6.11823600	-1.83223900	0.34823400
12	H	-5.16553100	-1.79664900	2.27278400
13	C	-5.95509000	-1.93391200	-1.03476500
14	H	-4.52477100	-2.16027400	-2.64682600
15	H	-7.11741100	-1.70556200	0.77705200
16	H	-6.82423300	-1.88620000	-1.69824300

17

18

TS1

19	Zero-point correction=		0.621104 (Hartree/Particle)
20	Thermal correction to Energy=		0.660905
21	Thermal correction to Enthalpy=		0.661849
22	Thermal correction to Gibbs Free Energy=		0.547310
23	Sum of electronic and zero-point Energies=		-2498.362546
24	Sum of electronic and thermal Energies=		-2498.322745
25	Sum of electronic and thermal Enthalpies=		-2498.321801
26	Sum of electronic and thermal Free Energies=		-2498.436340

27

Cartesian Coordinates

28	Atom	X	Y	Z
29	-----			
30	C	3.90984100	-1.62046800	-1.40258800
31	C	4.04632700	-0.32460900	-0.80343000
32	C	3.70733400	-0.07861300	0.54518500
33	C	2.99940300	-1.13751500	1.21300400
34	C	2.76468000	-2.38780000	0.59582200
35	C	3.29196000	-2.67073500	-0.71623100
36	H	4.21767700	-1.75660400	-2.44166000

1	H	4.47365900	0.47477300	-1.40951300
2	H	2.60028400	-0.97496800	2.21611800
3	H	2.20358000	-3.15372600	1.13403100
4	Ru	1.77810400	-0.77042800	-0.63249900
5	Cl	0.05876000	-2.27057700	-1.44114800
6	Cl	1.42572300	0.57857900	-2.61401200
7	C	0.43680600	0.10497400	0.50208900
8	C	0.42224000	1.48692500	0.96683500
9	C	-0.19978000	1.84920500	2.19273900
10	C	1.01674100	2.52068900	0.19969400
11	C	-0.19491900	3.16767300	2.63937000
12	H	-0.66753700	1.08368800	2.81567200
13	C	1.00038600	3.84090900	0.64330300
14	H	1.45524800	2.26264100	-0.76647000
15	C	0.40552000	4.17011800	1.86674200
16	H	-0.66810000	3.41896300	3.59346000
17	H	1.44811200	4.62409000	0.02428600
18	H	0.39842200	5.20805400	2.21387200
19	C	-0.39588500	-0.85034100	1.33640500
20	O	0.11488100	-1.42117500	2.28077800
21	O	-1.67278700	-0.94591500	0.97982300
22	C	-2.63026500	-1.88038200	1.62797800
23	C	4.08391600	1.18668900	1.30175800
24	H	3.17178800	1.54299500	1.81190500
25	C	5.12114300	0.84457200	2.39312800
26	H	6.06103500	0.47375500	1.94454300
27	H	5.35966400	1.74368400	2.98898300
28	H	4.74892600	0.07086400	3.08738000
29	C	4.59886100	2.32071800	0.40763700
30	H	3.88762700	2.56598400	-0.39795300
31	H	4.75122800	3.23305700	1.00994000
32	H	5.57001800	2.06439000	-0.05416700
33	C	3.06978100	-4.01806700	-1.33886500
34	H	3.46486300	-4.81738300	-0.68590000
35	H	1.98454500	-4.18321700	-1.47165900
36	H	3.55569500	-4.09192800	-2.32506700

1	C	-3.17982700	4.70930700	-1.18667900
2	C	-2.08083700	4.43114100	-2.00913500
3	C	-1.53692700	3.14906400	-2.07013000
4	C	-2.09444000	2.09506400	-1.30553700
5	C	-3.20620800	2.38384900	-0.47708400
6	C	-3.73477200	3.67186800	-0.42502300
7	H	-3.60251900	5.71752200	-1.14432600
8	H	-1.63784800	5.22773700	-2.61668800
9	H	-0.67887400	2.93687500	-2.71396400
10	H	-3.65187800	1.57847000	0.11479200
11	H	-4.59877400	3.86897100	0.21880700
12	N	-1.55545700	0.83758000	-1.34949900
13	H	-0.80807900	0.61586600	-2.00810800
14	H	-2.02046300	0.06455400	-0.88816400
15	C	-2.07470700	-3.31469200	1.62502500
16	H	-1.71185800	-3.58671300	0.62119700
17	H	-1.24352900	-3.42106600	2.33759100
18	H	-2.88481100	-4.00898000	1.90788000
19	C	-2.88139600	-1.38400700	3.05456000
20	H	-3.28219100	-0.35650900	3.05509300
21	H	-3.60182500	-2.04149300	3.56917200
22	H	-1.94005100	-1.40217500	3.62378900
23	C	-3.86453800	-1.80268800	0.72039100
24	C	-3.71688400	-2.02719400	-0.66154400
25	C	-5.15181300	-1.55485100	1.21994900
26	C	-4.82311000	-1.99832800	-1.51347300
27	H	-2.72326700	-2.21817100	-1.07779200
28	C	-6.26199300	-1.53291900	0.36648500
29	H	-5.30991100	-1.37553800	2.28526200
30	C	-6.10249000	-1.75247900	-1.00292000
31	H	-4.68156800	-2.16738500	-2.58544800
32	H	-7.25625300	-1.33715500	0.78047100
33	H	-6.96928000	-1.72988900	-1.67076000

34

35

CP2_{Assoc}

36 Zero-point correction=

0.625491 (Hartree/Particle)

1	Thermal correction to Energy=	0.664336
2	Thermal correction to Enthalpy=	0.665280
3	Thermal correction to Gibbs Free Energy=	0.553726
4	Sum of electronic and zero-point Energies=	-2498.388868
5	Sum of electronic and thermal Energies=	-2498.350023
6	Sum of electronic and thermal Enthalpies=	-2498.349079
7	Sum of electronic and thermal Free Energies=	-2498.460633

8 Cartesian Coordinates				
9 Atom	X	Y	Z	
10	-----			
11	C	3.05618200	-2.71452000	-1.00005600
12	C	3.74398000	-1.47987200	-0.88346200
13	C	3.64941500	-0.65306700	0.28062100
14	C	2.74004500	-1.08932000	1.28955000
15	C	2.03263300	-2.32369300	1.19380300
16	C	2.17955900	-3.14752700	0.04142200
17	H	3.12739700	-3.28934300	-1.92552600
18	H	4.32150600	-1.12993400	-1.74025800
19	H	2.55108200	-0.44727100	2.15242500
20	H	1.32176800	-2.59273300	1.97612200
21	Ru	1.58709900	-1.04932700	-0.57600000
22	Cl	-0.45542500	-2.04056400	-1.53232700
23	Cl	1.69683200	0.32715400	-2.63598400
24	C	0.17879200	0.55818700	0.26983200
25	C	0.95181900	1.76080900	0.77220500
26	C	1.20310100	1.98939900	2.14290700
27	C	1.44574500	2.72169400	-0.13717500
28	C	1.90623800	3.11890900	2.57546900
29	H	0.84015000	1.27536800	2.88151400
30	C	2.14275400	3.85037600	0.29855800
31	H	1.31593700	2.58055100	-1.21079000
32	C	2.37988600	4.06164200	1.66010300
33	H	2.07662500	3.26050400	3.64791000
34	H	2.50656100	4.56948200	-0.44237400
35	H	2.92521600	4.94704600	2.00114600
36	C	-0.64688500	-0.16814900	1.30275200

1	O	-0.21263900	-0.54829900	2.37419600
2	O	-1.92251500	-0.34158300	0.90944800
3	C	-2.92178300	-1.10574900	1.68393300
4	C	4.46680100	0.61518500	0.47785400
5	H	3.79889200	1.34844100	0.96121300
6	C	5.63089500	0.33313100	1.45085300
7	H	6.33134200	-0.41098900	1.02808900
8	H	6.19942300	1.25977000	1.64877500
9	H	5.26946600	-0.05546100	2.41965500
10	C	4.97941700	1.24148400	-0.82555100
11	H	4.16131000	1.38872200	-1.55001600
12	H	5.43557700	2.22414800	-0.61218200
13	H	5.75881000	0.61718300	-1.30125800
14	C	1.41943100	-4.43850200	-0.08713500
15	H	2.06058500	-5.27590200	0.24984800
16	H	0.50837500	-4.42930300	0.53124600
17	H	1.12207800	-4.62411900	-1.13089600
18	C	-3.39002700	4.17751000	-1.24683100
19	C	-2.89880100	3.53277400	-2.38616200
20	C	-2.00019900	2.47087800	-2.25597800
21	C	-1.60215600	2.05155100	-0.98257600
22	C	-2.08265300	2.69018800	0.16016900
23	C	-2.97771900	3.75558900	0.02064100
24	H	-4.09129800	5.01131800	-1.34667300
25	H	-3.21094400	3.85714400	-3.38325100
26	H	-1.60623700	1.96621400	-3.14384300
27	H	-1.76144500	2.37378200	1.15175700
28	H	-3.35330200	4.25951600	0.91613100
29	N	-0.67188200	0.91054100	-0.93286000
30	H	0.01400000	0.98026600	-1.73132700
31	H	-1.16418400	0.01721000	-1.15896800
32	C	-2.43234200	-2.54960100	1.89025400
33	H	-2.11080700	-2.98458700	0.92996700
34	H	-1.58804500	-2.58088300	2.59575100
35	H	-3.25990200	-3.15870000	2.29312300
36	C	-3.15434800	-0.40218400	3.02559800

1	H	-3.52029700	0.62772600	2.87645100
2	H	-3.90044500	-0.95342000	3.62177100
3	H	-2.21590000	-0.36954800	3.59645200
4	C	-4.16186400	-1.10355100	0.77726000
5	C	-4.03660500	-1.50606100	-0.56504000
6	C	-5.43642600	-0.75299100	1.24718900
7	C	-5.14969200	-1.55164800	-1.40715400
8	H	-3.05489000	-1.78540700	-0.95710800
9	C	-6.55406800	-0.80348700	0.40492600
10	H	-5.57966100	-0.43387100	2.28125000
11	C	-6.41607900	-1.20110600	-0.92602900
12	H	-5.02443000	-1.86562300	-2.44837300
13	H	-7.53742200	-0.52506000	0.79738900
14	H	-7.28902700	-1.23828500	-1.58546600

15

16

INT1_{Dis}

17	Zero-point correction=		0.406189 (Hartree/Particle)	
18	Thermal correction to Energy=		0.429031	
19	Thermal correction to Enthalpy=		0.429975	
20	Thermal correction to Gibbs Free Energy=		0.351071	
21	Sum of electronic and zero-point Energies=		-1094.212687	
22	Sum of electronic and thermal Energies=		-1094.189845	
23	Sum of electronic and thermal Enthalpies=		-1094.188901	
24	Sum of electronic and thermal Free Energies=		-1094.267805	

25

Cartesian Coordinates

26	Atom	X	Y	Z
27	-----			
28	C	1.30609900	-0.67327900	-0.18134500
29	C	2.72544200	-0.93301100	-0.31473200
30	C	3.30809700	-2.14029000	0.15895500
31	C	3.59917700	-0.00576500	-0.93939900
32	C	4.66784000	-2.39227300	0.00099500
33	H	2.66290400	-2.87174100	0.64605900
34	C	4.96351800	-0.27192200	-1.09346900
35	H	3.22726900	0.95634300	-1.30656300
36	C	5.51411900	-1.46606300	-0.62651200

1	H	5.07807600	-3.33582400	0.37740500
2	H	5.59962300	0.47410500	-1.58225000
3	H	6.58224500	-1.67285700	-0.74334700
4	C	0.29642700	-1.56130600	0.27909800
5	O	0.42337300	-2.64712400	0.82381300
6	O	-0.98353300	-1.01248200	0.00730900
7	C	-2.21966300	-1.55240500	0.55264600
8	C	1.39188200	4.32543800	1.17025500
9	C	1.14008000	4.27981200	-0.20499100
10	C	0.95723700	3.04827000	-0.84102000
11	C	1.03107200	1.87623900	-0.08827500
12	C	1.28413300	1.90209700	1.27968700
13	C	1.46355700	3.13874000	1.90755900
14	H	1.53766100	5.28897700	1.66741000
15	H	1.08744800	5.20383800	-0.78818500
16	H	0.76043000	3.00708300	-1.91815100
17	H	1.35260700	0.95997700	1.82864600
18	H	1.66814600	3.17191200	2.98171800
19	N	0.77963000	0.57428100	-0.77067000
20	H	1.06728000	0.67815000	-1.75923400
21	H	-0.25086800	0.39218000	-0.75788900
22	C	-2.45165900	-2.99026500	0.04873800
23	H	-2.42141100	-3.02317500	-1.05372400
24	H	-1.67603300	-3.66332400	0.44152600
25	H	-3.44806200	-3.33972200	0.37187800
26	C	-2.15010000	-1.51637900	2.08463600
27	H	-2.02262600	-0.48272900	2.44981200
28	H	-3.06628600	-1.93671300	2.53237000
29	H	-1.29537800	-2.12196800	2.42051800
30	C	-3.30372800	-0.63039100	-0.02870500
31	C	-3.28600900	-0.32692600	-1.40300300
32	C	-4.34509000	-0.10037600	0.74679200
33	C	-4.26935900	0.47965400	-1.97968300
34	H	-2.48746700	-0.73344000	-2.03000200
35	C	-5.33562500	0.70565600	0.17152600
36	H	-4.39732000	-0.31022700	1.81696400

1	C	-5.30231200	1.00129000	-1.19253000
2	H	-4.23232000	0.69864900	-3.05189800
3	H	-6.13689900	1.10608700	0.80084200
4	H	-6.07594700	1.63202400	-1.64152100
5				
6		[Ru(<i>p</i>-cymene)Cl₂]₂		
7	Zero-point correction=		0.216339	(Hartree/Particle)
8	Thermal correction to Energy=		0.231500	
9	Thermal correction to Enthalpy=		0.232444	
10	Thermal correction to Gibbs Free Energy=		0.172509	
11	Sum of electronic and zero-point Energies=		-1404.122899	
12	Sum of electronic and thermal Energies=		-1404.107737	
13	Sum of electronic and thermal Enthalpies=		-1404.106793	
14	Sum of electronic and thermal Free Energies=		-1404.166729	
15		Cartesian Coordinates		
16	Atom	X	Y	Z
17	-----			
18	C	0.22893500	-1.26339900	1.55327300
19	C	-1.03417700	-0.71188000	1.23545300
20	C	-1.45643800	-0.61500200	-0.12557200
21	C	-0.63511500	-1.23797400	-1.13280600
22	C	0.58961300	-1.86332400	-0.80537100
23	C	1.08282500	-1.81549300	0.53411000
24	H	0.60362800	-1.18530500	2.57715700
25	H	-1.59849900	-0.20423600	2.01860600
26	H	-0.92159200	-1.14386800	-2.18372300
27	H	1.23775200	-2.22754300	-1.60547200
28	Ru	0.55774000	0.23085900	-0.02326600
29	Cl	1.97803800	1.12325500	-1.63576700
30	Cl	0.60036600	2.25833600	1.12651900
31	C	-2.74368100	0.07993300	-0.54210800
32	H	-2.55512300	0.49035000	-1.55052300
33	C	-3.87346900	-0.96432600	-0.66390300
34	H	-4.09843800	-1.42091700	0.31728600
35	H	-4.79693100	-0.48502100	-1.03437200
36	H	-3.60884800	-1.77699400	-1.36365100

1	C	-3.14985400	1.24896200	0.36576000
2	H	-2.31375800	1.95439100	0.51096900
3	H	-3.99449200	1.79624000	-0.08796900
4	H	-3.48624900	0.89997900	1.35929500
5	C	2.45019300	-2.33989000	0.88113000
6	H	2.38134500	-3.40227200	1.18506700
7	H	3.13402600	-2.27123100	0.01995100
8	H	2.89074000	-1.77407800	1.71851300

9

10

CP3

11	Zero-point correction=		0.905126 (Hartree/Particle)	
12	Thermal correction to Energy=		0.959008	
13	Thermal correction to Enthalpy=		0.959952	
14	Thermal correction to Gibbs Free Energy=		0.811020	
15	Sum of electronic and zero-point Energies=		-3133.194757	
16	Sum of electronic and thermal Energies=		-3133.140876	
17	Sum of electronic and thermal Enthalpies=		-3133.139932	
18	Sum of electronic and thermal Free Energies=		-3133.288864	

19

Cartesian Coordinates

20	Atom	X	Y	Z
21	-----			
22	C	-2.83254400	-0.05812300	-3.66495900
23	C	-3.91581500	-0.54139900	-2.89994200
24	C	-4.28672800	0.03658200	-1.64030800
25	C	-3.43870100	1.06224800	-1.13962300
26	C	-2.34483300	1.57391100	-1.90300100
27	C	-2.02402000	1.01471800	-3.16749800
28	H	-2.55988100	-0.55702600	-4.59694900
29	H	-4.45447600	-1.41773700	-3.26327600
30	H	-3.62503300	1.47786400	-0.14607900
31	H	-1.72565600	2.36453500	-1.48214900
32	Ru	-2.09599100	-0.62920900	-1.60407500
33	Cl	0.18154000	-1.21480900	-2.31167800
34	Cl	-2.50191400	-3.07170400	-1.42000900
35	C	-1.26499200	-0.72711000	0.52024100
36	C	-2.28478500	-0.75660500	1.65080000

1	C	-2.07654000	-0.05909900	2.85749400
2	C	-3.42790800	-1.57406400	1.57090500
3	C	-2.98665200	-0.13931500	3.91637100
4	H	-1.18199100	0.55099200	2.98935800
5	C	-4.33263400	-1.66844300	2.63272100
6	H	-3.59425600	-2.15951600	0.66477900
7	C	-4.12517800	-0.94168100	3.80871500
8	H	-2.79233000	0.42115600	4.83643800
9	H	-5.20943400	-2.31699200	2.53478800
10	H	-4.83661600	-1.00961700	4.63779200
11	C	-0.22813900	0.36713900	0.61680900
12	O	0.96784900	0.15462000	0.55140900
13	O	-0.76155900	1.59282400	0.75415500
14	C	0.04574400	2.81108600	0.94695000
15	C	-5.55305700	-0.35139700	-0.89134400
16	H	-5.30609000	-0.32867300	0.18360400
17	C	-6.63872000	0.71832600	-1.13786600
18	H	-6.91570400	0.76404400	-2.20739300
19	H	-7.55125000	0.47996000	-0.56169000
20	H	-6.29800900	1.72397800	-0.83402600
21	C	-6.08471700	-1.75217200	-1.22580100
22	H	-5.29789300	-2.52035400	-1.14235400
23	H	-6.90676400	-2.01521300	-0.53652500
24	H	-6.49733200	-1.79589000	-2.25085900
25	C	-0.86347300	1.52652900	-3.97505700
26	H	-1.23328300	2.22966200	-4.74605800
27	H	-0.13598600	2.05752500	-3.34134000
28	H	-0.33655600	0.69991500	-4.47623600
29	C	0.66429300	-4.01603100	4.12986600
30	C	-0.46313500	-4.42802600	3.41261100
31	C	-0.82214800	-3.76942500	2.23400400
32	C	-0.05015200	-2.69562000	1.77768000
33	C	1.08639100	-2.28085400	2.47964500
34	C	1.43484300	-2.94874100	3.65838300
35	H	0.94554400	-4.53123900	5.05347000
36	H	-1.06807100	-5.26780300	3.76736200

1	H	-1.69594100	-4.09147400	1.66152400
2	H	1.70413100	-1.45729500	2.12103700
3	H	2.32439800	-2.62458000	4.20663900
4	N	-0.45942500	-2.04895100	0.52513000
5	H	-1.05426000	-2.71178500	-0.02965200
6	H	0.34887200	-1.84552200	-0.09442300
7	H	3.04180100	0.05582400	1.11426400
8	C	7.47023400	-0.73153200	-0.85920000
9	C	6.50344800	-0.12040100	-0.05527000
10	C	6.64875400	1.22404000	0.33128800
11	C	7.76206900	1.96013800	-0.08475300
12	C	8.72778200	1.34681300	-0.89198700
13	C	8.58425600	0.00673000	-1.27649900
14	H	7.36754000	-1.78151400	-1.15293400
15	H	7.88246000	3.00532900	0.21930500
16	H	9.60409200	1.91531600	-1.22000000
17	H	9.35027900	-0.46625000	-1.89927300
18	C	5.48674400	1.66165500	1.19308400
19	H	5.78418600	2.30727400	2.03773900
20	H	4.73841500	2.22650400	0.60406500
21	C	5.22749100	-0.71646900	0.52211700
22	H	5.42233500	-1.70165100	0.97513400
23	C	4.87001200	0.31674900	1.65866500
24	H	5.39429500	0.00255700	2.57994700
25	O	3.50036900	0.35102300	1.93687100
26	C	3.94741600	-0.07553100	-1.58595300
27	C	3.74133500	-2.25441300	-0.80983300
28	C	4.37059000	-0.97072000	-2.78630500
29	H	4.54520300	0.84473400	-1.50693700
30	H	2.88585700	0.20836900	-1.69418600
31	C	4.33873000	-2.41702200	-2.22708000
32	H	4.10099400	-3.00184300	-0.08403900
33	H	2.64113200	-2.34298200	-0.86853300
34	H	3.67419300	-0.84164000	-3.63116800
35	H	5.38018300	-0.70713000	-3.14262800
36	H	3.73672800	-3.10088900	-2.84820600

1	H	5.35849000	-2.83703100	-2.16875700
2	N	4.07962300	-0.89733400	-0.37407600
3	C	0.98463100	3.02309500	-0.24862600
4	H	1.62575100	3.90267800	-0.07407800
5	H	1.63577200	2.14769900	-0.37374700
6	H	0.42185400	3.18867600	-1.18240300
7	C	0.85025900	2.70886800	2.25625800
8	H	1.63835500	1.94088000	2.19577500
9	H	1.32635800	3.68377600	2.45929600
10	H	0.18066100	2.48739000	3.10492400
11	C	-1.00716000	3.92278100	1.08175600
12	C	-2.20844900	3.67876200	1.77194000
13	C	-0.78392800	5.21685300	0.58502900
14	C	-3.15220500	4.69275100	1.95617700
15	H	-2.40907900	2.68033500	2.16644000
16	C	-1.72719100	6.23431600	0.77080500
17	H	0.13523500	5.45102300	0.04402500
18	C	-2.91663100	5.97756500	1.45589000
19	H	-4.07949500	4.47493400	2.49580500
20	H	-1.52655800	7.23386500	0.37216100
21	H	-3.65535500	6.77225800	1.59955800

22

23

TS2

24	Zero-point correction=	0.902839 (Hartree/Particle)
25	Thermal correction to Energy=	0.955389
26	Thermal correction to Enthalpy=	0.956333
27	Thermal correction to Gibbs Free Energy=	0.815210
28	Sum of electronic and zero-point Energies=	-3133.176649
29	Sum of electronic and thermal Energies=	-3133.124099
30	Sum of electronic and thermal Enthalpies=	-3133.123155
31	Sum of electronic and thermal Free Energies=	-3133.264278

32

Cartesian Coordinates

33	Atom	X	Y	Z
34	-----			
35	C	-3.10289300	-0.94420300	-3.04371900
36	C	-3.15598800	-2.21282800	-2.43953000

1	C	-3.47903000	-2.37264400	-1.04601100
2	C	-3.66364000	-1.19063000	-0.29004900
3	C	-3.61043200	0.10505700	-0.89408800
4	C	-3.34357600	0.24851200	-2.27590500
5	H	-2.80267500	-0.85718800	-4.09018500
6	H	-2.88977600	-3.08706200	-3.03435600
7	H	-3.84127500	-1.26590300	0.78485700
8	H	-3.74282600	0.99288000	-0.27632200
9	Ru	-1.67728800	-0.95768000	-1.31537400
10	Cl	-0.09008900	0.36986000	-2.59969800
11	Cl	-0.08598400	-2.85768300	-1.49710700
12	C	-0.48756400	-0.26942200	0.59385500
13	C	-1.24555600	-0.82571100	1.78898700
14	C	-1.78840000	-0.02643100	2.81220100
15	C	-1.36625500	-2.22418800	1.94360100
16	C	-2.44828700	-0.58742500	3.91360100
17	H	-1.68537800	1.05737200	2.76790900
18	C	-2.00420900	-2.78693100	3.04884300
19	H	-0.95558300	-2.87920300	1.17185400
20	C	-2.56324300	-1.97203500	4.04129100
21	H	-2.85832600	0.07243700	4.68544200
22	H	-2.06834000	-3.87681700	3.13358400
23	H	-3.06926800	-2.41290100	4.90574800
24	C	-0.34681100	1.22727400	0.54995500
25	O	0.73093400	1.80426600	0.50612800
26	O	-1.50431700	1.90858300	0.55807800
27	C	-1.55677900	3.38398800	0.53192300
28	C	-3.70035500	-3.73392500	-0.39826600
29	H	-3.24282100	-3.68490000	0.60425900
30	C	-5.21567800	-3.95860500	-0.20269000
31	H	-5.74082800	-3.98873400	-1.17543100
32	H	-5.39763300	-4.92100700	0.30933600
33	H	-5.67450300	-3.15863500	0.40464500
34	C	-3.07216600	-4.91591200	-1.14840700
35	H	-1.99700000	-4.75339400	-1.32691800
36	H	-3.19277100	-5.83920000	-0.55384500

1	H	-3.56823000	-5.09148600	-2.12121400
2	C	-3.29889300	1.59250500	-2.94784200
3	H	-4.11332800	1.66591800	-3.69311600
4	H	-3.42596700	2.40837500	-2.21953900
5	H	-2.33578400	1.72669400	-3.46928500
6	C	2.82045600	-2.51796300	3.96910200
7	C	2.66800900	-3.27200300	2.80171400
8	C	2.01639300	-2.72534100	1.69202000
9	C	1.52391300	-1.41285800	1.73793900
10	C	1.67527800	-0.65662900	2.90611000
11	C	2.31810500	-1.21280000	4.01485300
12	H	3.32480100	-2.94576100	4.84093700
13	H	3.04724000	-4.29769500	2.75371900
14	H	1.87132300	-3.32179100	0.78634100
15	H	1.31516000	0.37010100	2.94576500
16	H	2.43206600	-0.61212000	4.92247700
17	N	0.92839600	-0.85212400	0.53465400
18	H	0.85190600	-1.62686800	-0.14961900
19	H	1.90047100	-0.13985800	-0.00031900
20	H	2.35449400	1.82970200	1.18430400
21	C	6.36099500	-0.83179200	-0.85808100
22	C	5.63713400	0.17813000	-0.21390500
23	C	6.24601400	1.41891600	0.05187900
24	C	7.55652400	1.66753300	-0.36496700
25	C	8.26329600	0.66799500	-1.04345600
26	C	7.67196400	-0.57981000	-1.27907100
27	H	5.92192500	-1.81953300	-1.02515000
28	H	8.03182300	2.63065700	-0.15221100
29	H	9.29034600	0.85443500	-1.37325300
30	H	8.24105200	-1.36644200	-1.78421600
31	C	5.32584400	2.30847300	0.84719200
32	H	5.83936700	2.83781300	1.66830100
33	H	4.84915800	3.08709500	0.22396700
34	C	4.22167400	0.12375500	0.35452800
35	H	4.05526800	-0.82534600	0.88387300
36	C	4.27676400	1.30165300	1.39617900

1	H	4.74264100	0.84010100	2.28659300
2	O	3.08481700	1.87524600	1.83615900
3	C	2.97895900	1.45018300	-1.43973400
4	C	3.14769800	-0.88848600	-1.68369300
5	C	3.84654800	1.24562400	-2.68842900
6	H	3.25091700	2.32113800	-0.83250900
7	H	1.92243800	1.54609900	-1.72180300
8	C	3.76836100	-0.27501900	-2.96053000
9	H	3.69411300	-1.75558200	-1.28501700
10	H	2.11710200	-1.20614400	-1.89383400
11	H	3.45969900	1.84201300	-3.53124000
12	H	4.88714500	1.55949300	-2.50943600
13	H	3.11430100	-0.49318000	-3.81954700
14	H	4.76289200	-0.69361000	-3.18016800
15	N	3.07988400	0.18999600	-0.63411300
16	C	-0.88449100	3.91020800	-0.74170600
17	H	-0.94455800	5.01066900	-0.77435200
18	H	0.17456600	3.62452800	-0.75127200
19	H	-1.36018600	3.49690200	-1.64426900
20	C	-0.88164200	3.96484200	1.78940400
21	H	0.19966100	3.76278400	1.79147600
22	H	-1.04209000	5.05655900	1.81304100
23	H	-1.32826600	3.54341200	2.70608000
24	C	-3.06217600	3.69789500	0.58785500
25	C	-3.88267400	3.03350900	1.51805400
26	C	-3.65523900	4.67405300	-0.22804400
27	C	-5.24248300	3.33307100	1.62860000
28	H	-3.45548200	2.25947900	2.15883700
29	C	-5.01759200	4.97956100	-0.11709300
30	H	-3.06030900	5.21362500	-0.96680700
31	C	-5.81838200	4.31095400	0.81041700
32	H	-5.85617100	2.79665800	2.35931200
33	H	-5.45155700	5.74590200	-0.76715700
34	H	-6.88341000	4.54796500	0.89583100

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36

CP4

1	Zero-point correction=		0.906621 (Hartree/Particle)	
2	Thermal correction to Energy=		0.959982	
3	Thermal correction to Enthalpy=		0.960926	
4	Thermal correction to Gibbs Free Energy=		0.816294	
5	Sum of electronic and zero-point Energies=		-3133.204233	
6	Sum of electronic and thermal Energies=		-3133.150873	
7	Sum of electronic and thermal Enthalpies=		-3133.149929	
8	Sum of electronic and thermal Free Energies=		-3133.294561	
9		Cartesian Coordinates		
10	Atom	X	Y	
11		-----		
12	C	-2.03567900	-3.31907200	-2.02339500
13	C	-2.00643700	-3.92090600	-0.75512000
14	C	-2.72196900	-3.35493700	0.35965100
15	C	-3.43477600	-2.15389200	0.12961000
16	C	-3.45681000	-1.52375100	-1.15396800
17	C	-2.75857900	-2.09364300	-2.24667400
18	H	-1.43110700	-3.73578400	-2.83212900
19	H	-1.37223700	-4.79416100	-0.60174900
20	H	-3.95147800	-1.67354800	0.96088500
21	H	-3.97989500	-0.57457400	-1.27734600
22	Ru	-1.33575500	-1.77799700	-0.52881600
23	Cl	0.33343600	-0.95793200	-2.17709200
24	Cl	0.58927300	-2.65246200	0.79325000
25	C	-1.18527900	0.29322300	0.61190900
26	C	-2.40848000	0.36217800	1.52320400
27	C	-3.64488700	0.96849100	1.21199200
28	C	-2.31506100	-0.24639100	2.79663100
29	C	-4.71878500	0.95668700	2.11152100
30	H	-3.77882100	1.44820900	0.24527800
31	C	-3.38432500	-0.26126800	3.69276000
32	H	-1.37750300	-0.72515800	3.08309700
33	C	-4.60306800	0.34139800	3.35950200
34	H	-5.65776300	1.44317100	1.82528800
35	H	-3.25879200	-0.74498100	4.66733300
36	H	-5.44161600	0.33717400	4.06283400

1	C	-1.05062700	1.33680800	-0.47336100
2	O	-0.01486400	1.92918000	-0.72155600
3	O	-2.17418000	1.61155400	-1.17602200
4	C	-2.17417900	2.67666700	-2.18789900
5	C	-2.78845800	-4.01388600	1.73409600
6	H	-2.58519400	-3.21631600	2.47030100
7	C	-4.22005300	-4.53253000	1.98873900
8	H	-4.49380900	-5.31615200	1.25782600
9	H	-4.29217200	-4.97338700	2.99934200
10	H	-4.97016400	-3.72571300	1.91952300
11	C	-1.76464700	-5.13438500	1.95675100
12	H	-0.73723700	-4.78086300	1.77446600
13	H	-1.82703700	-5.49060000	3.00042600
14	H	-1.96566900	-6.00493600	1.30420100
15	C	-2.77130000	-1.47291900	-3.61588400
16	H	-3.38236900	-2.09000000	-4.30198400
17	H	-3.20049600	-0.45950400	-3.59078900
18	H	-1.74864400	-1.40705400	-4.02211000
19	C	1.45063300	3.06297600	4.23028900
20	C	2.00376500	1.78080700	4.12489400
21	C	1.51646100	0.86908900	3.18918400
22	C	0.45565800	1.20897900	2.31118800
23	C	-0.10200000	2.50107200	2.43570400
24	C	0.39438000	3.40371800	3.37825900
25	H	1.83098000	3.77842200	4.96540900
26	H	2.82339600	1.47967000	4.78681400
27	H	1.94561000	-0.13783900	3.13428800
28	H	-0.92243600	2.80797800	1.78673200
29	H	-0.05848700	4.39918800	3.44142900
30	N	0.04255600	0.27288900	1.37992600
31	H	0.48213500	-0.64095300	1.45489300
32	H	2.35733500	-0.73619100	-1.54456100
33	H	1.63931700	1.69586000	-0.87760700
34	C	5.60958600	-1.58275500	1.18337000
35	C	4.99912200	-0.47345400	0.58530200
36	C	5.67974000	0.75500100	0.49554500

1	C	6.98963200	0.86526100	0.97065300
2	C	7.61004000	-0.25288900	1.54018100
3	C	6.92294000	-1.46889500	1.65346300
4	H	5.06418400	-2.52306600	1.30850200
5	H	7.52218200	1.81981300	0.91171000
6	H	8.63431700	-0.17187300	1.91778800
7	H	7.40861200	-2.32816700	2.12593300
8	C	4.80016300	1.82000700	-0.11009600
9	H	4.86098800	2.78339300	0.42399600
10	H	5.06796300	2.02573900	-1.16328300
11	C	3.59473000	-0.33924100	0.04786300
12	H	2.83709000	-0.82156900	0.68230100
13	C	3.37452300	1.21683800	-0.04434100
14	H	2.90979300	1.51097400	0.91311500
15	O	2.59546400	1.61223900	-1.12875800
16	C	4.19885200	-0.52020000	-2.46882300
17	C	3.44524600	-2.47539100	-1.35549700
18	C	3.85857500	-1.52173600	-3.58324400
19	H	5.25208700	-0.58757400	-2.15318500
20	H	3.93829400	0.52036700	-2.69511200
21	C	3.37870600	-2.80921900	-2.85277500
22	H	4.41630400	-2.75396200	-0.92023100
23	H	2.62452200	-2.88700200	-0.74861100
24	H	3.05113900	-1.12041200	-4.21575500
25	H	4.73270200	-1.69708800	-4.23039000
26	H	2.34231800	-3.04384800	-3.13736000
27	H	4.00491500	-3.68575400	-3.08354200
28	N	3.35820100	-0.97528700	-1.31073400
29	C	-3.63626600	2.70297500	-2.66577600
30	H	-3.76939900	3.49303500	-3.42371400
31	H	-3.91367300	1.73356700	-3.11615000
32	H	-4.32481900	2.91178200	-1.83047000
33	C	-1.26261200	2.29232500	-3.36019700
34	H	-1.48496800	1.25972000	-3.67027200
35	H	-1.44914000	2.95854900	-4.22016000
36	H	-0.20111100	2.33793400	-3.08500400

1	C	-1.83632800	4.03068000	-1.54499300
2	C	-0.98546000	4.95771600	-2.16400100
3	C	-2.44791300	4.40127000	-0.33469600
4	C	-0.75399100	6.21502800	-1.59507800
5	H	-0.48146700	4.70433900	-3.09847100
6	C	-2.21388400	5.65304400	0.23949400
7	H	-3.10870100	3.69780000	0.17891300
8	C	-1.36585000	6.56950000	-0.39080900
9	H	-0.08169300	6.91793200	-2.09758200
10	H	-2.69743400	5.91173300	1.18691600
11	H	-1.18065000	7.55100200	0.05683200

12

13

CP5

14	Zero-point correction=		0.905464 (Hartree/Particle)	
15	Thermal correction to Energy=			0.959275
16	Thermal correction to Enthalpy=			0.960219
17	Thermal correction to Gibbs Free Energy=			0.812392
18	Sum of electronic and zero-point Energies=			-3133.199878
19	Sum of electronic and thermal Energies=			-3133.146067
20	Sum of electronic and thermal Enthalpies=			-3133.145123
21	Sum of electronic and thermal Free Energies=			-3133.292949

22

Cartesian Coordinates

23	Atom	X	Y	Z
24	-----			
25	C	0.00940700	-2.29196500	0.30781700
26	C	-0.84617600	-3.48711800	0.11477200
27	C	-0.94705700	-4.26152800	-1.07047700
28	C	-1.66947700	-3.90350900	1.19574400
29	C	-1.82216600	-5.34616600	-1.16606700
30	H	-0.32490900	-4.01145700	-1.92504500
31	C	-2.54125800	-4.98813800	1.09476300
32	H	-1.61356000	-3.35039500	2.13537100
33	C	-2.63352800	-5.72400700	-0.09157100
34	H	-1.86018700	-5.91205600	-2.10396100
35	H	-3.15164500	-5.26440300	1.96196600
36	H	-3.31183700	-6.57944400	-0.17206700

1	C	0.80242900	-1.63347600	-0.65215000
2	O	1.42751400	-0.53220800	-0.51441500
3	O	0.92575000	-2.27176000	-1.85571300
4	C	1.35126600	-1.63581500	-3.08686000
5	C	0.37343200	-0.52209200	-3.47262800
6	H	-0.65491400	-0.91136500	-3.38359300
7	H	0.53104000	-0.21223500	-4.52063400
8	H	0.46432200	0.35725900	-2.81949600
9	C	1.25093200	-2.77758200	-4.11824000
10	H	1.61050300	-2.43285700	-5.10275800
11	H	0.20248800	-3.10776300	-4.21875100
12	H	1.86179600	-3.64155500	-3.80810900
13	C	2.81962900	-1.19721300	-3.00271700
14	C	3.28590300	-0.02107700	-3.60766600
15	C	3.75913200	-2.04332500	-2.38800500
16	C	4.65009800	0.29844900	-3.60488000
17	H	2.58340500	0.66533500	-4.08475600
18	C	5.11951400	-1.72647800	-2.37927500
19	H	3.41209600	-2.95899900	-1.90102300
20	C	5.57433600	-0.55186200	-2.99163200
21	H	4.98932500	1.22062500	-4.08852800
22	H	5.83056900	-2.40254800	-1.89317900
23	H	6.64084800	-0.30494200	-2.99284900
24	N	0.13490400	-1.81652800	1.64959400
25	H	-0.23041100	-0.89058200	1.86613000
26	C	1.00237800	-2.34630600	2.58323200
27	C	1.14456400	-1.71444000	3.84539700
28	C	1.75551200	-3.51985700	2.34662900
29	C	2.00935700	-2.22795100	4.81170500
30	H	0.55591700	-0.81474600	4.05264600
31	C	2.61598100	-4.02125800	3.32565600
32	H	1.65693500	-4.03114200	1.38684500
33	C	2.76056000	-3.38522600	4.56454700
34	H	2.09456500	-1.71648300	5.77737400
35	H	3.18497600	-4.93331300	3.11291200
36	H	3.43449300	-3.78851400	5.32621400

1	H	-2.02263400	1.52774400	-0.44899800
2	C	-6.09526100	1.51705400	1.08393900
3	C	-5.21194100	0.68907200	0.37884900
4	C	-5.70591900	-0.36627000	-0.41249100
5	C	-7.08416800	-0.56906300	-0.52984800
6	C	-7.96442000	0.28046300	0.14938900
7	C	-7.47393100	1.31399700	0.95844000
8	H	-5.72404700	2.30004200	1.75199900
9	H	-7.47193600	-1.39300700	-1.13700300
10	H	-9.04445500	0.12447100	0.06418400
11	H	-8.17034100	1.95404700	1.50854100
12	C	-4.58268400	-1.17322600	-1.01351300
13	H	-4.73863800	-2.26197400	-0.93087400
14	H	-4.44073300	-0.95539500	-2.08848900
15	C	-3.70089600	0.68131100	0.38559800
16	H	-3.26193100	0.80022400	1.38592600
17	C	-3.32834100	-0.71466000	-0.22884900
18	H	-3.17190000	-1.40089300	0.62103500
19	O	-2.18567000	-0.64905300	-1.02879100
20	H	-1.44166600	-1.15358500	-0.61225500
21	C	-3.46820600	1.97233400	-1.86554600
22	C	-3.09730000	3.15181500	0.23984300
23	C	-3.68536100	3.48286700	-2.05467800
24	H	-4.38013200	1.38876600	-2.04041100
25	H	-2.65611600	1.56736500	-2.48309700
26	C	-2.89246900	4.13261700	-0.90912500
27	H	-4.09777700	3.26351000	0.68165300
28	H	-2.33122600	3.17483400	1.02790300
29	H	-4.75839100	3.72698900	-1.96457800
30	H	-1.82064000	4.19060800	-1.15804600
31	N	-3.03350800	1.79240900	-0.41644100
32	C	3.74905100	1.33705400	0.00747000
33	C	3.23687000	2.64236800	-0.15592700
34	C	2.55451400	3.33017900	0.91174700
35	C	2.38293900	2.61330300	2.12387100
36	C	2.90447500	1.28808900	2.30242100

1	C	3.59740600	0.63622800	1.25517800
2	H	4.17826400	0.81756600	-0.85204800
3	H	3.28581600	3.11007100	-1.14242800
4	H	1.77137100	3.03772300	2.92057500
5	H	2.68755600	0.74149700	3.22257200
6	Ru	1.58803700	1.37166800	0.51017000
7	Cl	0.16250000	2.32479300	-1.26599200
8	Cl	-0.53642200	1.28430400	1.80401900
9	C	2.03626800	4.73984600	0.68163400
10	H	1.65550900	4.75677500	-0.35445100
11	C	0.87587700	5.13717600	1.60162200
12	H	1.19961900	5.24548700	2.65313000
13	H	0.46443800	6.11239200	1.28610100
14	H	0.06773500	4.38760200	1.56187300
15	C	3.20167300	5.74506900	0.78099400
16	H	4.01853400	5.49567300	0.08032800
17	H	2.85183300	6.76545300	0.54143800
18	H	3.62618100	5.76228700	1.80173800
19	C	4.10957600	-0.76701400	1.39819300
20	H	5.21017400	-0.74397900	1.51565200
21	H	3.67276700	-1.27491900	2.27118100
22	H	3.87711000	-1.35480000	0.49638500
23	H	-3.25339400	5.14229600	-0.65299000
24	H	-3.34935000	3.81564300	-3.04976100

25

26

TS3

27	Zero-point correction=		0.900393 (Hartree/Particle)
28	Thermal correction to Energy=		0.953428
29	Thermal correction to Enthalpy=		0.954372
30	Thermal correction to Gibbs Free Energy=		0.809647
31	Sum of electronic and zero-point Energies=		-3133.191313
32	Sum of electronic and thermal Energies=		-3133.138278
33	Sum of electronic and thermal Enthalpies=		-3133.137334
34	Sum of electronic and thermal Free Energies=		-3133.282058

35

Cartesian Coordinates

36	Atom	X	Y	Z
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1				
2	C	0.25678300	2.06529600	0.49284700
3	C	0.86964500	3.44342300	0.36197300
4	C	1.42291600	3.89992100	-0.85377700
5	C	1.03832400	4.26884100	1.49090400
6	C	2.06668500	5.13607900	-0.94335600
7	H	1.36723500	3.26594000	-1.73830800
8	C	1.68432100	5.50654100	1.40290100
9	H	0.66703200	3.93160500	2.45938700
10	C	2.19661600	5.95568600	0.18340500
11	H	2.48114700	5.45716100	-1.90538300
12	H	1.78707800	6.12231200	2.30290300
13	H	2.70080200	6.92495800	0.11261700
14	C	-0.72472700	1.56917500	-0.49086400
15	O	-1.32617200	0.48491400	-0.41655800
16	O	-0.88133800	2.35449200	-1.56585600
17	C	-1.39928900	1.90429200	-2.85780000
18	C	-0.54314100	0.74485900	-3.37680900
19	H	0.52204900	1.00571300	-3.25652700
20	H	-0.73357000	0.57992100	-4.45131000
21	H	-0.71684700	-0.19178600	-2.82842500
22	C	-1.19747800	3.14190900	-3.75051600
23	H	-1.60266300	2.94977200	-4.75831600
24	H	-0.12341200	3.37956800	-3.83594900
25	H	-1.71442100	4.01859800	-3.32672900
26	C	-2.89960900	1.60646300	-2.76882400
27	C	-3.49550600	0.57420100	-3.50885300
28	C	-3.73366700	2.44788800	-2.01251000
29	C	-4.88398200	0.38929500	-3.49702700
30	H	-2.87729900	-0.10019100	-4.10523100
31	C	-5.11837900	2.26302300	-1.99456600
32	H	-3.28846200	3.25451700	-1.42341400
33	C	-5.70238200	1.23225600	-2.74018600
34	H	-5.32583800	-0.42022300	-4.08730500
35	H	-5.74593300	2.93053700	-1.39540600
36	H	-6.78770600	1.09048700	-2.73321900

1	N	-0.03213200	1.64077400	1.84018400
2	H	0.34158700	0.72583700	2.08963300
3	C	-1.14098100	2.02659700	2.57005000
4	C	-1.43791300	1.36195200	3.78742400
5	C	-1.98379900	3.09532400	2.18493300
6	C	-2.51474300	1.75879900	4.57865900
7	H	-0.79759900	0.53212600	4.10185000
8	C	-3.05814000	3.48292000	2.99024300
9	H	-1.78117500	3.63477300	1.25713200
10	C	-3.34043400	2.82443800	4.19182400
11	H	-2.71022100	1.22863600	5.51766700
12	H	-3.68499600	4.32177800	2.66795500
13	H	-4.17994900	3.13846000	4.81904600
14	H	2.35418300	-1.13979900	-0.35908800
15	C	6.51924100	-1.33579000	0.87400500
16	C	5.50800800	-0.49514500	0.39412100
17	C	5.82646500	0.67398800	-0.32552000
18	C	7.16588300	0.99272400	-0.57276200
19	C	8.17575700	0.14313000	-0.10581200
20	C	7.85687600	-1.01518600	0.61574600
21	H	6.27668300	-2.22676500	1.46249300
22	H	7.42448100	1.90356900	-1.12222900
23	H	9.22504200	0.39120500	-0.29579600
24	H	8.65583500	-1.66265900	0.99014700
25	C	4.58304700	1.43077900	-0.72448700
26	H	4.67208000	2.51986700	-0.57197800
27	H	4.33823300	1.27728100	-1.79254200
28	C	4.01841100	-0.60456800	0.57694500
29	H	3.71489700	-0.86003800	1.60296300
30	C	3.44208200	0.80301300	0.13878700
31	H	3.36095700	1.40259300	1.07353500
32	O	2.24031000	0.64498600	-0.48964100
33	H	1.25078200	1.31836300	0.05290500
34	C	3.76690400	-1.80406100	-1.71612500
35	C	3.18552900	-2.99911300	0.33466000
36	C	4.07223200	-3.29786800	-1.86624300

1	H	4.63396100	-1.15992700	-1.90625300
2	H	2.93055200	-1.48052500	-2.35169200
3	C	3.13077100	-3.96039200	-0.84954100
4	H	4.09142400	-3.16817300	0.93870100
5	H	2.29964000	-3.00342500	0.98609300
6	H	5.12657600	-3.50143100	-1.60597900
7	H	2.10180400	-4.00329200	-1.24236300
8	N	3.29804900	-1.62693300	-0.28132700
9	C	-3.69459400	-1.53812900	-0.30122300
10	C	-3.12993300	-2.80072300	-0.57393200
11	C	-2.49825400	-3.58347700	0.45881200
12	C	-2.46217500	-3.01781000	1.76270400
13	C	-3.05920100	-1.74747900	2.05390600
14	C	-3.67486900	-0.99045000	1.03038400
15	H	-4.07428400	-0.92862700	-1.12445400
16	H	-3.08026700	-3.15005000	-1.60804100
17	H	-1.90019700	-3.51763400	2.55203400
18	H	-2.94896900	-1.31482400	3.05016900
19	Ru	-1.57617200	-1.58790000	0.39206100
20	Cl	-0.01824200	-2.26330300	-1.36617000
21	Cl	0.36611800	-1.53519000	1.89688500
22	C	-1.89577100	-4.93438900	0.11092800
23	H	-1.44688600	-4.81550400	-0.89020400
24	C	-0.77941500	-5.38413000	1.06083500
25	H	-1.16535400	-5.63033100	2.06721200
26	H	-0.29737300	-6.29575300	0.66560700
27	H	-0.01085500	-4.59999200	1.16372000
28	C	-3.01530700	-5.99075900	0.01586600
29	H	-3.79530000	-5.69799000	-0.70972800
30	H	-2.60040100	-6.96189300	-0.30889500
31	H	-3.50501400	-6.14158000	0.99565100
32	C	-4.26497500	0.36261700	1.29816000
33	H	-5.36747600	0.27291200	1.34988000
34	H	-3.90359000	0.78615800	2.24699900
35	H	-4.02434300	1.06331800	0.48410100
36	H	3.44436500	-4.97870900	-0.56534100

1	H	3.90886600	-3.64266100	-2.90042700
2				
3		CP6		
4	Zero-point correction=		0.624594	(Hartree/Particle)
5	Thermal correction to Energy=		0.664079	
6	Thermal correction to Enthalpy=		0.665023	
7	Thermal correction to Gibbs Free Energy=		0.549544	
8	Sum of electronic and zero-point Energies=		-2498.404770	
9	Sum of electronic and thermal Energies=		-2498.365285	
10	Sum of electronic and thermal Enthalpies=		-2498.364341	
11	Sum of electronic and thermal Free Energies=		-2498.479820	
12		Cartesian Coordinates		
13	Atom	X	Y	Z
14	-----			
15	C	1.52596600	-1.54765800	0.40315500
16	C	2.48061300	-2.52512900	-0.27560400
17	C	2.12023000	-3.08332400	-1.51424100
18	C	3.65434000	-2.96882500	0.34535800
19	C	2.93516300	-4.03304500	-2.13342700
20	H	1.17399900	-2.79225000	-1.98151600
21	C	4.47310700	-3.92069900	-0.27481100
22	H	3.92366100	-2.57605400	1.32787700
23	C	4.12174500	-4.45054100	-1.51853200
24	H	2.63535600	-4.46007700	-3.09593500
25	H	5.38902400	-4.25226600	0.22489200
26	H	4.76109400	-5.19596000	-2.00221500
27	C	1.07418100	-0.35233800	-0.45910400
28	O	0.03326500	0.26666600	-0.25226300
29	O	1.92373100	0.00119800	-1.40498900
30	C	1.60383000	0.96043900	-2.48516100
31	C	0.47420400	0.35747600	-3.32712500
32	H	0.74661600	-0.67150300	-3.61337200
33	H	0.33760300	0.93609400	-4.25542100
34	H	-0.47881500	0.31709100	-2.77916100
35	C	2.90966900	0.99339200	-3.29280100
36	H	2.80115700	1.67845700	-4.15017400

1	H	3.15491700	-0.01599300	-3.66492300
2	H	3.74439600	1.35052300	-2.66751700
3	C	1.31619200	2.35657500	-1.92517800
4	C	0.38538900	3.21182400	-2.53573800
5	C	2.06411400	2.85140400	-0.84356800
6	C	0.20831400	4.52468300	-2.08130300
7	H	-0.21026200	2.86542300	-3.38330000
8	C	1.88276700	4.15808800	-0.38355500
9	H	2.79010700	2.20736700	-0.34018500
10	C	0.95608200	5.00410700	-1.00296500
11	H	-0.51848400	5.17455200	-2.57928900
12	H	2.47424300	4.51372200	0.46572000
13	H	0.81939300	6.03034100	-0.64796300
14	N	1.89963700	-1.08989900	1.72987700
15	H	1.10587900	-1.15684000	2.36807900
16	C	2.82983900	-0.10818200	2.05103900
17	C	2.73992600	0.52004800	3.31588100
18	C	3.89243200	0.26967400	1.20081700
19	C	3.67262500	1.47634300	3.71134300
20	H	1.92287500	0.23969800	3.98895000
21	C	4.82044500	1.23292600	1.61052600
22	H	3.99928000	-0.19705500	0.22086200
23	C	4.72420200	1.84677200	2.86260100
24	H	3.57472000	1.94076000	4.69838200
25	H	5.63827700	1.50021500	0.93254900
26	H	5.45755900	2.59548600	3.17588800
27	H	0.58062800	-2.09236100	0.56558300
28	C	-2.63177900	1.76685500	-0.35861400
29	C	-3.52786600	0.78927100	-0.84157700
30	C	-4.19973500	-0.11025000	0.06271300
31	C	-3.95381500	0.05526300	1.45291200
32	C	-3.07950700	1.08407700	1.94083100
33	C	-2.39296100	1.94291600	1.05308800
34	H	-2.03745700	2.34891900	-1.06809400
35	H	-3.62724400	0.63414900	-1.91839100
36	H	-4.36602200	-0.65817700	2.16662000

1	H	-2.85070700	1.11855200	3.00807800
2	Ru	-2.03532400	-0.19879000	0.46372400
3	Cl	-1.76251200	-2.06816600	-1.04923000
4	Cl	-1.22936000	-1.59571400	2.27689300
5	C	-5.10948900	-1.19172300	-0.49617500
6	H	-4.63336400	-1.53233700	-1.43127800
7	C	-5.25536400	-2.41977900	0.41047000
8	H	-5.81338900	-2.18919200	1.33671000
9	H	-5.81875900	-3.20671000	-0.12083600
10	H	-4.26810800	-2.83044900	0.68011800
11	C	-6.48020700	-0.57563900	-0.84379900
12	H	-6.38482700	0.27492500	-1.54261600
13	H	-7.12798800	-1.33277900	-1.32047400
14	H	-6.99585400	-0.21151100	0.06395500
15	C	-1.40067900	2.96233100	1.54152600
16	H	-1.86100000	3.96875300	1.55134000
17	H	-1.06236900	2.72865800	2.56404800
18	H	-0.51730200	3.00295300	0.88384800

19
20

6

21	Zero-point correction=		0.278778 (Hartree/Particle)	
22	Thermal correction to Energy=		0.291292	
23	Thermal correction to Enthalpy=		0.292236	
24	Thermal correction to Gibbs Free Energy=		0.239295	
25	Sum of electronic and zero-point Energies=		-634.799406	
26	Sum of electronic and thermal Energies=		-634.786892	
27	Sum of electronic and thermal Enthalpies=		-634.785948	
28	Sum of electronic and thermal Free Energies=		-634.838890	

29

Cartesian Coordinates

30	Atom	X	Y	Z
31	-----			
32	H	1.77963300	2.25803100	0.16344400
33	C	-1.16217900	-1.41979700	-0.89966000
34	C	-0.81945100	-0.11996600	-0.51486700
35	C	-1.72248400	0.66365700	0.22681200
36	C	-2.96988000	0.14537800	0.58759100

1	C	-3.30884600	-1.15843300	0.20613400
2	C	-2.41121100	-1.93758800	-0.53639700
3	H	-0.46974600	-2.02701900	-1.49245700
4	H	-3.67906400	0.75321300	1.15908400
5	H	-4.28500800	-1.56986600	0.48254500
6	H	-2.69165500	-2.95096500	-0.84069500
7	C	-1.13915900	2.02758700	0.51601200
8	H	-1.87242000	2.84694700	0.42029900
9	H	-0.72586100	2.08527900	1.54137100
10	C	0.45724200	0.65358600	-0.80000800
11	H	0.75704900	0.55702600	-1.85542000
12	C	0.02038800	2.14128400	-0.50919500
13	H	-0.39258900	2.56011700	-1.44673600
14	O	1.10232000	2.92462600	-0.10835300
15	C	1.50282900	-0.29469900	1.31680500
16	C	2.73686700	-0.41988200	-0.64818400
17	C	1.81272900	-1.80812300	1.13391500
18	H	0.49957800	-0.11023900	1.72650000
19	H	2.23261300	0.15947700	2.01303900
20	C	2.54333400	-1.89696100	-0.23204700
21	H	2.73161200	-0.25770800	-1.73782700
22	H	3.70817800	-0.04846700	-0.26745400
23	H	2.43204000	-2.18829200	1.96372400
24	H	0.88324300	-2.39995000	1.12220300
25	H	3.50260800	-2.43818300	-0.17178900
26	H	1.91964600	-2.42475200	-0.97411300
27	N	1.65864500	0.33458300	-0.00290800

28

29

TS3_{major}

30	Zero-point correction=	0.981536 (Hartree/Particle)
31	Thermal correction to Energy=	1.039188
32	Thermal correction to Enthalpy=	1.040132
33	Thermal correction to Gibbs Free Energy=	0.883902
34	Sum of electronic and zero-point Energies=	-3363.989305
35	Sum of electronic and thermal Energies=	-3363.931653
36	Sum of electronic and thermal Enthalpies=	-3363.930709

1	Sum of electronic and thermal Free Energies=			-3364.086939
2		Cartesian Coordinates		
3	Atom	X	Y	Z
4	-----			
5	C	1.16559400	2.28967800	-0.02264400
6	C	1.09990500	3.71653600	0.47891500
7	C	0.48253500	4.04841000	1.70423800
8	C	1.52874000	4.78621800	-0.33120600
9	C	0.34556200	5.37605600	2.11566000
10	H	0.08387200	3.25427200	2.33503000
11	C	1.39074300	6.11644200	0.07906600
12	H	1.96867600	4.57431400	-1.30646400
13	C	0.80584000	6.42349000	1.30991500
14	H	-0.13697000	5.59377700	3.07488000
15	H	1.74514200	6.91881300	-0.57693500
16	H	0.69874500	7.46403700	1.63312000
17	C	1.61772200	1.19221700	0.85336700
18	O	1.76954300	0.01031600	0.50125500
19	O	1.78917900	1.53885000	2.13660400
20	C	1.78850300	0.60170200	3.25974300
21	C	0.47818400	-0.19167700	3.26700700
22	H	-0.36266700	0.50536900	3.11147700
23	H	0.33465900	-0.68389400	4.24428800
24	H	0.43266800	-0.94584000	2.46896600
25	C	1.83737300	1.53928000	4.47957300
26	H	1.89763800	0.94693800	5.40812700
27	H	0.93099100	2.16755300	4.51439700
28	H	2.71737200	2.20143000	4.42889100
29	C	3.05872500	-0.25506900	3.25143500
30	C	3.05476400	-1.58980100	3.68376000
31	C	4.29042700	0.32705100	2.90562200
32	C	4.24604700	-2.32154900	3.77079900
33	H	2.11527100	-2.07399200	3.95887000
34	C	5.47978300	-0.40150900	2.98683300
35	H	4.31454900	1.36439900	2.56044700
36	C	5.46425500	-1.73155000	3.42281500

1	H	4.21776500	-3.36017900	4.11640100
2	H	6.42590100	0.07410600	2.70930900
3	H	6.39595400	-2.30157700	3.49398400
4	N	1.59466800	2.13282900	-1.39011200
5	H	0.97733500	1.56587400	-1.96981800
6	C	2.90903900	2.17073100	-1.81668300
7	C	3.22297400	1.76687200	-3.13966100
8	C	3.96906300	2.63997300	-1.00616100
9	C	4.52818100	1.84236600	-3.62329900
10	H	2.41620200	1.40063800	-3.78191000
11	C	5.27196400	2.71208200	-1.50635400
12	H	3.76284300	2.96674700	0.01540300
13	C	5.57139900	2.31543500	-2.81408000
14	H	4.73386300	1.53005700	-4.65343300
15	H	6.06811000	3.09054000	-0.85565800
16	H	6.59320100	2.38080200	-3.19935300
17	H	-2.12702400	0.23181600	-0.55994800
18	C	-5.63889400	2.20966900	-2.19167600
19	C	-4.52913700	2.35731800	-1.35137800
20	C	-4.54051100	3.29938800	-0.30334800
21	C	-5.67626700	4.08834600	-0.09310000
22	C	-6.79131800	3.92933100	-0.92447600
23	C	-6.77491000	2.99660800	-1.97032400
24	H	-5.62027500	1.50254500	-3.02756000
25	H	-5.69240300	4.82990000	0.71200200
26	H	-7.68081400	4.54703700	-0.76372000
27	H	-7.64669600	2.89345700	-2.62382900
28	C	-3.23548100	3.29462900	0.45494200
29	H	-2.86634300	4.30787200	0.68800900
30	H	-3.32803800	2.75869700	1.41846900
31	C	-3.19489300	1.66508400	-1.41400500
32	H	-2.77954300	1.59427000	-2.43035300
33	C	-2.24867900	2.50049800	-0.45942800
34	H	-1.72913100	3.23709500	-1.11264600
35	O	-1.38030100	1.66680100	0.18624300
36	H	-0.11322500	1.96112000	0.02361000

1	C	-3.96042200	-0.10384100	0.32945100
2	C	-3.40604100	-0.81771600	-1.93743200
3	C	-4.81714000	-1.32480000	-0.06275000
4	H	-4.56798100	0.75852500	0.62970700
5	H	-3.24352100	-0.33444100	1.12938000
6	C	-3.96183700	-2.00162700	-1.15591100
7	H	-4.15690700	-0.41550500	-2.63611300
8	H	-2.46475400	-1.01036200	-2.47254300
9	H	-5.73871400	-0.94836300	-0.54150500
10	H	-3.13288700	-2.57101200	-0.70636300
11	N	-3.13839400	0.24024900	-0.89731200
12	C	3.15877600	-2.73943800	0.01019700
13	C	2.11199200	-3.65641300	-0.21543500
14	C	1.50619600	-3.80574500	-1.51506300
15	C	2.00527300	-2.97627100	-2.55599300
16	C	3.08536900	-2.05877600	-2.34058900
17	C	3.67081100	-1.92362500	-1.05993000
18	H	3.52736400	-2.58113100	1.02634400
19	H	1.68348500	-4.19546800	0.63292400
20	H	1.50832900	-2.97095800	-3.52634200
21	H	3.39212300	-1.38749600	-3.14507600
22	Ru	1.41662100	-1.69242100	-0.90791500
23	Cl	-0.67039500	-2.04379800	0.32934400
24	Cl	0.06667000	-0.43599100	-2.53040200
25	C	0.37258400	-4.80041700	-1.70213000
26	H	-0.23829800	-4.73677700	-0.78518700
27	C	-0.54749500	-4.48343900	-2.88695000
28	H	-0.03899200	-4.63192200	-3.85744200
29	H	-1.42197300	-5.15759600	-2.87138700
30	H	-0.90955300	-3.44281400	-2.83811500
31	C	0.94770500	-6.22794700	-1.80123100
32	H	1.56640100	-6.48343400	-0.92228200
33	H	0.12939200	-6.96759200	-1.86344100
34	H	1.57777300	-6.34220400	-2.70261300
35	C	4.77146700	-0.93853000	-0.79788400
36	H	5.73631300	-1.47948000	-0.74637100

1	H	4.83831100	-0.17900200	-1.59098900
2	H	4.62133800	-0.42996800	0.16663400
3	C	-5.22384500	-2.20141100	1.10704300
4	C	-6.58005300	-2.37293500	1.42478100
5	C	-4.26381300	-2.85951500	1.89729600
6	C	-6.97428900	-3.17858100	2.49852400
7	H	-7.34169900	-1.86713100	0.82140700
8	C	-4.65536800	-3.66408500	2.97063000
9	H	-3.19730100	-2.74734000	1.67552800
10	C	-6.01144000	-3.82741700	3.27595100
11	H	-8.03822600	-3.29743200	2.72703800
12	H	-3.89305600	-4.16782200	3.57346700
13	H	-6.31527800	-4.45799600	4.11747800
14	H	-4.55255600	-2.67995900	-1.79345800

15

16

TS3_{minor}

17	Zero-point correction=		0.981379 (Hartree/Particle)
18	Thermal correction to Energy=		1.039167
19	Thermal correction to Enthalpy=		1.040111
20	Thermal correction to Gibbs Free Energy=		0.883402
21	Sum of electronic and zero-point Energies=		-3363.988712
22	Sum of electronic and thermal Energies=		-3363.930923
23	Sum of electronic and thermal Enthalpies=		-3363.929979
24	Sum of electronic and thermal Free Energies=		-3364.086688

25

Cartesian Coordinates

26	Atom	X	Y	Z
27	-----			
28	O	-1.49233900	1.67218500	0.74744800
29	H	-0.21493900	1.77081500	0.93234500
30	C	1.04167400	1.67356400	1.36443200
31	C	1.22379700	2.97386300	2.12187700
32	C	2.28366100	3.88350200	1.95321600
33	C	0.25796800	3.27889000	3.10313200
34	C	2.36859500	5.04909500	2.72316700
35	H	3.05740900	3.68144600	1.21135600
36	C	0.34269200	4.43882300	3.87480400

1	H	-0.57263800	2.58413200	3.25081300
2	C	1.39986300	5.33670900	3.68787700
3	H	3.20934300	5.73426200	2.56939000
4	H	-0.42545600	4.64465300	4.62803300
5	H	1.46967500	6.24744600	4.29143300
6	C	1.69047200	1.42174200	0.07296800
7	O	1.81412000	0.32274500	-0.49376200
8	O	2.03072000	2.55116600	-0.57756900
9	C	2.27635500	2.64631300	-2.01960000
10	C	1.02838100	2.19989000	-2.78513500
11	H	0.16321400	2.77391400	-2.41009900
12	H	1.14142200	2.43038000	-3.85847600
13	H	0.82286700	1.12518100	-2.67486200
14	C	2.47111200	4.15867400	-2.22627100
15	H	2.68503100	4.36935600	-3.28784200
16	H	1.55590800	4.69916100	-1.93049000
17	H	3.30545000	4.54676700	-1.62059900
18	C	3.56255500	1.90330100	-2.41001200
19	C	3.59039400	0.93176400	-3.42174800
20	C	4.77760100	2.24924000	-1.79148400
21	C	4.79819400	0.34699900	-3.82242900
22	H	2.66426100	0.60488100	-3.89651100
23	C	5.98393600	1.66580800	-2.18682100
24	H	4.78488300	2.98769100	-0.98463100
25	C	6.00114900	0.71527400	-3.21371600
26	H	4.79307000	-0.40240400	-4.62080600
27	H	6.91550900	1.95743600	-1.69125600
28	H	6.94549200	0.26312300	-3.53325800
29	N	0.87672000	0.51852800	2.20631700
30	H	0.07118500	-0.06838400	1.99807400
31	C	1.76755800	0.02583200	3.13082000
32	C	1.39387800	-1.09039800	3.92400700
33	C	3.05739400	0.57077400	3.33507100
34	C	2.27196300	-1.63653700	4.85770200
35	H	0.39543200	-1.51891500	3.78890800
36	C	3.92412600	0.01478200	4.28086900

1	H	3.37449900	1.43887300	2.75525500
2	C	3.55136200	-1.09407000	5.04782000
3	H	1.94939100	-2.49813600	5.45294200
4	H	4.91404000	0.46391800	4.41790000
5	H	4.23594500	-1.51994400	5.78705900
6	H	-2.12621100	0.34994700	-0.30678800
7	C	-5.33684100	4.53513000	-0.42834500
8	C	-4.25471900	3.64928300	-0.40554200
9	C	-4.04178100	2.77884800	-1.49283700
10	C	-4.89581400	2.79712500	-2.60167600
11	C	-5.98133300	3.68040600	-2.61422800
12	C	-6.19914200	4.54284200	-1.53121200
13	H	-5.50707900	5.22154000	0.40721700
14	H	-4.71367000	2.14410300	-3.46147900
15	H	-6.65365300	3.70712800	-3.47728800
16	H	-7.04611000	5.23614500	-1.55296800
17	C	-2.80093800	1.95817600	-1.26843200
18	H	-2.14064100	1.91615400	-2.14785900
19	C	-2.07883600	2.63008400	-0.02843000
20	H	-1.34231400	3.34900300	-0.45516600
21	C	-3.05254300	-0.45539900	-2.05484100
22	C	-4.14604300	0.16234400	0.04021600
23	C	-3.79401700	-1.66791100	-1.50872600
24	H	-3.61969200	0.03284700	-2.86398200
25	H	-2.02312200	-0.66673500	-2.38695800
26	H	-4.80516500	1.03258800	0.15263800
27	H	-3.69758300	-0.06986400	1.01589500
28	H	-3.09561000	-2.29261000	-0.92968400
29	N	-3.00003900	0.50314100	-0.89276200
30	C	3.38874300	-2.67445100	-1.34497700
31	C	2.33070000	-3.62306300	-1.50362200
32	C	1.53813900	-4.06225800	-0.40419700
33	C	1.84516900	-3.48922800	0.87816100
34	C	2.88980700	-2.55534300	1.05596000
35	C	3.66620100	-2.11862400	-0.06671900
36	H	3.91949900	-2.30424200	-2.22433000

1	H	2.06936400	-3.93996600	-2.51380700
2	H	1.19523600	-3.71312600	1.72748600
3	H	3.03953400	-2.09640400	2.03448300
4	Ru	1.47873100	-1.86727700	-0.55450300
5	Cl	0.42280900	-1.39256300	-2.70697200
6	Cl	-0.77269900	-1.68081000	0.44958100
7	C	0.39925000	-5.06250200	-0.52739700
8	H	-0.39776400	-4.69242100	0.14109500
9	C	0.85768400	-6.44067400	-0.00911200
10	H	1.66707500	-6.85320300	-0.63957800
11	H	0.01670500	-7.15704800	-0.02610500
12	H	1.23291800	-6.38551100	1.02855300
13	C	-0.19488700	-5.16432400	-1.93793400
14	H	-0.46816100	-4.16966200	-2.32900800
15	H	-1.10224800	-5.79355900	-1.91558600
16	H	0.50981000	-5.63637200	-2.64771300
17	C	4.72836500	-1.07378400	0.11380800
18	H	4.46775900	-0.38459800	0.93276600
19	H	4.88694700	-0.49381300	-0.80728500
20	H	5.68230400	-1.56857200	0.38091100
21	C	-3.20571400	3.46093700	0.66307200
22	H	-2.83210400	4.41369400	1.07584700
23	H	-3.59678200	2.87502300	1.51603000
24	C	-4.87205000	-1.04661700	-0.59237300
25	H	-5.67679100	-0.65381300	-1.23842500
26	C	-5.50124600	-1.98818200	0.41808600
27	C	-6.88775100	-2.20309800	0.42208500
28	C	-4.71659600	-2.66678000	1.36838800
29	C	-7.48110100	-3.07090700	1.34550200
30	H	-7.51487000	-1.68273000	-0.31001100
31	C	-5.30683400	-3.53277600	2.29237400
32	H	-3.63098700	-2.52275400	1.38897300
33	C	-6.69129600	-3.73868600	2.28491200
34	H	-8.56498800	-3.22318000	1.32957400
35	H	-4.67923000	-4.05104800	3.02426200
36	H	-7.15154200	-4.41725800	3.00996600

1	H	-4.23013300	-2.28462300	-2.31144000
2				
3		TS_Ru-N_{ylide}		
4	Zero-point correction=		0.653291	(Hartree/Particle)
5	Thermal correction to Energy=		0.695907	
6	Thermal correction to Enthalpy=		0.696852	
7	Thermal correction to Gibbs Free Energy=		0.575065	
8	Sum of electronic and zero-point Energies=		-2612.757477	
9	Sum of electronic and thermal Energies=		-2612.714860	
10	Sum of electronic and thermal Enthalpies=		-2612.713916	
11	Sum of electronic and thermal Free Energies=		-2612.835702	
12		Cartesian Coordinates		
13	Atom	X	Y	Z
14	-----			
15	C	4.48631700	-0.27475900	-1.43053400
16	C	4.14911500	0.97208600	-0.80695500
17	C	3.75252900	1.05516500	0.54616700
18	C	3.47875700	-0.19948300	1.19374600
19	C	3.70707500	-1.43921900	0.55269100
20	C	4.29295600	-1.48927700	-0.76410300
21	H	4.81581200	-0.27240800	-2.47185000
22	H	4.25418300	1.88241800	-1.39789000
23	H	3.05342700	-0.20963600	2.19911400
24	H	3.46140500	-2.36531500	1.07527800
25	Ru	2.20215100	-0.26451300	-0.64507200
26	Cl	1.13258500	-2.26962000	-1.48608500
27	Cl	1.36877200	0.90625500	-2.59936100
28	C	0.63366700	0.04746300	0.50447300
29	C	0.12009400	1.32001700	0.99385400
30	C	-0.60322000	1.40740500	2.21503000
31	C	0.30543000	2.51508000	0.25295400
32	C	-1.08377700	2.62766000	2.68102800
33	H	-0.76806900	0.51183300	2.81806900
34	C	-0.19351300	3.72983200	0.71690300
35	H	0.81585500	2.45345700	-0.71031200
36	C	-0.88174100	3.79527000	1.93385500

1	H	-1.62880900	2.67022000	3.62877100
2	H	-0.05515100	4.63463500	0.11751200
3	H	-1.27329000	4.75126300	2.29481400
4	C	0.21709500	-1.15875900	1.32558800
5	O	0.90840700	-1.51640500	2.25967000
6	O	-0.93807100	-1.71422500	0.97008400
7	C	-1.47670900	-2.94567800	1.60455000
8	C	3.65134000	2.35733100	1.32690000
9	H	2.67426200	2.35206000	1.84111100
10	C	4.74672400	2.39203400	2.41452200
11	H	5.75526500	2.39327900	1.96170100
12	H	4.64762800	3.30551600	3.02780900
13	H	4.68132200	1.52351000	3.09315400
14	C	3.71991700	3.61691500	0.45549500
15	H	2.96414300	3.60500800	-0.34674000
16	H	3.53710500	4.51178200	1.07531800
17	H	4.71605300	3.73526300	-0.00912100
18	C	4.56870900	-2.81453800	-1.41239500
19	H	5.23162700	-3.42771500	-0.77523400
20	H	3.61612000	-3.35927200	-1.54771600
21	H	5.04086400	-2.68988900	-2.40019600
22	C	-4.36436700	3.07727800	-1.01748700
23	C	-3.25431900	3.20938700	-1.86433300
24	C	-2.29561500	2.20395800	-1.97565700
25	C	-2.42024600	1.00858500	-1.22921300
26	C	-3.53717100	0.87753900	-0.36756700
27	C	-4.48375400	1.89156100	-0.27160100
28	H	-3.13074300	4.12618500	-2.45241300
29	H	-1.43443400	2.32759900	-2.63775100
30	H	-3.65055500	-0.03869300	0.21999400
31	H	-5.33482100	1.77540300	0.40551600
32	N	-1.47204200	0.02542000	-1.31213400
33	H	-0.70829700	0.09692300	-1.98555600
34	H	-1.62214900	-0.87063300	-0.86330500
35	C	-0.43039400	-4.07290700	1.57569800
36	H	-0.00060500	-4.17544200	0.56665600

1	H	0.38680600	-3.87560800	2.28503500
2	H	-0.92425200	-5.02189200	1.84747900
3	C	-1.88164500	-2.59896900	3.04002300
4	H	-2.63592300	-1.79454900	3.05923100
5	H	-2.30103700	-3.48465200	3.54583500
6	H	-0.99598000	-2.27361300	3.60585400
7	C	-2.65994600	-3.31715300	0.70150400
8	C	-2.45274300	-3.44805100	-0.68483500
9	C	-3.94212300	-3.57473400	1.20922800
10	C	-3.49830600	-3.81981100	-1.53274900
11	H	-1.46349200	-3.24906400	-1.10765800
12	C	-4.98875400	-3.95433500	0.35966900
13	H	-4.14547600	-3.48414800	2.27808400
14	C	-4.77217700	-4.07682200	-1.01400700
15	H	-3.31412700	-3.90707500	-2.60804900
16	H	-5.98032800	-4.14966100	0.78026900
17	H	-5.59133900	-4.36850600	-1.67868900
18	C	-5.42579800	4.14650700	-0.94142500
19	H	-6.29755300	3.85333200	-1.56901300
20	H	-5.02727600	5.08923600	-1.37362700
21	O	-5.83738800	4.32942500	0.40502400
22	H	-6.64561500	4.86686500	0.40490800

23

24

Ru-N_{ytide}

25	Zero-point correction=		0.657449 (Hartree/Particle)
26	Thermal correction to Energy=		0.699292
27	Thermal correction to Enthalpy=		0.700237
28	Thermal correction to Gibbs Free Energy=		0.580656
29	Sum of electronic and zero-point Energies=		-2612.784711
30	Sum of electronic and thermal Energies=		-2612.742867
31	Sum of electronic and thermal Enthalpies=		-2612.741923
32	Sum of electronic and thermal Free Energies=		-2612.861504

33

Cartesian Coordinates

34	Atom	X	Y	Z
35	-----			
36	C	3.89348900	-1.98854900	-1.14004200

1	C	4.24710900	-0.62492500	-0.98041200
2	C	3.97301100	0.10596100	0.21916100
3	C	3.22980800	-0.58553100	1.22115700
4	C	2.85826100	-1.95538700	1.08286600
5	C	3.18125200	-2.66993300	-0.10562300
6	H	4.08607000	-2.49095900	-2.09004000
7	H	4.69575500	-0.10695000	-1.82920800
8	H	2.90464800	-0.04602100	2.11318700
9	H	2.25899400	-2.42646000	1.86300900
10	Ru	2.05924900	-0.77082300	-0.62473800
11	Cl	0.32195900	-2.21416200	-1.60806800
12	Cl	1.76451800	0.67425700	-2.61836700
13	C	0.30682800	0.38240000	0.31250700
14	C	0.75777300	1.72247500	0.85804800
15	C	0.97898100	1.95268400	2.23359600
16	C	0.96368700	2.81415500	-0.01372600
17	C	1.38050000	3.20670200	2.70645800
18	H	0.83025800	1.14047200	2.94436600
19	C	1.35976500	4.06557000	0.46225200
20	H	0.84469200	2.68803200	-1.09036300
21	C	1.57183000	4.27565300	1.82810200
22	H	1.53714900	3.34407900	3.78153900
23	H	1.50622200	4.88352400	-0.25048500
24	H	1.88056500	5.25718800	2.20085600
25	C	-0.27705400	-0.57390300	1.32258300
26	O	0.26503500	-0.86822800	2.37184100
27	O	-1.47038700	-1.06192500	0.93578100
28	C	-2.21823400	-2.08780000	1.69014600
29	C	4.44532700	1.53244100	0.45918100
30	H	3.62295700	2.05298900	0.97867400
31	C	5.66220000	1.52099600	1.40811400
32	H	6.52030000	0.99599600	0.94859100
33	H	5.98018900	2.55408200	1.63771200
34	H	5.43092600	1.01797900	2.36397500
35	C	4.75584400	2.31641900	-0.82261400
36	H	3.91282200	2.27791600	-1.53230600

1	H	4.95197900	3.37414900	-0.57353700
2	H	5.65845300	1.92893300	-1.33127200
3	C	2.77246300	-4.10658300	-0.27871600
4	H	3.61686400	-4.76425700	0.00474700
5	H	1.90995500	-4.35643900	0.35861700
6	H	2.49841500	-4.31995600	-1.32353700
7	C	-4.13876200	3.00317200	-0.97507300
8	C	-3.52041000	2.54316800	-2.14735100
9	C	-2.37304300	1.75378200	-2.08448800
10	C	-1.83409800	1.40994800	-0.83987800
11	C	-2.43109100	1.86352700	0.33342600
12	C	-3.58000800	2.65843300	0.26012400
13	H	-3.93529000	2.80583400	-3.12664900
14	H	-1.89320400	1.40351800	-3.00383500
15	H	-2.00874600	1.61383400	1.30626500
16	H	-4.05346300	3.02167200	1.17357900
17	N	-0.63704100	0.55152500	-0.85979000
18	H	-0.01454400	0.83209500	-1.66288600
19	H	-0.88662700	-0.42832000	-1.12096400
20	C	-1.36303300	-3.35855700	1.83508100
21	H	-0.95589900	-3.65727400	0.85530600
22	H	-0.52761600	-3.19245500	2.53218100
23	H	-1.99395400	-4.17873900	2.21903400
24	C	-2.60056600	-1.51640100	3.05996700
25	H	-3.22696300	-0.61469000	2.95366400
26	H	-3.16315500	-2.26466200	3.64273600
27	H	-1.69226000	-1.25704600	3.62156800
28	C	-3.43359500	-2.38219900	0.79759200
29	C	-3.23481300	-2.69358300	-0.55998400
30	C	-4.74542700	-2.39622700	1.29473500
31	C	-4.31382800	-3.00509000	-1.39001100
32	H	-2.22287900	-2.68984100	-0.97400800
33	C	-5.82752500	-2.71348100	0.46441500
34	H	-4.94613900	-2.15900700	2.34114300
35	C	-5.61745000	-3.01792200	-0.88160700
36	H	-4.13179100	-3.24126700	-2.44336700

1	H	-6.84101100	-2.71753100	0.87842800
2	H	-6.46321900	-3.26417300	-1.53155500
3	C	-5.38816300	3.85234800	-1.06336700
4	H	-6.18426200	3.26202500	-1.56798800
5	H	-5.18031900	4.72786700	-1.71648200
6	O	-5.79279800	4.25804300	0.22481800
7	H	-6.60464700	4.78210600	0.14645100

8

9

TS_Ru-O_{ylide}

10	Zero-point correction=		0.653886 (Hartree/Particle)	
11	Thermal correction to Energy=			0.696034
12	Thermal correction to Enthalpy=			0.696978
13	Thermal correction to Gibbs Free Energy=			0.576585
14	Sum of electronic and zero-point Energies=			-2612.750471
15	Sum of electronic and thermal Energies=			-2612.708323
16	Sum of electronic and thermal Enthalpies=			-2612.707378
17	Sum of electronic and thermal Free Energies=			-2612.827772

18

Cartesian Coordinates

19	Atom	X	Y	Z
20	-----			
21	C	3.63276700	0.25562800	-2.60226500
22	C	3.92012200	0.92404200	-1.36750500
23	C	4.00226900	0.23510900	-0.13415700
24	C	3.53116200	-1.12098100	-0.14942400
25	C	3.14907300	-1.77039000	-1.35061700
26	C	3.27140000	-1.09809000	-2.61863300
27	H	3.61736700	0.83402000	-3.52856000
28	H	4.12973100	1.99367000	-1.40437100
29	H	3.44320700	-1.67632800	0.78653900
30	H	2.78068100	-2.79666900	-1.31024800
31	Ru	1.84313300	0.01779800	-1.03833200
32	Cl	0.00494900	-0.95029100	-2.27572000
33	Cl	0.88321900	2.24028200	-1.44793900
34	C	0.77175300	-0.29179400	0.63109700
35	C	1.04156700	0.38703000	1.92014700
36	C	0.96810200	-0.30045700	3.15433800

1	C	1.36976800	1.76162900	1.94787500
2	C	1.23250300	0.35399000	4.35879900
3	H	0.72743900	-1.36503400	3.17485900
4	C	1.60773200	2.41788600	3.15540800
5	H	1.40552600	2.30725200	1.00145100
6	C	1.54902300	1.71650900	4.36568700
7	H	1.18445100	-0.20412500	5.29894000
8	H	1.84571600	3.48618100	3.15188000
9	H	1.74586300	2.23070900	5.31174600
10	C	0.25121200	-1.71285700	0.78383100
11	O	1.07523000	-2.59087300	0.97357900
12	O	-1.05596800	-1.87707400	0.77068600
13	C	-1.70380500	-3.20332400	0.78671000
14	C	4.59160600	0.83253900	1.13468600
15	H	3.89485300	0.60104600	1.95875500
16	C	5.93218700	0.13676700	1.45535600
17	H	6.67645300	0.32361500	0.65949700
18	H	6.34587700	0.52010100	2.40553000
19	H	5.81307700	-0.95628600	1.55682200
20	C	4.77530700	2.35406100	1.08334900
21	H	3.84019500	2.87315400	0.81606900
22	H	5.09822100	2.72704100	2.07093200
23	H	5.55159600	2.64459100	0.35183900
24	C	2.90564600	-1.81305500	-3.88634300
25	H	3.48506800	-2.74897900	-3.98410000
26	H	1.83022600	-2.06864600	-3.86008800
27	H	3.09158000	-1.18463500	-4.77225800
28	H	-0.73122300	1.28325900	-0.48676700
29	C	-1.10935200	-4.11432100	-0.30260300
30	H	-1.07055200	-3.57828000	-1.26469700
31	H	-0.09272100	-4.44333300	-0.04047300
32	H	-1.75833000	-4.99963600	-0.41716500
33	C	-1.52327800	-3.80428800	2.18497300
34	H	-1.99511300	-3.16791300	2.95288600
35	H	-1.97517500	-4.80861900	2.23828200
36	H	-0.45022300	-3.90785000	2.40699800

1	C	-3.16357400	-2.89237200	0.43474600
2	C	-3.44581300	-1.94676400	-0.56719100
3	C	-4.23318100	-3.57617200	1.03261500
4	C	-4.76433700	-1.70061500	-0.95948200
5	H	-2.62622100	-1.39351200	-1.03244200
6	C	-5.55340800	-3.32892000	0.63818300
7	H	-4.05143300	-4.31587500	1.81585800
8	C	-5.82435100	-2.39077100	-0.36057500
9	H	-4.96134400	-0.95803500	-1.73901800
10	H	-6.37186100	-3.87459900	1.11887800
11	H	-6.85641800	-2.19734700	-0.67060100
12	O	-1.12318000	0.69021100	0.20392000
13	C	-1.87220900	1.45380500	1.15341700
14	H	-2.33349300	0.71410100	1.82559300
15	H	-1.19222300	2.08902100	1.75187700
16	C	-2.92328200	2.30798200	0.48802800
17	C	-2.59680500	3.56512000	-0.04765300
18	C	-4.24685500	1.86282400	0.34668200
19	C	-3.55003800	4.35074300	-0.69170800
20	H	-1.56954500	3.93608400	0.03143900
21	C	-5.21196000	2.64193000	-0.28894200
22	H	-4.53067700	0.88275100	0.74311100
23	C	-4.88081900	3.90349900	-0.82495800
24	H	-3.26490200	5.32481900	-1.10339100
25	H	-6.23815500	2.26986000	-0.38070700
26	N	-5.82476000	4.66199700	-1.50232400
27	H	-6.80139600	4.45264300	-1.32360500
28	H	-5.62896200	5.65123000	-1.61490900

29

30

Ru-O_{ylide}

31	Zero-point correction=		0.654603 (Hartree/Particle)
32	Thermal correction to Energy=		0.696528
33	Thermal correction to Enthalpy=		0.697473
34	Thermal correction to Gibbs Free Energy=		0.578085
35	Sum of electronic and zero-point Energies=		-2612.766570
36	Sum of electronic and thermal Energies=		-2612.724644

1	Sum of electronic and thermal Enthalpies=			-2612.723700
2	Sum of electronic and thermal Free Energies=			-2612.843087
3	Cartesian Coordinates			
4	Atom	X	Y	Z
5	-----			
6	C	3.15766800	-1.11540000	-2.63221200
7	C	3.69118600	-0.06086400	-1.84483800
8	C	3.84434800	-0.15965600	-0.42663700
9	C	3.29589900	-1.32674600	0.18142800
10	C	2.72991000	-2.38953100	-0.58372200
11	C	2.66498000	-2.29642800	-2.00451100
12	H	3.03835500	-0.98155900	-3.70908300
13	H	3.96527200	0.86800000	-2.34779400
14	H	3.28577600	-1.40542400	1.27116800
15	H	2.28896200	-3.24330900	-0.06783100
16	Ru	1.66746800	-0.49322100	-1.03637500
17	Cl	-0.37632600	-1.26073000	-2.11042900
18	Cl	0.96885800	1.80279500	-1.72118800
19	C	0.39918600	-0.13642100	0.78398400
20	C	1.15461000	0.56704700	1.89735100
21	C	1.62192700	-0.09326600	3.05250100
22	C	1.41164200	1.95221500	1.79604800
23	C	2.30428900	0.60206000	4.05753200
24	H	1.45172200	-1.16402700	3.16546800
25	C	2.08236400	2.64474500	2.80606000
26	H	1.09965000	2.49298100	0.90024100
27	C	2.53529700	1.97522600	3.94800300
28	H	2.65006100	0.05643500	4.94171800
29	H	2.26049300	3.71894400	2.69073400
30	H	3.06291200	2.51679500	4.73921200
31	C	-0.18899500	-1.47640600	1.16432400
32	O	0.49434000	-2.38345200	1.60206500
33	O	-1.51480200	-1.54184800	1.00561400
34	C	-2.29462800	-2.77781400	1.19323000
35	C	4.56024000	0.88690900	0.41320200
36	H	4.00585600	0.96429100	1.36376100

1	C	5.98561900	0.39757900	0.74555600
2	H	6.59143200	0.28418300	-0.17266100
3	H	6.49878700	1.12245700	1.40336600
4	H	5.97131100	-0.57822700	1.26293300
5	C	4.59390100	2.28390800	-0.22093600
6	H	3.58726100	2.61175500	-0.52984900
7	H	4.99015500	3.01528700	0.50548100
8	H	5.25497800	2.31541200	-1.10699000
9	C	2.06634700	-3.40664600	-2.82198300
10	H	2.87400200	-4.07987800	-3.16969400
11	H	1.35151800	-3.99714600	-2.22859600
12	H	1.53357800	-3.01174600	-3.70053500
13	H	-0.32527100	1.31299200	-0.51165400
14	C	-1.71686100	-3.92122400	0.33944200
15	H	-1.54784600	-3.57522400	-0.69320100
16	H	-0.76238500	-4.28009800	0.75236300
17	H	-2.43978200	-4.75527500	0.32176800
18	C	-2.28776700	-3.13587200	2.68334100
19	H	-2.74040200	-2.33223700	3.28895200
20	H	-2.85198600	-4.06673800	2.86064500
21	H	-1.25251100	-3.29689500	3.01791300
22	C	-3.68449400	-2.40314400	0.65966600
23	C	-3.78798500	-1.75170100	-0.58379300
24	C	-4.86574600	-2.73443600	1.33954900
25	C	-5.03890000	-1.44725900	-1.12657600
26	H	-2.87695700	-1.48033600	-1.12592700
27	C	-6.11936500	-2.42838500	0.79472700
28	H	-4.82639800	-3.23905000	2.30729200
29	C	-6.21177100	-1.78367200	-0.44007400
30	H	-5.09580100	-0.94596000	-2.09841700
31	H	-7.02684000	-2.69702400	1.34509300
32	H	-7.19129400	-1.54557700	-0.86706200
33	O	-0.68583600	0.75963300	0.29975200
34	C	-1.72140400	1.40858200	1.15785100
35	H	-2.42925400	0.60046000	1.37277700
36	H	-1.21393500	1.73282300	2.07722100

1	C	-2.34129600	2.54825900	0.41932500
2	C	-1.90944700	3.87039000	0.62145300
3	C	-3.36838800	2.32658400	-0.51576600
4	C	-2.47800600	4.93275600	-0.07400100
5	H	-1.11336600	4.07411300	1.34537000
6	C	-3.94090000	3.37908000	-1.22078500
7	H	-3.72584300	1.30682800	-0.69056300
8	C	-3.50491100	4.70726500	-1.01654600
9	H	-2.12361700	5.95332300	0.10370200
10	H	-4.73737700	3.17955200	-1.94501400
11	N	-4.04302500	5.74891700	-1.74222800
12	H	-4.91672000	5.59573400	-2.23268300
13	H	-3.88590500	6.69649700	-1.41864700

14

15

S₀-2a

16	Zero-point correction=		0.295672 (Hartree/Particle)	
17	Thermal correction to Energy=			0.314549
18	Thermal correction to Enthalpy=			0.315493
19	Thermal correction to Gibbs Free Energy=			0.245413
20	Sum of electronic and zero-point Energies=			-917.067720
21	Sum of electronic and thermal Energies=			-917.048844
22	Sum of electronic and thermal Enthalpies=			-917.047900
23	Sum of electronic and thermal Free Energies=			-917.117980

24

Cartesian Coordinates

25	Atom	X	Y	Z
26	-----			
27	C	0.63206800	-0.73765800	0.00013100
28	C	1.61828500	0.36077600	-0.00004600
29	O	-0.62944200	-0.24576100	0.00019600
30	C	3.09360900	0.23734400	-0.00001600
31	C	3.72161200	-1.02145400	-0.00036800
32	C	3.90268700	1.38974000	0.00034400
33	C	5.11316600	-1.11056600	-0.00035400
34	H	3.11690600	-1.91777000	-0.00062800
35	C	5.29076200	1.28785400	0.00034300
36	H	3.45156700	2.37819500	0.00064700

1	C	5.90752400	0.03572100	-0.00000600
2	H	5.57645600	-2.09379000	-0.00063200
3	H	5.89016400	2.19433500	0.00062900
4	H	6.99096600	-0.04360900	-0.00000200
5	O	0.93084400	-1.91760100	0.00021100
6	N	0.69011500	2.63327500	-0.00032300
7	N	1.10629800	1.57338200	-0.00019500
8	C	-1.80746800	-1.12792900	0.00006600
9	C	-1.79718400	-1.98031500	1.27910000
10	H	-2.71912200	-2.56562100	1.34410300
11	H	-0.94653900	-2.66336600	1.28375200
12	H	-1.74696500	-1.33239700	2.16001800
13	C	-1.79705000	-1.98020200	-1.27903200
14	H	-0.94638800	-2.66324700	-1.28367400
15	H	-2.71892300	-2.56563200	-1.34406900
16	H	-1.74686800	-1.33227900	-2.15993300
17	C	-3.01382000	-0.17970500	0.00003300
18	C	-2.88252600	1.21375100	0.00005300
19	C	-4.30812800	-0.72370100	-0.00002800
20	C	-4.01084800	2.03773700	-0.00000300
21	H	-1.89733300	1.66152100	0.00012400
22	C	-5.43404900	0.09750400	-0.00008500
23	H	-4.44604700	-1.80164900	-0.00003000
24	C	-5.29047800	1.48615200	-0.00007800
25	H	-3.88168800	3.11693500	0.00001400
26	H	-6.42440400	-0.35019300	-0.00013800
27	H	-6.16684800	2.12857600	-0.00012800
28				
29			*S_n-2a	
30	Zero-point correction=		0.294007 (Hartree/Particle)	
31	Thermal correction to Energy=			0.311111
32	Thermal correction to Enthalpy=			0.312056
33	Thermal correction to Gibbs Free Energy=			0.248521
34	Sum of electronic and zero-point Energies=			-916.976833
35	Sum of electronic and thermal Energies=			-916.959728
36	Sum of electronic and thermal Enthalpies=			-916.958784

1	Sum of electronic and thermal Free Energies=			-917.022318
2		Cartesian Coordinates		
3	Atom	X	Y	Z
4	-----			
5	C	0.63206800	-0.73765800	0.00013100
6	C	1.61828500	0.36077600	-0.00004600
7	O	-0.62944200	-0.24576100	0.00019600
8	C	3.09360900	0.23734400	-0.00001600
9	C	3.72161200	-1.02145400	-0.00036800
10	C	3.90268700	1.38974000	0.00034400
11	C	5.11316600	-1.11056600	-0.00035400
12	H	3.11690600	-1.91777000	-0.00062800
13	C	5.29076200	1.28785400	0.00034300
14	H	3.45156700	2.37819500	0.00064700
15	C	5.90752400	0.03572100	-0.00000600
16	H	5.57645600	-2.09379000	-0.00063200
17	H	5.89016400	2.19433500	0.00062900
18	H	6.99096600	-0.04360900	-0.00000200
19	O	0.93084400	-1.91760100	0.00021100
20	N	0.69011500	2.63327500	-0.00032300
21	N	1.10629800	1.57338200	-0.00019500
22	C	-1.80746800	-1.12792900	0.00006600
23	C	-1.79718400	-1.98031500	1.27910000
24	H	-2.71912200	-2.56562100	1.34410300
25	H	-0.94653900	-2.66336600	1.28375200
26	H	-1.74696500	-1.33239700	2.16001800
27	C	-1.79705000	-1.98020200	-1.27903200
28	H	-0.94638800	-2.66324700	-1.28367400
29	H	-2.71892300	-2.56563200	-1.34406900
30	H	-1.74686800	-1.33227900	-2.15993300
31	C	-3.01382000	-0.17970500	0.00003300
32	C	-2.88252600	1.21375100	0.00005300
33	C	-4.30812800	-0.72370100	-0.00002800
34	C	-4.01084800	2.03773700	-0.00000300
35	H	-1.89733300	1.66152100	0.00012400
36	C	-5.43404900	0.09750400	-0.00008500

1	H	-4.44604700	-1.80164900	-0.00003000
2	C	-5.29047800	1.48615200	-0.00007800
3	H	-3.88168800	3.11693500	0.00001400
4	H	-6.42440400	-0.35019300	-0.00013800
5	H	-6.16684800	2.12857600	-0.00012800
6				
7			S_I-2a	
8	Zero-point correction=		0.295197 (Hartree/Particle)	
9	Thermal correction to Energy=			0.313867
10	Thermal correction to Enthalpy=			0.314811
11	Thermal correction to Gibbs Free Energy=			0.246057
12	Sum of electronic and zero-point Energies=			-917.006484
13	Sum of electronic and thermal Energies=			-916.987814
14	Sum of electronic and thermal Enthalpies=			-916.986870
15	Sum of electronic and thermal Free Energies=			-917.055625
16			Cartesian Coordinates	
17	Atom	X	Y	Z
18	-----			
19	C	-0.61160500	-0.70019500	0.00044000
20	C	-1.59669500	0.40871300	0.00018900
21	O	0.65278500	-0.23189900	0.00011300
22	C	-3.01855100	0.23741800	0.00001900
23	C	-3.61638200	-1.06535200	-0.00039500
24	C	-3.90862300	1.35808000	0.00021400
25	C	-4.99142400	-1.21941000	-0.00060000
26	H	-2.96952200	-1.93006700	-0.00054000
27	C	-5.28163700	1.18121600	0.00002000
28	H	-3.50536200	2.36033700	0.00052300
29	C	-5.83875500	-0.10367200	-0.00039200
30	H	-5.41323600	-2.22051000	-0.00093200
31	H	-5.92893800	2.05363200	0.00020000
32	H	-6.91729100	-0.23355300	-0.00054500
33	O	-0.90622900	-1.88747700	0.00072700
34	N	-1.38259600	2.79311500	-0.00005600
35	N	-0.96692200	1.68849200	0.00011700
36	C	1.81890200	-1.12263100	0.00017100

1	C	1.80661900	-1.97614600	-1.27858400
2	H	2.72756400	-2.56337600	-1.34245900
3	H	0.95427100	-2.65701100	-1.28349200
4	H	1.75877500	-1.32799400	-2.15946800
5	C	1.80670700	-1.97578900	1.27915900
6	H	0.95432400	-2.65661100	1.28433500
7	H	2.72762600	-2.56305100	1.34310700
8	H	1.75897800	-1.32739500	2.15987100
9	C	3.02802700	-0.17700100	-0.00002100
10	C	2.89128700	1.21647300	-0.00019200
11	C	4.32251000	-0.71965700	-0.00004900
12	C	4.01911400	2.04129400	-0.00038400
13	H	1.90225800	1.65692000	-0.00016600
14	C	5.44708600	0.10376900	-0.00024100
15	H	4.46208800	-1.79759700	0.00007600
16	C	5.30009100	1.49205400	-0.00041000
17	H	3.88873200	3.12046000	-0.00051100
18	H	6.43857300	-0.34167000	-0.00025900
19	H	6.17531800	2.13625700	-0.00056000

20

21

T_n-2a

22	Zero-point correction=		0.293214 (Hartree/Particle)
23	Thermal correction to Energy=		0.310757
24	Thermal correction to Enthalpy=		0.311701
25	Thermal correction to Gibbs Free Energy=		0.246257
26	Sum of electronic and zero-point Energies=		-917.019944
27	Sum of electronic and thermal Energies=		-917.002401
28	Sum of electronic and thermal Enthalpies=		-917.001457
29	Sum of electronic and thermal Free Energies=		-917.066901

30

Cartesian Coordinates

31	Atom	X	Y	Z
32	-----			
33	C	-0.61150900	-0.70047100	0.00023300
34	C	-1.59651400	0.40855100	0.00019600
35	O	0.65296600	-0.23233800	0.00011400
36	C	-3.01839600	0.23742000	-0.00000500

1	C	-3.61637000	-1.06527100	-0.00073200
2	C	-3.90837100	1.35815300	0.00047700
3	C	-4.99143300	-1.21918100	-0.00094900
4	H	-2.96961300	-1.93006200	-0.00110000
5	C	-5.28141500	1.18144200	0.00026900
6	H	-3.50502400	2.36036400	0.00102700
7	C	-5.83866600	-0.10337400	-0.00044900
8	H	-5.41333000	-2.22024200	-0.00152200
9	H	-5.92863300	2.05392200	0.00067700
10	H	-6.91721700	-0.23313300	-0.00061600
11	O	-0.90626800	-1.88769500	0.00042600
12	N	-1.38215500	2.79295800	0.00046900
13	N	-0.96663900	1.68827300	0.00041600
14	C	1.81908500	-1.12308400	0.00025300
15	C	1.80694000	-1.97664000	-1.27849900
16	H	2.72786800	-2.56390400	-1.34225400
17	H	0.95458100	-2.65748600	-1.28350700
18	H	1.75922600	-1.32852600	-2.15942100
19	C	1.80707000	-1.97608800	1.27936600
20	H	0.95471800	-2.65693800	1.28474500
21	H	2.72800800	-2.56332000	1.34329100
22	H	1.75943200	-1.32760100	2.16001800
23	C	3.02789700	-0.17712200	-0.00003200
24	C	2.89058500	1.21628000	-0.00041200
25	C	4.32258700	-0.71928600	0.00007800
26	C	4.01807700	2.04155700	-0.00068100
27	H	1.90135900	1.65631000	-0.00048800
28	C	5.44682900	0.10459400	-0.00018900
29	H	4.46259400	-1.79716800	0.00037600
30	C	5.29927200	1.49282400	-0.00057400
31	H	3.88725900	3.12067000	-0.00097500
32	H	6.43849500	-0.34044400	-0.00009400
33	H	6.17424100	2.13737700	-0.00078500
34				
35			T_I-2a	
36	Zero-point correction=			0.293443 (Hartree/Particle)

1	Thermal correction to Energy=			0.312462
2	Thermal correction to Enthalpy=			0.313406
3	Thermal correction to Gibbs Free Energy=			0.243275
4	Sum of electronic and zero-point Energies=			-917.023262
5	Sum of electronic and thermal Energies=			-917.004242
6	Sum of electronic and thermal Enthalpies=			-917.003298
7	Sum of electronic and thermal Free Energies=			-917.073430
8	Cartesian Coordinates			
9	Atom	X	Y	Z
10	-----			
11	C	-0.65989800	-0.63094300	0.49945800
12	C	-1.66453000	0.48294200	0.43206800
13	O	0.56757700	-0.19842800	0.19196900
14	C	-3.02856100	0.27451600	0.01868500
15	C	-3.50548800	-0.98720600	-0.42769600
16	C	-3.93879500	1.36737900	0.02030900
17	C	-4.82036700	-1.13613900	-0.84693900
18	H	-2.83856700	-1.83867100	-0.42539000
19	C	-5.24933500	1.20277700	-0.39953000
20	H	-3.58964600	2.33651400	0.35654000
21	C	-5.70082800	-0.04881900	-0.83642800
22	H	-5.16455400	-2.10989900	-1.18388400
23	H	-5.92665200	2.05208100	-0.38771000
24	H	-6.72879900	-0.17467000	-1.16474200
25	O	-0.96606600	-1.77261900	0.79789200
26	N	-0.27159800	2.19726300	1.22617000
27	N	-1.32782600	1.78529600	0.81815000
28	C	1.74774600	-1.08671700	0.22485500
29	C	1.55046500	-2.19641400	-0.81901000
30	H	2.44491500	-2.82283500	-0.87626500
31	H	0.70222300	-2.82915800	-0.55365000
32	H	1.38209100	-1.75692300	-1.80724900
33	C	1.92827700	-1.63680100	1.64819500
34	H	2.86695500	-2.19659200	1.70496900
35	H	1.98544500	-0.80993300	2.36293400
36	H	1.10516200	-2.29844900	1.92340200

1	C	2.93070100	-0.18268700	-0.14328600
2	C	2.81082500	1.20888400	-0.24033200
3	C	4.19193900	-0.76044000	-0.35753700
4	C	3.92085800	1.99660500	-0.55526600
5	H	1.85300400	1.67983000	-0.05942300
6	C	5.29884900	0.02679400	-0.67045300
7	H	4.32137300	-1.83643700	-0.27697000
8	C	5.16720100	1.41254100	-0.77439800
9	H	3.80399400	3.07495300	-0.62518700
10	H	6.26423000	-0.44538400	-0.83310400
11	H	6.02836000	2.02839600	-1.01957400

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14	Zero-point correction=	0.290874 (Hartree/Particle)
15	Thermal correction to Energy=	0.310337
16	Thermal correction to Enthalpy=	0.311282
17	Thermal correction to Gibbs Free Energy=	0.239725
18	Sum of electronic and zero-point Energies=	-917.009530
19	Sum of electronic and thermal Energies=	-916.990067
20	Sum of electronic and thermal Enthalpies=	-916.989123
21	Sum of electronic and thermal Free Energies=	-917.060679

22

Cartesian Coordinates

23	Atom	X	Y	Z
24	-----			
25	C	-0.66481100	-0.74735200	0.30763000
26	C	-1.67089100	0.31422800	0.25933900
27	O	0.57315600	-0.26037800	0.10613700
28	C	-3.05553800	0.22944200	-0.01995700
29	C	-3.65976800	-1.00993400	-0.39280600
30	C	-3.88755500	1.38592000	0.02180500
31	C	-5.00946900	-1.07084900	-0.70444200
32	H	-3.04721900	-1.90211800	-0.41433900
33	C	-5.23515000	1.30356700	-0.29173600
34	H	-3.45298700	2.33743300	0.30175900
35	C	-5.80759200	0.07879500	-0.65743600
36	H	-5.44847900	-2.02479200	-0.98397200

1	H	-5.84872000	2.19943900	-0.25241000
2	H	-6.86459900	0.02110400	-0.90155000
3	O	-0.94614500	-1.92222300	0.50886700
4	N	-0.16780100	2.15819600	1.37798500
5	N	-1.19192900	1.95627100	0.92265500
6	C	1.77046600	-1.11340200	0.17820500
7	C	1.68064500	-2.21088200	-0.89516000
8	H	2.61769600	-2.77491300	-0.92501100
9	H	0.86060900	-2.89844700	-0.68397000
10	H	1.52974400	-1.75812900	-1.88042200
11	C	1.88264900	-1.68412900	1.60039700
12	H	2.81405900	-2.24793900	1.70644500
13	H	1.89517100	-0.86812500	2.32963900
14	H	1.04597700	-2.35097200	1.81666000
15	C	2.94537900	-0.17543200	-0.12724600
16	C	2.76821300	1.17144200	-0.46408300
17	C	4.25307100	-0.68423000	-0.08624200
18	C	3.86766800	1.98543000	-0.74775100
19	H	1.77004800	1.58750100	-0.49825800
20	C	5.34987300	0.12758500	-0.36976200
21	H	4.42483600	-1.72668200	0.16880700
22	C	5.16173000	1.47022300	-0.70262300
23	H	3.70504900	3.02923000	-1.00369700
24	H	6.35205300	-0.29121800	-0.32984700
25	H	6.01526700	2.10563500	-0.92314000

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28	Zero-point correction=	0.284213 (Hartree/Particle)
29	Thermal correction to Energy=	0.301281
30	Thermal correction to Enthalpy=	0.302225
31	Thermal correction to Gibbs Free Energy=	0.236644
32	Sum of electronic and zero-point Energies=	-807.515685
33	Sum of electronic and thermal Energies=	-807.498618
34	Sum of electronic and thermal Enthalpies=	-807.497674
35	Sum of electronic and thermal Free Energies=	-807.563255

36

Cartesian Coordinates

1	Atom	X	Y	Z
2	-----			
3	C	-0.72691400	-0.66791000	-0.00031000
4	C	-1.72529600	0.37304100	-0.00029900
5	O	0.51891900	-0.14786200	-0.00030200
6	C	-3.12929400	0.41321600	-0.00012100
7	C	-3.92883800	-0.76998800	0.00006100
8	C	-3.79299400	1.67316800	-0.00012700
9	C	-5.31282600	-0.67632600	0.00022900
10	H	-3.42852100	-1.73112900	0.00006600
11	C	-5.17778200	1.74511500	0.00004200
12	H	-3.19316200	2.57830300	-0.00026700
13	C	-5.94602700	0.57352700	0.00022100
14	H	-5.90938200	-1.58483400	0.00036800
15	H	-5.66694900	2.71536100	0.00003500
16	H	-7.03074100	0.63426700	0.00035400
17	O	-1.00632100	-1.86330900	0.00000700
18	C	1.72038400	-0.98861600	-0.00004700
19	C	1.74000700	-1.84311600	-1.27813600
20	H	2.67963300	-2.40007600	-1.34175200
21	H	0.91037700	-2.55215900	-1.28191600
22	H	1.66893900	-1.19848600	-2.15997500
23	C	1.73969900	-1.84282100	1.27824400
24	H	2.67933200	-2.39973000	1.34222100
25	H	1.66839400	-1.19798900	2.15991700
26	H	0.91009200	-2.55189000	1.28198500
27	C	2.89130100	0.00323100	-0.00000400
28	C	2.70003600	1.39006700	-0.00008700
29	C	4.20651700	-0.48676900	0.00015100
30	C	3.79311600	2.26012600	-0.00002000
31	H	1.69329400	1.78871000	-0.00020800
32	C	5.29716400	0.38111000	0.00021700
33	H	4.38879700	-1.55827000	0.00022400
34	C	5.09500600	1.76245700	0.00013100
35	H	3.62010500	3.33334600	-0.00008900
36	H	6.30569000	-0.02419900	0.00033700

1	H	5.94377100	2.44108300	0.00018300
2				
3				
3				
4	Zero-point correction=			0.291550 (Hartree/Particle)
5	Thermal correction to Energy=			0.311007
6	Thermal correction to Enthalpy=			0.311952
7	Thermal correction to Gibbs Free Energy=			0.241418
8	Sum of electronic and zero-point Energies=			-917.015110
9	Sum of electronic and thermal Energies=			-916.995653
10	Sum of electronic and thermal Enthalpies=			-916.994709
11	Sum of electronic and thermal Free Energies=			-917.065242
12				
12				
13	Atom	X	Y	Z
14				
15	C	0.66769700	-0.82298800	0.59886200
16	C	1.74008600	0.09342000	0.90250000
17	O	-0.53676200	-0.29693200	0.29428700
18	C	3.00339300	0.08413900	0.19530600
19	C	3.27348900	-0.77657400	-0.89503600
20	C	4.03756100	0.93574400	0.64719800
21	C	4.52736400	-0.78819700	-1.49492500
22	H	2.50038400	-1.45857600	-1.23262400
23	C	5.27729900	0.95227500	0.01902400
24	H	3.84038500	1.58077400	1.49838400
25	C	5.52573200	0.08474200	-1.04962700
26	H	4.72717600	-1.46605200	-2.32020500
27	H	6.05760700	1.62146800	0.37035000
28	H	6.50034700	0.08297000	-1.53060700
29	O	0.91395200	-2.01641100	0.77407200
30	N	0.73541600	2.86733400	1.08287900
31	N	0.97629400	1.88850800	0.61034000
32	C	-1.74806400	-1.12970900	0.25250100
33	C	-1.97914400	-1.73944900	1.64418900
34	H	-2.92038300	-2.29679300	1.66236800
35	H	-1.16538500	-2.41860700	1.90357800
36	H	-2.04067900	-0.94545000	2.39510700

1	C	-1.59834400	-2.20019300	-0.84184100
2	H	-0.80795700	-2.90731000	-0.58654000
3	H	-2.54005500	-2.74509300	-0.95995100
4	H	-1.36348900	-1.72407500	-1.79949600
5	C	-2.88265600	-0.16420700	-0.11450900
6	C	-2.65710700	1.18165400	-0.42548800
7	C	-4.20141100	-0.64324300	-0.16273600
8	C	-3.71779400	2.02362100	-0.76889800
9	H	-1.64888300	1.57355500	-0.39848800
10	C	-5.26022900	0.19576600	-0.50547000
11	H	-4.41134900	-1.68421500	0.06802000
12	C	-5.02315400	1.53735700	-0.81015300
13	H	-3.51663400	3.06565800	-1.00432200
14	H	-6.27170700	-0.20112300	-0.53373400
15	H	-5.84718600	2.19374700	-1.07663000

16

17

¹carbene

18	Zero-point correction=		0.284230 (Hartree/Particle)	
19	Thermal correction to Energy=			0.301422
20	Thermal correction to Enthalpy=			0.302366
21	Thermal correction to Gibbs Free Energy=			0.236916
22	Sum of electronic and zero-point Energies=			-807.508606
23	Sum of electronic and thermal Energies=			-807.491414
24	Sum of electronic and thermal Enthalpies=			-807.490470
25	Sum of electronic and thermal Free Energies=			-807.555920

26

Cartesian Coordinates

27	Atom	X	Y	Z
28	-----			
29	C	0.78665400	1.22911500	-0.50962000
30	C	1.85732500	0.56101300	-1.18780100
31	O	-0.32866800	0.48559000	-0.35018300
32	C	2.94697100	-0.00725300	-0.46473200
33	C	3.09035100	0.04382300	0.95075200
34	C	3.94373100	-0.68650900	-1.21397200
35	C	4.17489300	-0.55260200	1.57553800
36	H	2.34600100	0.57911800	1.53280500

1	C	5.01450900	-1.30905500	-0.58424400
2	H	3.82998500	-0.70742400	-2.29315000
3	C	5.12980000	-1.23551000	0.80800000
4	H	4.28393300	-0.50185800	2.65516700
5	H	5.76478600	-1.83741300	-1.16513500
6	H	5.97328400	-1.71041700	1.30287700
7	O	0.92664900	2.42136900	-0.23616900
8	C	-1.61060800	1.06998300	0.06115800
9	C	-2.02459000	2.14574100	-0.95579300
10	H	-3.02388000	2.52291600	-0.71712400
11	H	-1.31921900	2.97862500	-0.94270800
12	H	-2.05537000	1.71604400	-1.96195000
13	C	-1.46972800	1.63409600	1.48471400
14	H	-0.76174200	2.46469100	1.49624200
15	H	-2.43806500	1.98891200	1.85067900
16	H	-1.11959000	0.85019200	2.16441600
17	C	-2.60449400	-0.09805100	0.03869800
18	C	-2.23636900	-1.38766300	-0.36264100
19	C	-3.93582700	0.12331100	0.42410000
20	C	-3.17188600	-2.42512500	-0.37498600
21	H	-1.21494000	-1.57771700	-0.66739900
22	C	-4.86974800	-0.91136600	0.41154400
23	H	-4.25434600	1.11411900	0.73742900
24	C	-4.49098700	-2.19419600	0.01160800
25	H	-2.86265900	-3.41832500	-0.69088200
26	H	-5.89463600	-0.71319300	0.71460600
27	H	-5.21738300	-3.00245100	0.00100100

28

29

MECP

30	Zero-point correction=	0.284007 (Hartree/Particle)
31	Thermal correction to Energy=	0.292172
32	Thermal correction to Enthalpy=	0.292790
33	Thermal correction to Gibbs Free Energy=	0.257011
34	Sum of electronic and zero-point Energies=	-807.504969
35	Sum of electronic and thermal Energies=	-807.496804
36	Sum of electronic and thermal Enthalpies=	-807.496187

1	Sum of electronic and thermal Free Energies=			-807.531966
2		Cartesian Coordinates		
3	Atom	X	Y	Z
4		-----		
5	C	-0.74140200	-1.06966900	-0.51511000
6	C	-1.80422700	-0.23166200	-0.99800400
7	O	0.41442400	-0.38853200	-0.35622100
8	C	-3.02352500	0.14227100	-0.40709700
9	C	-3.46825600	-0.37702000	0.84594300
10	C	-3.85311800	1.08830100	-1.07319900
11	C	-4.67539900	0.03414600	1.38954100
12	H	-2.85593800	-1.11695800	1.35145900
13	C	-5.04296000	1.51610100	-0.50249600
14	H	-3.52127900	1.47227600	-2.03295000
15	C	-5.45973300	0.98807700	0.72578200
16	H	-5.00900000	-0.37667200	2.33840400
17	H	-5.65746100	2.25249900	-1.01247100
18	H	-6.39796000	1.31689100	1.16422600
19	O	-0.90156400	-2.27811400	-0.36310900
20	C	1.68368100	-1.05373900	-0.04069000
21	C	2.03849100	-2.00944900	-1.19141900
22	H	3.02871200	-2.44599600	-1.02880700
23	H	1.30599300	-2.81596200	-1.26098400
24	H	2.06258800	-1.45972700	-2.13782100
25	C	1.56336100	-1.77645500	1.31128400
26	H	0.84007400	-2.59121900	1.25001300
27	H	2.53465500	-2.18563500	1.60498700
28	H	1.24817400	-1.06980400	2.08605500
29	C	2.71188800	0.08110600	0.05048600
30	C	2.36743900	1.42404200	-0.14221100
31	C	4.05061300	-0.22688100	0.33811000
32	C	3.33361700	2.42859700	-0.04587100
33	H	1.34069000	1.68249800	-0.36890100
34	C	5.01489500	0.77482100	0.43381800
35	H	4.35094700	-1.26018700	0.49036600
36	C	4.65980100	2.11142400	0.24314800

1	H	3.04194000	3.46453500	-0.19869800
2	H	6.04446100	0.50809700	0.65790300
3	H	5.40953100	2.89445500	0.31976800
4				
5			TS5	
6	Zero-point correction=		0.402693 (Hartree/Particle)	
7	Thermal correction to Energy=			0.426748
8	Thermal correction to Enthalpy=			0.427692
9	Thermal correction to Gibbs Free Energy=			0.343837
10	Sum of electronic and zero-point Energies=			-1095.001561
11	Sum of electronic and thermal Energies=			-1094.977507
12	Sum of electronic and thermal Enthalpies=			-1094.976562
13	Sum of electronic and thermal Free Energies=			-1095.060418
14			Cartesian Coordinates	
15	Atom	X	Y	Z
16	-----			
17	C	0.59716800	0.37079900	-0.18079100
18	C	0.88367500	1.75324700	-0.02018400
19	C	0.22420800	2.60129000	0.91408000
20	C	1.85880800	2.32877600	-0.87873100
21	C	0.52015400	3.95488800	0.97361900
22	H	-0.52818100	2.17335400	1.56994100
23	C	2.16700200	3.68021200	-0.80376200
24	H	2.35857800	1.67019600	-1.58150800
25	C	1.49421300	4.49021400	0.11882100
26	H	0.00697200	4.59963700	1.68143600
27	H	2.91996100	4.11054100	-1.45737900
28	H	1.72847800	5.55046300	0.17310700
29	C	-0.29711800	-0.36165500	0.66708500
30	O	0.10185100	-1.13528700	1.54194500
31	O	-1.59007400	-0.19679500	0.29117600
32	C	-2.64923600	-1.14610700	0.66195600
33	C	-2.24424900	-2.56033100	0.21775200
34	H	-1.36619000	-2.90217700	0.76877100
35	H	-3.06752900	-3.25840800	0.39753800
36	H	-2.02259400	-2.56688400	-0.85415000

1	C	-2.88575700	-1.05351900	2.17820500
2	H	-3.73193800	-1.68307400	2.47055700
3	H	-1.99650300	-1.37878300	2.72043100
4	H	-3.12141100	-0.02136500	2.45756000
5	C	-3.88886000	-0.67806700	-0.11067300
6	C	-5.10552300	-1.35528700	0.06606800
7	C	-3.85471300	0.40189800	-1.00074600
8	C	-6.25264500	-0.96475700	-0.62274900
9	H	-5.16444100	-2.20007200	0.74734100
10	C	-5.00430600	0.79402600	-1.69095000
11	H	-2.92500300	0.93527800	-1.15395500
12	C	-6.20755700	0.11517400	-1.50635500
13	H	-7.18221200	-1.50643200	-0.46801100
14	H	-4.95322700	1.63549100	-2.37735400
15	H	-7.10063400	0.42141300	-2.04450500
16	N	3.03717800	-0.65335600	1.29847200
17	H	3.38333100	-0.45091900	2.22836100
18	H	2.13777400	-1.12694000	1.32326100
19	C	3.99341100	-1.10449200	0.39338600
20	C	5.36716500	-0.94284100	0.65120500
21	C	3.60310500	-1.68197500	-0.83089300
22	C	6.31766300	-1.35485500	-0.28082700
23	H	5.68433200	-0.49515100	1.59139100
24	C	4.56280200	-2.09466600	-1.75075200
25	H	2.54397000	-1.77571200	-1.05386700
26	C	5.92712700	-1.93771300	-1.48782600
27	H	7.37348500	-1.22311100	-0.05582600
28	H	4.23907500	-2.54125700	-2.68808900
29	H	6.67021800	-2.26149900	-2.21094200

30

31

IN1

32	Zero-point correction=	0.407439 (Hartree/Particle)
33	Thermal correction to Energy=	0.430229
34	Thermal correction to Enthalpy=	0.431173
35	Thermal correction to Gibbs Free Energy=	0.352604
36	Sum of electronic and zero-point Energies=	-1095.057121

1	Sum of electronic and thermal Energies=			-1095.034331
2	Sum of electronic and thermal Enthalpies=			-1095.033387
3	Sum of electronic and thermal Free Energies=			-1095.111956
4	Cartesian Coordinates			
5	Atom	X	Y	Z
6	-----			
7	C	-0.79725900	0.21162800	-0.10834400
8	C	-1.29118500	1.57133000	-0.12708700
9	C	-0.64059400	2.62644900	0.56268300
10	C	-2.45637200	1.91651400	-0.85577200
11	C	-1.12002400	3.92954000	0.50370100
12	H	0.24415400	2.40561900	1.14480200
13	C	-2.92766100	3.22772800	-0.90673100
14	H	-3.02506100	1.15271500	-1.37949400
15	C	-2.26529000	4.25112000	-0.23196200
16	H	-0.58888900	4.70863700	1.04629600
17	H	-3.82685300	3.44321000	-1.47967500
18	H	-2.63387300	5.27227200	-0.27000800
19	C	0.41163100	-0.39067500	0.31373300
20	O	0.68074800	-1.58700500	0.02431000
21	O	1.25306500	0.38747100	1.04464800
22	C	2.58732400	-0.10462100	1.39499900
23	C	3.19873600	1.09142600	2.14421800
24	H	2.60832700	1.32156900	3.03771400
25	H	4.22339900	0.85659900	2.44911000
26	H	3.22544700	1.97786600	1.50401000
27	C	2.46879400	-1.30165600	2.34722300
28	H	3.43806000	-1.52462800	2.80594200
29	H	1.77283300	-1.04277500	3.15189600
30	H	2.09628000	-2.18564700	1.83011500
31	C	3.40001200	-0.37406000	0.12482400
32	C	4.30963200	-1.43318800	0.03308500
33	C	3.29749300	0.51127900	-0.95868700
34	C	5.09352800	-1.60659700	-1.10995400
35	H	4.40897000	-2.13920900	0.85100500
36	C	4.07453700	0.33686800	-2.10232000

1	H	2.59127100	1.33501200	-0.90776600
2	C	4.97967100	-0.72364900	-2.18278200
3	H	5.79073800	-2.43921700	-1.15990600
4	H	3.97343700	1.03211900	-2.93204700
5	H	5.58793200	-0.86010400	-3.07313400
6	N	-1.51491300	-0.81135800	-0.90385600
7	H	-1.61800900	-0.52989600	-1.88753200
8	H	-0.77145200	-1.57824100	-0.84872800
9	C	-2.81453100	-1.34091800	-0.42978600
10	C	-3.73459800	-1.80001700	-1.36837200
11	C	-3.06386800	-1.42197300	0.93517700
12	C	-4.93905900	-2.35030200	-0.92735300
13	H	-3.51920600	-1.72888700	-2.43274500
14	C	-4.26925700	-1.97697900	1.36548200
15	H	-2.32816700	-1.03824500	1.63387100
16	C	-5.20648500	-2.44069200	0.43953300
17	H	-5.66505700	-2.70484000	-1.65315100
18	H	-4.47665400	-2.04226600	2.42959500
19	H	-6.14478900	-2.86722700	0.78208600

20

21

TS6

22	Zero-point correction=		0.403703 (Hartree/Particle)
23	Thermal correction to Energy=		0.426172
24	Thermal correction to Enthalpy=		0.427116
25	Thermal correction to Gibbs Free Energy=		0.349369
26	Sum of electronic and zero-point Energies=		-1095.058632
27	Sum of electronic and thermal Energies=		-1095.036163
28	Sum of electronic and thermal Enthalpies=		-1095.035219
29	Sum of electronic and thermal Free Energies=		-1095.112966

30

Cartesian Coordinates

31	Atom	X	Y	Z
32	-----			
33	C	-0.79056500	0.25210300	-0.12241100
34	C	-1.32061400	1.59979800	-0.16004300
35	C	-0.70275100	2.67388700	0.52633200
36	C	-2.48476600	1.90115900	-0.90456900

1	C	-1.21711000	3.96381400	0.45263900
2	H	0.18282700	2.48214100	1.11887500
3	C	-2.99247900	3.19746100	-0.96968700
4	H	-3.01303000	1.11180500	-1.43163800
5	C	-2.36442800	4.24387800	-0.29546300
6	H	-0.71382200	4.76283100	0.99259100
7	H	-3.89077300	3.38509200	-1.55346800
8	H	-2.76144800	5.25387200	-0.34566200
9	C	0.40327500	-0.30061900	0.35417000
10	O	0.63951600	-1.53979200	0.08757300
11	O	1.26084100	0.45174400	1.06650300
12	C	2.59881100	-0.05371600	1.40682900
13	C	3.23106500	1.14704300	2.12871400
14	H	2.65417300	1.39815600	3.02523800
15	H	4.25626400	0.90448700	2.42498300
16	H	3.26059200	2.02242500	1.47381600
17	C	2.47269000	-1.23361300	2.37798700
18	H	3.44566500	-1.46700000	2.82298600
19	H	1.79541700	-0.95076800	3.19026000
20	H	2.07702100	-2.11987500	1.88199800
21	C	3.38439300	-0.35322000	0.12737000
22	C	4.26355800	-1.43731900	0.03091100
23	C	3.28428400	0.52382300	-0.96316400
24	C	5.02201900	-1.64211400	-1.12393500
25	H	4.35935500	-2.13750400	0.85419200
26	C	4.03536300	0.31728900	-2.11874700
27	H	2.60084800	1.36637400	-0.90915300
28	C	4.91115200	-0.76717200	-2.20363700
29	H	5.69646600	-2.49290200	-1.17774100
30	H	3.93683300	1.00605000	-2.95400300
31	H	5.49924000	-0.92846400	-3.10324500
32	N	-1.44620100	-0.84813700	-0.85606900
33	H	-1.48708900	-0.67726500	-1.86538500
34	H	-0.51709300	-1.58689100	-0.60085200
35	C	-2.72673300	-1.38078200	-0.40172300
36	C	-3.59794700	-1.94006200	-1.33685400

1	C	-3.03960300	-1.38608200	0.95623300
2	C	-4.79765800	-2.50867200	-0.90782100
3	H	-3.34247200	-1.93227800	-2.39476100
4	C	-4.24052100	-1.95789400	1.37553000
5	H	-2.35307600	-0.93218800	1.66290900
6	C	-5.12183300	-2.52020700	0.44951900
7	H	-5.47743100	-2.93955000	-1.63747300
8	H	-4.48851100	-1.95942400	2.43321500
9	H	-6.05701900	-2.96048600	0.78311300

10

11 **IN2**

12	Zero-point correction=		0.407314 (Hartree/Particle)	
13	Thermal correction to Energy=			0.430140
14	Thermal correction to Enthalpy=			0.431084
15	Thermal correction to Gibbs Free Energy=			0.352835
16	Sum of electronic and zero-point Energies=			-1095.072755
17	Sum of electronic and thermal Energies=			-1095.049929
18	Sum of electronic and thermal Enthalpies=			-1095.048985
19	Sum of electronic and thermal Free Energies=			-1095.127234

20 Cartesian Coordinates

21	Atom	X	Y	Z
22	-----			
23	C	-0.69481200	0.05310300	-0.02633800
24	C	-1.03283600	1.48627800	-0.06799800
25	C	-0.43180000	2.45482200	0.76733000
26	C	-2.00277300	1.94350900	-0.98545000
27	C	-0.76850000	3.80274000	0.66414400
28	H	0.29108800	2.14367000	1.50914100
29	C	-2.33760300	3.29246600	-1.08085200
30	H	-2.51295900	1.23393900	-1.62814000
31	C	-1.71969300	4.23662700	-0.26090500
32	H	-0.28622200	4.51974900	1.32452100
33	H	-3.09048600	3.60340500	-1.80105800
34	H	-1.98111700	5.28874900	-0.33408800
35	C	0.37320100	-0.53920800	0.59234200
36	O	0.59505700	-1.86329000	0.47825500

1	O	1.23835000	0.12479200	1.36902000
2	C	2.66624800	-0.25969500	1.44803600
3	C	3.29746100	0.96630800	2.12548000
4	H	2.84661600	1.12761200	3.11045900
5	H	4.37262500	0.80677600	2.25263800
6	H	3.15150400	1.86534500	1.52097800
7	C	2.80982700	-1.48122000	2.36289600
8	H	3.86067500	-1.63271200	2.63141700
9	H	2.25128700	-1.29757000	3.28567400
10	H	2.42399800	-2.38860900	1.89827700
11	C	3.23867100	-0.43292400	0.04084200
12	C	4.11330900	-1.47624300	-0.28379900
13	C	2.92508800	0.51027800	-0.95067500
14	C	4.66506600	-1.57423400	-1.56310100
15	H	4.37049800	-2.22419700	0.45883400
16	C	3.46885100	0.40844500	-2.23014600
17	H	2.24210900	1.32341200	-0.72204200
18	C	4.34439800	-0.63391000	-2.54139200
19	H	5.34311900	-2.39200800	-1.79295700
20	H	3.20865300	1.14675800	-2.98415200
21	H	4.77135200	-0.71213500	-3.53769400
22	N	-1.48732100	-0.90021200	-0.77050100
23	H	-1.39626900	-0.79904900	-1.77833300
24	H	-0.12832500	-2.15950600	-0.12359200
25	C	-2.81871600	-1.21248600	-0.39300600
26	C	-3.70127400	-1.73376700	-1.35167000
27	C	-3.25722700	-1.06946800	0.93049100
28	C	-4.99447700	-2.10699100	-0.99148600
29	H	-3.36785400	-1.84930100	-2.38171900
30	C	-4.55402200	-1.44405900	1.27928000
31	H	-2.58240500	-0.65937500	1.67472600
32	C	-5.43174000	-1.96552900	0.32692700
33	H	-5.66326000	-2.50762100	-1.74910000
34	H	-4.87965400	-1.32304200	2.30936900
35	H	-6.44087000	-2.25386400	0.60644000
36				

1	TS7_{major_298K}			
2	Zero-point correction=			0.766034 (Hartree/Particle)
3	Thermal correction to Energy=			0.807413
4	Thermal correction to Enthalpy=			0.808357
5	Thermal correction to Gibbs Free Energy=			0.688209
6	Sum of electronic and zero-point Energies=			-1961.339466
7	Sum of electronic and thermal Energies=			-1961.298087
8	Sum of electronic and thermal Enthalpies=			-1961.297143
9	Sum of electronic and thermal Free Energies=			-1961.417292
10	Cartesian Coordinates			
11	Atom	X	Y	Z
12	-----			
13	C	2.32846800	-0.81256500	-0.38720400
14	C	3.61310100	-1.45483800	0.06678500
15	C	3.72764800	-1.96970900	1.37037000
16	C	4.74391700	-1.52020200	-0.76235300
17	C	4.91244000	-2.55389300	1.81382900
18	H	2.87450300	-1.90145200	2.03922300
19	C	5.93457400	-2.09723200	-0.31790100
20	H	4.69153600	-1.10908300	-1.76669300
21	C	6.02516900	-2.62257000	0.97135700
22	H	4.97155700	-2.94632000	2.82654600
23	H	6.79389900	-2.13502600	-0.98364000
24	H	6.95269200	-3.06980000	1.31982300
25	C	1.16463900	-1.66956300	-0.63189000
26	O	0.15543600	-1.30577500	-1.25538000
27	O	1.25344900	-2.87575900	-0.01837200
28	C	0.21978400	-3.89638000	-0.11823800
29	C	0.88250600	-5.09343600	0.58862900
30	H	1.80212600	-5.37636800	0.06638900
31	H	0.20122300	-5.94988400	0.60385800
32	H	1.13512000	-4.83162300	1.62003100
33	C	-0.03891900	-4.24052500	-1.59439600
34	H	-0.61509800	-5.16721000	-1.67849800
35	H	0.92181000	-4.40291600	-2.09427700
36	H	-0.57124600	-3.43758800	-2.10379600

1	C	-1.04327000	-3.50681600	0.65713500
2	C	-1.03037900	-2.48584800	1.61771000
3	C	-2.21852600	-4.25841700	0.50210300
4	C	-2.16423200	-2.22449200	2.39122200
5	H	-0.14749500	-1.87340500	1.76137200
6	C	-3.34768000	-4.00085600	1.28166300
7	H	-2.25661300	-5.06539700	-0.22403600
8	C	-3.32688400	-2.97916900	2.23152400
9	H	-2.12823500	-1.42714200	3.12982400
10	H	-4.24173100	-4.60503000	1.14776900
11	H	-4.20466800	-2.77591300	2.83909300
12	N	2.43392500	0.16498100	-1.45774000
13	H	2.26034700	-0.17716000	-2.39578600
14	C	3.15197300	1.34801400	-1.39981000
15	C	3.27334900	2.13895500	-2.56548400
16	C	3.75106600	1.82327500	-0.21392900
17	C	3.94429300	3.35684100	-2.53852600
18	H	2.83778400	1.77989300	-3.49718600
19	C	4.41473700	3.05052000	-0.20336800
20	H	3.71647600	1.21703700	0.68349500
21	C	4.51863100	3.83171600	-1.35519200
22	H	4.02071400	3.93932500	-3.45393700
23	H	4.87043000	3.38967100	0.72408100
24	H	5.04472800	4.78157700	-1.33662900
25	H	-0.17159600	0.51556600	-0.34157300
26	C	-1.09053200	4.73252800	0.23569500
27	C	-0.63292900	3.58338300	0.88434300
28	C	-0.81349000	3.41936600	2.26960100
29	C	-1.46987500	4.40671900	3.00503400
30	C	-1.94308800	5.54828900	2.35230500
31	C	-1.75372400	5.71376500	0.97638800
32	H	-0.91766800	4.87887400	-0.82797000
33	H	-1.60747900	4.29435000	4.07764900
34	H	-2.45279300	6.32135200	2.92144900
35	H	-2.11062500	6.61467000	0.48495000
36	C	-0.21450500	2.11766400	2.74700900

1	H	0.32227500	2.21269500	3.69712800
2	H	-0.98464000	1.34716900	2.89154000
3	C	0.13316700	2.41875100	0.31828400
4	H	0.92771200	2.70812200	-0.37356300
5	C	0.72171700	1.68086500	1.58338300
6	H	1.70673300	2.15096900	1.74847300
7	O	0.80046400	0.31603700	1.42427400
8	H	1.66088500	-0.12194600	0.67126100
9	C	-2.11507900	1.11120700	-0.00475000
10	C	-0.75662500	1.68514500	-1.95376100
11	C	-3.00356600	1.22856800	-1.26362300
12	H	-2.39660600	1.81905100	0.77304100
13	H	-2.10453900	0.10332200	0.41157200
14	C	-2.00918800	0.95462600	-2.41438500
15	H	-0.84789200	2.76636500	-2.08840100
16	H	0.17743300	1.33424200	-2.39074300
17	H	-3.32752900	2.27431500	-1.34590200
18	H	-1.80238700	-0.11578700	-2.50161400
19	N	-0.69561300	1.40839200	-0.47075000
20	C	-4.23988400	0.35194200	-1.25274900
21	C	-5.50781200	0.92679000	-1.40405000
22	C	-4.14499600	-1.04102400	-1.11758000
23	C	-6.65697100	0.13474200	-1.42688300
24	H	-5.59631900	2.00636800	-1.50691500
25	C	-5.29213700	-1.83349400	-1.13923600
26	H	-3.17436800	-1.51471300	-0.99135200
27	C	-6.55134900	-1.24990800	-1.29541300
28	H	-7.63163000	0.60067000	-1.54610400
29	H	-5.19722000	-2.90952200	-1.02684800
30	H	-7.44337700	-1.87044600	-1.31188400
31	H	-2.37443000	1.32208300	-3.37785000

32

33

TS7*minor_298K*

34 Zero-point correction= 0.765695 (Hartree/Particle)

35 Thermal correction to Energy= 0.807157

36 Thermal correction to Enthalpy= 0.808101

1	Thermal correction to Gibbs Free Energy=	0.685179
2	Sum of electronic and zero-point Energies=	-1961.338569
3	Sum of electronic and thermal Energies=	-1961.297108
4	Sum of electronic and thermal Enthalpies=	-1961.296164
5	Sum of electronic and thermal Free Energies=	-1961.419086

6 Cartesian Coordinates

7	Atom	X	Y	Z
8	-----			
9	C	1.62165700	-1.10109500	0.45583300
10	C	2.50979900	-1.84518100	1.41389700
11	C	2.98557900	-1.23932400	2.59281300
12	C	2.84970300	-3.19237300	1.19677600
13	C	3.78849900	-1.93766300	3.49230100
14	H	2.72060100	-0.20811500	2.80210500
15	C	3.64685300	-3.89465700	2.10172600
16	H	2.48054500	-3.68983900	0.30551600
17	C	4.12627400	-3.27241800	3.25460300
18	H	4.14221300	-1.43891600	4.39208300
19	H	3.89357000	-4.93497600	1.90109200
20	H	4.74455100	-3.81951700	3.96178200
21	C	2.14194300	0.06676000	-0.24801700
22	O	1.71681100	0.46665500	-1.34076800
23	O	3.11267900	0.74194600	0.44280600
24	C	3.93636400	1.74895800	-0.21909400
25	C	3.09460900	2.97474000	-0.60146500
26	H	2.48154700	3.26610800	0.25841300
27	H	3.74108800	3.82484300	-0.84514700
28	H	2.44259100	2.76023700	-1.44804000
29	C	4.93783300	2.13718300	0.88284000
30	H	5.65599500	2.86836900	0.49811500
31	H	4.41059500	2.57561300	1.73744300
32	H	5.48698600	1.25731000	1.22840900
33	C	4.69617500	1.11726500	-1.39106500
34	C	5.19212700	-0.18959000	-1.26720600
35	C	4.98532800	1.82998100	-2.56035800
36	C	5.94477700	-0.76785100	-2.28797100

1	H	4.97409200	-0.76109200	-0.36970100
2	C	5.74463900	1.25369700	-3.58149400
3	H	4.61528000	2.84211700	-2.68898300
4	C	6.22677000	-0.04778900	-3.45082900
5	H	6.31190500	-1.78453600	-2.17283900
6	H	5.95344100	1.82571800	-4.48219600
7	H	6.81476900	-0.49784000	-4.24650200
8	N	0.89450100	-1.92106200	-0.49322000
9	H	1.16031100	-1.80154400	-1.46266900
10	H	-1.25448200	0.05389700	0.22524700
11	C	-0.18763100	-2.73698300	-0.25693500
12	C	-0.79664600	-3.40784700	-1.34687800
13	C	-0.72030700	-2.96046700	1.03372100
14	C	-1.88627500	-4.25088500	-1.15406200
15	H	-0.38678500	-3.27014300	-2.34640400
16	C	-1.81502600	-3.80545400	1.20588100
17	H	-0.27193400	-2.47476500	1.89132100
18	C	-2.41403700	-4.45981800	0.12511500
19	H	-2.32304100	-4.75507100	-2.01338800
20	H	-2.19799800	-3.96159000	2.21206600
21	H	-3.25462500	-5.13110400	0.27636400
22	C	-2.02738400	4.27512500	-0.24357900
23	C	-1.60031100	3.25745600	0.61228500
24	C	-1.78364100	3.35954700	2.00219600
25	C	-2.40714000	4.48671400	2.53801900
26	C	-2.84567100	5.49959500	1.68082000
27	C	-2.65751900	5.39752400	0.29819000
28	H	-1.86039600	4.20700200	-1.31610100
29	H	-2.54707600	4.58117600	3.61194900
30	H	-3.32963000	6.38095500	2.09325300
31	H	-2.99096900	6.19956600	-0.35436000
32	C	-1.23253200	2.14897900	2.71987400
33	H	-0.67918500	2.40340300	3.63023700
34	H	-2.03258700	1.45758200	3.01752200
35	C	-0.87188400	1.98920700	0.27298000
36	H	-0.06069700	2.11260100	-0.44682900

1	C	-0.33615200	1.45148700	1.66227900
2	H	0.69699500	1.81519300	1.76189000
3	O	-0.39909700	0.06244500	1.71783600
4	H	0.55738000	-0.41547800	1.24598100
5	C	-3.18751000	0.76509400	0.04038700
6	C	-1.57454700	0.65229700	-1.79255800
7	C	-3.90825300	0.41570900	-1.28444900
8	H	-3.52058500	1.71179200	0.46418700
9	H	-3.29296100	-0.01909300	0.79247600
10	C	-2.78340600	-0.20362300	-2.14746700
11	H	-1.63401500	1.63991500	-2.26146500
12	H	-0.58863300	0.22477900	-1.98458200
13	H	-4.20477500	1.36044300	-1.75796900
14	H	-2.60468500	-1.24943600	-1.87476000
15	H	-3.01472900	-0.16759200	-3.21594400
16	N	-1.71002700	0.85093000	-0.30298400
17	C	-5.15437300	-0.43006200	-1.10468000
18	C	-6.40362400	0.07213600	-1.48891900
19	C	-5.08834300	-1.72026100	-0.55687300
20	C	-7.56261600	-0.69063600	-1.33396300
21	H	-6.47052100	1.07108000	-1.91505000
22	C	-6.24519600	-2.48317300	-0.40153300
23	H	-4.13427600	-2.14523300	-0.25348300
24	C	-7.48613300	-1.97205400	-0.78857000
25	H	-8.52230800	-0.28211300	-1.63925100
26	H	-6.17290600	-3.48146200	0.02149300
27	H	-8.38573100	-2.56918500	-0.66626900
28				
29			TS11_{298K}	
30	Zero-point correction=		0.880552 (Hartree/Particle)	
31	Thermal correction to Energy=			0.932335
32	Thermal correction to Enthalpy=			0.933279
33	Thermal correction to Gibbs Free Energy=			0.782722
34	Sum of electronic and zero-point Energies=			-2245.040665
35	Sum of electronic and thermal Energies=			-2244.988883
36	Sum of electronic and thermal Enthalpies=			-2244.987939

1	Sum of electronic and thermal Free Energies=			-2245.138496
2		Cartesian Coordinates		
3	Atom	X	Y	Z
4	-----			
5	C	-2.09364000	0.72313600	-0.83658700
6	C	-3.06447700	1.86468600	-0.87604600
7	C	-3.76397300	2.34808500	0.25463200
8	C	-3.26984500	2.56100700	-2.08717400
9	C	-4.62677000	3.44304000	0.16696400
10	H	-3.64692100	1.85242600	1.20989100
11	C	-4.12722500	3.65622300	-2.16819800
12	H	-2.75389200	2.22003300	-2.97699300
13	C	-4.81665500	4.11100500	-1.04283000
14	H	-5.15318500	3.77336700	1.06011300
15	H	-4.25861200	4.15564800	-3.12550600
16	H	-5.48537700	4.96509700	-1.10689600
17	C	-2.39720900	-0.50735800	-0.12733500
18	O	-2.05525000	-1.63831600	-0.49904200
19	O	-3.03859800	-0.31222900	1.07695800
20	N	-1.46971200	0.40096600	-2.10196800
21	H	-1.65848100	-0.54644200	-2.40836800
22	H	0.10930700	-3.88524100	1.08520900
23	C	-0.31815900	0.96045100	-2.61456100
24	C	0.34903900	0.31981100	-3.68633400
25	C	0.20761900	2.18604200	-2.15327000
26	C	1.49484300	0.86993000	-4.24971500
27	H	-0.05643500	-0.61102200	-4.07879500
28	C	1.36158800	2.72288100	-2.72403000
29	H	-0.30565200	2.72980400	-1.36924000
30	C	2.02435300	2.07528700	-3.77061800
31	H	1.98203000	0.35177400	-5.07255900
32	H	1.73806300	3.67115000	-2.34698000
33	H	2.91641600	2.50525000	-4.21614800
34	H	-0.55447100	-2.75168000	0.03404100
35	H	0.38654700	0.73603700	1.32215900
36	H	-1.00413400	1.24142600	0.31271700

1	C	-3.75790200	-1.40896600	1.73425700
2	N	0.30658700	-3.18115800	0.38228000
3	C	1.19504700	-3.61057300	-0.61711200
4	C	2.17117000	-4.58416600	-0.35003000
5	C	3.09587300	-4.94443000	-1.32920200
6	C	3.07108900	-4.34432900	-2.59069800
7	C	2.09780500	-3.37785800	-2.86070400
8	C	1.16728700	-3.01107900	-1.88845000
9	H	2.20724500	-5.05132400	0.63190600
10	H	3.84119500	-5.70257900	-1.10218500
11	H	3.79134700	-4.62954200	-3.35168400
12	H	2.05534600	-2.90534900	-3.83904700
13	H	0.41088400	-2.26079200	-2.10018200
14	N	-0.38641300	1.46382200	1.29349900
15	C	-4.45914900	-0.69798100	2.90485400
16	H	-5.05926200	-1.41573800	3.47269900
17	H	-3.72053600	-0.24994000	3.57995000
18	H	-5.12239200	0.08952700	2.53716700
19	C	-2.76657600	-2.44157900	2.28812600
20	H	-2.35933600	-3.06779100	1.49523500
21	H	-1.94433400	-1.91655100	2.78611900
22	H	-3.25331300	-3.07862700	3.03433000
23	C	-4.81386600	-1.99505500	0.79180800
24	C	-5.11809200	-3.36135400	0.78068000
25	C	-5.56004100	-1.13858100	-0.03181900
26	C	-6.13574700	-3.86168200	-0.03463700
27	H	-4.56121300	-4.05193800	1.40571800
28	C	-6.57082000	-1.63819000	-0.85135400
29	H	-5.34020500	-0.07504300	-0.04235200
30	C	-6.86504900	-3.00307200	-0.85566600
31	H	-6.35156900	-4.92703200	-0.02902700
32	H	-7.12853900	-0.95705100	-1.48872600
33	H	-7.65346900	-3.39265800	-1.49415300
34	H	1.14417600	-1.45085200	1.15168200
35	H	2.26541100	-0.38969600	0.53440400
36	N	1.66250400	-0.58294300	1.34700400

1	C	2.38600500	-0.65538500	2.56252700
2	C	1.82009700	-1.28566800	3.68297700
3	C	2.49864200	-1.30878300	4.89978700
4	C	3.74935700	-0.69971400	5.02797200
5	C	4.31628600	-0.07458900	3.91630700
6	C	3.64765400	-0.05234700	2.69185800
7	H	0.84526400	-1.76026500	3.59049800
8	H	2.04543600	-1.80602400	5.75396400
9	H	4.27520100	-0.71756300	5.97820700
10	H	5.29476100	0.39255000	3.99415700
11	H	4.11226400	0.41119700	1.82487100
12	H	3.04672700	-1.12811100	-1.64789800
13	H	2.82578600	0.50838800	-1.82204700
14	N	3.28792600	-0.21377200	-1.27327900
15	C	4.67406100	-0.01028800	-1.12744900
16	C	5.53982700	-1.09721800	-0.92188000
17	C	6.90069200	-0.88206200	-0.71370300
18	C	7.42692000	0.41193000	-0.70434200
19	C	6.56789300	1.49372400	-0.90818600
20	C	5.20434700	1.29062400	-1.11665800
21	H	5.13787200	-2.10794600	-0.92896100
22	H	7.55534600	-1.73634900	-0.55986800
23	H	8.48884300	0.57397600	-0.54365100
24	H	6.96032000	2.50778200	-0.90971500
25	H	4.54090100	2.13663200	-1.28097600
26	C	0.13311200	2.81764600	1.46045000
27	C	-0.72484700	3.90918100	1.30882000
28	C	1.48457800	3.00614200	1.75440400
29	C	-0.21895300	5.20059600	1.45924200
30	H	-1.77145200	3.75144800	1.06501900
31	C	1.97913200	4.30347700	1.89742300
32	H	2.14116100	2.15292800	1.88932300
33	C	1.13148500	5.40227800	1.75114300
34	H	-0.88566300	6.04976700	1.33956200
35	H	3.03006300	4.44963200	2.13023500
36	H	1.52066500	6.41026400	1.86334800

1	H	-1.05642200	1.22375700	2.02949600
2				
3		TS10_{298K}		
4	Zero-point correction=		0.761558 (Hartree/Particle)	
5	Thermal correction to Energy=			0.805772
6	Thermal correction to Enthalpy=			0.806716
7	Thermal correction to Gibbs Free Energy=			0.676050
8	Sum of electronic and zero-point Energies=			-1957.548122
9	Sum of electronic and thermal Energies=			-1957.503908
10	Sum of electronic and thermal Enthalpies=			-1957.502964
11	Sum of electronic and thermal Free Energies=			-1957.633630
12		Cartesian Coordinates		
13	Atom	X	Y	Z
14	-----			
15	C	1.82091000	-0.75888200	1.17630900
16	C	3.30564300	-0.75589900	1.35189700
17	C	4.20514000	-1.11572400	0.32396800
18	C	3.87157600	-0.32239700	2.56799200
19	C	5.58551200	-1.05535400	0.51057900
20	H	3.81880400	-1.47121200	-0.62382800
21	C	5.25262700	-0.26078700	2.75061500
22	H	3.20922400	-0.04211600	3.37940800
23	C	6.12468100	-0.62567700	1.72458900
24	H	6.24436000	-1.34937400	-0.30383400
25	H	5.64708900	0.07333700	3.70764600
26	H	7.20101400	-0.57610100	1.86638800
27	C	1.11701000	-1.88327300	0.59487900
28	O	-0.09177500	-2.11008600	0.78149700
29	O	1.86155500	-2.65799200	-0.25447500
30	N	1.04997700	-0.23735800	2.29296100
31	H	0.30491400	-0.86684500	2.56819800
32	H	-3.06152500	-1.51514900	-0.99270400
33	C	0.76488300	1.09586100	2.52486000
34	C	-0.35094000	1.43709100	3.32667900
35	C	1.56780600	2.14700400	2.03112500
36	C	-0.64849700	2.76698500	3.61195800

1	H	-0.97770200	0.64225300	3.72719700
2	C	1.25096600	3.47375900	2.31894800
3	H	2.44773900	1.91767300	1.44103200
4	C	0.14513400	3.80354200	3.10687900
5	H	-1.51197300	2.99416500	4.23286800
6	H	1.88828600	4.26098200	1.92313500
7	H	-0.08420500	4.83976600	3.33753400
8	H	-1.87215300	-1.64810600	0.16564600
9	H	-0.08220300	1.18268400	-0.54062100
10	H	1.36913000	0.21672300	-0.06477900
11	C	1.24403400	-3.76816800	-0.97710600
12	N	-2.80445000	-1.28014100	-0.03850700
13	C	-3.77542500	-1.66904800	0.90860500
14	C	-5.14298500	-1.62405100	0.59555400
15	C	-6.09791300	-1.95526800	1.55520100
16	C	-5.71185200	-2.33204100	2.84325900
17	C	-4.35157200	-2.37806900	3.15668200
18	C	-3.38850900	-2.05381400	2.20277900
19	H	-5.45399600	-1.32030100	-0.40210300
20	H	-7.15220800	-1.91579500	1.29240200
21	H	-6.45863700	-2.58795400	3.58931800
22	H	-4.03303500	-2.67731800	4.15231200
23	H	-2.32971000	-2.10971900	2.44186400
24	N	0.82983300	0.82304900	-0.93589300
25	C	0.69971200	-4.81630600	0.00228200
26	H	0.44073000	-5.73706100	-0.53185600
27	H	1.48527300	-5.05924600	0.72451000
28	H	-0.17062000	-4.45243300	0.54667600
29	C	2.42915400	-4.37493900	-1.74842800
30	H	2.88803300	-3.64030600	-2.41613200
31	H	3.19125900	-4.72319600	-1.04443600
32	H	2.08979900	-5.22263100	-2.35223000
33	C	0.21153500	-3.22059600	-1.97119500
34	C	-1.06311900	-3.77486000	-2.12486600
35	C	0.57154100	-2.15183200	-2.81141300
36	C	-1.95659300	-3.27170800	-3.07674800

1	H	-1.37511300	-4.60180400	-1.49633100
2	C	-0.31874200	-1.64126300	-3.75670100
3	H	1.56977000	-1.72804700	-2.73181600
4	C	-1.59332600	-2.19983700	-3.89173400
5	H	-2.93890500	-3.72618600	-3.17939300
6	H	-0.01258600	-0.81965000	-4.39975800
7	H	-2.28651600	-1.81178500	-4.63299500
8	H	-2.23562500	0.68903500	0.09140300
9	H	-1.54070600	1.83170500	1.09920200
10	N	-1.76374000	1.60453900	0.13036500
11	C	-2.47339700	2.63324700	-0.53044000
12	C	-3.29213000	2.33526300	-1.63178400
13	C	-3.94468700	3.35576000	-2.32156000
14	C	-3.79254300	4.68847400	-1.93296100
15	C	-2.97593900	4.98744800	-0.84018500
16	C	-2.31863000	3.97441500	-0.14273100
17	H	-3.41817600	1.29896500	-1.93545100
18	H	-4.58017400	3.10477700	-3.16729300
19	H	-4.30445000	5.48082200	-2.47137900
20	H	-2.84984100	6.01920500	-0.52145500
21	H	-1.68464000	4.21165000	0.70863500
22	C	1.62133400	1.88558600	-1.54894400
23	C	1.00229700	3.07283600	-1.94366000
24	C	2.99324200	1.70017300	-1.72804900
25	C	1.76805100	4.07924700	-2.53399600
26	H	-0.06335700	3.21354900	-1.79075900
27	C	3.74795300	2.71267700	-2.32212900
28	H	3.47269000	0.78867300	-1.38373700
29	C	3.13879800	3.90112700	-2.72834500
30	H	1.28700600	5.00374100	-2.84044000
31	H	4.81660700	2.57170300	-2.45624500
32	H	3.73110300	4.68787500	-3.18700600
33	H	0.57921000	0.10283300	-1.62343100
34				
35			TS9_{298K}	
36	Zero-point correction=			0.643668 (Hartree/Particle)

1	Thermal correction to Energy=			0.680243
2	Thermal correction to Enthalpy=			0.681187
3	Thermal correction to Gibbs Free Energy=			0.569163
4	Sum of electronic and zero-point Energies=			-1670.045102
5	Sum of electronic and thermal Energies=			-1670.008528
6	Sum of electronic and thermal Enthalpies=			-1670.007583
7	Sum of electronic and thermal Free Energies=			-1670.119608
8	Cartesian Coordinates			
9	Atom	X	Y	Z
10	-----			
11	C	-0.88927900	-0.92276300	0.74542000
12	C	-1.47950800	-2.23730900	0.38606000
13	C	-1.94196700	-2.57039000	-0.91054500
14	C	-1.53017600	-3.26361100	1.35651800
15	C	-2.43624900	-3.84287700	-1.20212800
16	H	-1.93287800	-1.81981400	-1.69076000
17	C	-2.02219100	-4.53182200	1.05745700
18	H	-1.18556600	-3.04082700	2.36026000
19	C	-2.48097600	-4.83834100	-0.22527800
20	H	-2.79133600	-4.05288800	-2.20914800
21	H	-2.04962800	-5.28717800	1.83985600
22	H	-2.86377100	-5.82840200	-0.45785700
23	C	-1.34322500	0.35294200	0.26102300
24	O	-1.15428200	1.43573100	0.84308800
25	O	-1.90461800	0.32044400	-1.00738700
26	N	-0.37878600	-0.78971500	2.09797900
27	H	-0.76942600	0.02825200	2.55489700
28	H	0.84240500	1.95161700	0.71311500
29	C	0.95252300	-0.99998000	2.43562800
30	C	1.53962900	-0.25607100	3.48424500
31	C	1.74940900	-1.96625500	1.78602200
32	C	2.86797400	-0.46151100	3.85163200
33	H	0.93857500	0.48543700	4.00735600
34	C	3.07927300	-2.15565300	2.15957100
35	H	1.31088300	-2.58414900	1.00979300
36	C	3.65621500	-1.40707600	3.18814000

1	H	3.29069000	0.12906800	4.66119200
2	H	3.66844100	-2.90719000	1.63928000
3	H	4.69148500	-1.56476200	3.47608900
4	H	2.15733900	1.20485200	1.38142300
5	H	1.57117700	0.39588600	-0.69222800
6	H	0.42593000	-0.81717800	-0.40272400
7	C	-2.75264800	1.42565200	-1.46203300
8	N	1.82823200	1.71327700	0.56086500
9	C	2.66067300	2.80297800	0.20933500
10	C	2.13967400	3.90434800	-0.48535800
11	C	2.98084600	4.94000800	-0.88927400
12	C	4.34877500	4.89695800	-0.61110500
13	C	4.86759600	3.80196500	0.08259100
14	C	4.03472400	2.76080500	0.49079900
15	H	1.07460300	3.94592100	-0.70106500
16	H	2.56047400	5.78921200	-1.42196600
17	H	4.99971000	5.70735700	-0.92584900
18	H	5.92868900	3.75671700	0.31424400
19	H	4.44150000	1.91353500	1.03916400
20	N	1.13575800	-0.42831800	-1.19581600
21	C	-3.31582600	0.89894600	-2.79346600
22	H	-3.99250100	1.63859400	-3.23295100
23	H	-2.50319600	0.70502500	-3.50351300
24	H	-3.87312600	-0.02872800	-2.63795900
25	C	-1.90260300	2.67626400	-1.72684300
26	H	-1.54804000	3.11651800	-0.79524100
27	H	-1.03813200	2.39728800	-2.34049900
28	H	-2.47497100	3.42019500	-2.29127500
29	C	-3.90515700	1.64295700	-0.47650500
30	C	-4.39621700	2.91799400	-0.17381200
31	C	-4.54440900	0.52967100	0.09036800
32	C	-5.49441700	3.07919200	0.67403700
33	H	-3.92212800	3.80044500	-0.59086100
34	C	-5.63612400	0.68977900	0.94193600
35	H	-4.17471600	-0.46861000	-0.12549400
36	C	-6.11842000	1.96668100	1.23640700

1	H	-5.85582600	4.07967200	0.89793200
2	H	-6.10941700	-0.18667900	1.37690900
3	H	-6.96999700	2.09223100	1.89990200
4	C	2.10809500	-1.36689700	-1.74011600
5	C	3.45375700	-1.00574500	-1.79638700
6	C	1.67412000	-2.61800900	-2.18021300
7	C	4.37985100	-1.91371700	-2.31179500
8	H	3.77352100	-0.02863200	-1.44432300
9	C	2.60932900	-3.51470000	-2.69718200
10	H	0.62424900	-2.88968700	-2.10255600
11	C	3.96006600	-3.16555400	-2.76487500
12	H	5.42943900	-1.63846600	-2.35919100
13	H	2.27953500	-4.49122100	-3.03946400
14	H	4.68402500	-3.86949100	-3.16503900
15	H	0.49793700	-0.06318200	-1.90989300

16

17

TS8_{298K}

18	Zero-point correction=		0.523803 (Hartree/Particle)	
19	Thermal correction to Energy=			0.553185
20	Thermal correction to Enthalpy=			0.554129
21	Thermal correction to Gibbs Free Energy=			0.461008
22	Sum of electronic and zero-point Energies=			-1382.542753
23	Sum of electronic and thermal Energies=			-1382.513372
24	Sum of electronic and thermal Enthalpies=			-1382.512427
25	Sum of electronic and thermal Free Energies=			-1382.605548

26

Cartesian Coordinates

27	Atom	X	Y	Z
28	-----			
29	C	-1.06245100	-1.00376400	-0.33874900
30	C	-1.51821900	-1.93998200	0.72259300
31	C	-0.80432700	-2.08228800	1.92928900
32	C	-2.70880100	-2.67748800	0.58558800
33	C	-1.24179900	-2.94162300	2.93314500
34	H	0.10378300	-1.50487700	2.07610600
35	C	-3.15278600	-3.53084600	1.59619300
36	H	-3.28397600	-2.57889900	-0.32972600

1	C	-2.42203200	-3.67417500	2.77579300
2	H	-0.66409400	-3.03126400	3.85048600
3	H	-4.07581300	-4.08901500	1.45612500
4	H	-2.76877300	-4.33734000	3.56401600
5	C	0.25809600	-1.07328800	-0.91219100
6	O	0.63624500	-0.33900900	-1.85752900
7	O	1.08947000	-1.98827300	-0.33821900
8	C	2.45054100	-2.19340500	-0.83070200
9	C	2.92188700	-3.40244400	-0.00271100
10	H	2.28673600	-4.26854700	-0.21357600
11	H	3.95778200	-3.65020700	-0.25566400
12	H	2.86819800	-3.19191300	1.06859100
13	C	2.43231800	-2.58673600	-2.31412000
14	H	3.41676200	-2.95864600	-2.61842900
15	H	1.71205500	-3.39955200	-2.45161400
16	H	2.14188900	-1.75339000	-2.95260700
17	C	3.32821100	-0.98051200	-0.50153800
18	C	4.19246000	-0.39756600	-1.43630200
19	C	3.33474100	-0.47692100	0.80892600
20	C	5.04671200	0.64640900	-1.07176900
21	H	4.20605600	-0.75492600	-2.46017200
22	C	4.18865300	0.56147600	1.17798000
23	H	2.66396000	-0.90576700	1.54778500
24	C	5.05452800	1.12635900	0.23801600
25	H	5.71053200	1.07971700	-1.81560000
26	H	4.17841900	0.92802000	2.20124500
27	H	5.73020900	1.92820900	0.52487600
28	N	-2.03615500	-0.62686600	-1.34135200
29	H	-1.74379800	-0.76689100	-2.30062200
30	H	-0.01621600	1.32789200	-1.32034900
31	C	-3.11136100	0.22491900	-1.17374100
32	C	-3.80518900	0.70510100	-2.30996500
33	C	-3.55367600	0.65068800	0.10076700
34	C	-4.89028500	1.56338500	-2.17454500
35	H	-3.48303000	0.38678700	-3.29983000
36	C	-4.64375700	1.51610200	0.21495400

1	H	-3.06153100	0.27283900	0.99003900
2	C	-5.32298200	1.98206300	-0.91128000
3	H	-5.40193400	1.91244400	-3.06834400
4	H	-4.96981000	1.81689000	1.20810700
5	H	-6.17325700	2.64980500	-0.81037300
6	C	1.44040700	4.67598700	1.73789100
7	C	2.17541400	3.76533700	0.97666500
8	C	1.52723400	2.78241700	0.22816000
9	C	0.13442900	2.72770000	0.25061700
10	C	-0.61568900	3.62549300	1.01218600
11	C	0.04537800	4.60275800	1.75497500
12	H	1.95148000	5.43999300	2.31653400
13	H	3.26002600	3.81181100	0.96030300
14	H	2.09323700	2.06748700	-0.36118400
15	H	-1.70074600	3.55781400	1.02176300
16	H	-0.53218000	5.30757800	2.34608200
17	N	-0.54715300	1.69623600	-0.50256900
18	H	-0.71023600	0.68617300	0.00412900
19	H	-1.48422400	1.97948800	-0.80141200

20

21 **TS7_{major_195K}**

22	Zero-point correction=		0.766034 (Hartree/Particle)	
23	Thermal correction to Energy=		0.785067	
24	Thermal correction to Enthalpy=		0.785685	
25	Thermal correction to Gibbs Free Energy=		0.725040	
26	Sum of electronic and zero-point Energies=			-1961.339466
27	Sum of electronic and thermal Energies=			-1961.320433
28	Sum of electronic and thermal Enthalpies=			-1961.319816
29	Sum of electronic and thermal Free Energies=			-1961.380460

30 Cartesian Coordinates

31	Atom	X	Y	Z
32	-----			
33	C	2.32846800	-0.81256500	-0.38720400
34	C	3.61310100	-1.45483800	0.06678500
35	C	3.72764800	-1.96970900	1.37037000
36	C	4.74391700	-1.52020200	-0.76235300

1	C	4.91244000	-2.55389300	1.81382900
2	H	2.87450300	-1.90145200	2.03922300
3	C	5.93457400	-2.09723200	-0.31790100
4	H	4.69153600	-1.10908300	-1.76669300
5	C	6.02516900	-2.62257000	0.97135700
6	H	4.97155700	-2.94632000	2.82654600
7	H	6.79389900	-2.13502600	-0.98364000
8	H	6.95269200	-3.06980000	1.31982300
9	C	1.16463900	-1.66956300	-0.63189000
10	O	0.15543600	-1.30577500	-1.25538000
11	O	1.25344900	-2.87575900	-0.01837200
12	C	0.21978400	-3.89638000	-0.11823800
13	C	0.88250600	-5.09343600	0.58862900
14	H	1.80212600	-5.37636800	0.06638900
15	H	0.20122300	-5.94988400	0.60385800
16	H	1.13512000	-4.83162300	1.62003100
17	C	-0.03891900	-4.24052500	-1.59439600
18	H	-0.61509800	-5.16721000	-1.67849800
19	H	0.92181000	-4.40291600	-2.09427700
20	H	-0.57124600	-3.43758800	-2.10379600
21	C	-1.04327000	-3.50681600	0.65713500
22	C	-1.03037900	-2.48584800	1.61771000
23	C	-2.21852600	-4.25841700	0.50210300
24	C	-2.16423200	-2.22449200	2.39122200
25	H	-0.14749500	-1.87340500	1.76137200
26	C	-3.34768000	-4.00085600	1.28166300
27	H	-2.25661300	-5.06539700	-0.22403600
28	C	-3.32688400	-2.97916900	2.23152400
29	H	-2.12823500	-1.42714200	3.12982400
30	H	-4.24173100	-4.60503000	1.14776900
31	H	-4.20466800	-2.77591300	2.83909300
32	N	2.43392500	0.16498100	-1.45774000
33	H	2.26034700	-0.17716000	-2.39578600
34	C	3.15197300	1.34801400	-1.39981000
35	C	3.27334900	2.13895500	-2.56548400
36	C	3.75106600	1.82327500	-0.21392900

1	C	3.94429300	3.35684100	-2.53852600
2	H	2.83778400	1.77989300	-3.49718600
3	C	4.41473700	3.05052000	-0.20336800
4	H	3.71647600	1.21703700	0.68349500
5	C	4.51863100	3.83171600	-1.35519200
6	H	4.02071400	3.93932500	-3.45393700
7	H	4.87043000	3.38967100	0.72408100
8	H	5.04472800	4.78157700	-1.33662900
9	H	-0.17159600	0.51556600	-0.34157300
10	C	-1.09053200	4.73252800	0.23569500
11	C	-0.63292900	3.58338300	0.88434300
12	C	-0.81349000	3.41936600	2.26960100
13	C	-1.46987500	4.40671900	3.00503400
14	C	-1.94308800	5.54828900	2.35230500
15	C	-1.75372400	5.71376500	0.97638800
16	H	-0.91766800	4.87887400	-0.82797000
17	H	-1.60747900	4.29435000	4.07764900
18	H	-2.45279300	6.32135200	2.92144900
19	H	-2.11062500	6.61467000	0.48495000
20	C	-0.21450500	2.11766400	2.74700900
21	H	0.32227500	2.21269500	3.69712800
22	H	-0.98464000	1.34716900	2.89154000
23	C	0.13316700	2.41875100	0.31828400
24	H	0.92771200	2.70812200	-0.37356300
25	C	0.72171700	1.68086500	1.58338300
26	H	1.70673300	2.15096900	1.74847300
27	O	0.80046400	0.31603700	1.42427400
28	H	1.66088500	-0.12194600	0.67126100
29	C	-2.11507900	1.11120700	-0.00475000
30	C	-0.75662500	1.68514500	-1.95376100
31	C	-3.00356600	1.22856800	-1.26362300
32	H	-2.39660600	1.81905100	0.77304100
33	H	-2.10453900	0.10332200	0.41157200
34	C	-2.00918800	0.95462600	-2.41438500
35	H	-0.84789200	2.76636500	-2.08840100
36	H	0.17743300	1.33424200	-2.39074300

1	H	-3.32752900	2.27431500	-1.34590200
2	H	-1.80238700	-0.11578700	-2.50161400
3	N	-0.69561300	1.40839200	-0.47075000
4	C	-4.23988400	0.35194200	-1.25274900
5	C	-5.50781200	0.92679000	-1.40405000
6	C	-4.14499600	-1.04102400	-1.11758000
7	C	-6.65697100	0.13474200	-1.42688300
8	H	-5.59631900	2.00636800	-1.50691500
9	C	-5.29213700	-1.83349400	-1.13923600
10	H	-3.17436800	-1.51471300	-0.99135200
11	C	-6.55134900	-1.24990800	-1.29541300
12	H	-7.63163000	0.60067000	-1.54610400
13	H	-5.19722000	-2.90952200	-1.02684800
14	H	-7.44337700	-1.87044600	-1.31188400
15	H	-2.37443000	1.32208300	-3.37785000

16

17

TS7_{minor_195K}

18	Zero-point correction=	0.765695 (Hartree/Particle)
19	Thermal correction to Energy=	0.784845
20	Thermal correction to Enthalpy=	0.785462
21	Thermal correction to Gibbs Free Energy=	0.722975
22	Sum of electronic and zero-point Energies=	-1961.338569
23	Sum of electronic and thermal Energies=	-1961.319420
24	Sum of electronic and thermal Enthalpies=	-1961.318802
25	Sum of electronic and thermal Free Energies=	-1961.381290

26

Cartesian Coordinates

27	Atom	X	Y	Z
28	-----			
29	C	1.62165700	-1.10109500	0.45583300
30	C	2.50979900	-1.84518100	1.41389700
31	C	2.98557900	-1.23932400	2.59281300
32	C	2.84970300	-3.19237300	1.19677600
33	C	3.78849900	-1.93766300	3.49230100
34	H	2.72060100	-0.20811500	2.80210500
35	C	3.64685300	-3.89465700	2.10172600
36	H	2.48054500	-3.68983900	0.30551600

1	C	4.12627400	-3.27241800	3.25460300
2	H	4.14221300	-1.43891600	4.39208300
3	H	3.89357000	-4.93497600	1.90109200
4	H	4.74455100	-3.81951700	3.96178200
5	C	2.14194300	0.06676000	-0.24801700
6	O	1.71681100	0.46665500	-1.34076800
7	O	3.11267900	0.74194600	0.44280600
8	C	3.93636400	1.74895800	-0.21909400
9	C	3.09460900	2.97474000	-0.60146500
10	H	2.48154700	3.26610800	0.25841300
11	H	3.74108800	3.82484300	-0.84514700
12	H	2.44259100	2.76023700	-1.44804000
13	C	4.93783300	2.13718300	0.88284000
14	H	5.65599500	2.86836900	0.49811500
15	H	4.41059500	2.57561300	1.73744300
16	H	5.48698600	1.25731000	1.22840900
17	C	4.69617500	1.11726500	-1.39106500
18	C	5.19212700	-0.18959000	-1.26720600
19	C	4.98532800	1.82998100	-2.56035800
20	C	5.94477700	-0.76785100	-2.28797100
21	H	4.97409200	-0.76109200	-0.36970100
22	C	5.74463900	1.25369700	-3.58149400
23	H	4.61528000	2.84211700	-2.68898300
24	C	6.22677000	-0.04778900	-3.45082900
25	H	6.31190500	-1.78453600	-2.17283900
26	H	5.95344100	1.82571800	-4.48219600
27	H	6.81476900	-0.49784000	-4.24650200
28	N	0.89450100	-1.92106200	-0.49322000
29	H	1.16031100	-1.80154400	-1.46266900
30	H	-1.25448200	0.05389700	0.22524700
31	C	-0.18763100	-2.73698300	-0.25693500
32	C	-0.79664600	-3.40784700	-1.34687800
33	C	-0.72030700	-2.96046700	1.03372100
34	C	-1.88627500	-4.25088500	-1.15406200
35	H	-0.38678500	-3.27014300	-2.34640400
36	C	-1.81502600	-3.80545400	1.20588100

1	H	-0.27193400	-2.47476500	1.89132100
2	C	-2.41403700	-4.45981800	0.12511500
3	H	-2.32304100	-4.75507100	-2.01338800
4	H	-2.19799800	-3.96159000	2.21206600
5	H	-3.25462500	-5.13110400	0.27636400
6	C	-2.02738400	4.27512500	-0.24357900
7	C	-1.60031100	3.25745600	0.61228500
8	C	-1.78364100	3.35954700	2.00219600
9	C	-2.40714000	4.48671400	2.53801900
10	C	-2.84567100	5.49959500	1.68082000
11	C	-2.65751900	5.39752400	0.29819000
12	H	-1.86039600	4.20700200	-1.31610100
13	H	-2.54707600	4.58117600	3.61194900
14	H	-3.32963000	6.38095500	2.09325300
15	H	-2.99096900	6.19956600	-0.35436000
16	C	-1.23253200	2.14897900	2.71987400
17	H	-0.67918500	2.40340300	3.63023700
18	H	-2.03258700	1.45758200	3.01752200
19	C	-0.87188400	1.98920700	0.27298000
20	H	-0.06069700	2.11260100	-0.44682900
21	C	-0.33615200	1.45148700	1.66227900
22	H	0.69699500	1.81519300	1.76189000
23	O	-0.39909700	0.06244500	1.71783600
24	H	0.55738000	-0.41547800	1.24598100
25	C	-3.18751000	0.76509400	0.04038700
26	C	-1.57454700	0.65229700	-1.79255800
27	C	-3.90825300	0.41570900	-1.28444900
28	H	-3.52058500	1.71179200	0.46418700
29	H	-3.29296100	-0.01909300	0.79247600
30	C	-2.78340600	-0.20362300	-2.14746700
31	H	-1.63401500	1.63991500	-2.26146500
32	H	-0.58863300	0.22477900	-1.98458200
33	H	-4.20477500	1.36044300	-1.75796900
34	H	-2.60468500	-1.24943600	-1.87476000
35	H	-3.01472900	-0.16759200	-3.21594400
36	N	-1.71002700	0.85093000	-0.30298400

1	C	-5.15437300	-0.43006200	-1.10468000
2	C	-6.40362400	0.07213600	-1.48891900
3	C	-5.08834300	-1.72026100	-0.55687300
4	C	-7.56261600	-0.69063600	-1.33396300
5	H	-6.47052100	1.07108000	-1.91505000
6	C	-6.24519600	-2.48317300	-0.40153300
7	H	-4.13427600	-2.14523300	-0.25348300
8	C	-7.48613300	-1.97205400	-0.78857000
9	H	-8.52230800	-0.28211300	-1.63925100
10	H	-6.17290600	-3.48146200	0.02149300
11	H	-8.38573100	-2.56918500	-0.66626900

12

13

TS11_{195K}

14	Zero-point correction=		0.880552 (Hartree/Particle)	
15	Thermal correction to Energy=			0.905036
16	Thermal correction to Enthalpy=			0.905653
17	Thermal correction to Gibbs Free Energy=			0.829050
18	Sum of electronic and zero-point Energies=			-2245.040665
19	Sum of electronic and thermal Energies=			-2245.016182
20	Sum of electronic and thermal Enthalpies=			-2245.015564
21	Sum of electronic and thermal Free Energies=			-2245.092168

22

Cartesian Coordinates

23	Atom	X	Y	Z
24	-----			
25	C	-2.09364000	0.72313600	-0.83658700
26	C	-3.06447700	1.86468600	-0.87604600
27	C	-3.76397300	2.34808500	0.25463200
28	C	-3.26984500	2.56100700	-2.08717400
29	C	-4.62677000	3.44304000	0.16696400
30	H	-3.64692100	1.85242600	1.20989100
31	C	-4.12722500	3.65622300	-2.16819800
32	H	-2.75389200	2.22003300	-2.97699300
33	C	-4.81665500	4.11100500	-1.04283000
34	H	-5.15318500	3.77336700	1.06011300
35	H	-4.25861200	4.15564800	-3.12550600
36	H	-5.48537700	4.96509700	-1.10689600

1	C	-2.39720900	-0.50735800	-0.12733500
2	O	-2.05525000	-1.63831600	-0.49904200
3	O	-3.03859800	-0.31222900	1.07695800
4	N	-1.46971200	0.40096600	-2.10196800
5	H	-1.65848100	-0.54644200	-2.40836800
6	H	0.10930700	-3.88524100	1.08520900
7	C	-0.31815900	0.96045100	-2.61456100
8	C	0.34903900	0.31981100	-3.68633400
9	C	0.20761900	2.18604200	-2.15327000
10	C	1.49484300	0.86993000	-4.24971500
11	H	-0.05643500	-0.61102200	-4.07879500
12	C	1.36158800	2.72288100	-2.72403000
13	H	-0.30565200	2.72980400	-1.36924000
14	C	2.02435300	2.07528700	-3.77061800
15	H	1.98203000	0.35177400	-5.07255900
16	H	1.73806300	3.67115000	-2.34698000
17	H	2.91641600	2.50525000	-4.21614800
18	H	-0.55447100	-2.75168000	0.03404100
19	H	0.38654700	0.73603700	1.32215900
20	H	-1.00413400	1.24142600	0.31271700
21	C	-3.75790200	-1.40896600	1.73425700
22	N	0.30658700	-3.18115800	0.38228000
23	C	1.19504700	-3.61057300	-0.61711200
24	C	2.17117000	-4.58416600	-0.35003000
25	C	3.09587300	-4.94443000	-1.32920200
26	C	3.07108900	-4.34432900	-2.59069800
27	C	2.09780500	-3.37785800	-2.86070400
28	C	1.16728700	-3.01107900	-1.88845000
29	H	2.20724500	-5.05132400	0.63190600
30	H	3.84119500	-5.70257900	-1.10218500
31	H	3.79134700	-4.62954200	-3.35168400
32	H	2.05534600	-2.90534900	-3.83904700
33	H	0.41088400	-2.26079200	-2.10018200
34	N	-0.38641300	1.46382200	1.29349900
35	C	-4.45914900	-0.69798100	2.90485400
36	H	-5.05926200	-1.41573800	3.47269900

1	H	-3.72053600	-0.24994000	3.57995000
2	H	-5.12239200	0.08952700	2.53716700
3	C	-2.76657600	-2.44157900	2.28812600
4	H	-2.35933600	-3.06779100	1.49523500
5	H	-1.94433400	-1.91655100	2.78611900
6	H	-3.25331300	-3.07862700	3.03433000
7	C	-4.81386600	-1.99505500	0.79180800
8	C	-5.11809200	-3.36135400	0.78068000
9	C	-5.56004100	-1.13858100	-0.03181900
10	C	-6.13574700	-3.86168200	-0.03463700
11	H	-4.56121300	-4.05193800	1.40571800
12	C	-6.57082000	-1.63819000	-0.85135400
13	H	-5.34020500	-0.07504300	-0.04235200
14	C	-6.86504900	-3.00307200	-0.85566600
15	H	-6.35156900	-4.92703200	-0.02902700
16	H	-7.12853900	-0.95705100	-1.48872600
17	H	-7.65346900	-3.39265800	-1.49415300
18	H	1.14417600	-1.45085200	1.15168200
19	H	2.26541100	-0.38969600	0.53440400
20	N	1.66250400	-0.58294300	1.34700400
21	C	2.38600500	-0.65538500	2.56252700
22	C	1.82009700	-1.28566800	3.68297700
23	C	2.49864200	-1.30878300	4.89978700
24	C	3.74935700	-0.69971400	5.02797200
25	C	4.31628600	-0.07458900	3.91630700
26	C	3.64765400	-0.05234700	2.69185800
27	H	0.84526400	-1.76026500	3.59049800
28	H	2.04543600	-1.80602400	5.75396400
29	H	4.27520100	-0.71756300	5.97820700
30	H	5.29476100	0.39255000	3.99415700
31	H	4.11226400	0.41119700	1.82487100
32	H	3.04672700	-1.12811100	-1.64789800
33	H	2.82578600	0.50838800	-1.82204700
34	N	3.28792600	-0.21377200	-1.27327900
35	C	4.67406100	-0.01028800	-1.12744900
36	C	5.53982700	-1.09721800	-0.92188000

1	C	6.90069200	-0.88206200	-0.71370300
2	C	7.42692000	0.41193000	-0.70434200
3	C	6.56789300	1.49372400	-0.90818600
4	C	5.20434700	1.29062400	-1.11665800
5	H	5.13787200	-2.10794600	-0.92896100
6	H	7.55534600	-1.73634900	-0.55986800
7	H	8.48884300	0.57397600	-0.54365100
8	H	6.96032000	2.50778200	-0.90971500
9	H	4.54090100	2.13663200	-1.28097600
10	C	0.13311200	2.81764600	1.46045000
11	C	-0.72484700	3.90918100	1.30882000
12	C	1.48457800	3.00614200	1.75440400
13	C	-0.21895300	5.20059600	1.45924200
14	H	-1.77145200	3.75144800	1.06501900
15	C	1.97913200	4.30347700	1.89742300
16	H	2.14116100	2.15292800	1.88932300
17	C	1.13148500	5.40227800	1.75114300
18	H	-0.88566300	6.04976700	1.33956200
19	H	3.03006300	4.44963200	2.13023500
20	H	1.52066500	6.41026400	1.86334800
21	H	-1.05642200	1.22375700	2.02949600

22

23

TS10_{195K}

24	Zero-point correction=		0.761557 (Hartree/Particle)
25	Thermal correction to Energy=		0.782318
26	Thermal correction to Enthalpy=		0.782936
27	Thermal correction to Gibbs Free Energy=		0.716296
28	Sum of electronic and zero-point Energies=		-1957.548122
29	Sum of electronic and thermal Energies=		-1957.527362
30	Sum of electronic and thermal Enthalpies=		-1957.526744
31	Sum of electronic and thermal Free Energies=		-1957.593384

32

Cartesian Coordinates

33	Atom	X	Y	Z
34	-----			
35	C	1.82095300	-0.75867800	1.17619800
36	C	3.30568000	-0.75546400	1.35187000

1	C	4.20529000	-1.11504100	0.32395400
2	C	3.87147400	-0.32198400	2.56803600
3	C	5.58564300	-1.05446300	0.51064600
4	H	3.81906200	-1.47050000	-0.62389700
5	C	5.25250500	-0.26016500	2.75074100
6	H	3.20902900	-0.04188600	3.37944000
7	C	6.12467500	-0.62481400	1.72472600
8	H	6.24458300	-1.34829600	-0.30376000
9	H	5.64686200	0.07393300	3.70782500
10	H	7.20099200	-0.57507500	1.86658800
11	C	1.11730000	-1.88320900	0.59472100
12	O	-0.09142500	-2.11032200	0.78134400
13	O	1.86201100	-2.65770000	-0.25469100
14	N	1.04988300	-0.23737000	2.29286300
15	H	0.30492800	-0.86701800	2.56802600
16	H	-3.06156300	-1.51574100	-0.99244800
17	C	0.76449600	1.09578200	2.52480400
18	C	-0.35148600	1.43674800	3.32651400
19	C	1.56726800	2.14710800	2.03121700
20	C	-0.64934200	2.76656900	3.61182100
21	H	-0.97814700	0.64176700	3.72690500
22	C	1.25012700	3.47378700	2.31906200
23	H	2.44731400	1.91798100	1.44121400
24	C	0.14413700	3.80331000	3.10687900
25	H	-1.51293600	2.99354600	4.23264100
26	H	1.88733500	4.26115600	1.92335900
27	H	-0.08543900	4.83947700	3.33755400
28	H	-1.87194000	-1.64852300	0.16567300
29	H	-0.08230800	1.18264100	-0.54071700
30	H	1.36913800	0.21689000	-0.06482900
31	C	1.24472100	-3.76795300	-0.97740800
32	N	-2.80430000	-1.28063900	-0.03832500
33	C	-3.77506200	-1.66949900	0.90902600
34	C	-5.14269200	-1.62450200	0.59628100
35	C	-6.09740600	-1.95566800	1.55615700
36	C	-5.71106000	-2.33238500	2.84414600

1	C	-4.35071000	-2.37841500	3.15726400
2	C	-3.38785700	-2.05421500	2.20312900
3	H	-5.45392400	-1.32078800	-0.40131800
4	H	-7.15176000	-1.91619600	1.29359400
5	H	-6.45767900	-2.58825700	3.59038500
6	H	-4.03195100	-2.67762500	4.15283600
7	H	-2.32900500	-2.11013400	2.44197400
8	N	0.82982600	0.82321800	-0.93594500
9	C	0.70067000	-4.81630300	0.00190300
10	H	0.44185400	-5.73705800	-0.53231500
11	H	1.48631800	-5.05914900	0.72406800
12	H	-0.16971200	-4.45266600	0.54637700
13	C	2.42995800	-4.37438500	-1.74881700
14	H	2.88865500	-3.63959100	-2.41646800
15	H	3.19216000	-4.72253300	-1.04487600
16	H	2.09077800	-5.22210100	-2.35268400
17	C	0.21206400	-3.22051900	-1.97141000
18	C	-1.06251000	-3.77498600	-2.12501300
19	C	0.57182900	-2.15165300	-2.81160000
20	C	-1.95613900	-3.27193500	-3.07680200
21	H	-1.37431900	-4.60201400	-1.49649700
22	C	-0.31861000	-1.64118400	-3.75679500
23	H	1.56999100	-1.72770200	-2.73205200
24	C	-1.59311000	-2.19996200	-3.89176100
25	H	-2.93838200	-3.72657200	-3.17939800
26	H	-0.01263900	-0.81948700	-4.39983300
27	H	-2.28642000	-1.81198800	-4.63295100
28	H	-2.23570700	0.68860200	0.09125800
29	H	-1.54108000	1.83151200	1.09897500
30	N	-1.76400500	1.60420500	0.13014600
31	C	-2.47382300	2.63270200	-0.53080700
32	C	-3.29235500	2.33445800	-1.63223100
33	C	-3.94507400	3.35475900	-2.32214400
34	C	-3.79329200	4.68753300	-1.93360800
35	C	-2.97688400	4.98676700	-0.84075700
36	C	-2.31941800	3.97393100	-0.14316400

1	H	-3.41811200	1.29811300	-1.93585600
2	H	-4.58040200	3.10357400	-3.16793800
3	H	-4.30532400	5.47972600	-2.47213300
4	H	-2.85106600	6.01857300	-0.52207600
5	H	-1.68558100	4.21136800	0.70825900
6	C	1.62117200	1.88598200	-1.54881100
7	C	1.00186800	3.07301700	-1.94375600
8	C	2.99318800	1.70099600	-1.72752600
9	C	1.76746600	4.07964600	-2.53392200
10	H	-0.06387400	3.21339800	-1.79115700
11	C	3.74774200	2.71371500	-2.32143900
12	H	3.47282700	0.78965600	-1.38305700
13	C	3.13832500	3.90195300	-2.72787600
14	H	1.28621400	5.00397400	-2.84054100
15	H	4.81647900	2.57307300	-2.45525200
16	H	3.73050800	4.68887000	-3.18640600
17	H	0.57939000	0.10304200	-1.62359200

18

19

TS9_{195K}

20	Zero-point correction=		0.643668 (Hartree/Particle)
21	Thermal correction to Energy=		0.660719
22	Thermal correction to Enthalpy=		0.661337
23	Thermal correction to Gibbs Free Energy=		0.603777
24	Sum of electronic and zero-point Energies=		-1670.045102
25	Sum of electronic and thermal Energies=		-1670.028051
26	Sum of electronic and thermal Enthalpies=		-1670.027434
27	Sum of electronic and thermal Free Energies=		-1670.084994

28

Cartesian Coordinates

29	Atom	X	Y	Z
30	-----			
31	C	-0.88927900	-0.92276300	0.74542000
32	C	-1.47950800	-2.23730900	0.38606000
33	C	-1.94196700	-2.57039000	-0.91054500
34	C	-1.53017600	-3.26361100	1.35651800
35	C	-2.43624900	-3.84287700	-1.20212800
36	H	-1.93287800	-1.81981400	-1.69076000

1	C	-2.02219100	-4.53182200	1.05745700
2	H	-1.18556600	-3.04082700	2.36026000
3	C	-2.48097600	-4.83834100	-0.22527800
4	H	-2.79133600	-4.05288800	-2.20914800
5	H	-2.04962800	-5.28717800	1.83985600
6	H	-2.86377100	-5.82840200	-0.45785700
7	C	-1.34322500	0.35294200	0.26102300
8	O	-1.15428200	1.43573100	0.84308800
9	O	-1.90461800	0.32044400	-1.00738700
10	N	-0.37878600	-0.78971500	2.09797900
11	H	-0.76942600	0.02825200	2.55489700
12	H	0.84240500	1.95161700	0.71311500
13	C	0.95252300	-0.99998000	2.43562800
14	C	1.53962900	-0.25607100	3.48424500
15	C	1.74940900	-1.96625500	1.78602200
16	C	2.86797400	-0.46151100	3.85163200
17	H	0.93857500	0.48543700	4.00735600
18	C	3.07927300	-2.15565300	2.15957100
19	H	1.31088300	-2.58414900	1.00979300
20	C	3.65621500	-1.40707600	3.18814000
21	H	3.29069000	0.12906800	4.66119200
22	H	3.66844100	-2.90719000	1.63928000
23	H	4.69148500	-1.56476200	3.47608900
24	H	2.15733900	1.20485200	1.38142300
25	H	1.57117700	0.39588600	-0.69222800
26	H	0.42593000	-0.81717800	-0.40272400
27	C	-2.75264800	1.42565200	-1.46203300
28	N	1.82823200	1.71327700	0.56086500
29	C	2.66067300	2.80297800	0.20933500
30	C	2.13967400	3.90434800	-0.48535800
31	C	2.98084600	4.94000800	-0.88927400
32	C	4.34877500	4.89695800	-0.61110500
33	C	4.86759600	3.80196500	0.08259100
34	C	4.03472400	2.76080500	0.49079900
35	H	1.07460300	3.94592100	-0.70106500
36	H	2.56047400	5.78921200	-1.42196600

1	H	4.99971000	5.70735700	-0.92584900
2	H	5.92868900	3.75671700	0.31424400
3	H	4.44150000	1.91353500	1.03916400
4	N	1.13575800	-0.42831800	-1.19581600
5	C	-3.31582600	0.89894600	-2.79346600
6	H	-3.99250100	1.63859400	-3.23295100
7	H	-2.50319600	0.70502500	-3.50351300
8	H	-3.87312600	-0.02872800	-2.63795900
9	C	-1.90260300	2.67626400	-1.72684300
10	H	-1.54804000	3.11651800	-0.79524100
11	H	-1.03813200	2.39728800	-2.34049900
12	H	-2.47497100	3.42019500	-2.29127500
13	C	-3.90515700	1.64295700	-0.47650500
14	C	-4.39621700	2.91799400	-0.17381200
15	C	-4.54440900	0.52967100	0.09036800
16	C	-5.49441700	3.07919200	0.67403700
17	H	-3.92212800	3.80044500	-0.59086100
18	C	-5.63612400	0.68977900	0.94193600
19	H	-4.17471600	-0.46861000	-0.12549400
20	C	-6.11842000	1.96668000	1.23640700
21	H	-5.85582600	4.07967200	0.89793200
22	H	-6.10941700	-0.18668000	1.37690900
23	H	-6.96999700	2.09223000	1.89990200
24	C	2.10809500	-1.36689700	-1.74011600
25	C	3.45375700	-1.00574500	-1.79638700
26	C	1.67412000	-2.61800900	-2.18021300
27	C	4.37985100	-1.91371700	-2.31179500
28	H	3.77352100	-0.02863200	-1.44432300
29	C	2.60932900	-3.51470000	-2.69718200
30	H	0.62424900	-2.88968700	-2.10255600
31	C	3.96006600	-3.16555400	-2.76487500
32	H	5.42943900	-1.63846600	-2.35919100
33	H	2.27953500	-4.49122100	-3.03946400
34	H	4.68402500	-3.86949100	-3.16503900
35	H	0.49793700	-0.06318200	-1.90989300
36				

1	TS8_{195K}			
2	Zero-point correction=			0.523803 (Hartree/Particle)
3	Thermal correction to Energy=			0.537312
4	Thermal correction to Enthalpy=			0.537930
5	Thermal correction to Gibbs Free Energy=			0.489844
6	Sum of electronic and zero-point Energies=			-1382.542753
7	Sum of electronic and thermal Energies=			-1382.529244
8	Sum of electronic and thermal Enthalpies=			-1382.528626
9	Sum of electronic and thermal Free Energies=			-1382.576712
10	Cartesian Coordinates			
11	Atom	X	Y	Z
12	-----			
13	C	-1.06245100	-1.00376400	-0.33874900
14	C	-1.51821900	-1.93998200	0.72259300
15	C	-0.80432700	-2.08228800	1.92928900
16	C	-2.70880100	-2.67748800	0.58558800
17	C	-1.24179900	-2.94162300	2.93314500
18	H	0.10378300	-1.50487700	2.07610600
19	C	-3.15278600	-3.53084600	1.59619300
20	H	-3.28397600	-2.57889900	-0.32972600
21	C	-2.42203200	-3.67417500	2.77579300
22	H	-0.66409400	-3.03126400	3.85048600
23	H	-4.07581300	-4.08901500	1.45612500
24	H	-2.76877300	-4.33734000	3.56401600
25	C	0.25809600	-1.07328800	-0.91219100
26	O	0.63624500	-0.33900900	-1.85752900
27	O	1.08947000	-1.98827300	-0.33821900
28	C	2.45054100	-2.19340500	-0.83070200
29	C	2.92188700	-3.40244400	-0.00271100
30	H	2.28673600	-4.26854700	-0.21357600
31	H	3.95778200	-3.65020700	-0.25566400
32	H	2.86819800	-3.19191300	1.06859100
33	C	2.43231800	-2.58673600	-2.31412000
34	H	3.41676200	-2.95864600	-2.61842900
35	H	1.71205500	-3.39955200	-2.45161400
36	H	2.14188900	-1.75339000	-2.95260700

1	C	3.32821100	-0.98051200	-0.50153800
2	C	4.19246000	-0.39756600	-1.43630200
3	C	3.33474100	-0.47692100	0.80892600
4	C	5.04671200	0.64640900	-1.07176900
5	H	4.20605600	-0.75492600	-2.46017200
6	C	4.18865300	0.56147600	1.17798000
7	H	2.66396000	-0.90576700	1.54778500
8	C	5.05452800	1.12635900	0.23801600
9	H	5.71053200	1.07971700	-1.81560000
10	H	4.17841900	0.92802000	2.20124500
11	H	5.73020900	1.92820900	0.52487600
12	N	-2.03615500	-0.62686600	-1.34135200
13	H	-1.74379800	-0.76689100	-2.30062200
14	H	-0.01621600	1.32789200	-1.32034900
15	C	-3.11136100	0.22491900	-1.17374100
16	C	-3.80518900	0.70510100	-2.30996500
17	C	-3.55367600	0.65068800	0.10076700
18	C	-4.89028500	1.56338500	-2.17454500
19	H	-3.48303000	0.38678700	-3.29983000
20	C	-4.64375700	1.51610200	0.21495400
21	H	-3.06153100	0.27283900	0.99003900
22	C	-5.32298200	1.98206300	-0.91128000
23	H	-5.40193400	1.91244400	-3.06834400
24	H	-4.96981000	1.81689000	1.20810700
25	H	-6.17325700	2.64980500	-0.81037300
26	C	1.44040700	4.67598700	1.73789100
27	C	2.17541400	3.76533700	0.97666500
28	C	1.52723400	2.78241700	0.22816000
29	C	0.13442900	2.72770000	0.25061700
30	C	-0.61568900	3.62549300	1.01218600
31	C	0.04537800	4.60275800	1.75497500
32	H	1.95148000	5.43999300	2.31653400
33	H	3.26002600	3.81181100	0.96030300
34	H	2.09323700	2.06748700	-0.36118400
35	H	-1.70074600	3.55781400	1.02176300
36	H	-0.53218000	5.30757800	2.34608200

1	N	-0.54715300	1.69623600	-0.50256900
2	H	-0.71023600	0.68617300	0.00412900
3	H	-1.48422400	1.97948800	-0.80141200
4				
5			7	
6	Zero-point correction=		0.361746	(Hartree/Particle)
7	Thermal correction to Energy=			0.378732
8	Thermal correction to Enthalpy=			0.379676
9	Thermal correction to Gibbs Free Energy=			0.315413
10	Sum of electronic and zero-point Energies=			-866.268698
11	Sum of electronic and thermal Energies=			-866.251712
12	Sum of electronic and thermal Enthalpies=			-866.250768
13	Sum of electronic and thermal Free Energies=			-866.315031
14			Cartesian Coordinates	
15	Atom	X	Y	Z
16	-----			
17	H	0.22343600	-1.50529100	1.57016800
18	C	-3.36488100	1.39097200	0.13705100
19	C	-2.68633300	0.17733800	0.25660400
20	C	-2.93146400	-0.86904300	-0.64637300
21	C	-3.86135800	-0.70414600	-1.67266900
22	C	-4.53622300	0.51364700	-1.79606700
23	C	-4.29070100	1.55625800	-0.89681000
24	H	-3.18876000	2.19710300	0.84559400
25	H	-4.06367000	-1.51412700	-2.36969000
26	H	-5.26334600	0.64901900	-2.59263500
27	H	-4.82959900	2.49481200	-0.99647200
28	C	-2.08494300	-2.07979500	-0.31984000
29	H	-2.63786000	-3.02321900	-0.39409200
30	H	-1.22013100	-2.16408300	-0.99160100
31	C	-1.64325900	-0.22919700	1.28146500
32	H	-1.94786700	0.03532000	2.30012900
33	C	-1.59627600	-1.79412700	1.12433500
34	H	-2.32959300	-2.22108400	1.82337000
35	O	-0.32157500	-2.31256900	1.42914500
36	C	0.22615800	0.54647400	-0.24258200

1	C	0.05123800	1.53216200	1.86744400
2	C	1.56403900	1.31464100	-0.04076400
3	H	-0.47069500	1.15983200	-0.83412500
4	H	0.35785500	-0.40287000	-0.76801600
5	C	1.50743100	1.76959900	1.45670700
6	H	-0.58184400	2.39095400	1.57601200
7	H	-0.07637000	1.36809200	2.94289200
8	H	1.54889600	2.20445300	-0.67932000
9	H	2.16707900	1.13820400	2.05967900
10	N	-0.28440000	0.31760000	1.11969000
11	C	2.82248300	0.53183500	-0.37334900
12	C	3.91487000	1.18279600	-0.96131000
13	C	2.94615900	-0.83359500	-0.07392300
14	C	5.09958600	0.49836700	-1.23818500
15	H	3.83494300	2.23973800	-1.20790700
16	C	4.12735900	-1.52154000	-0.35240300
17	H	2.11022500	-1.37235000	0.36474800
18	C	5.21041600	-0.85842400	-0.93309700
19	H	5.93235400	1.02507400	-1.69736500
20	H	4.19909900	-2.58019000	-0.11672700
21	H	6.12940500	-1.39617300	-1.15056700
22	H	1.82404100	2.80881000	1.58752600

23

24 **aniline₄**

25 Zero-point correction= 0.475228 (Hartree/Particle)

26 Thermal correction to Energy= 0.503232

27 Thermal correction to Enthalpy= 0.504176

28 Thermal correction to Gibbs Free Energy= 0.407126

29 Sum of electronic and zero-point Energies= -1149.968502

30 Sum of electronic and thermal Energies= -1149.940498

31 Sum of electronic and thermal Enthalpies= -1149.939554

32 Sum of electronic and thermal Free Energies= -1150.036604

33

Cartesian Coordinates

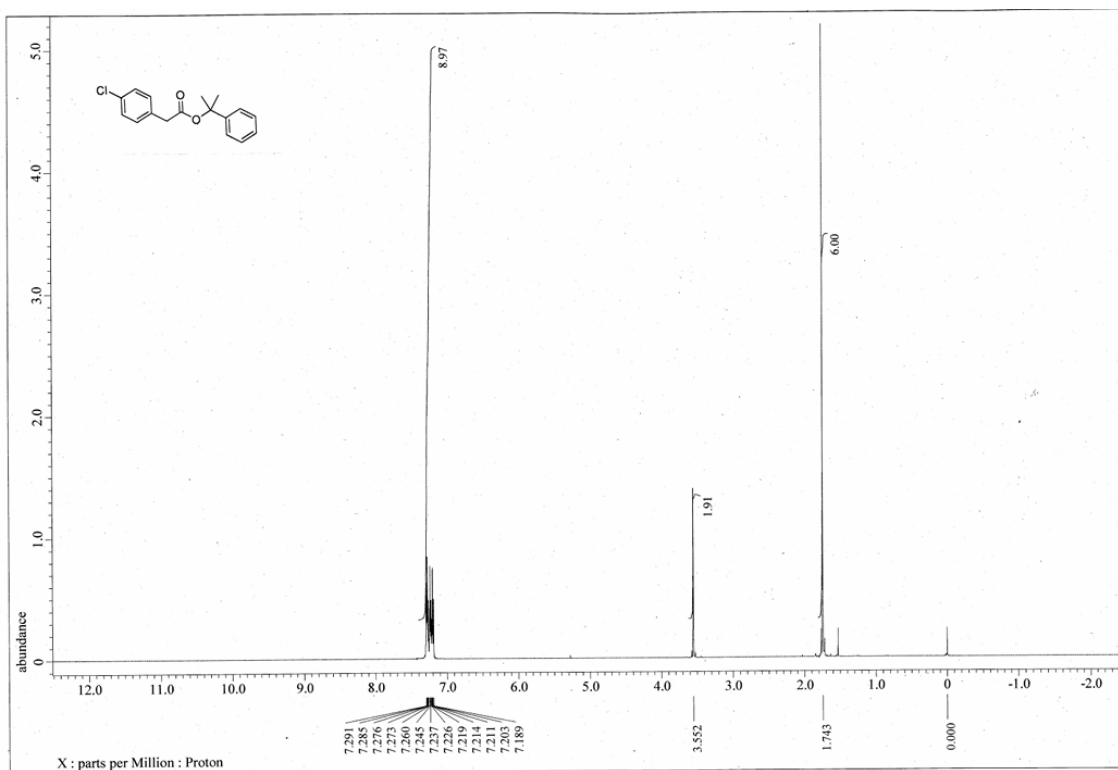
34	Atom	X	Y	Z
35	-----			
36	H	1.03898500	-2.83988400	1.22356300

1	H	-0.02451800	-1.54730800	1.09076000
2	H	1.96157900	-0.86781700	-0.15837300
3	N	0.58815700	-2.19583200	0.58079500
4	C	-0.02415900	-2.84645800	-0.51077700
5	C	0.53064300	-4.02269800	-1.04079200
6	C	-0.03503200	-4.62850700	-2.16102100
7	C	-1.15808400	-4.07432300	-2.77912200
8	C	-1.71255900	-2.90580900	-2.25315200
9	C	-1.15788900	-2.29429100	-1.12939600
10	H	1.41098400	-4.45749900	-0.57137000
11	H	0.40784200	-5.54098100	-2.55258400
12	H	-1.59678000	-4.54871900	-3.65213700
13	H	-2.59434200	-2.46668400	-2.71305000
14	H	-1.61260000	-1.39807000	-0.71539600
15	C	3.73342800	0.12455600	0.17089900
16	C	4.86102700	0.67175600	-0.46315300
17	C	3.79446200	-0.12669500	1.55245200
18	C	6.01398100	0.95703100	0.26586100
19	H	4.82756700	0.87374500	-1.53189200
20	C	4.95223400	0.16062800	2.27262700
21	H	2.92707900	-0.54976200	2.05362500
22	C	6.07103800	0.70496600	1.63817200
23	H	6.87563500	1.37772200	-0.24652100
24	H	4.97932100	-0.04577200	3.33988100
25	H	6.97185500	0.92686700	2.20275800
26	N	2.54212900	-0.10901100	-0.53964600
27	H	2.68799600	-0.24111200	-1.53562800
28	H	0.96910000	2.85383100	0.62802300
29	H	1.19585100	1.40533800	-0.17508100
30	N	0.50413500	2.10630100	0.12140800
31	C	-0.30825100	2.58244000	-0.92628100
32	C	-0.81867400	3.89073300	-0.91122400
33	C	-1.66732100	4.33139100	-1.92513000
34	C	-2.02513200	3.48223200	-2.97425400
35	C	-1.52168300	2.17966000	-2.99206000
36	C	-0.67387700	1.72822600	-1.98163400

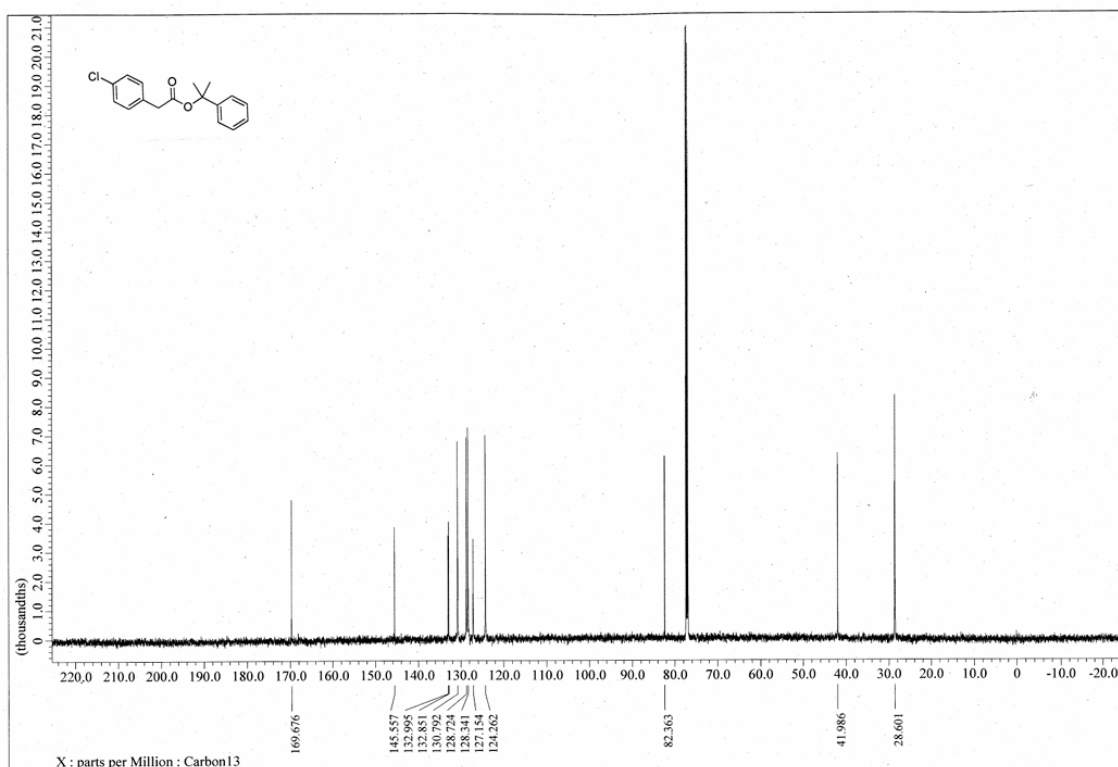
1	H	-0.54647400	4.56146200	-0.09863200
2	H	-2.04817100	5.34920100	-1.89408900
3	H	-2.68488800	3.82941800	-3.76403300
4	H	-1.78852000	1.50387200	-3.80084400
5	H	-0.29319900	0.70995200	-2.00219900
6	H	-0.43880800	0.14440600	2.97398300
7	C	-2.29893300	0.09630500	2.16310500
8	C	-3.08910800	0.59463300	1.11402300
9	C	-2.93517700	-0.46189800	3.28327200
10	C	-4.47967200	0.52744100	1.19009000
11	H	-2.61033100	1.04214300	0.24657200
12	C	-4.32586000	-0.52134000	3.35020800
13	H	-2.33303800	-0.85337300	4.10117500
14	C	-5.10993000	-0.02934100	2.30471900
15	H	-5.07355800	0.92220800	0.36952700
16	H	-4.79806900	-0.95550200	4.22806100
17	H	-6.19365800	-0.07671500	2.35944000
18	N	-0.89081000	0.10204100	2.06501700
19	H	-0.51495800	0.84070500	1.45684300
20				
21				

1 9. Copy of NMR and HPLC Spectra

2 e1



3

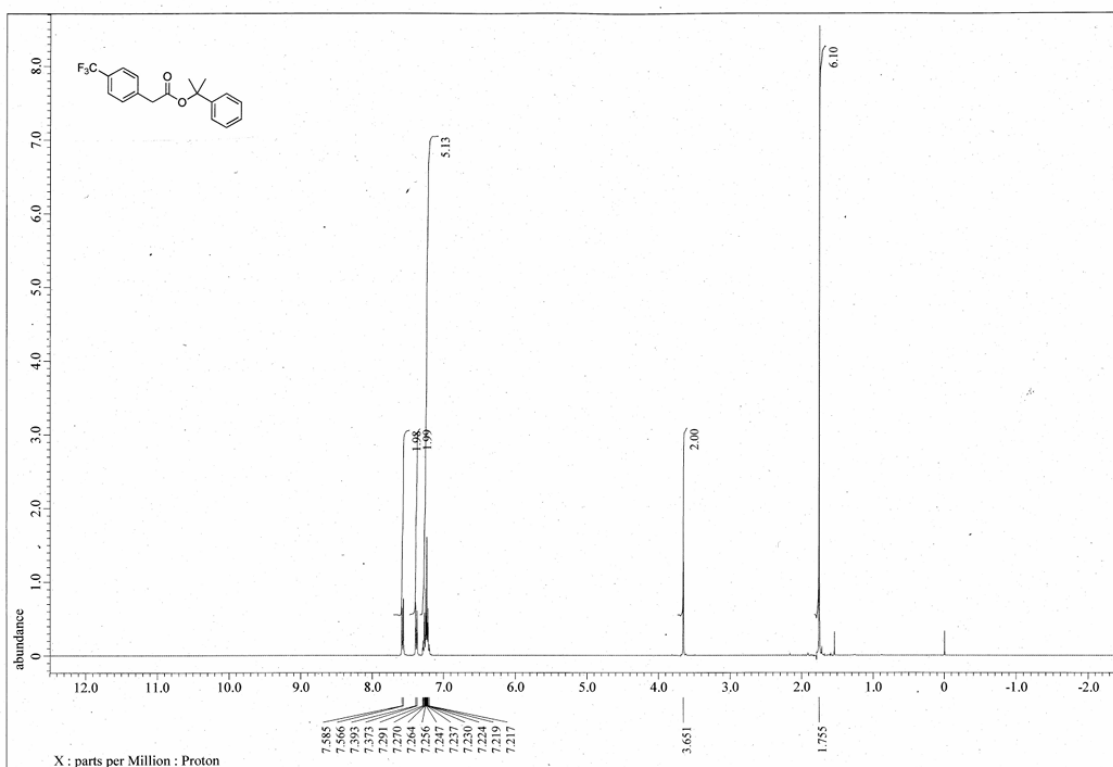


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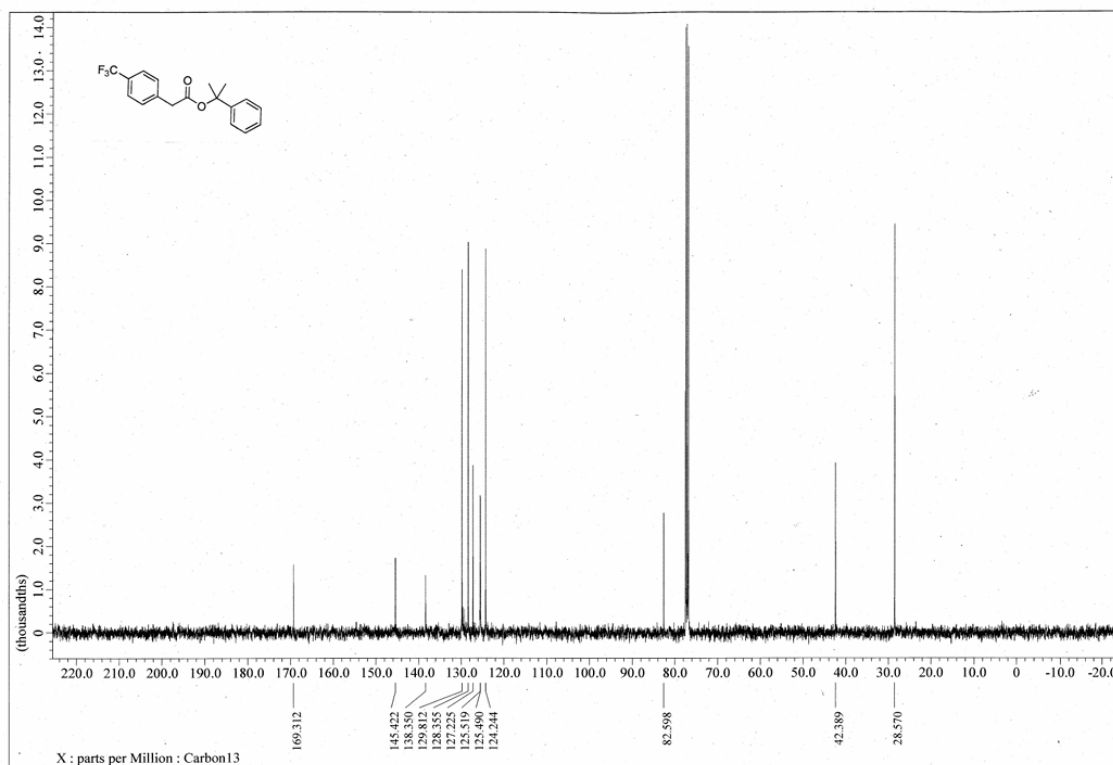
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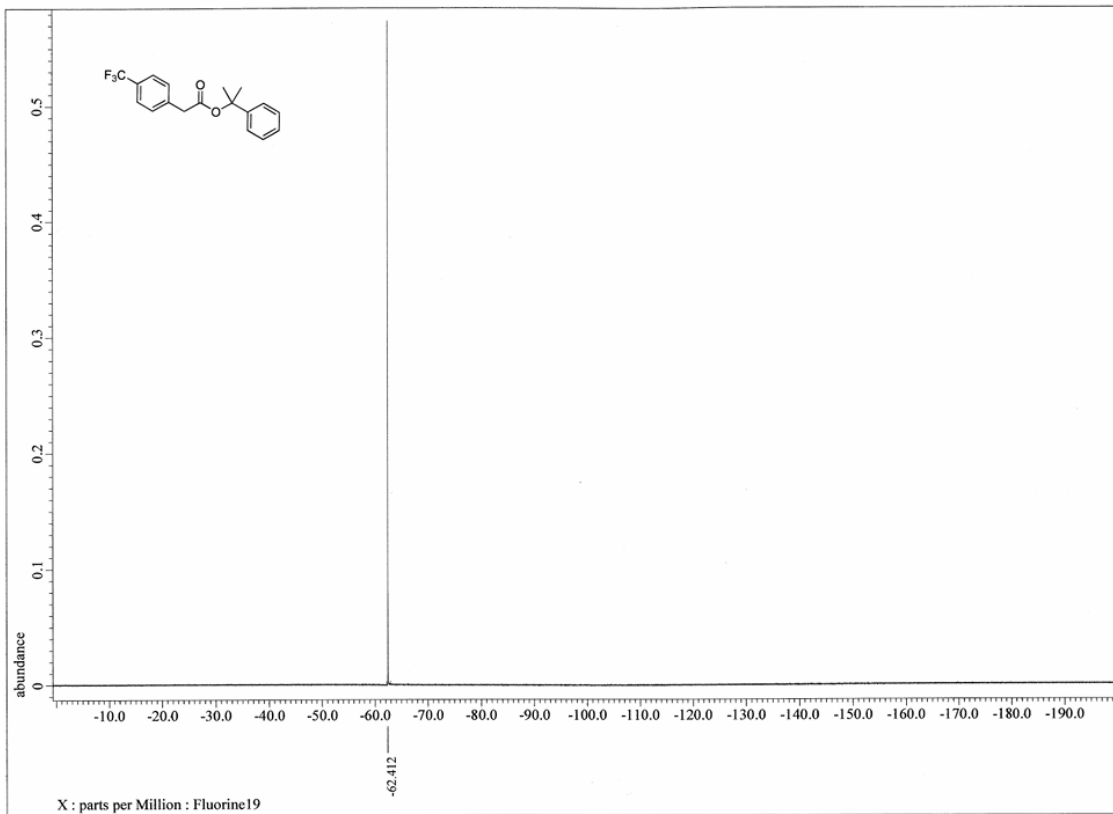


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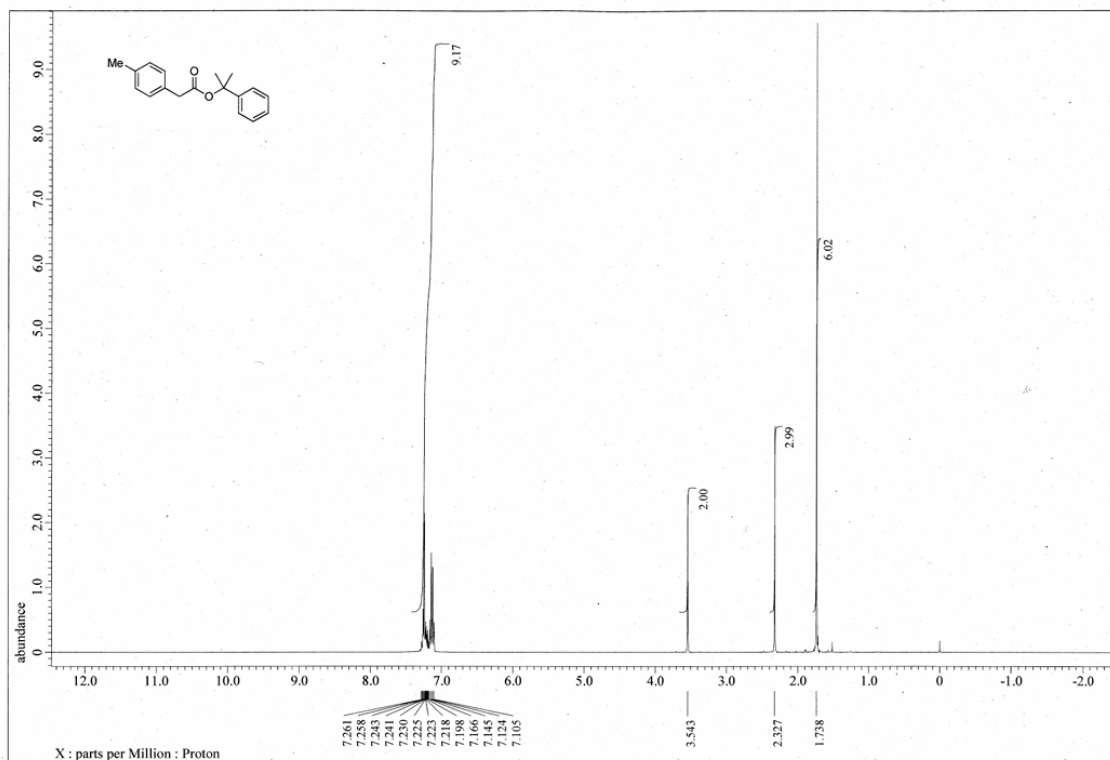


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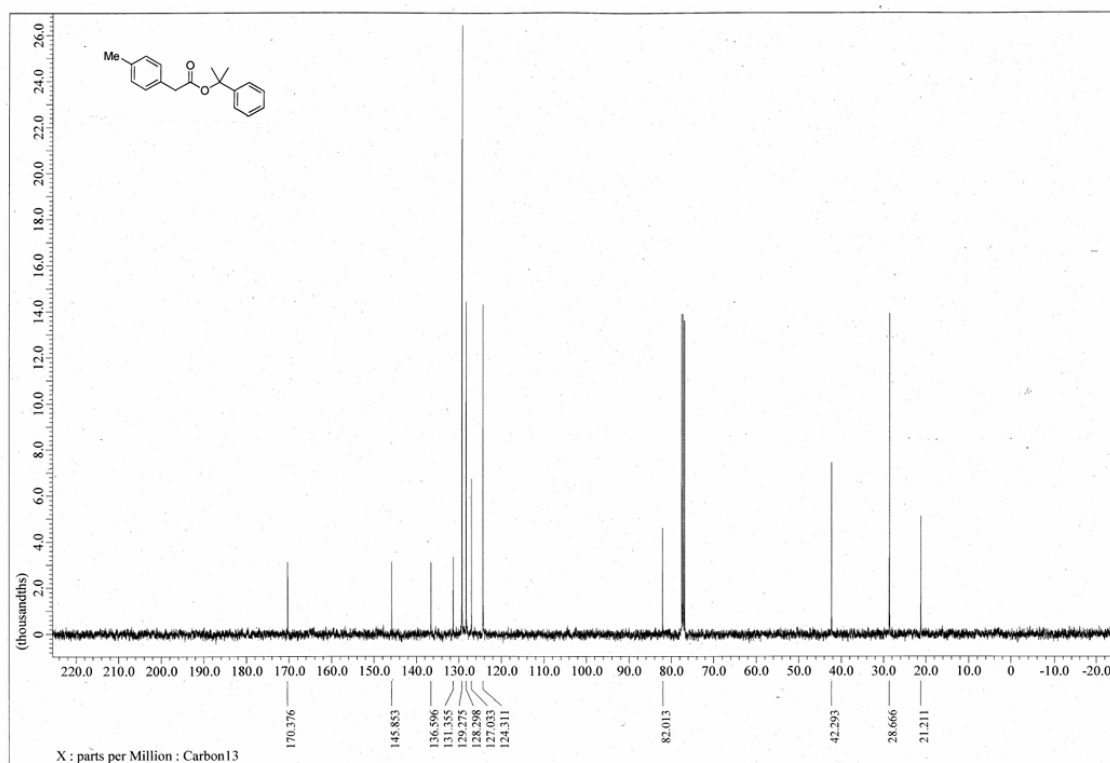
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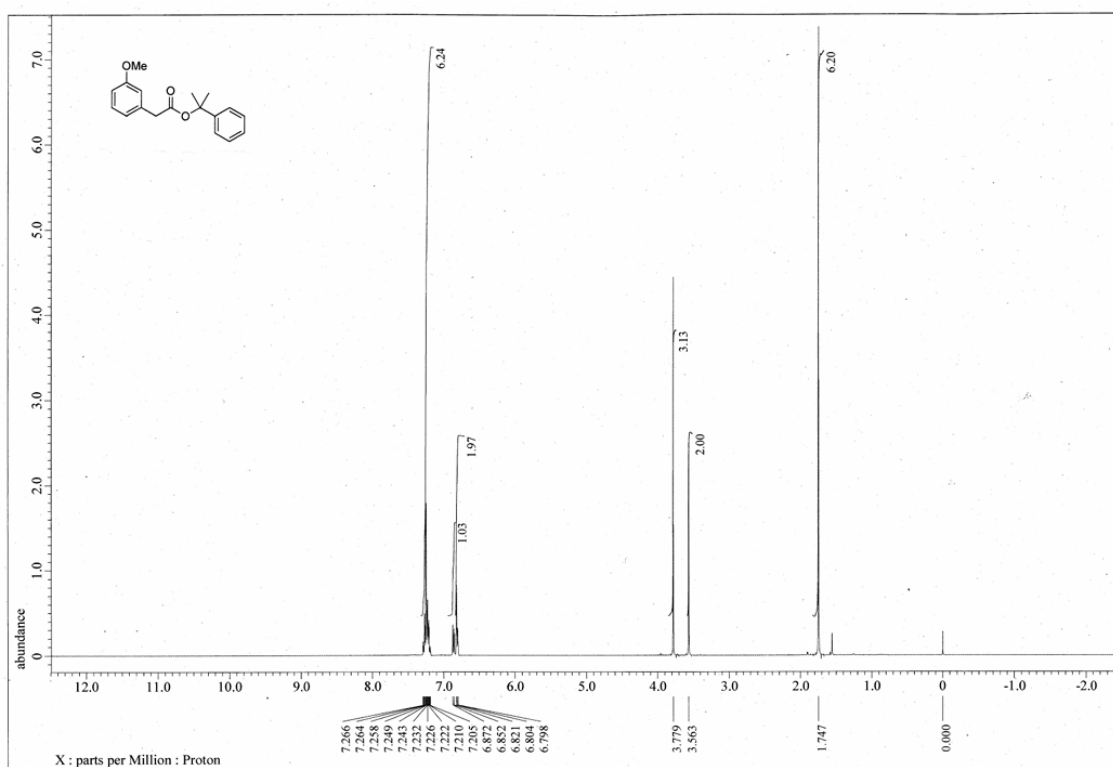


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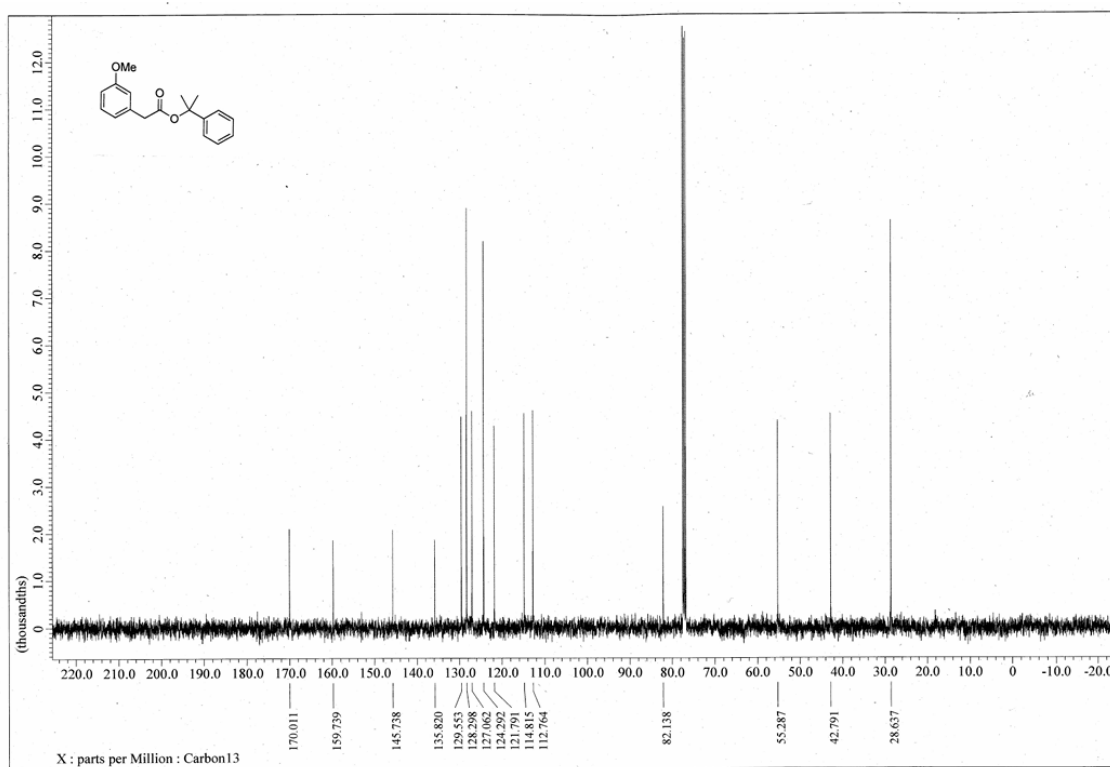
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e4



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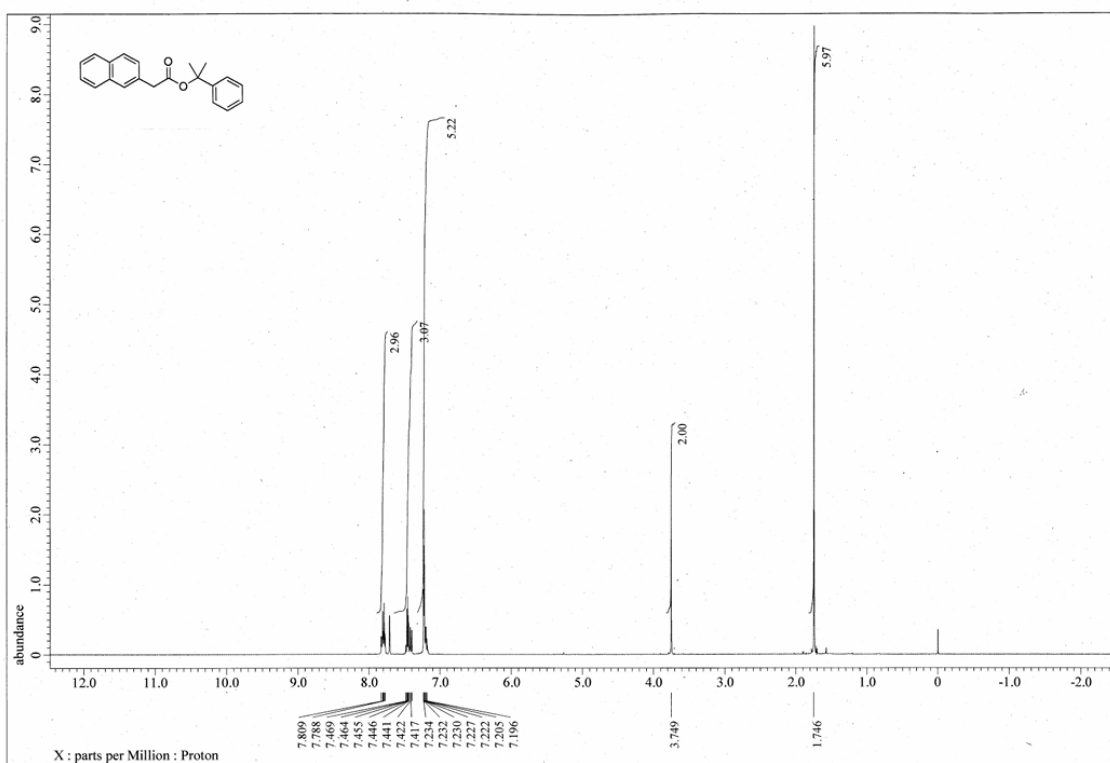


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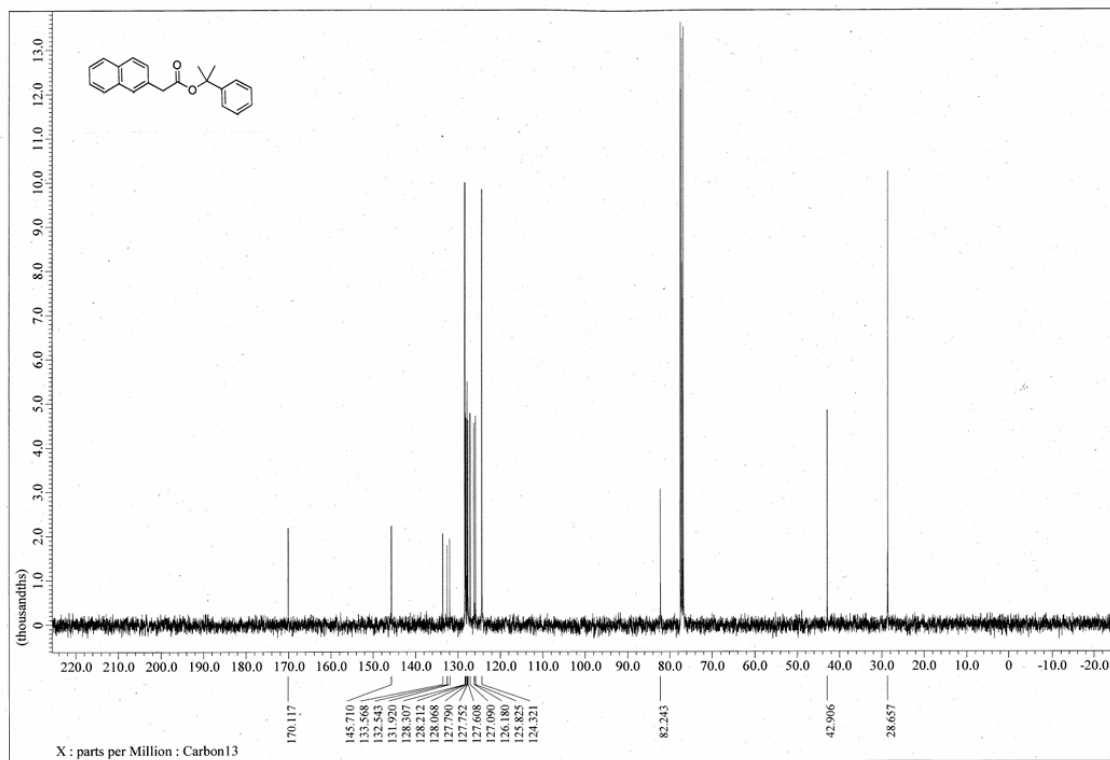
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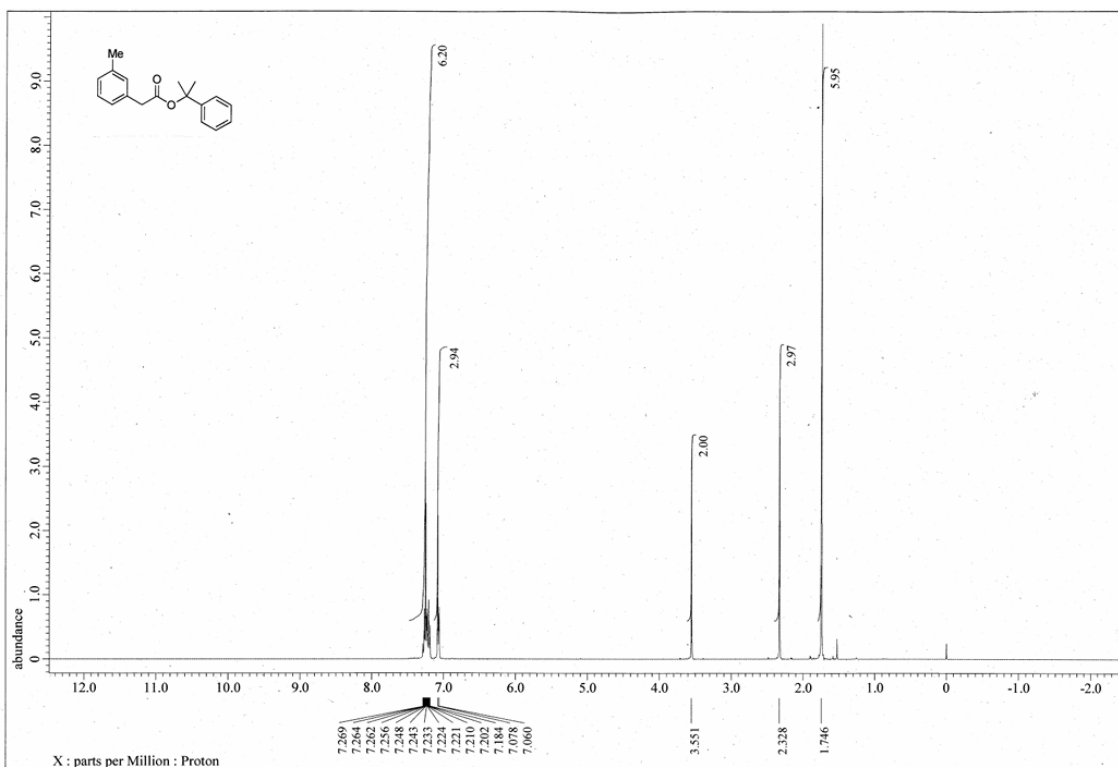


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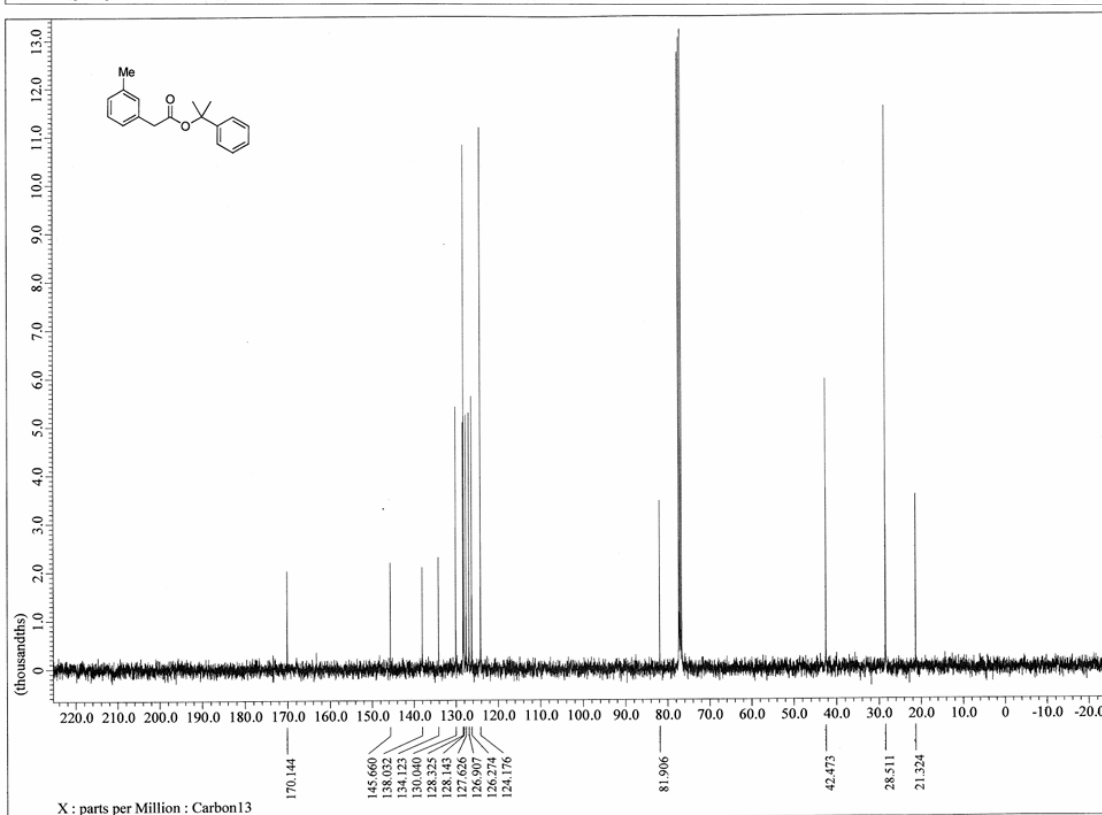
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e6



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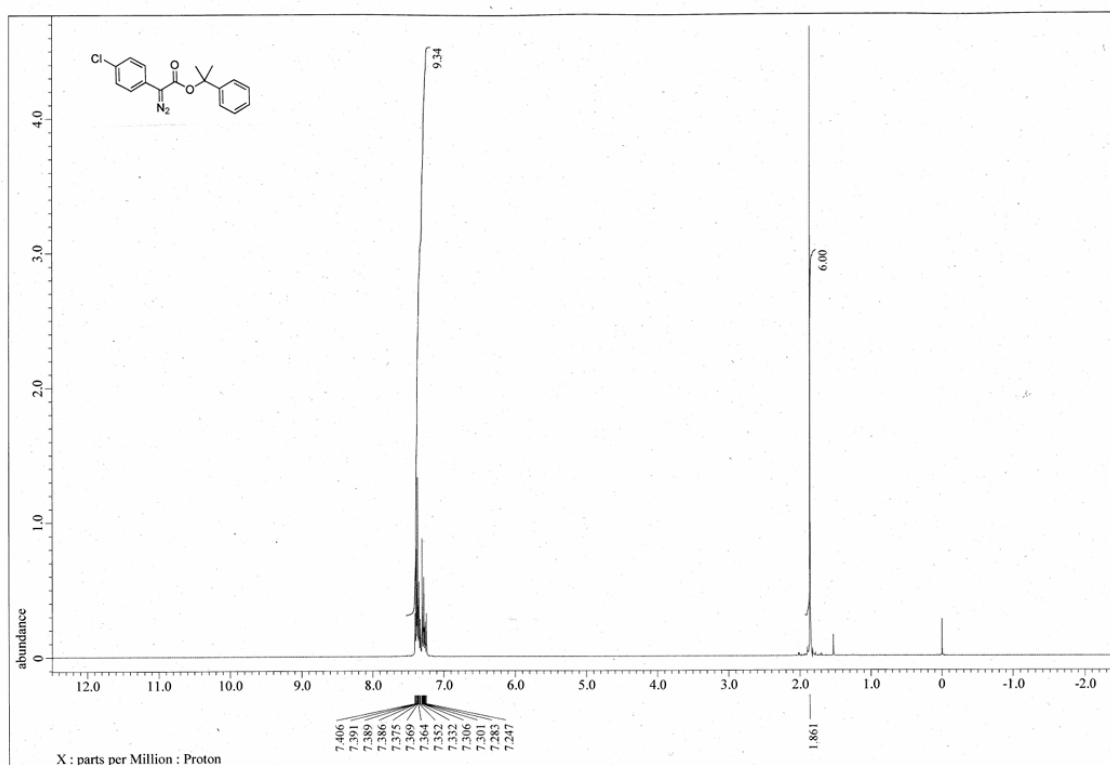


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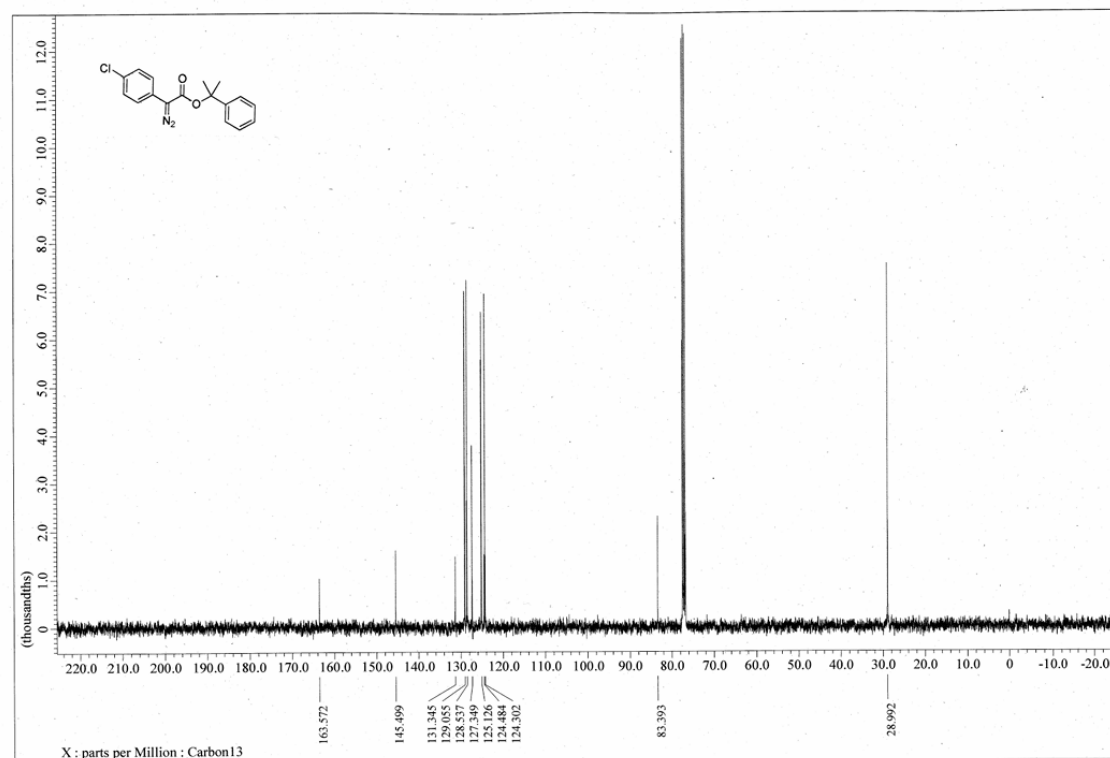
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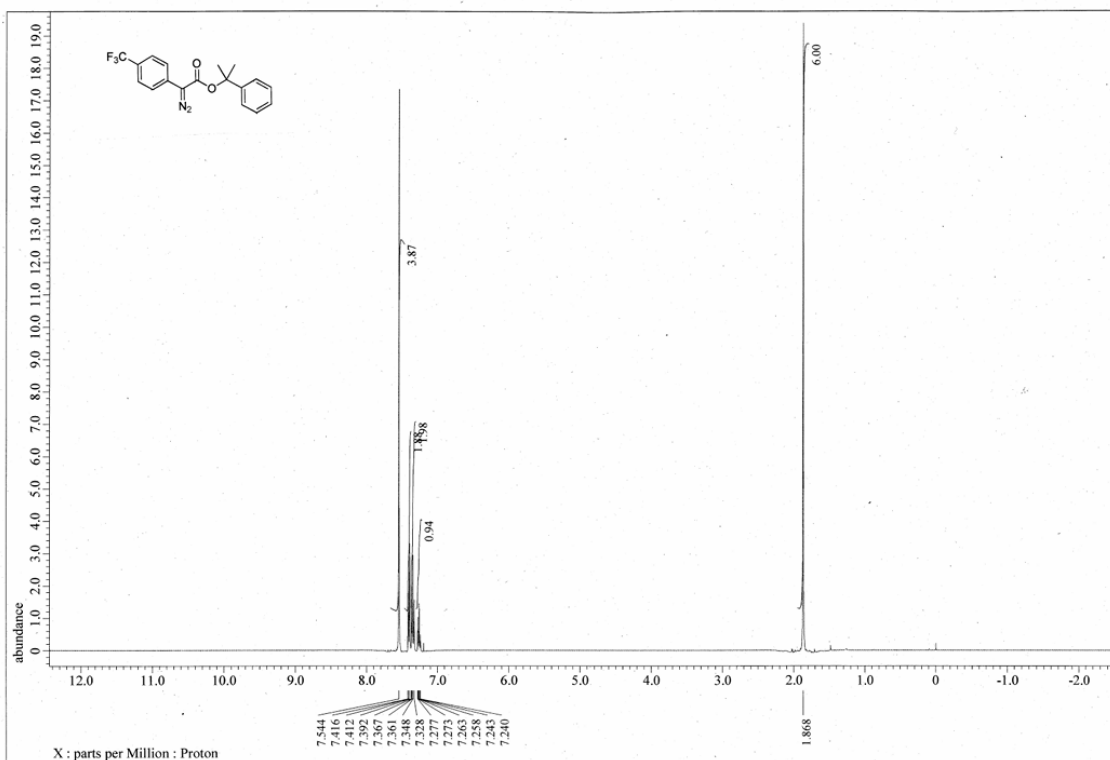


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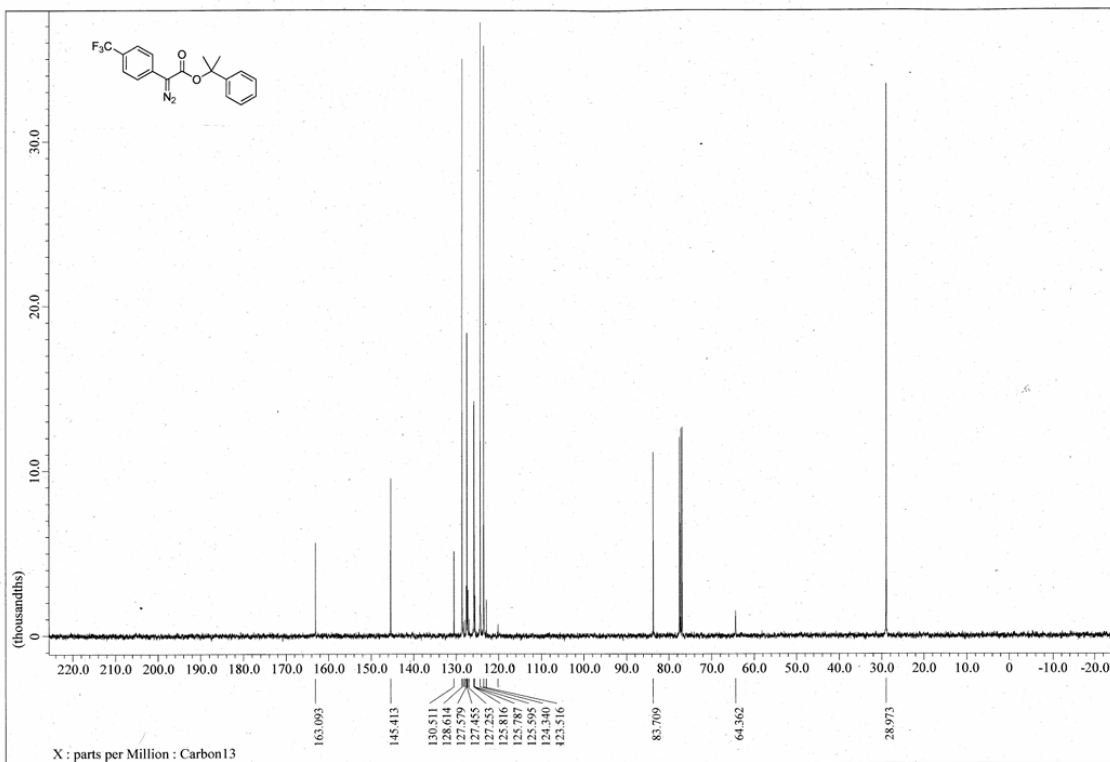
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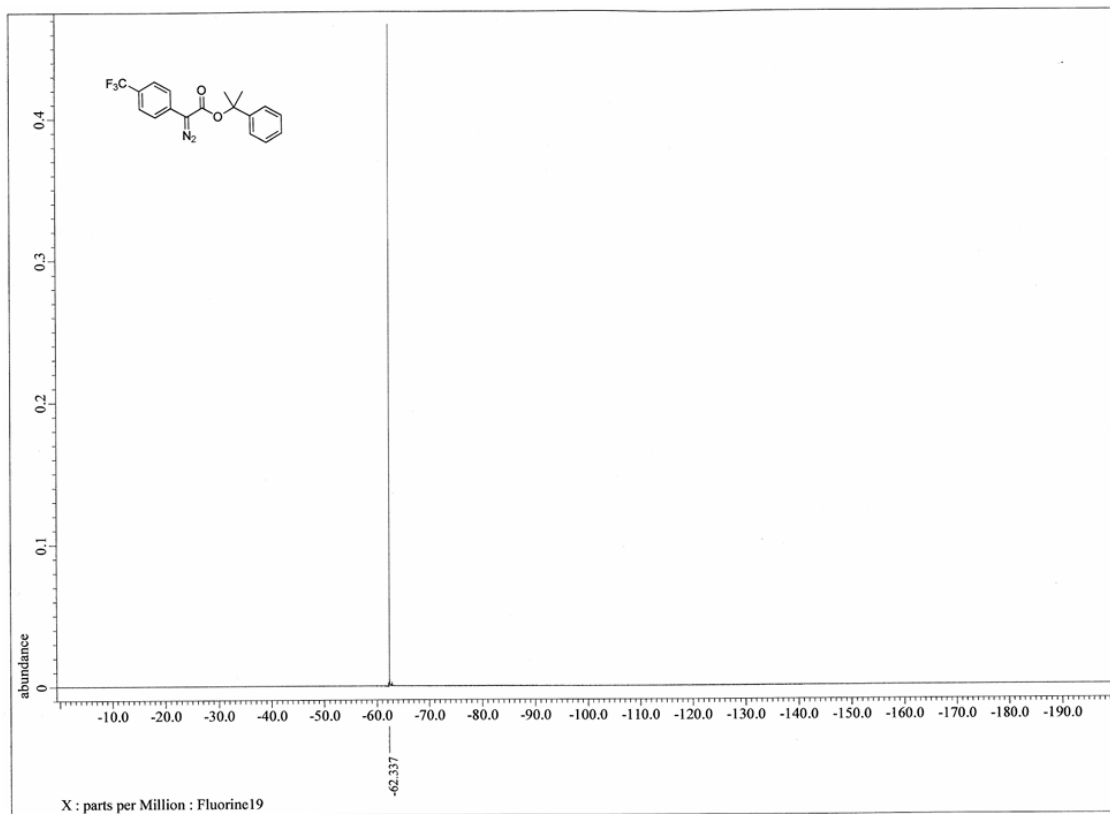


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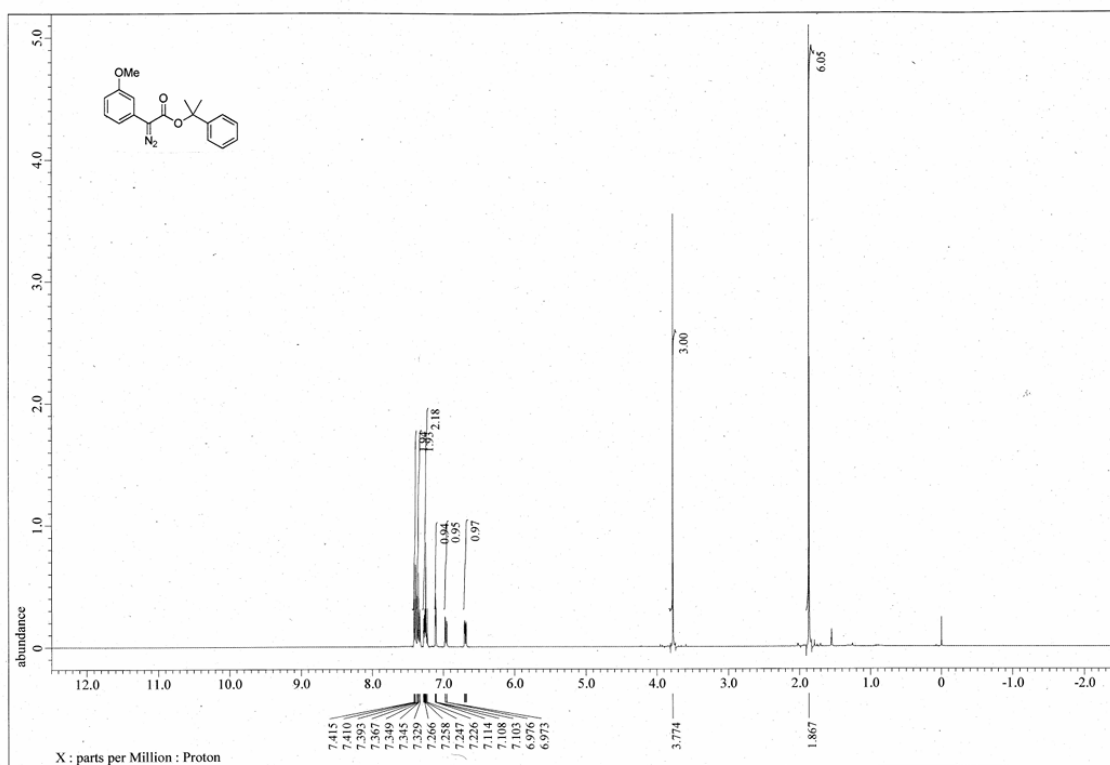


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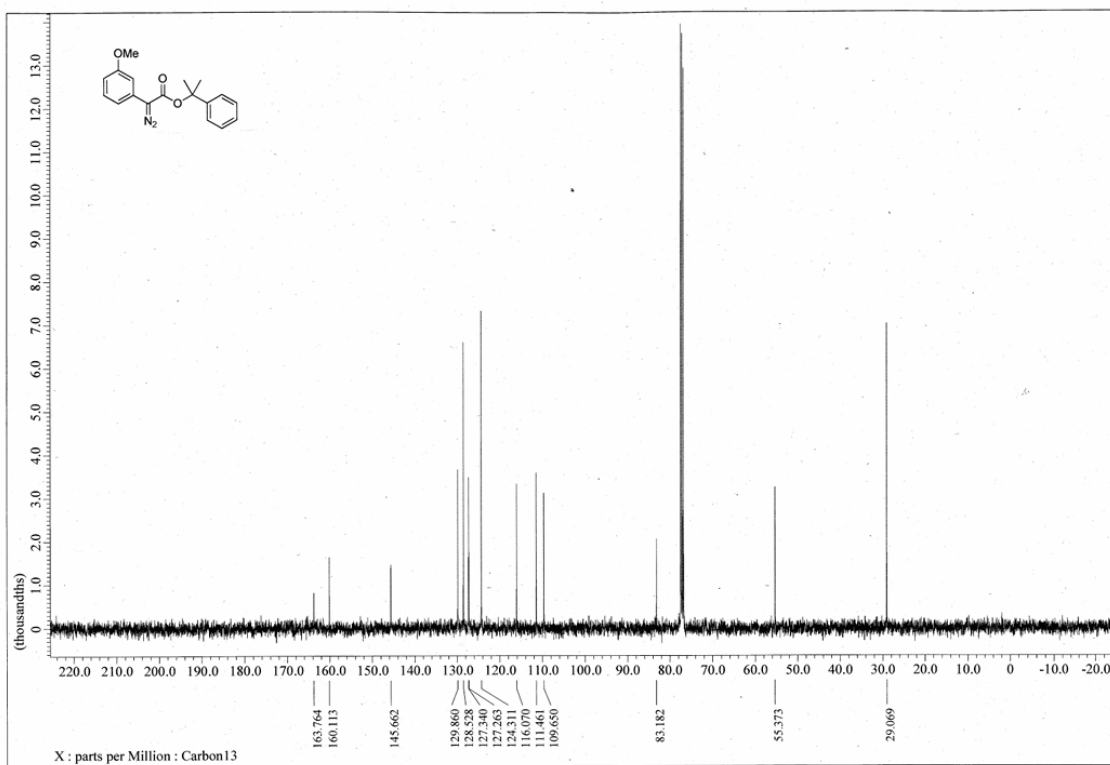
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d4



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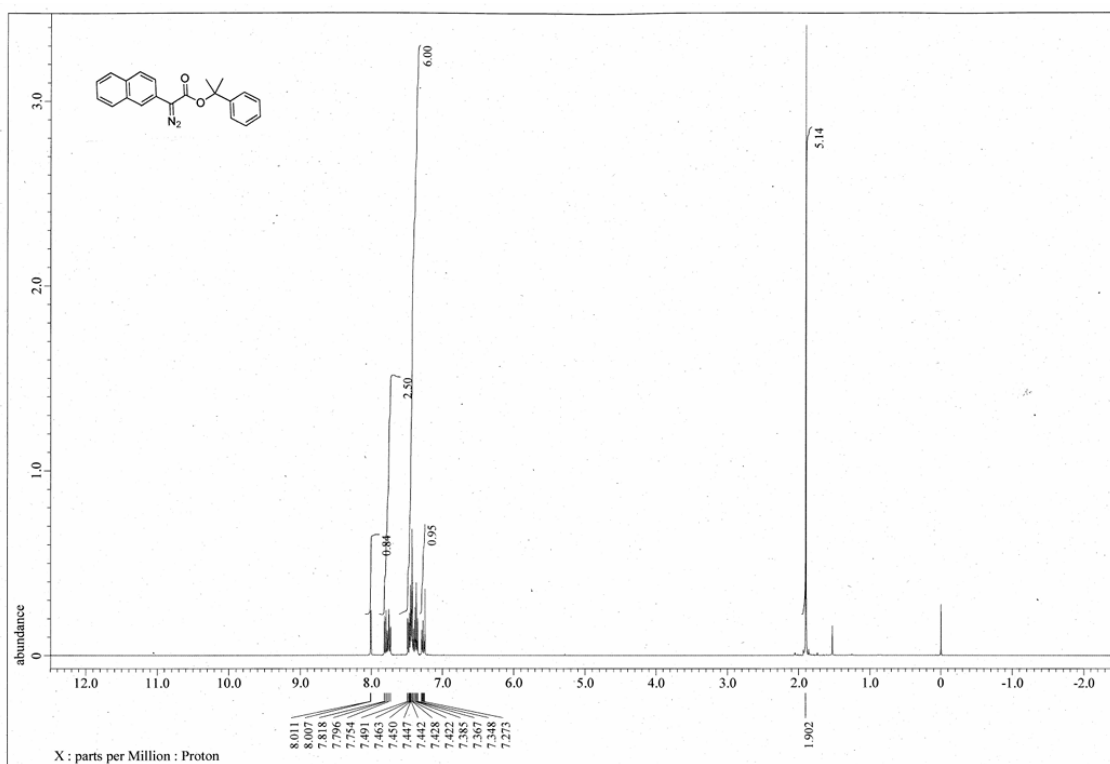


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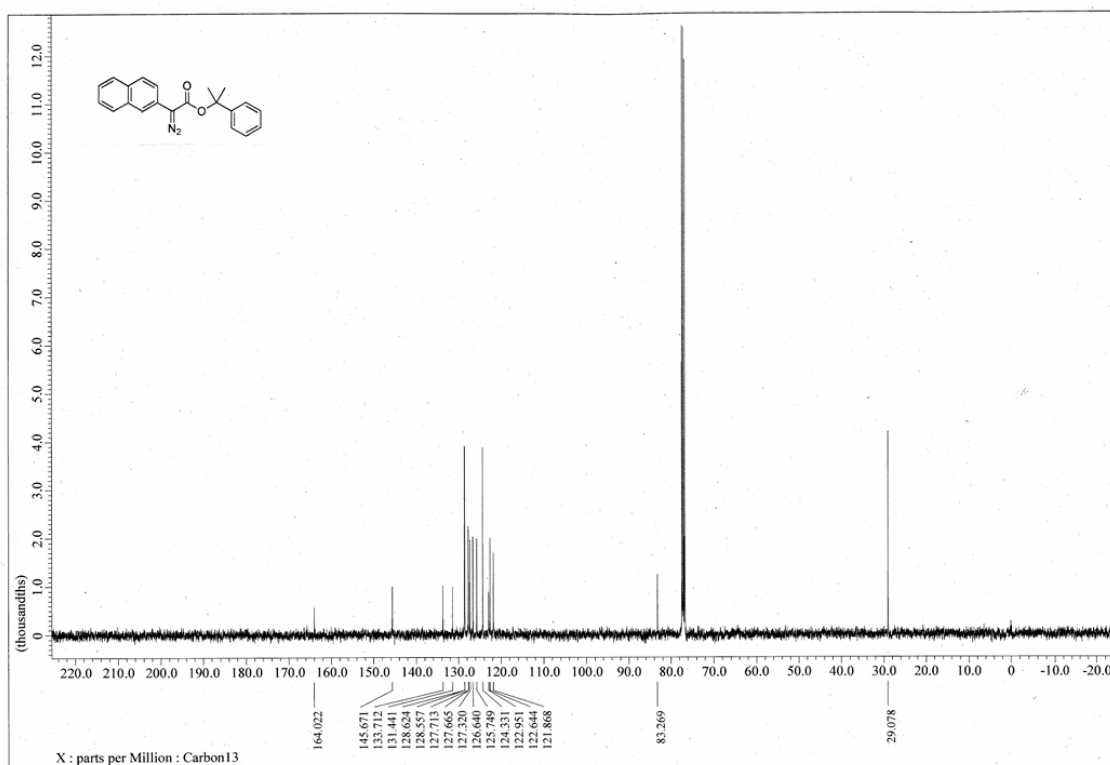
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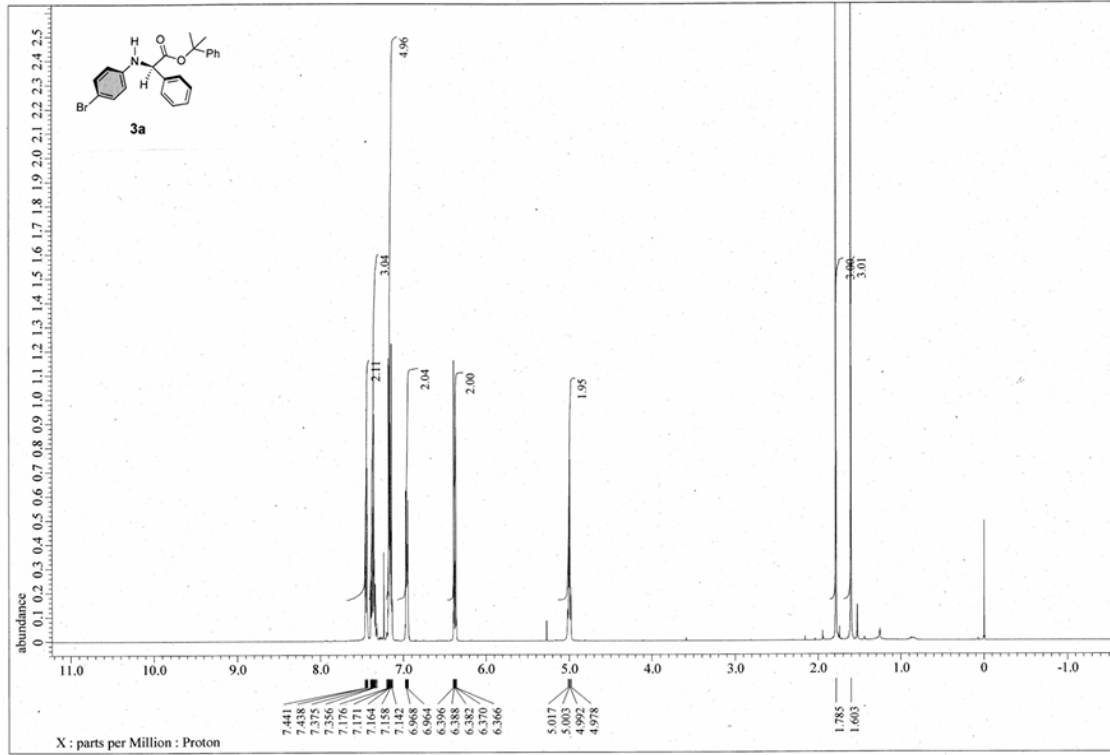


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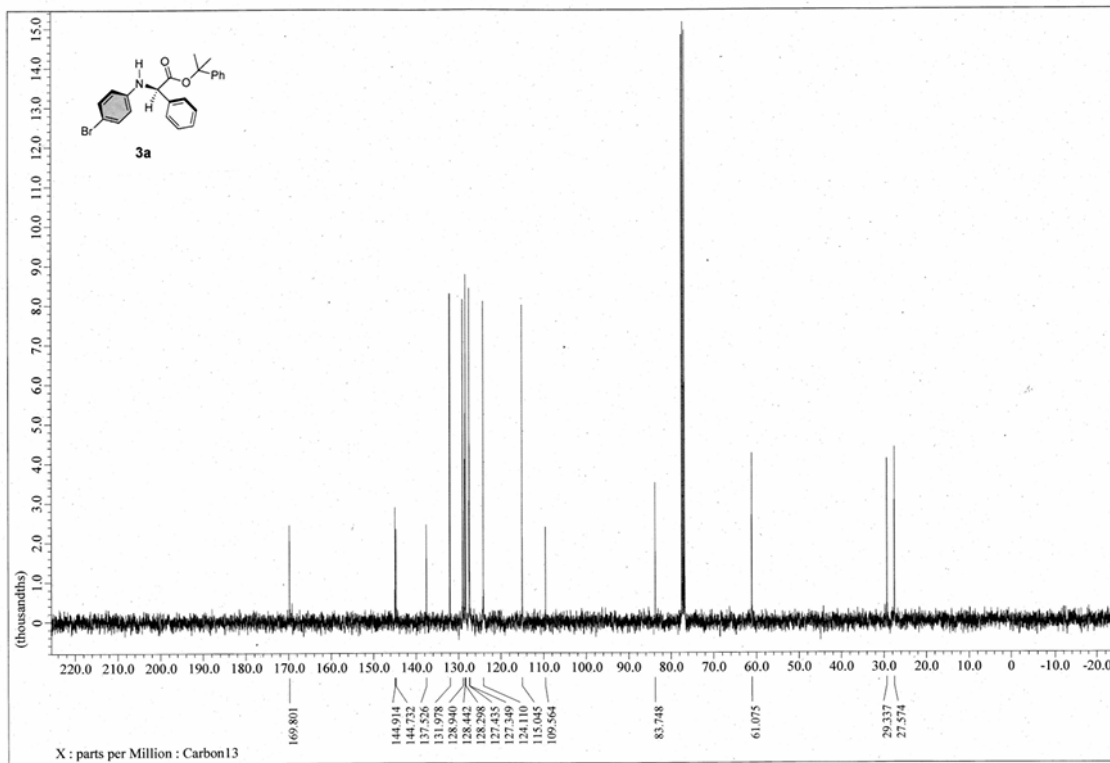
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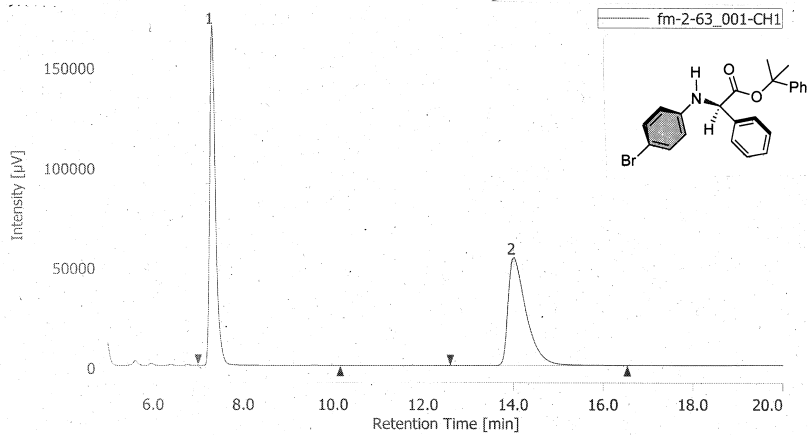
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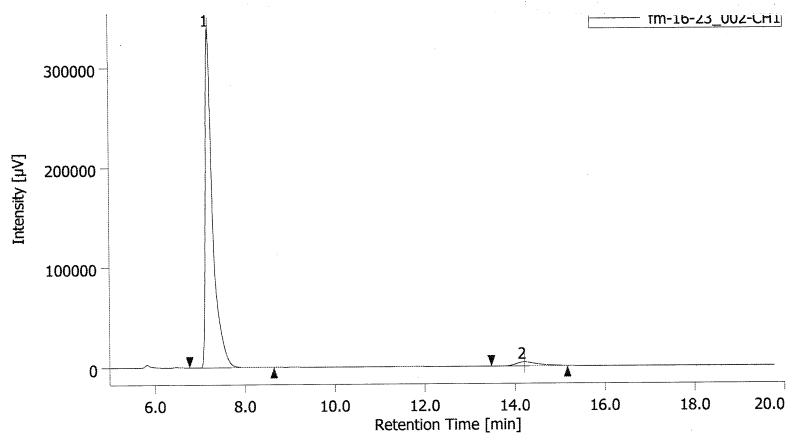
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4



#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	7.317	1528404	50.375	170252	75.966
2	14.017	1505678	49.625	53884	24.034

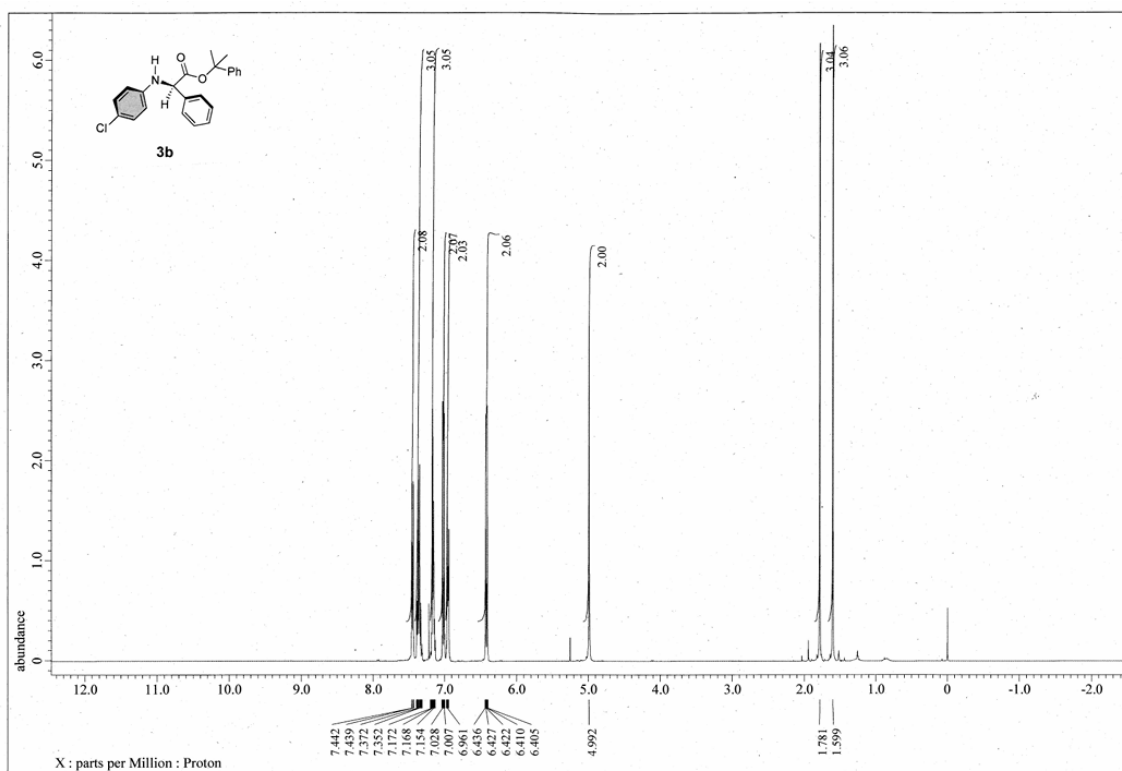


#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	7.208	3799117	96.691	340223	98.858
2	14.208	130007	3.309	3930	1.142

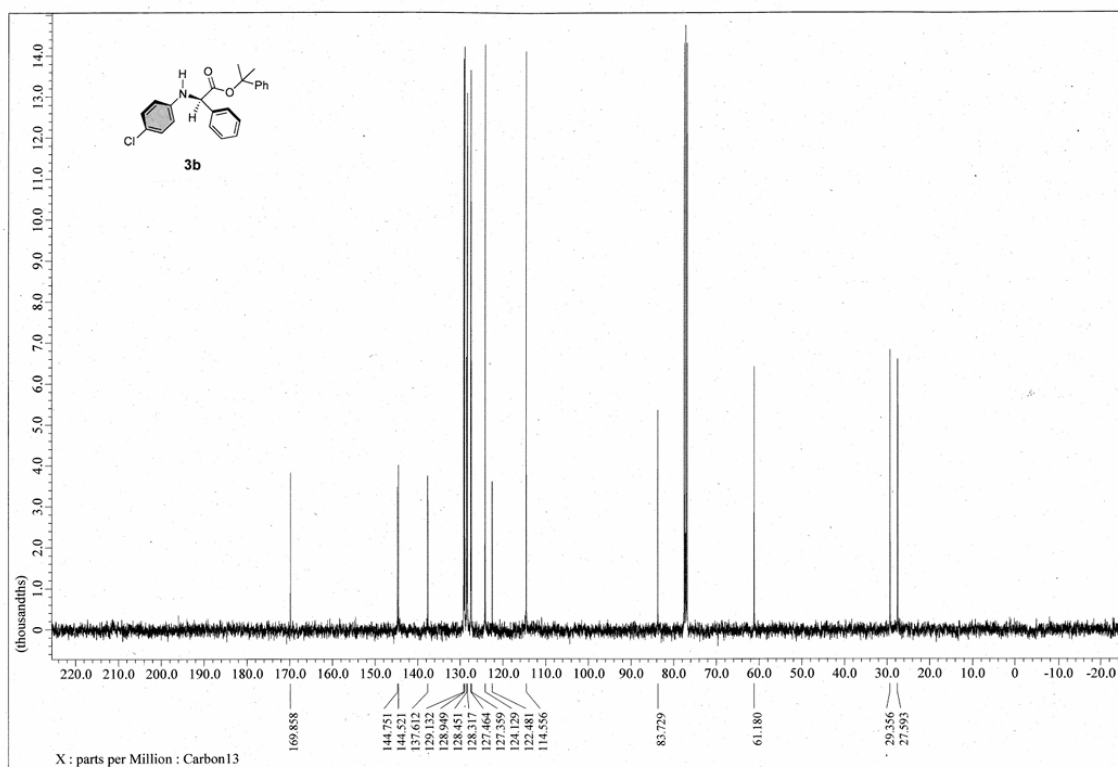
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3b

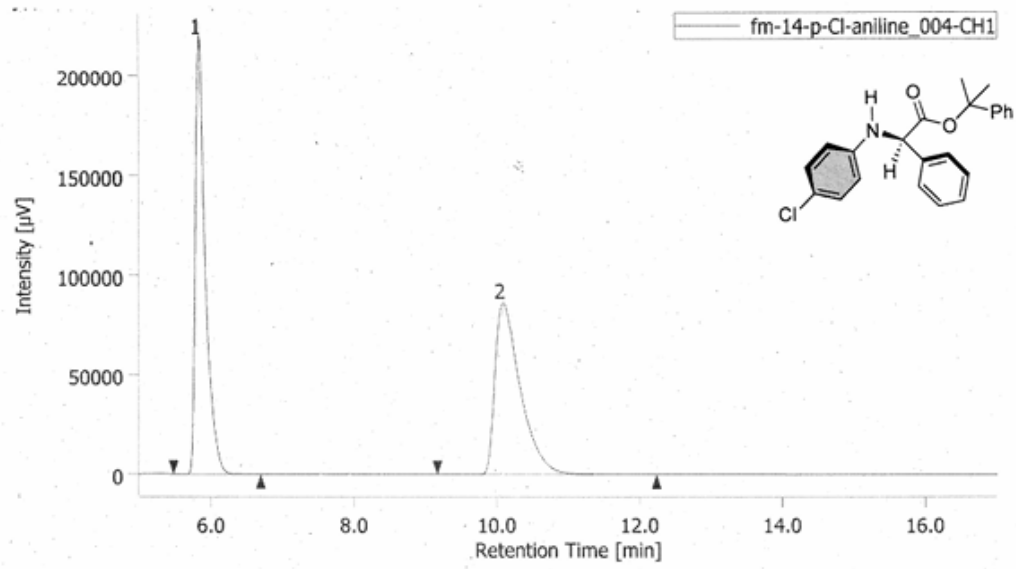


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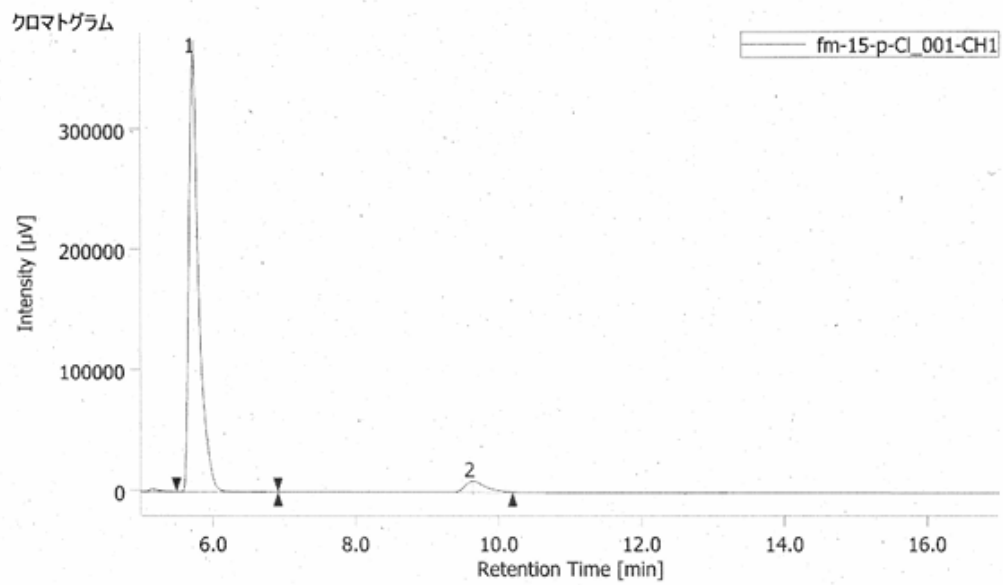
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4



#	tR [min]	Area [$\mu\text{V}\cdot\text{sec}$]	Area%	Height [μV]	Height%
1	5.842	2130996	50.098	220009	71.734
2	10.092	2122625	49.902	86694	28.266

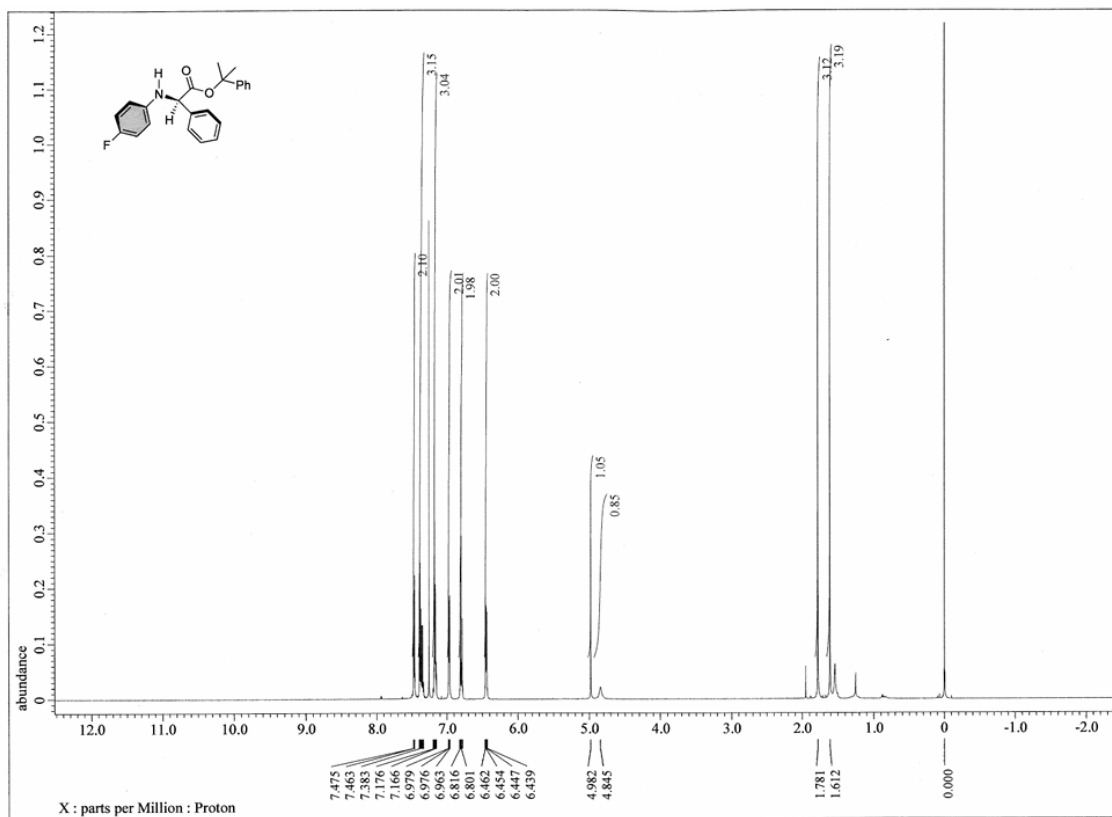
228 fm-15-p-Cl_001 2025/03/13 12:55:28



#	tR [min]	Area [$\mu\text{V}\cdot\text{sec}$]	Area%	Height [μV]	Height%
1	5.725	3404020	94.989	362464	97.533
2	9.642	179571	5.011	9166	2.467

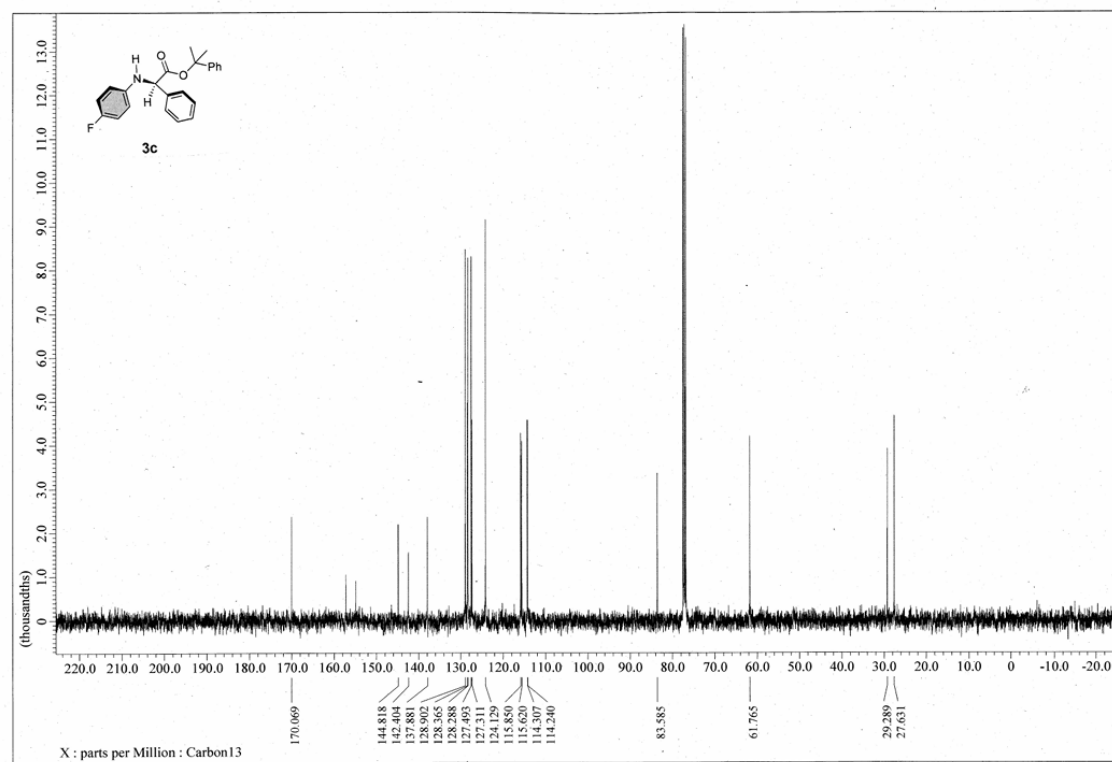
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3c

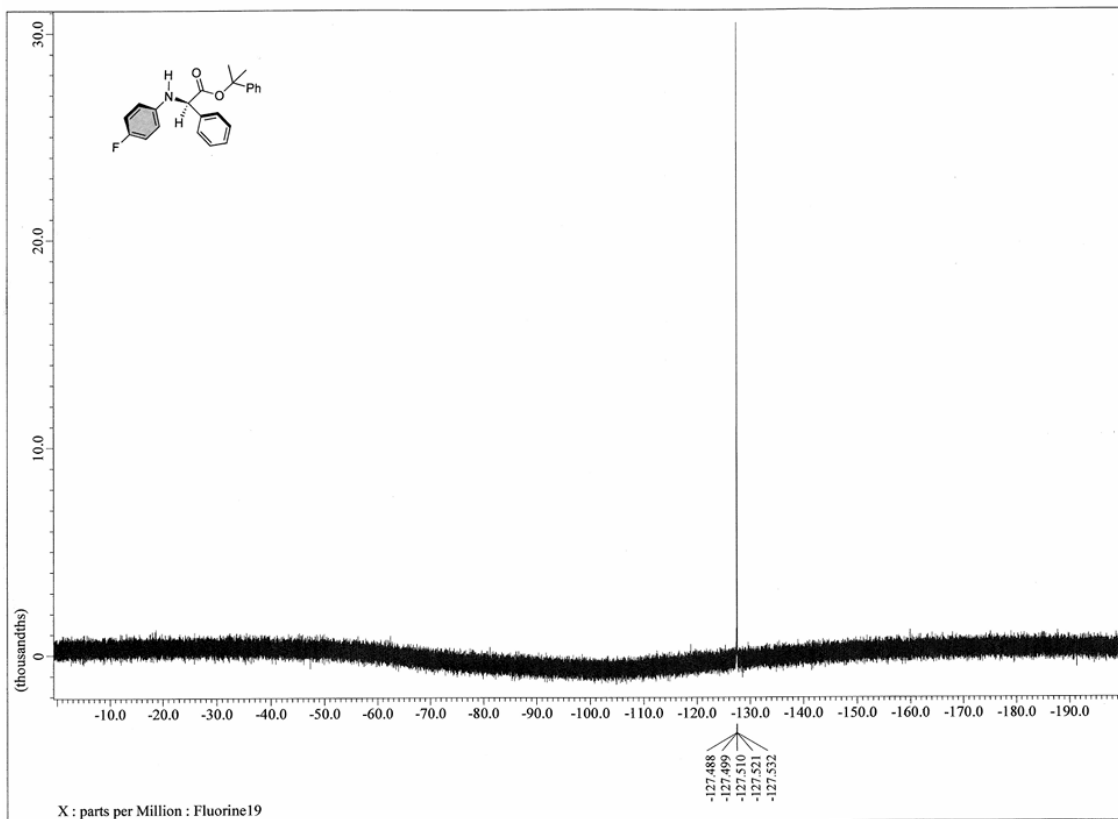


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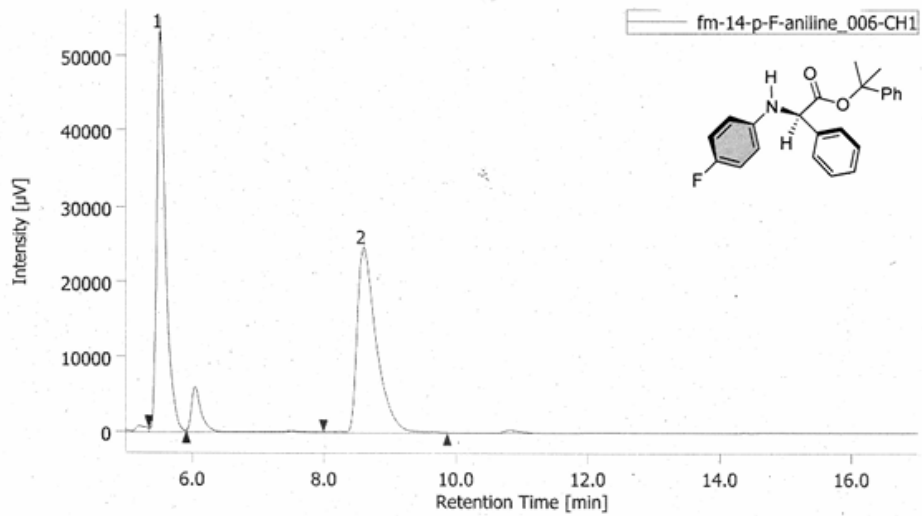


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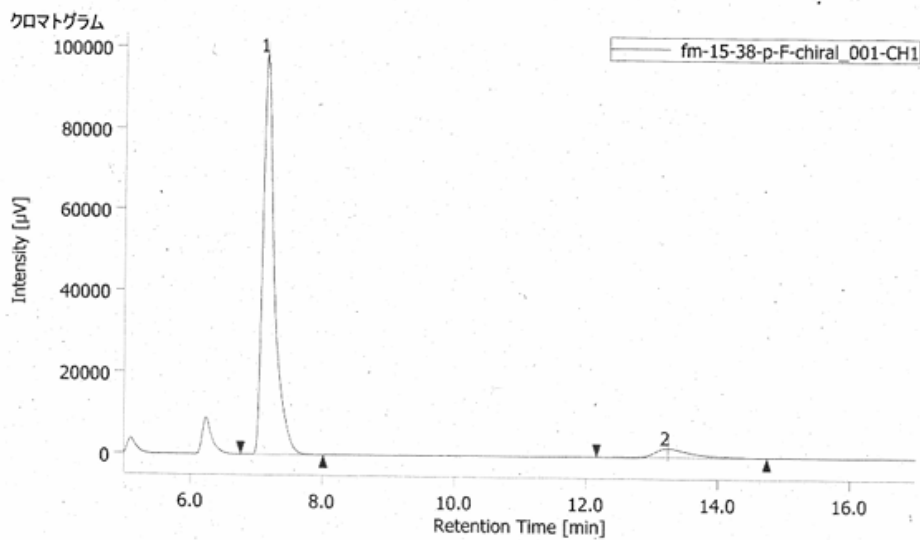
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2



#	tR [min]	Area [μV-sec]	Area%	Height [μV]	Height%
1	5.517	495834	49.935	53367	68.397
2	8.600	497126	50.065	24658	31.603

0110 fm-15-38-p-F-chiral_001 2025/03/13 13:03:48

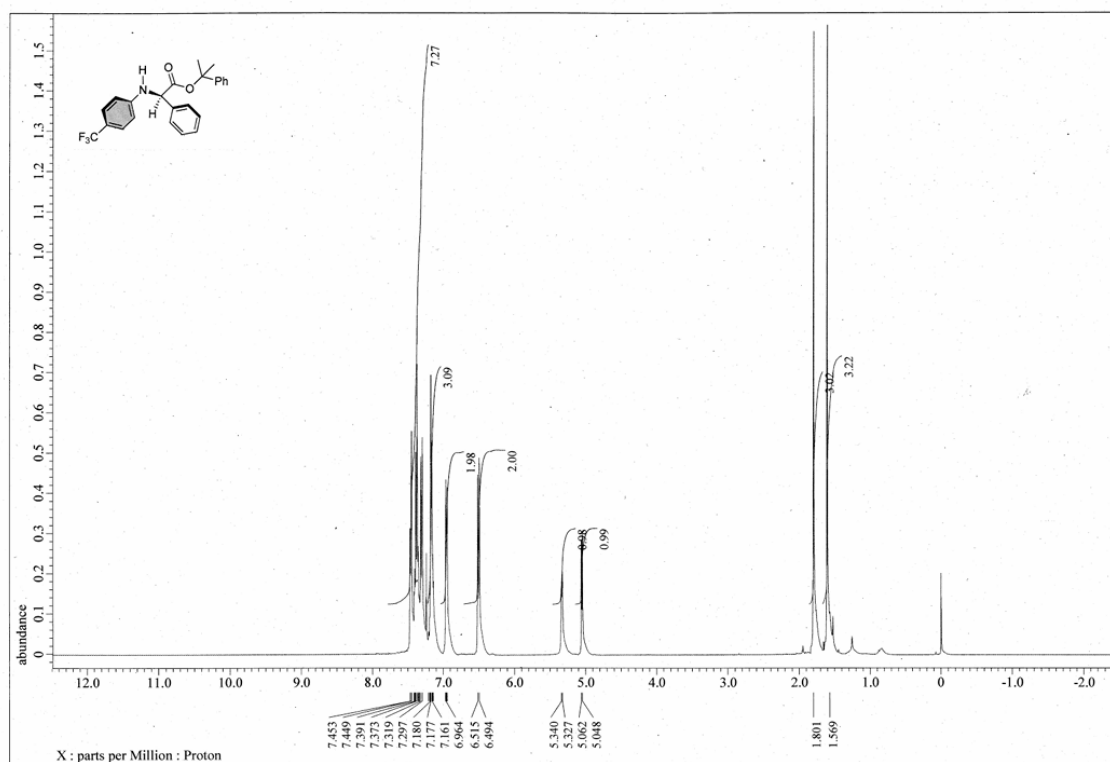


#	tR [min]	Area [μV-sec]	Area%	Height [μV]	Height%
1	7.142	1200720	93.774	98522	97.856
2	13.242	79715	6.226	2158	2.144

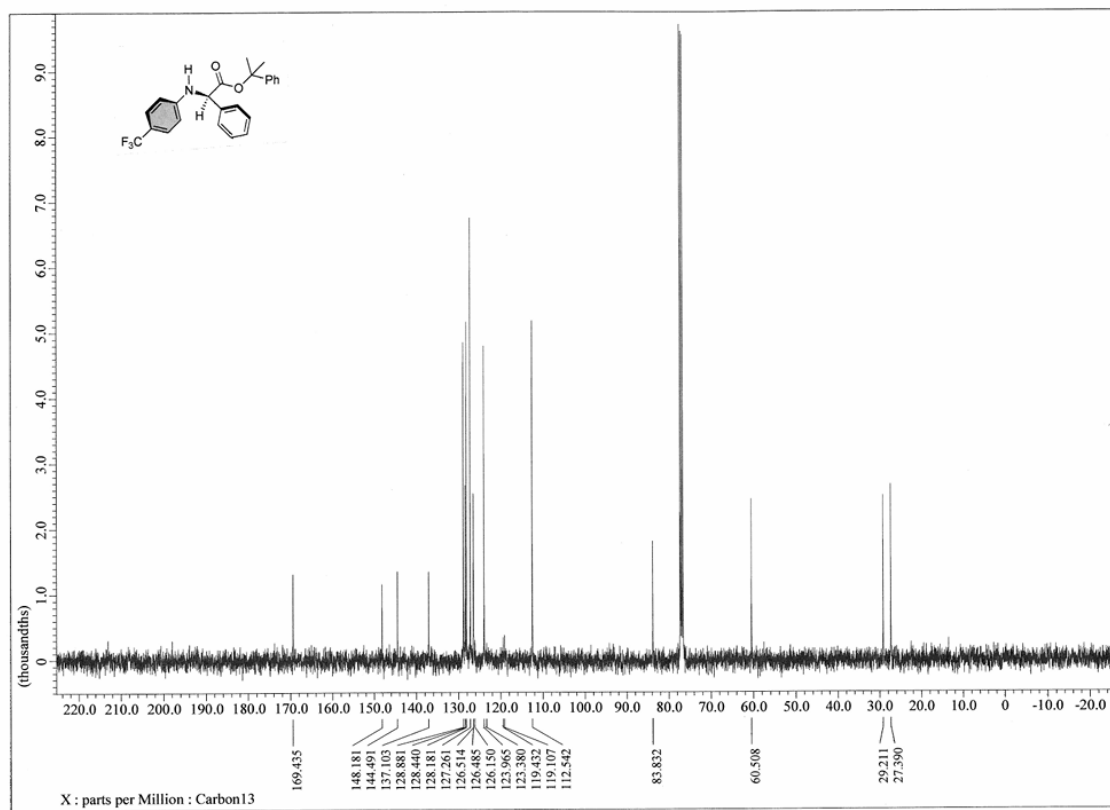
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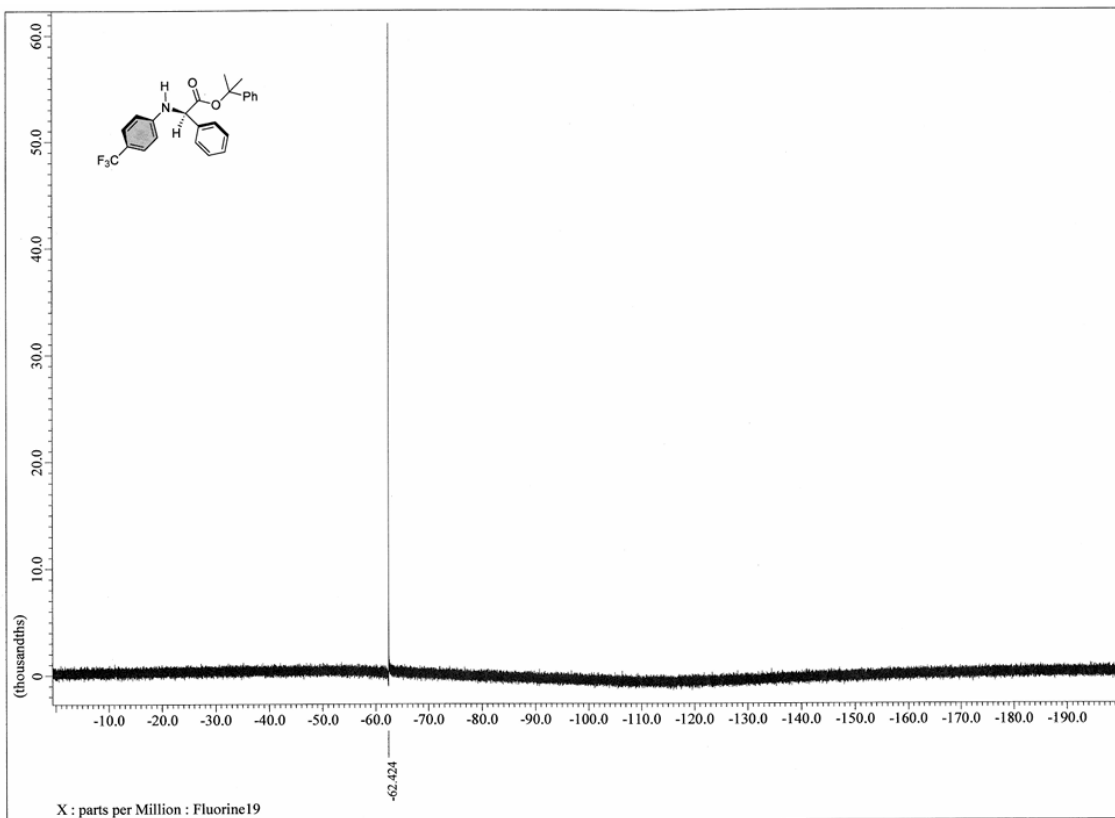
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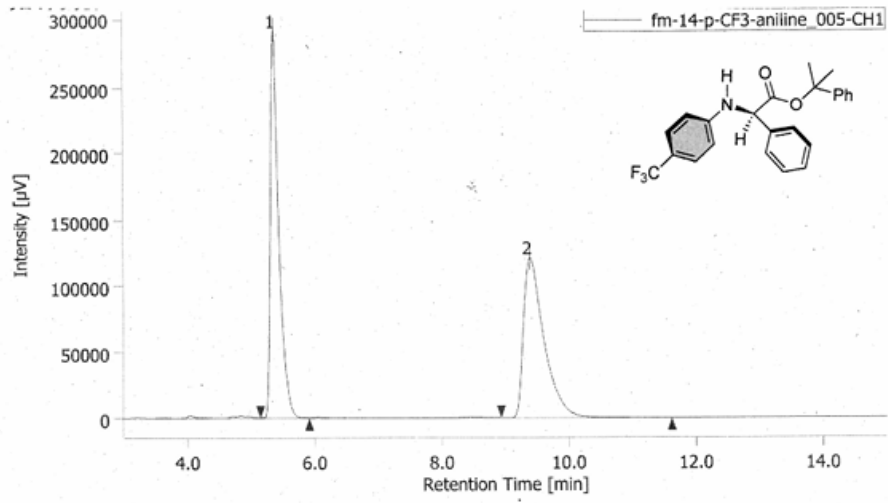
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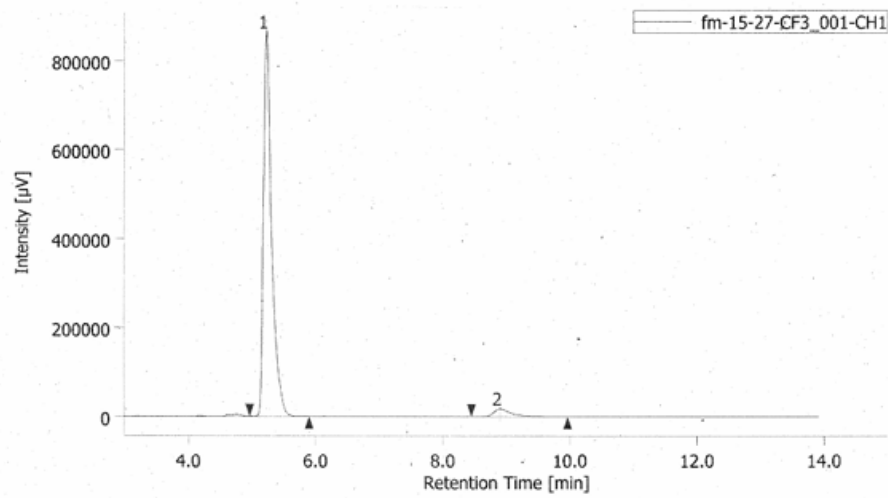
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#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	5.367	2696655	50.043	293053	70.774
2	9.392	2692015	49.957	121013	29.226

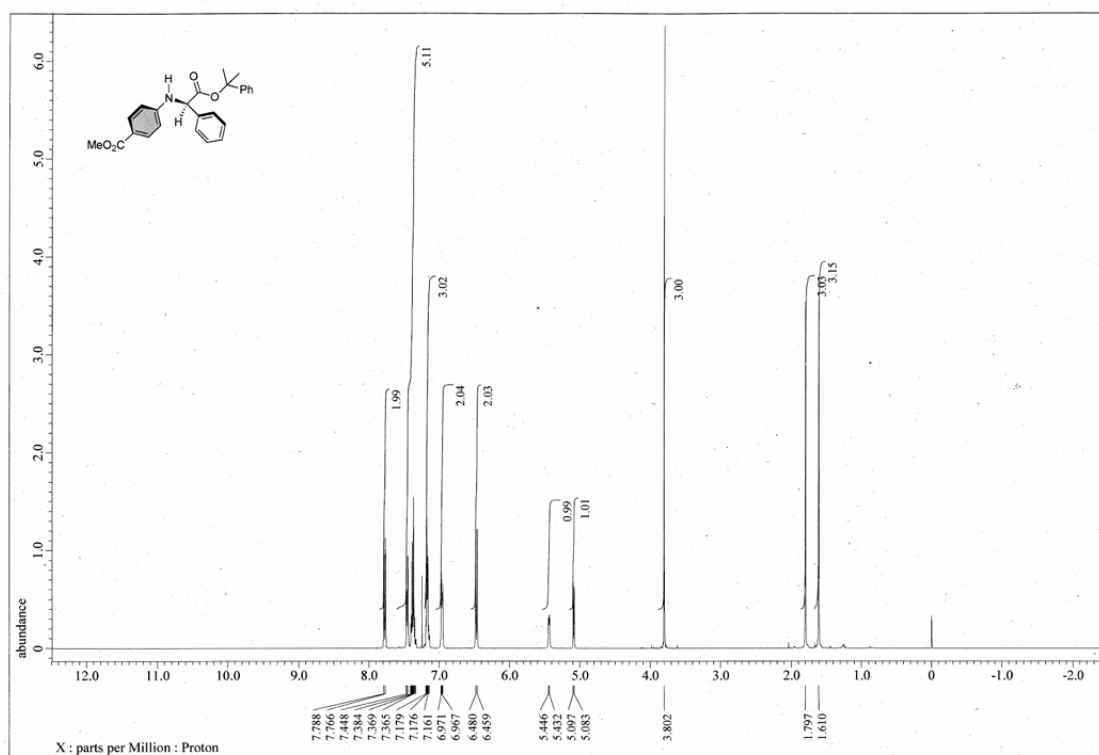


#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	5.233	7764055	96.065	867919	98.084
2	8.900	318008	3.935	16955	1.916

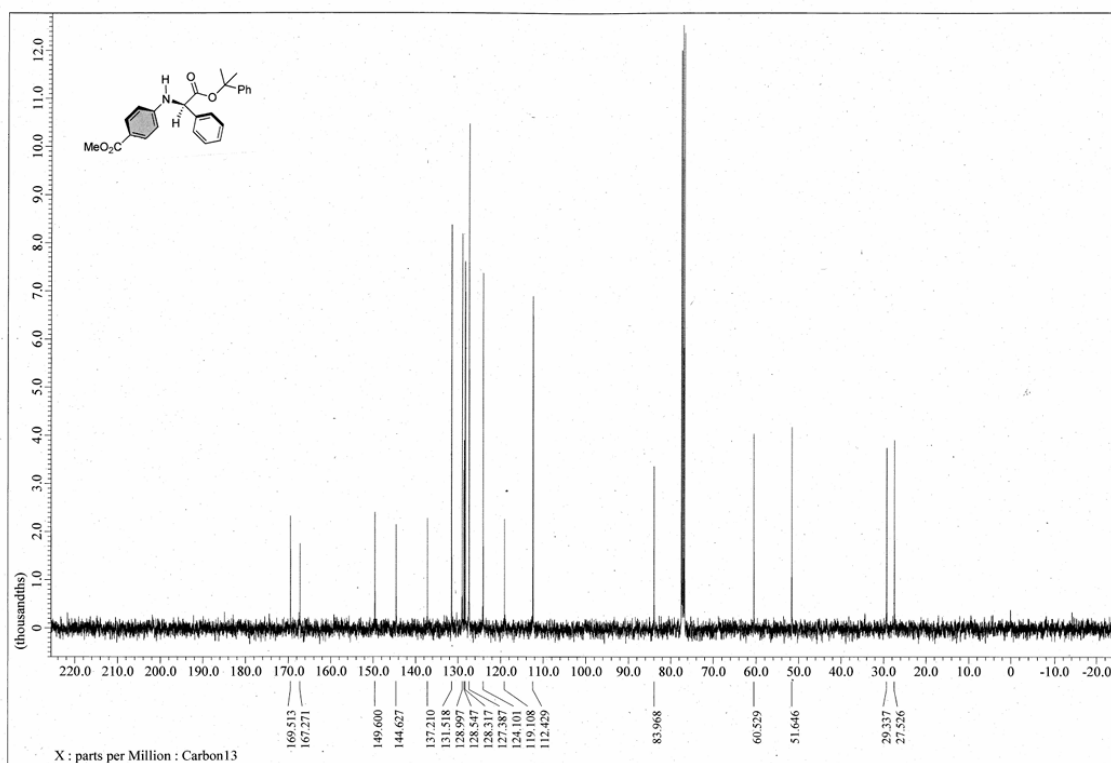
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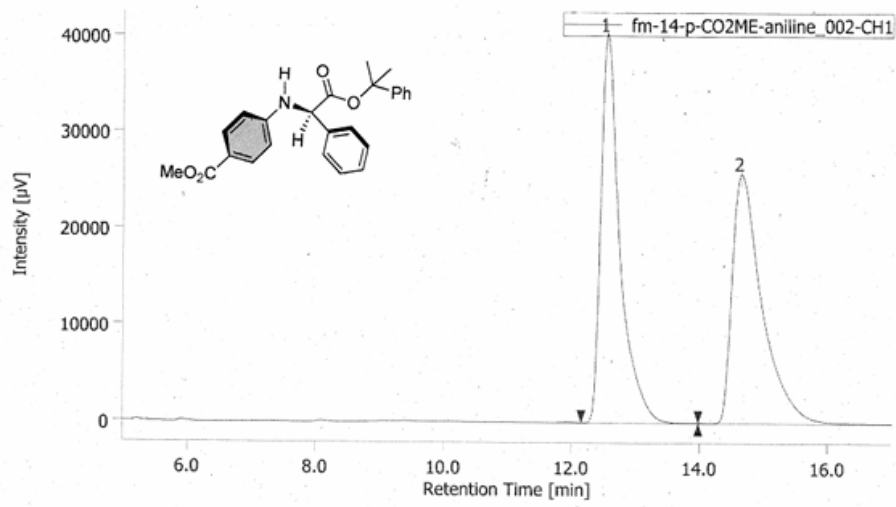


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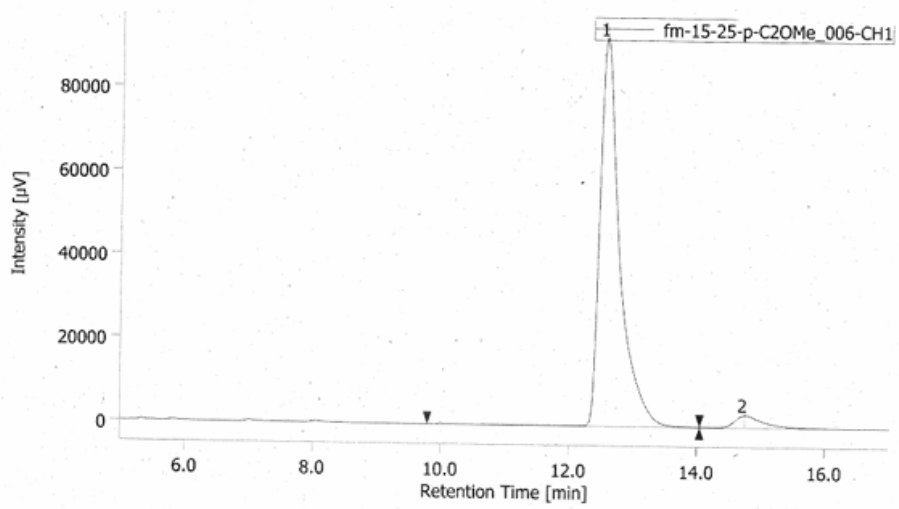


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4



#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	12.550	838630	50.032	40423	60.915
2	14.650	837546	49.968	25937	39.085

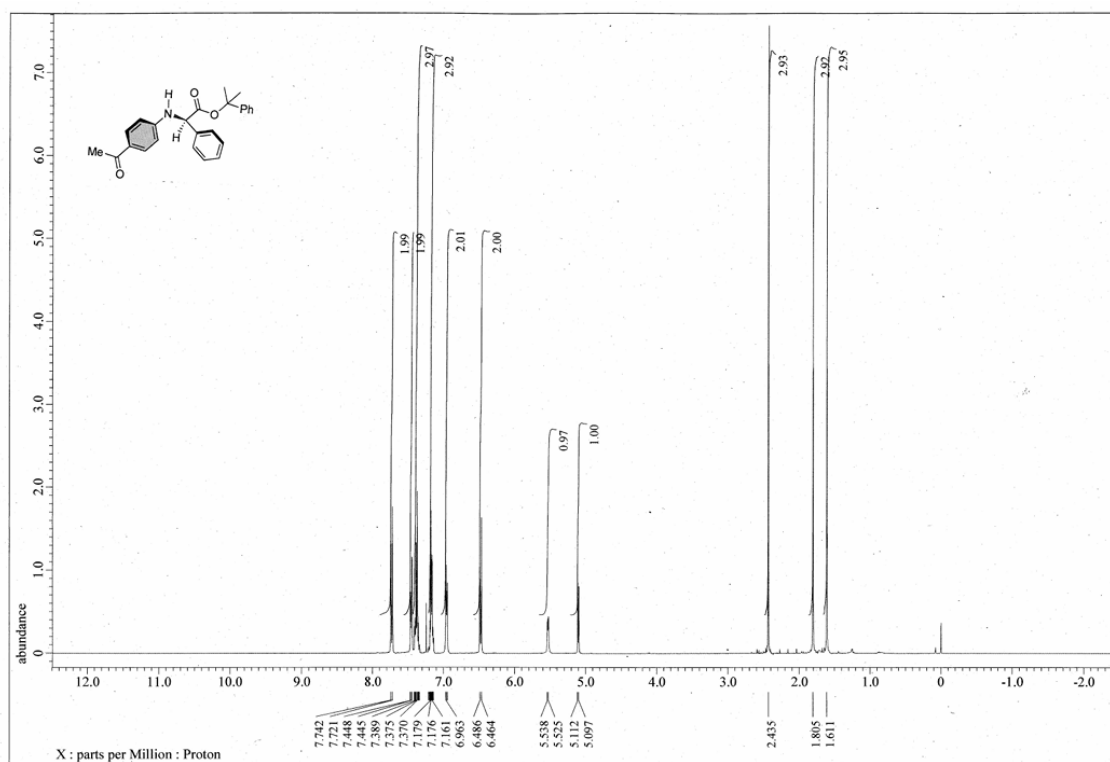


#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	12.558	2000823	95.567	93037	96.933
2	14.750	92803	4.433	2943	3.067

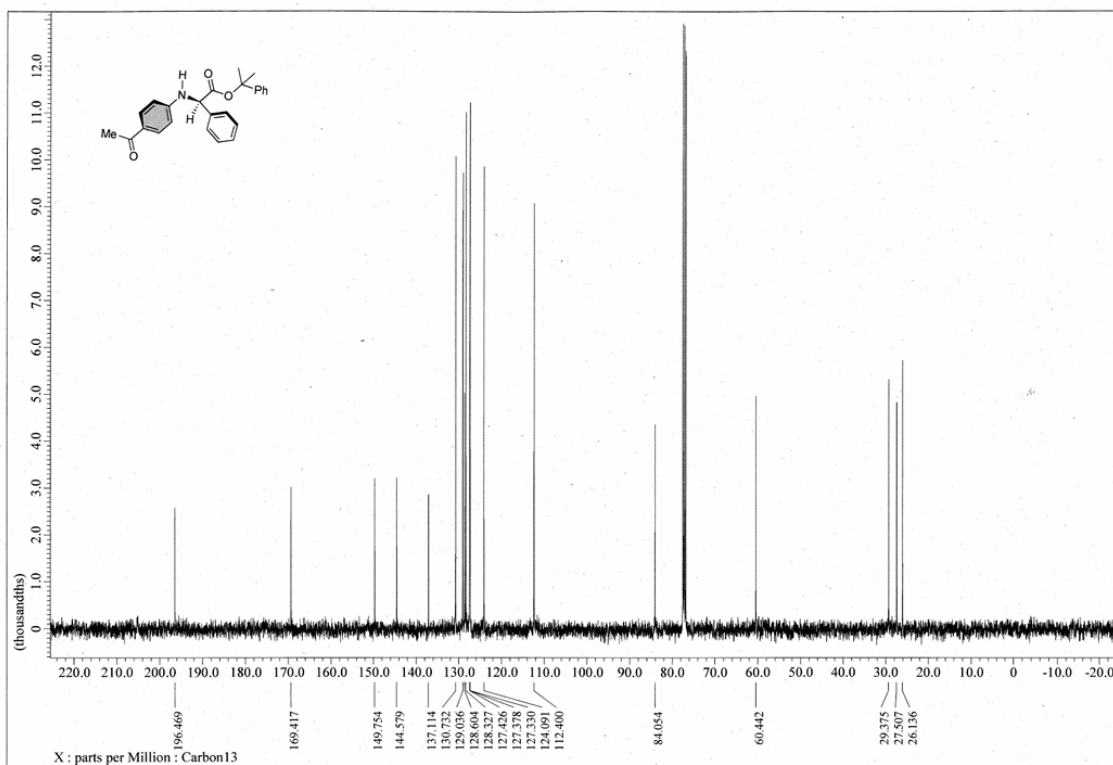
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- 2
- 3

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3f

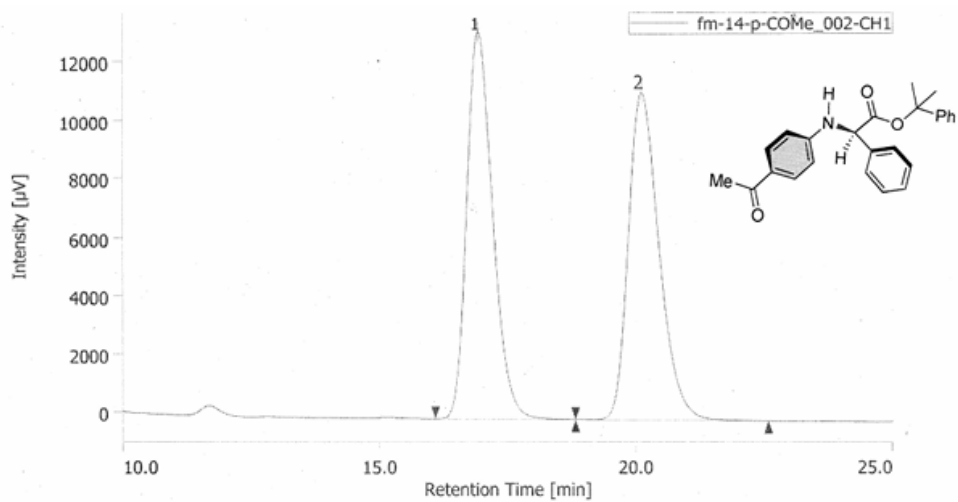


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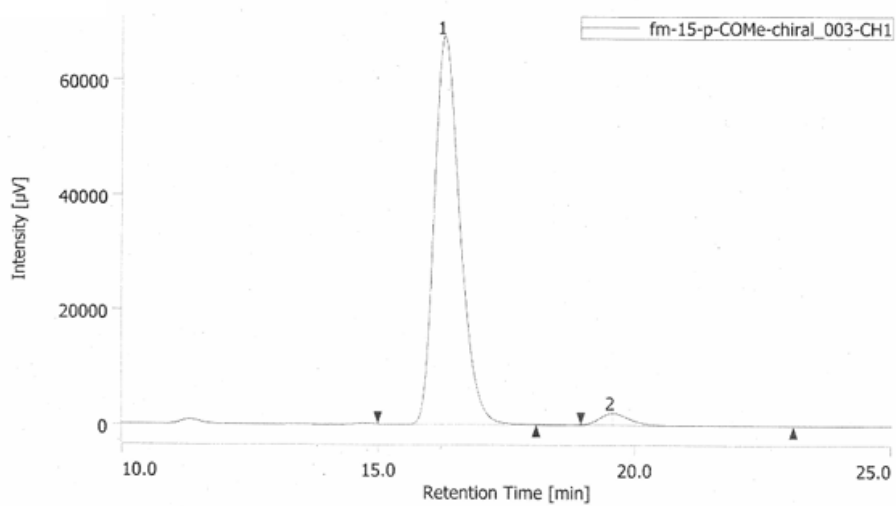
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4



#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	16.925	466207	49.840	13282	54.159
2	20.108	469205	50.160	11242	45.841

1229 fm-15-p-COMe-chiral_003 2025/03/13 12:18:35

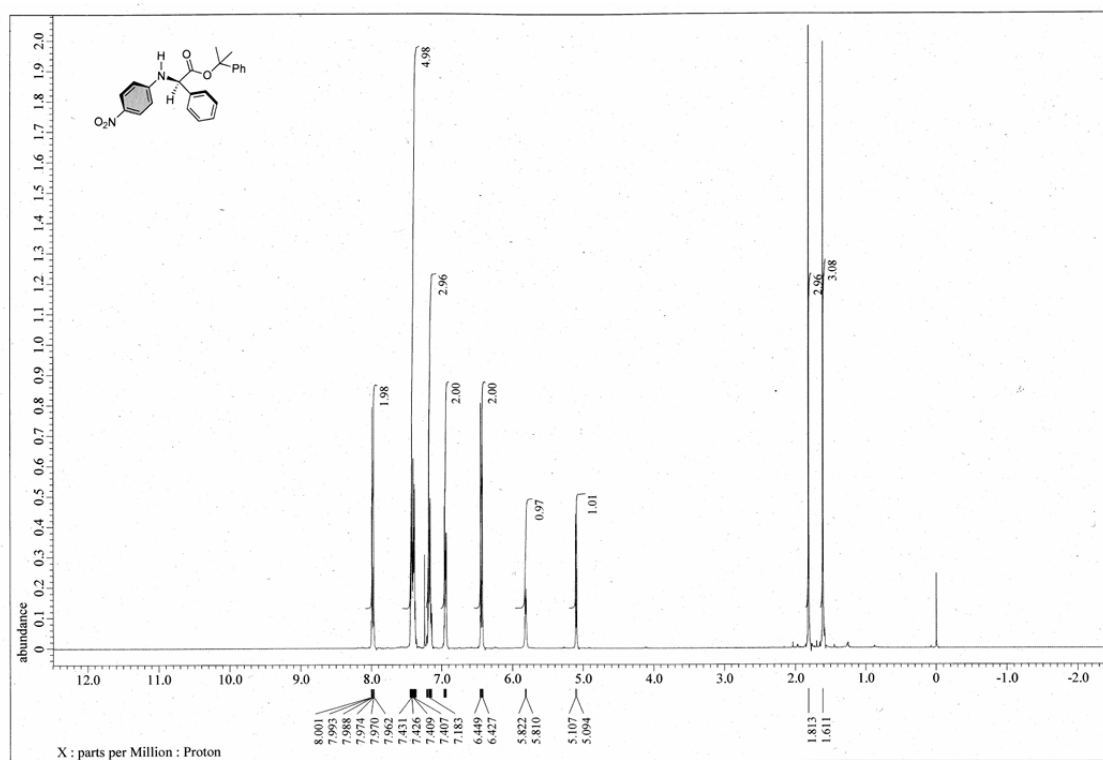


#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	16.283	2342353	96.589	67536	97.068
2	19.567	82716	3.411	2040	2.932

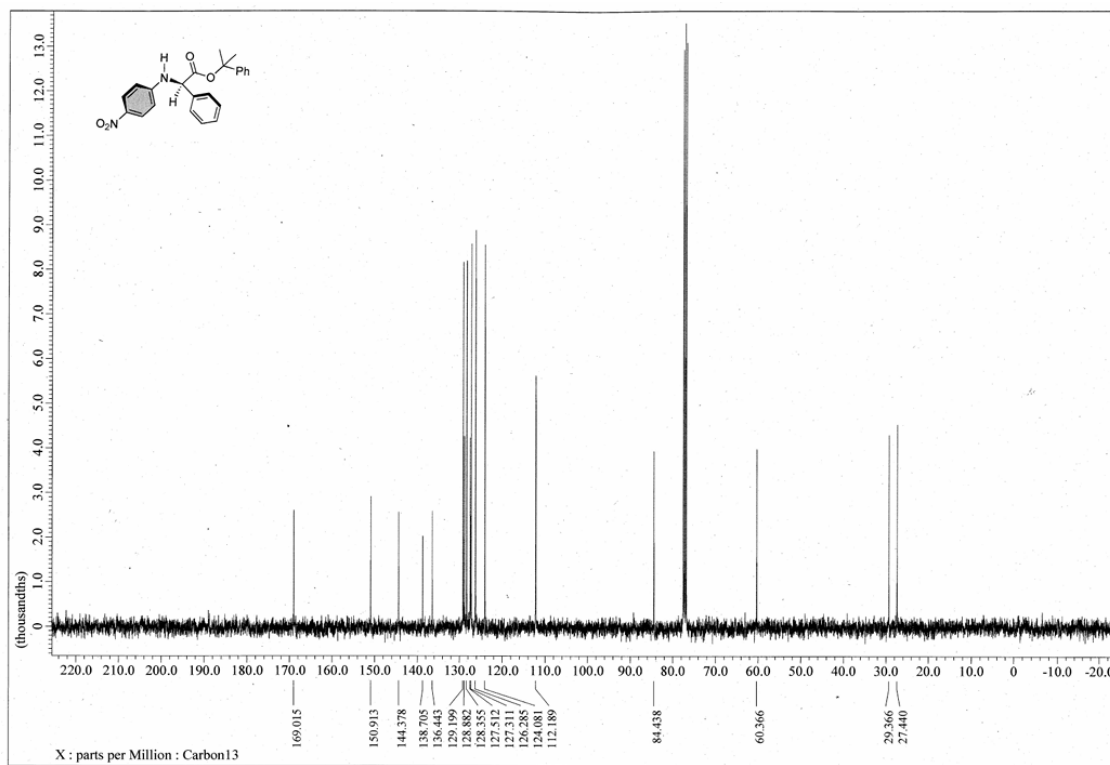
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- 2
- 3

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3g

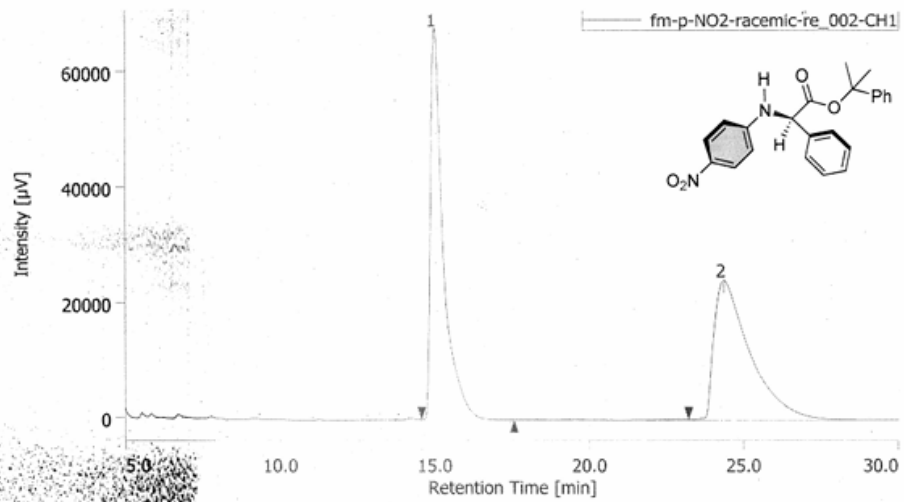


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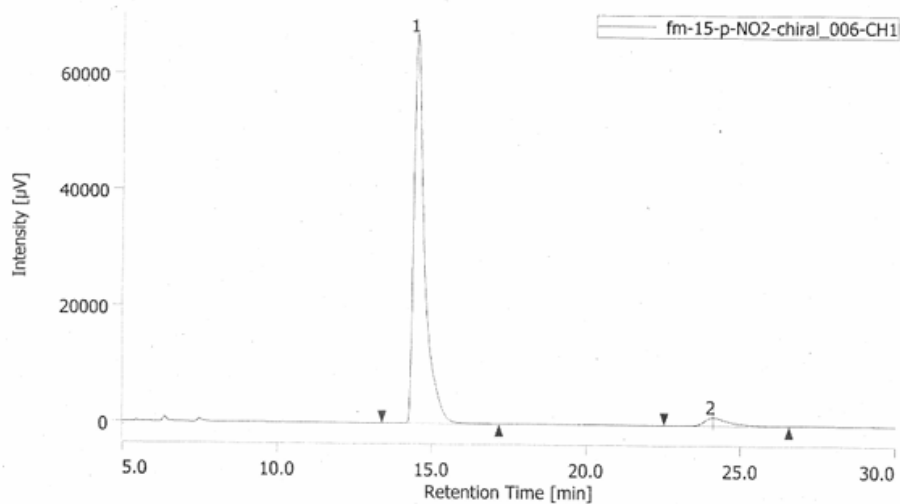


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#	tR [min]	Area [$\mu\text{V}\cdot\text{sec}$]	Area%	Height [μV]	Height%
1	14.992	1961513	49.921	67884	73.730
2	24.350	1967713	50.079	24188	26.270

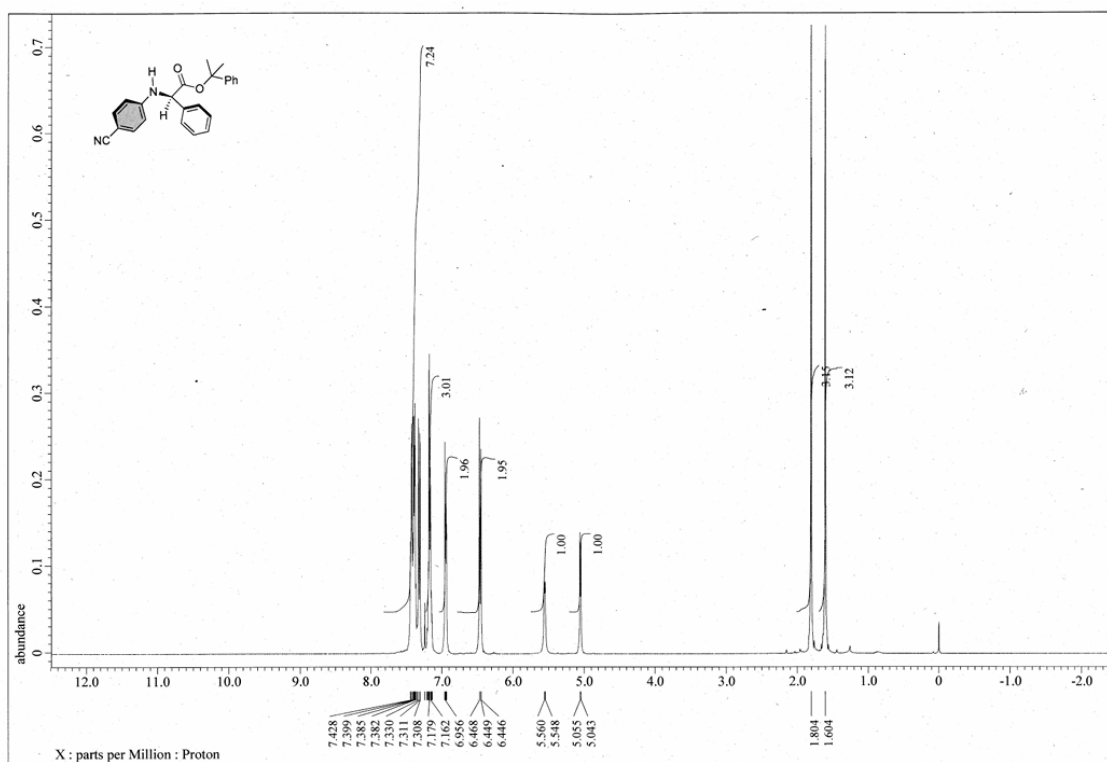


#	tR [min]	Area [$\mu\text{V}\cdot\text{sec}$]	Area%	Height [μV]	Height%
1	14.500	1616330	95.665	67072	97.968
2	24.108	73241	4.335	1391	2.032

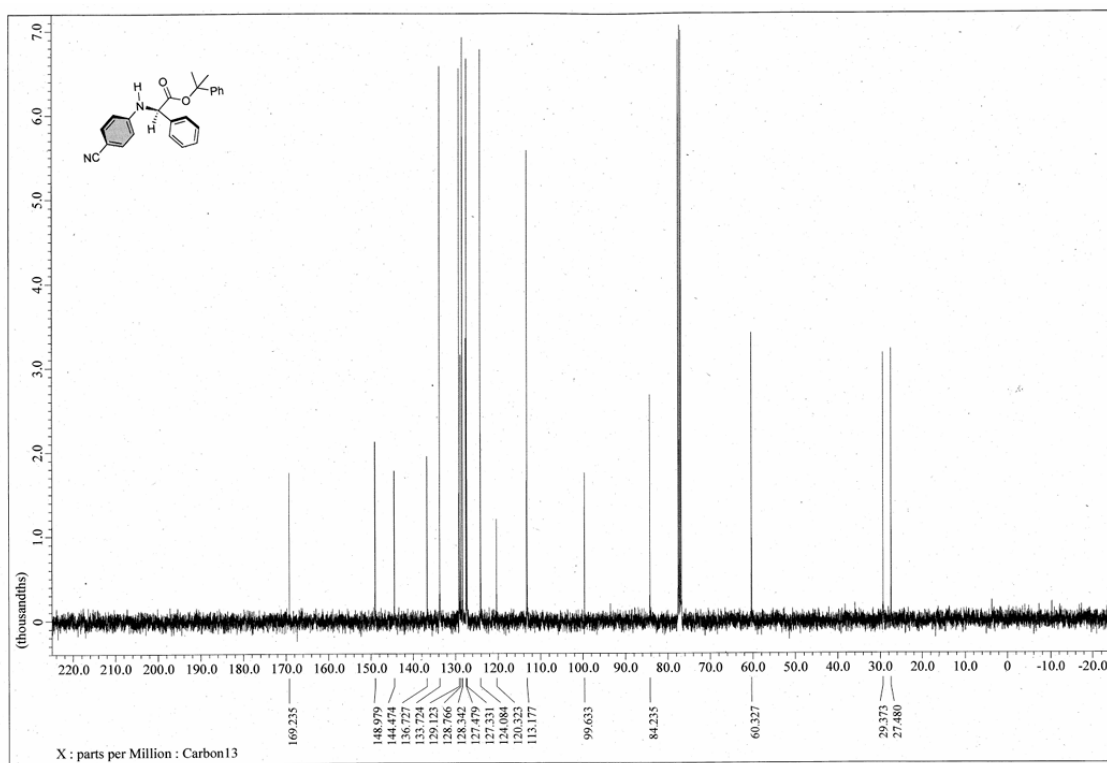
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- 4

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3h



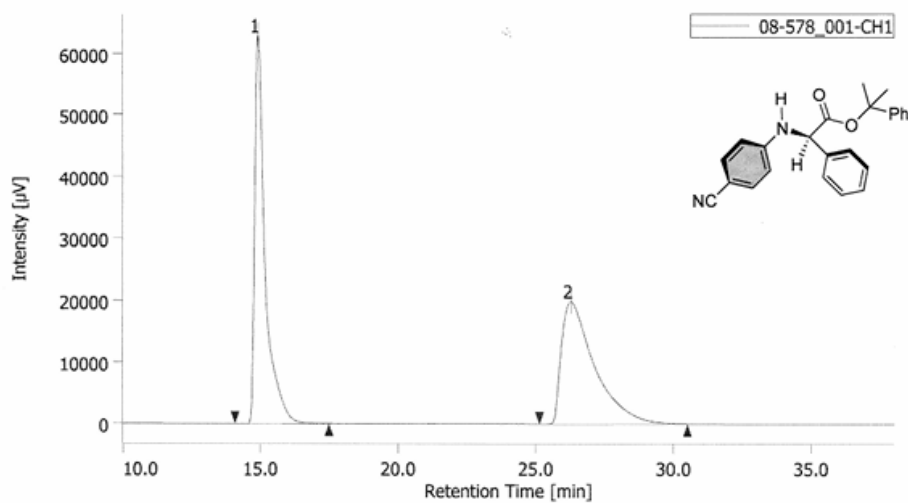
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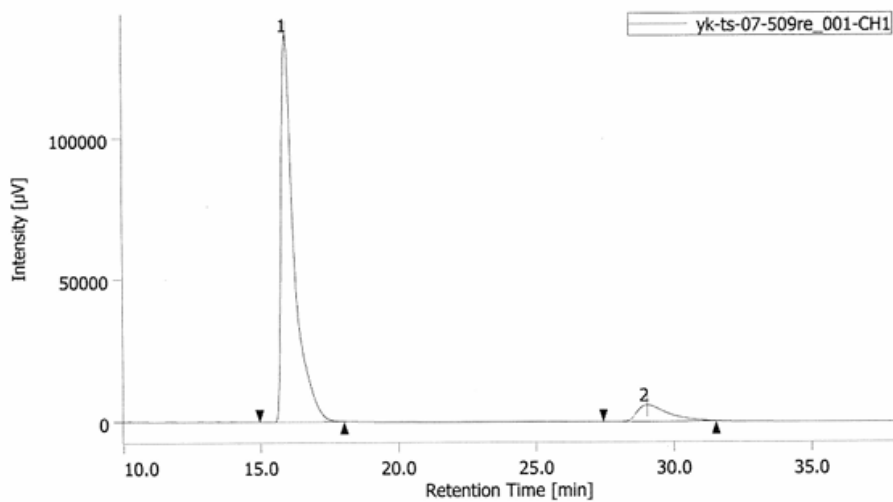
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0614 08-578_001 2026/06/15 15:18:56



#	tR [min]	Area [$\mu\text{V}\cdot\text{sec}$]	Area%	Height [μV] [μV]	Height%
1	14.925	1658442	50.087	63145	76.007
2	26.275	1652661	49.913	19932	23.993

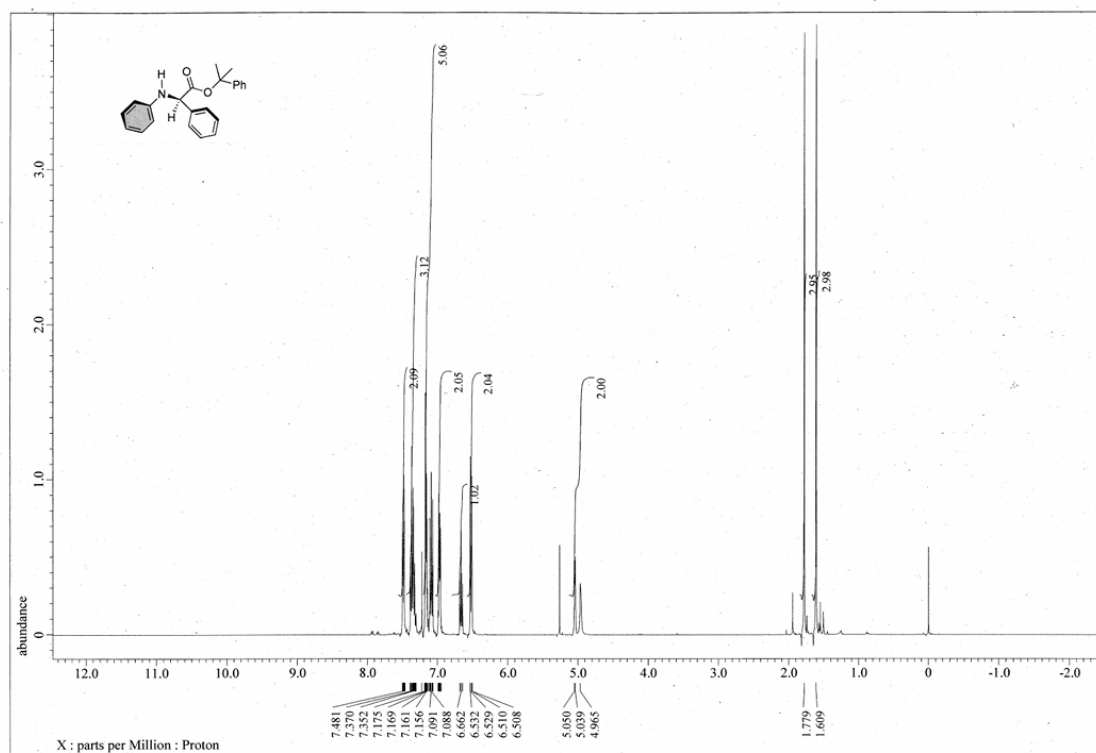
0416 yk-ts-07-509re_001 2026/06/14 2:26:56



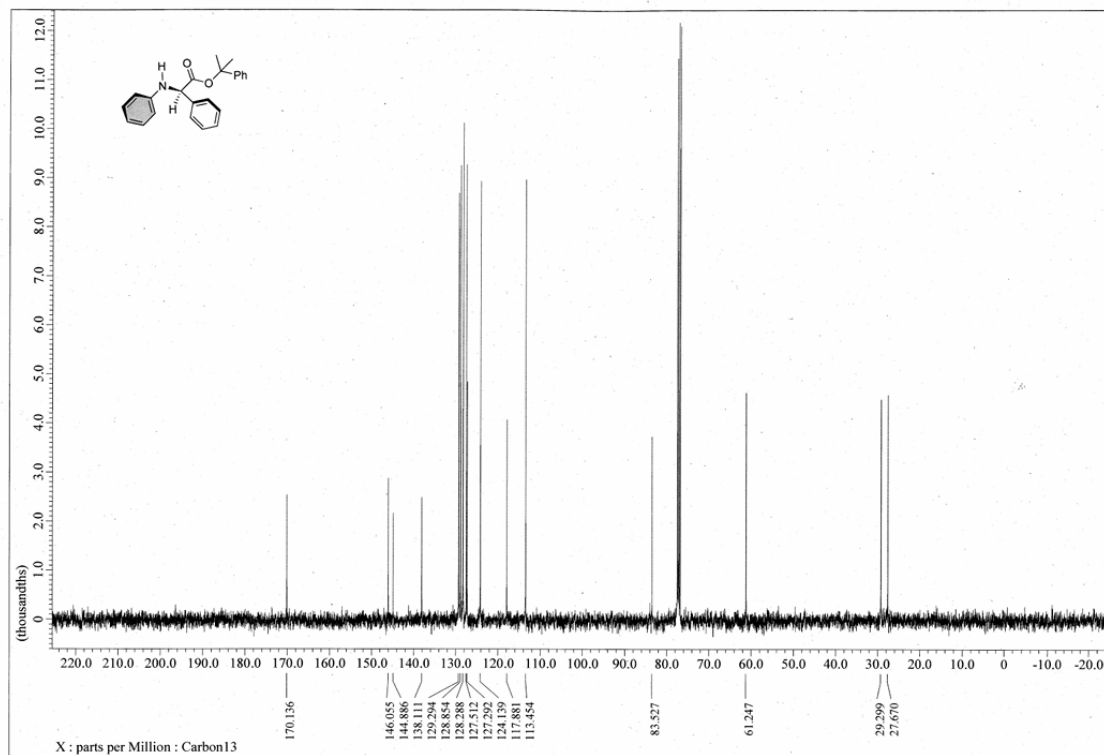
#	tR [min]	Area [$\mu\text{V}\cdot\text{sec}$]	Area%	Height [μV] [μV]	Height%
1	15.933	4409963	90.810	137137	95.966
2	29.017	446312	9.190	5764	4.034

1

3i

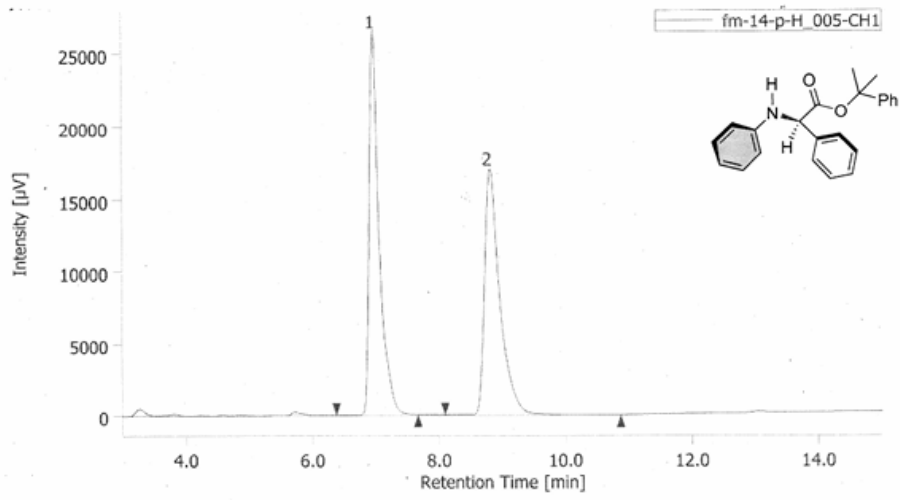


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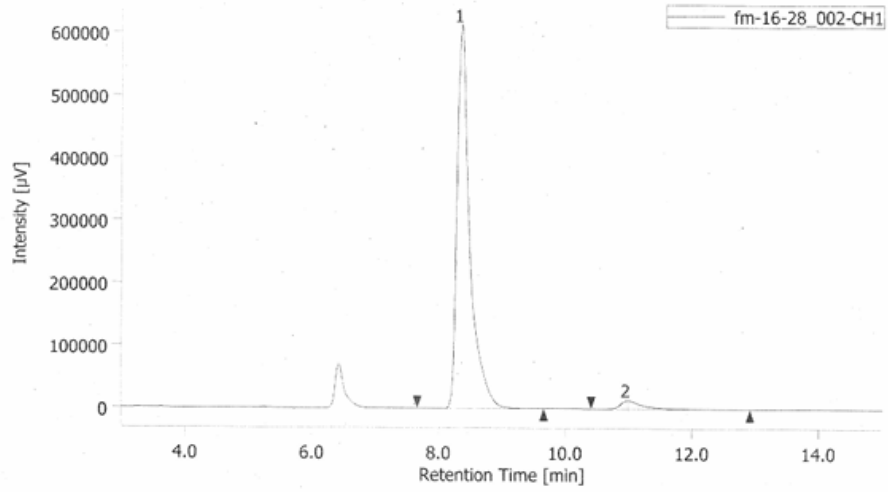


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#	tR [min]	Area [µV.sec]	Area%	Height [µV]	Height%
1	6.967	295666	50.895	26660	61.091
2	8.808	285272	49.105	16980	38.909

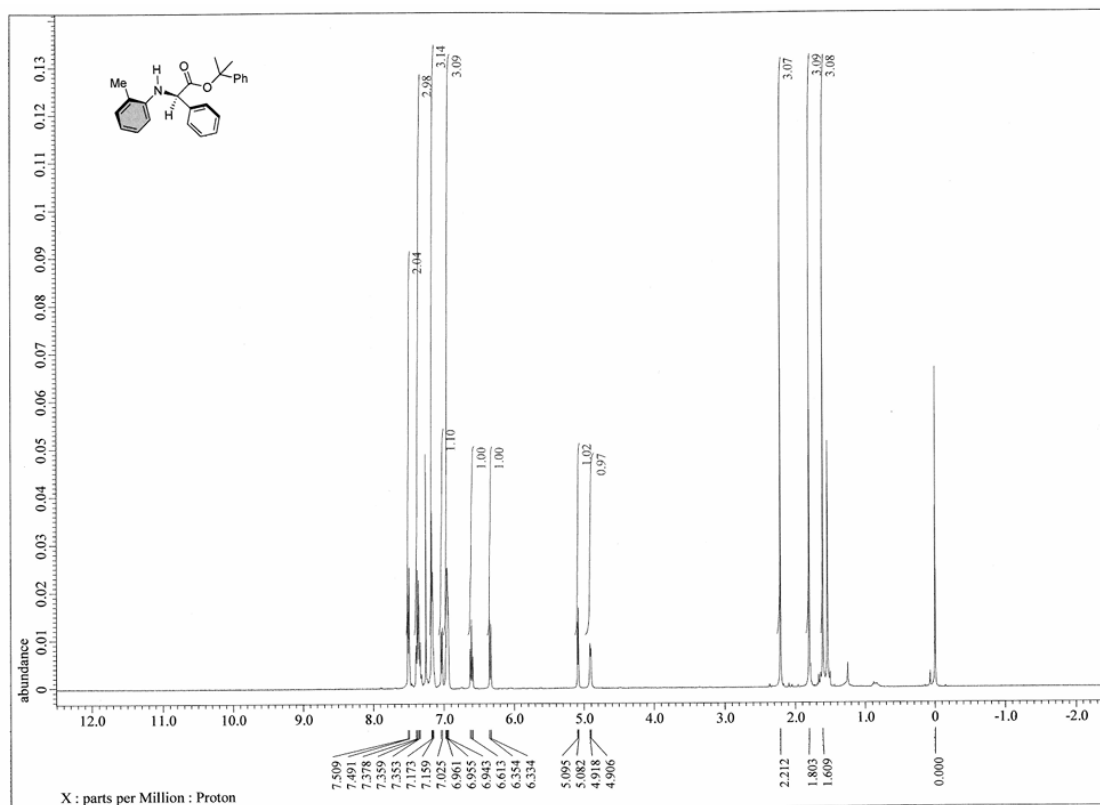


#	tR [min]	Area [µV.sec]	Area%	Height [µV]	Height%
1	8.350	8578580	96.564	614210	97.907
2	10.992	305278	3.436	13128	2.093

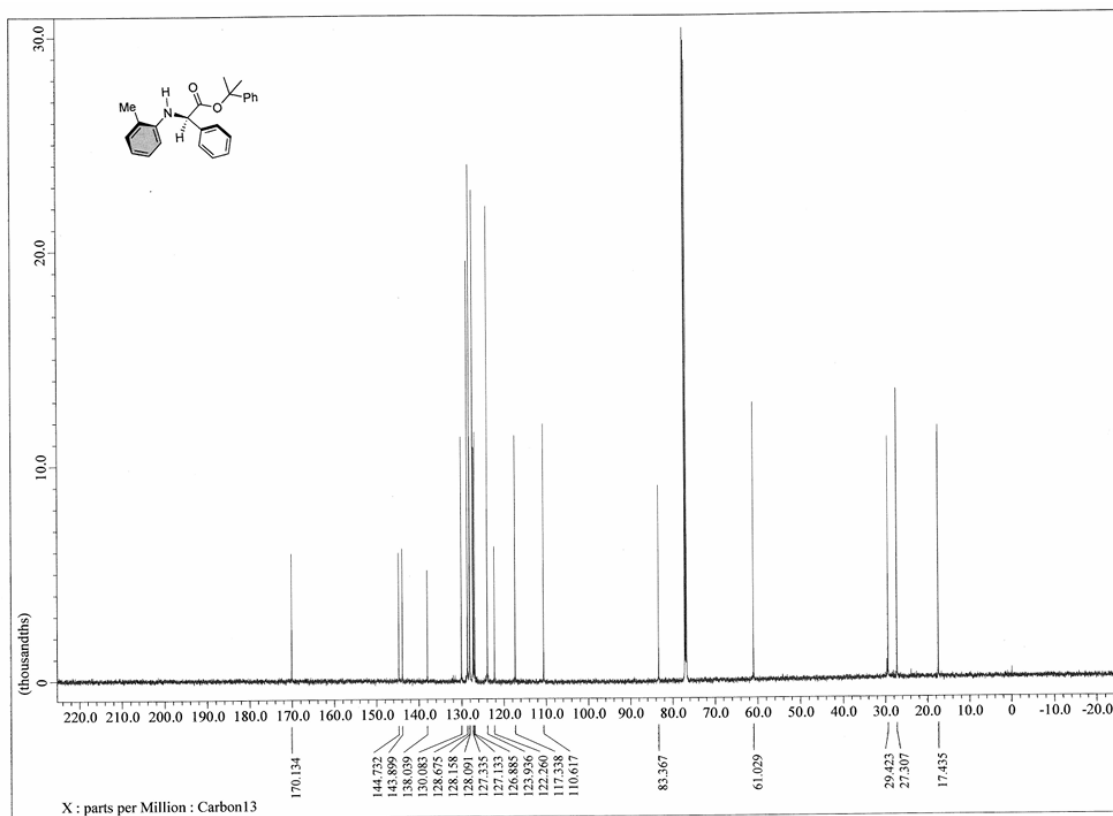
- 1
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- 4

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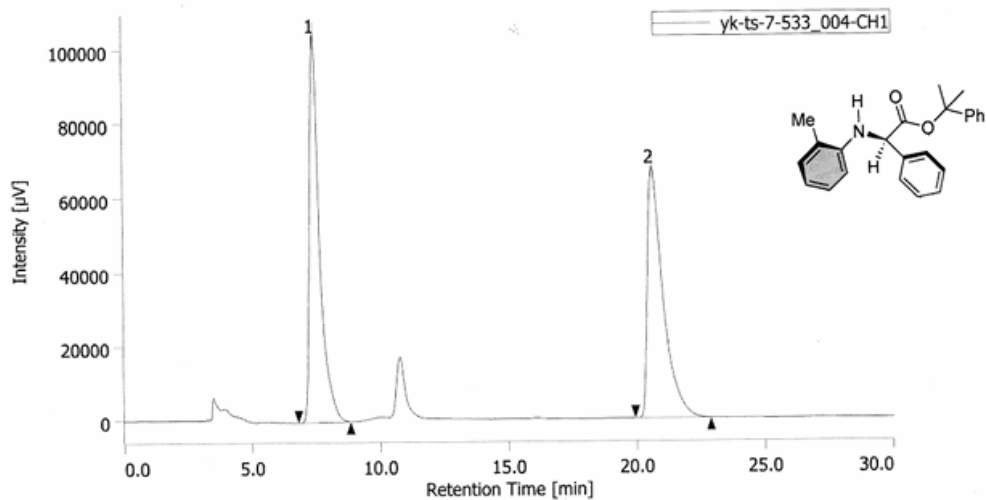


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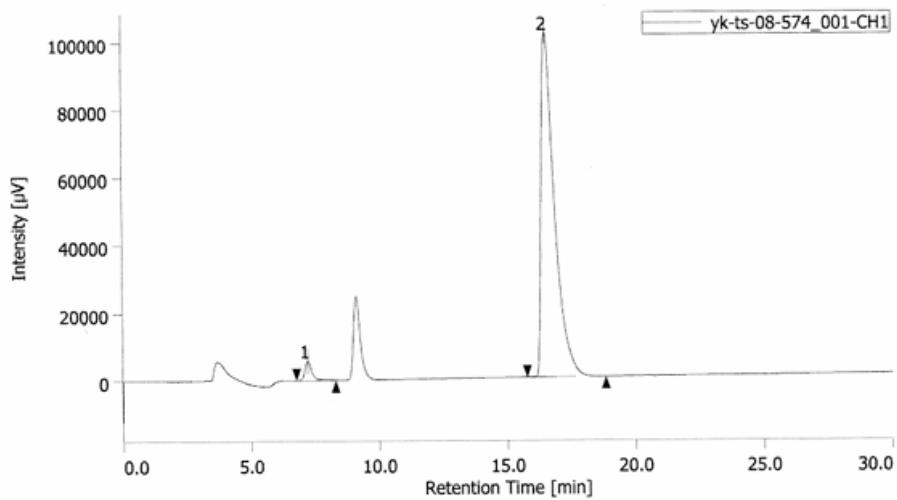
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0508 yk-ts-7-533_004 2026/05/08 13:32:36



#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	7.450	2843651	49.785	104655	60.608
2	20.633	2868223	50.215	68020	39.392

0614 yk-ts-08-574_001 2026/06/14 19:32:19

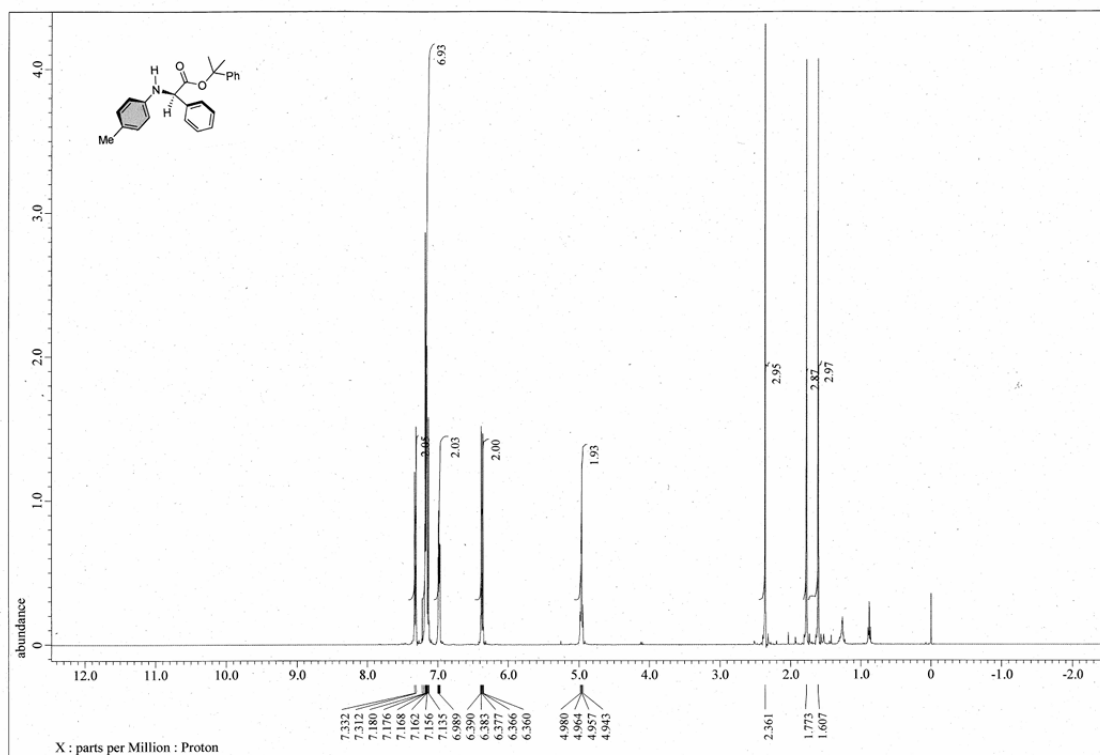


#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	7.208	110868	2.930	5748	5.323
2	16.517	3673204	97.070	102248	94.677

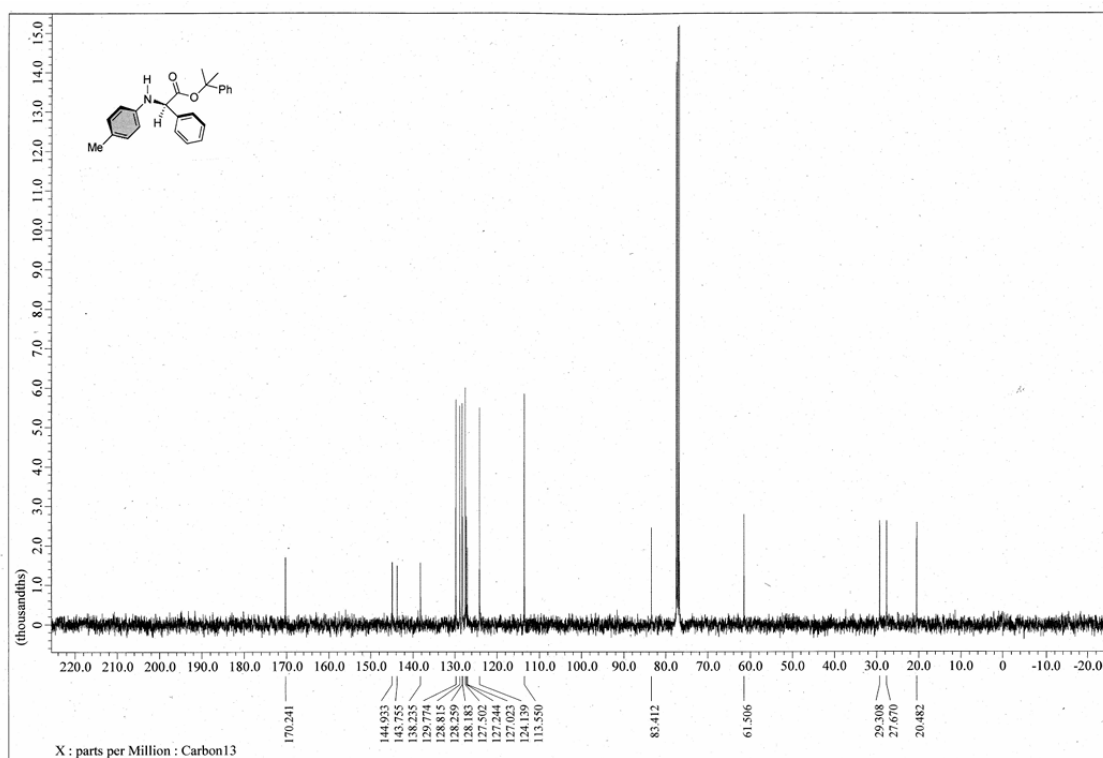
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3k



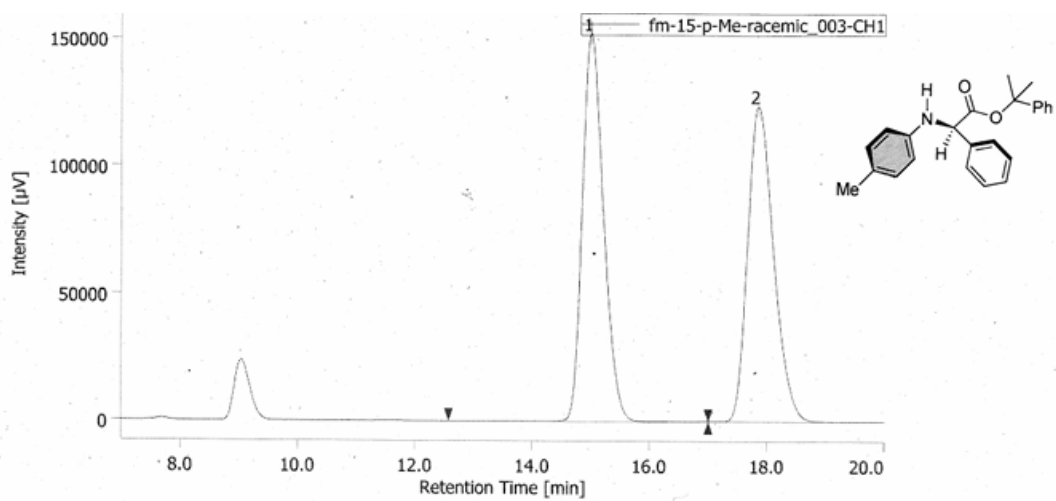
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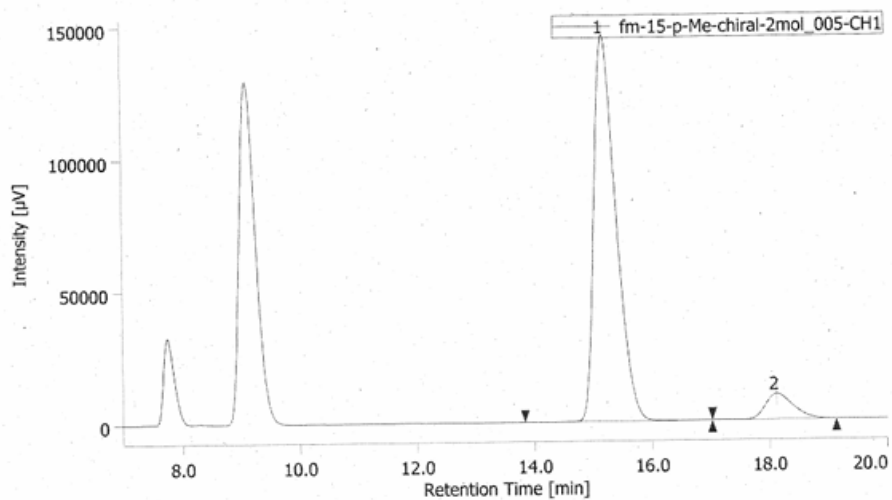
3

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1



#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	14.992	3834097	49.958	152988	55.145
2	17.842	3840523	50.042	124441	44.855



#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	15.192	3779079	92.257	145770	93.796
2	18.117	317183	7.743	9642	6.204

2

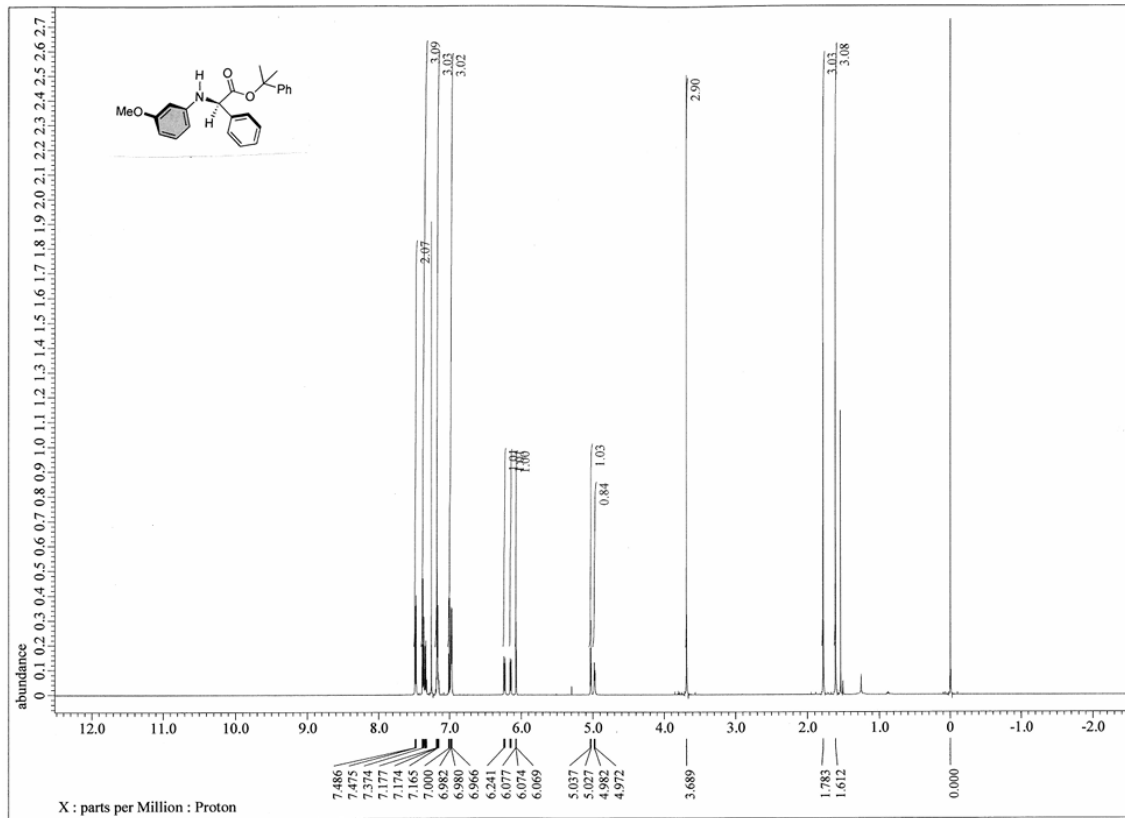
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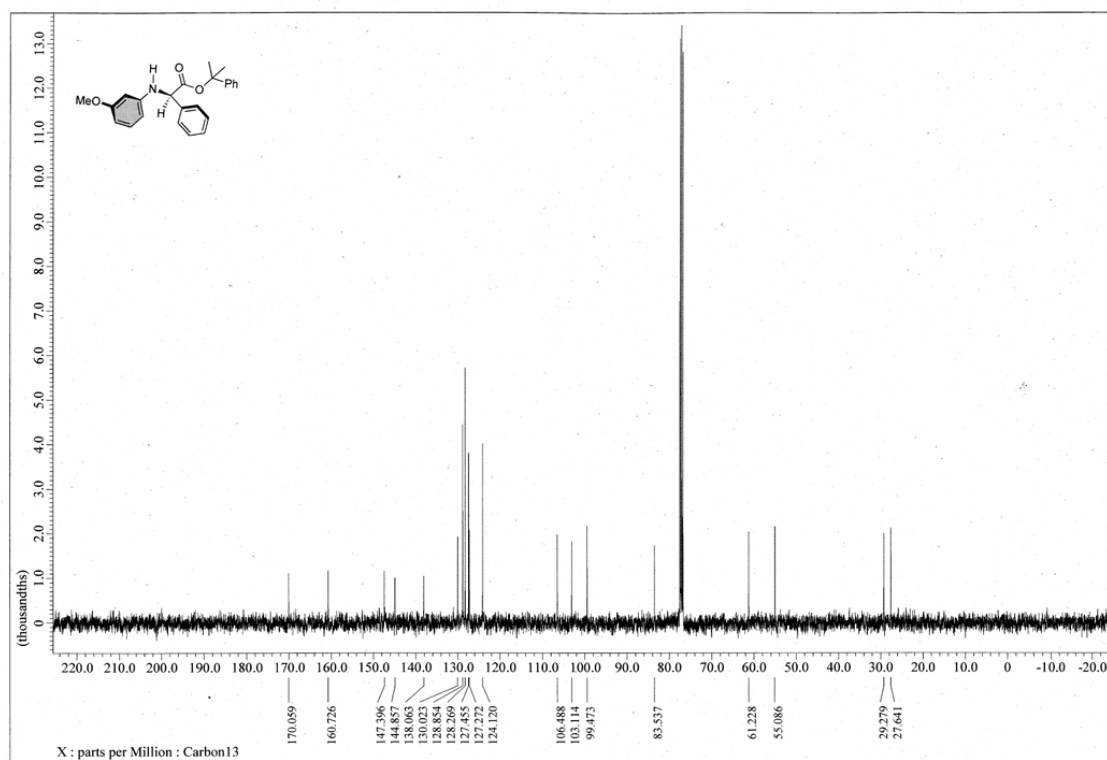
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31

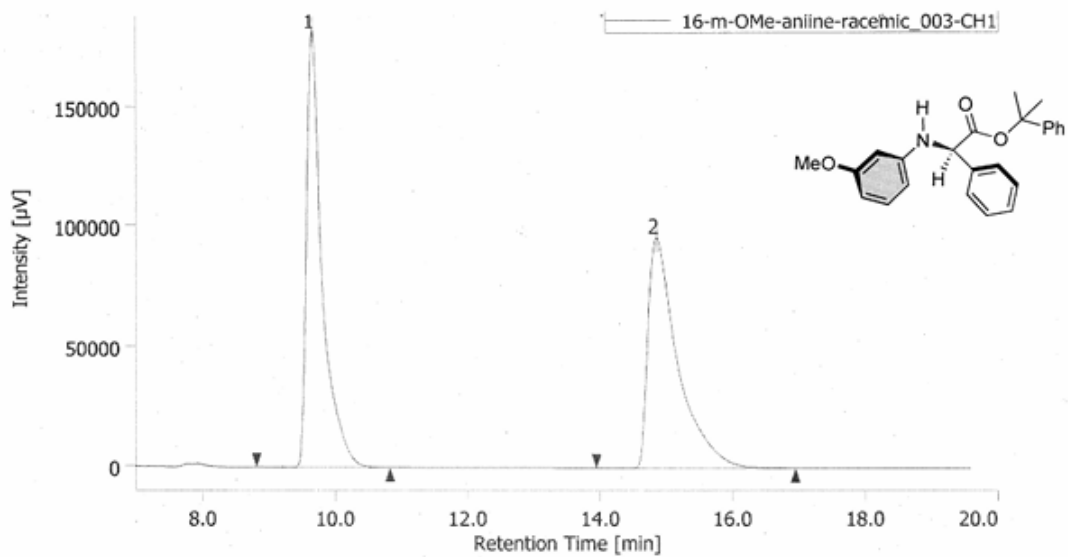


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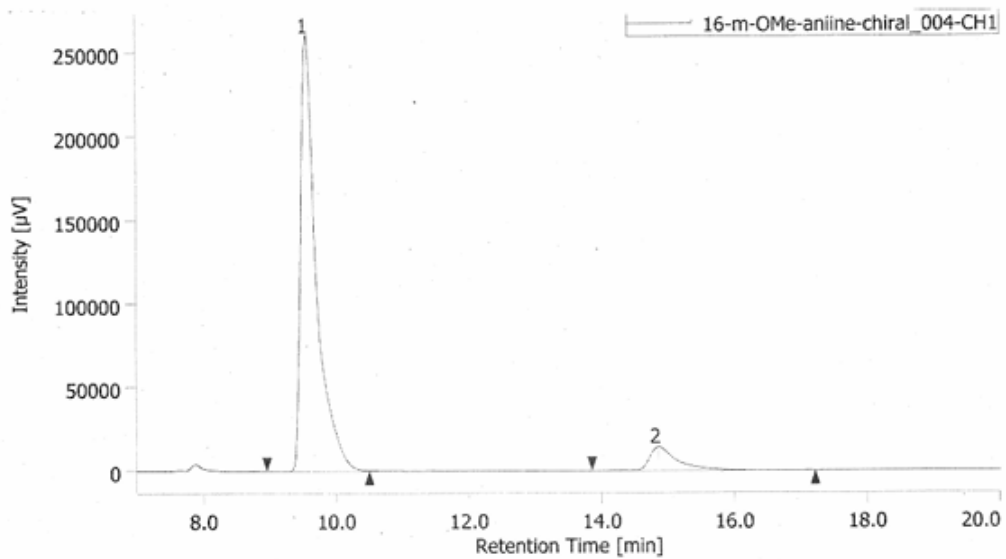


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2



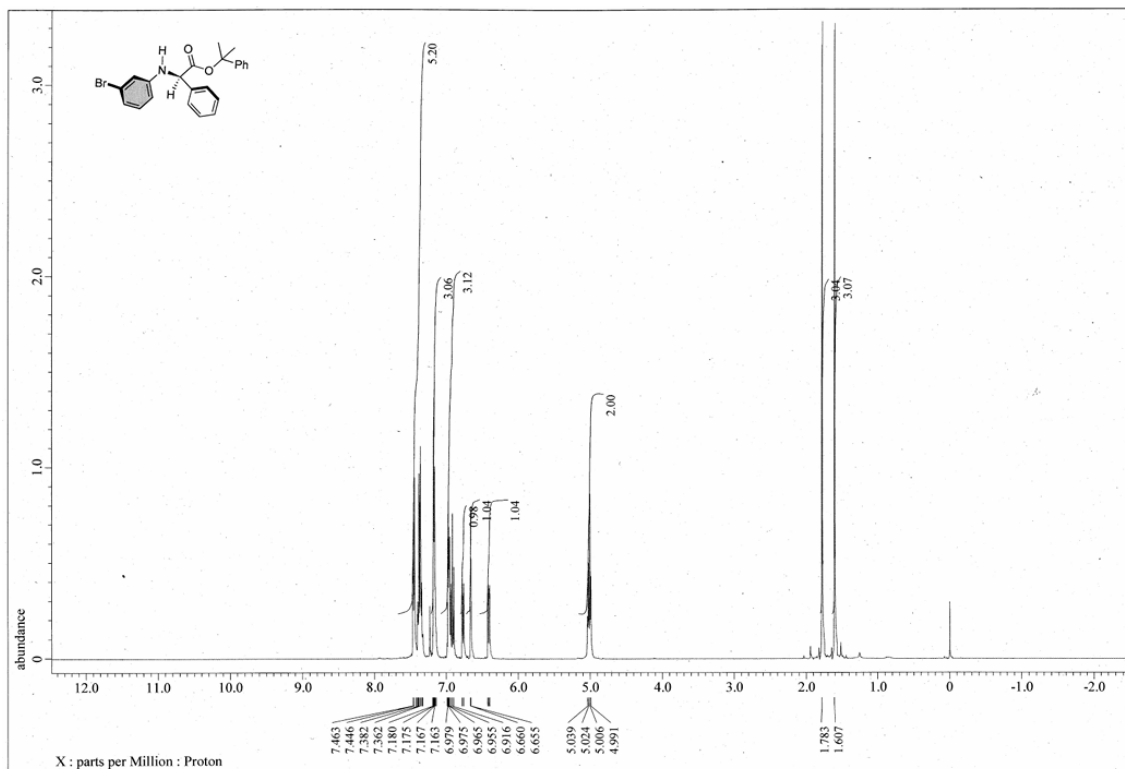
#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	9.650	2968762	49.877	181665	65.504
2	14.850	2983421	50.123	95668	34.496



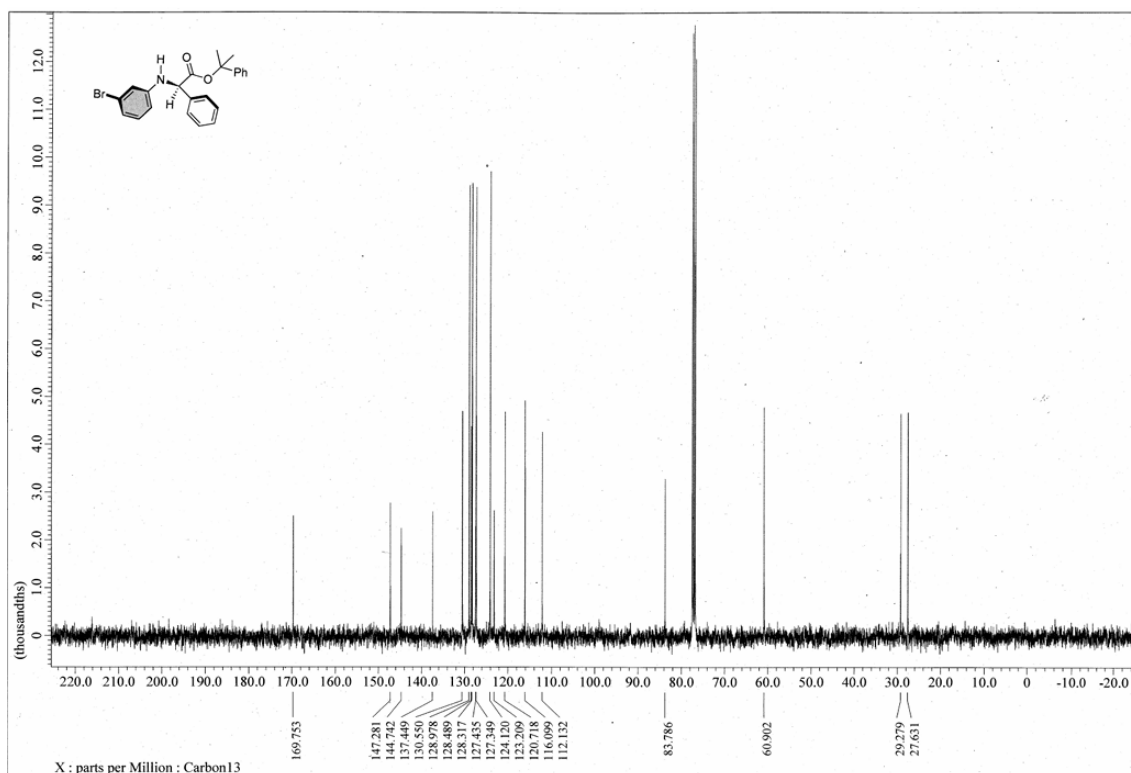
#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	9.558	4279117	91.676	261180	94.941
2	14.850	388538	8.324	13916	5.059

1
2
3

3m

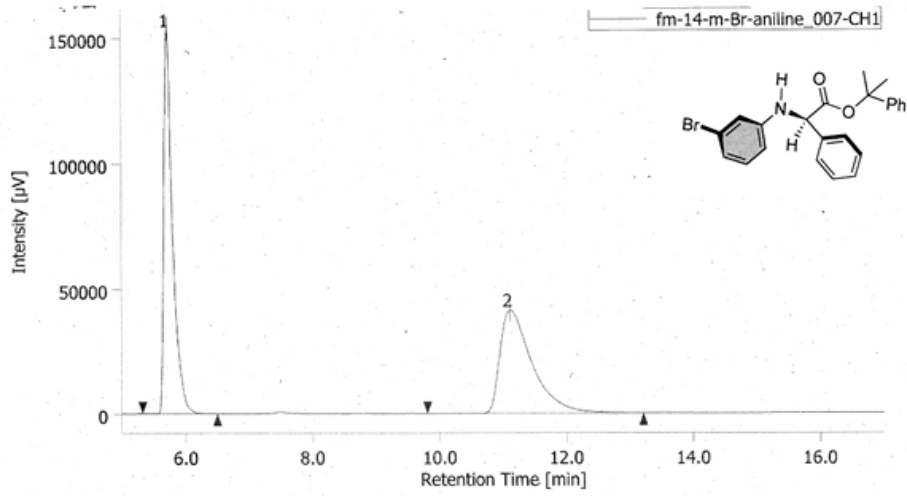


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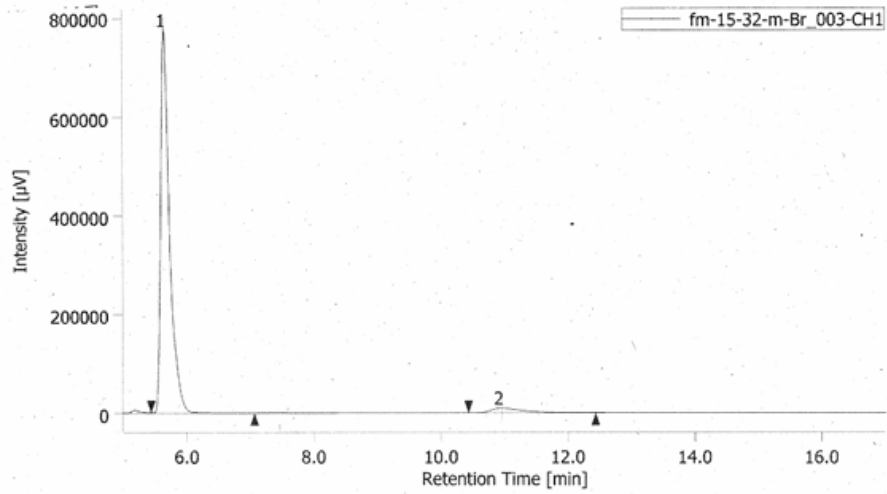


2

3



#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	5.725	1463262	50.242	153780	78.857
2	11.117	1449182	49.758	41231	21.143

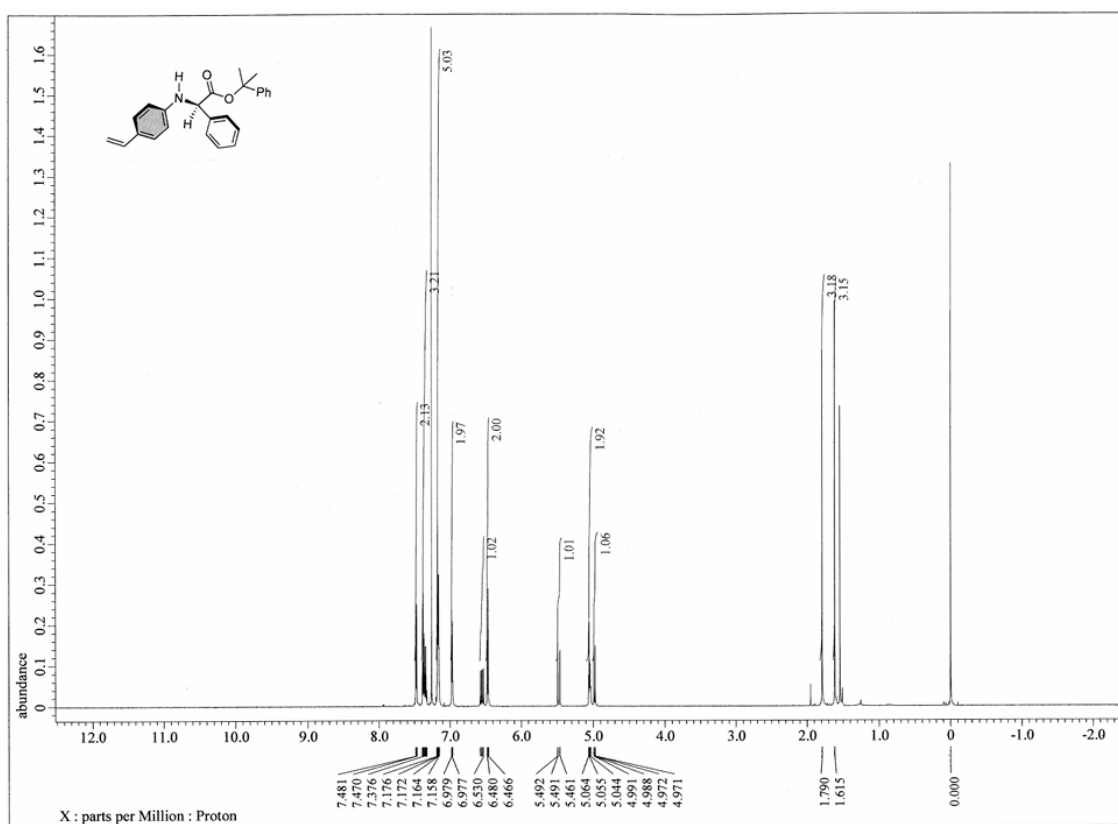


#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	5.650	7525734	95.716	780083	98.745
2	10.950	336842	4.284	9911	1.255

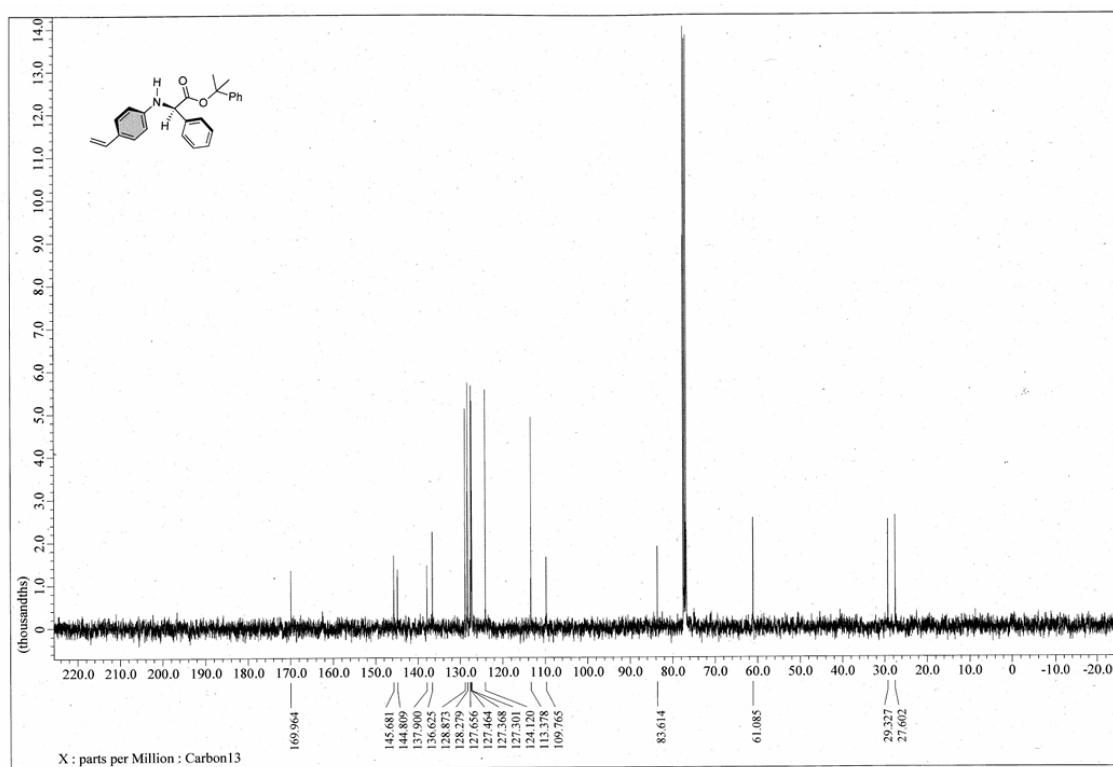
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- 5

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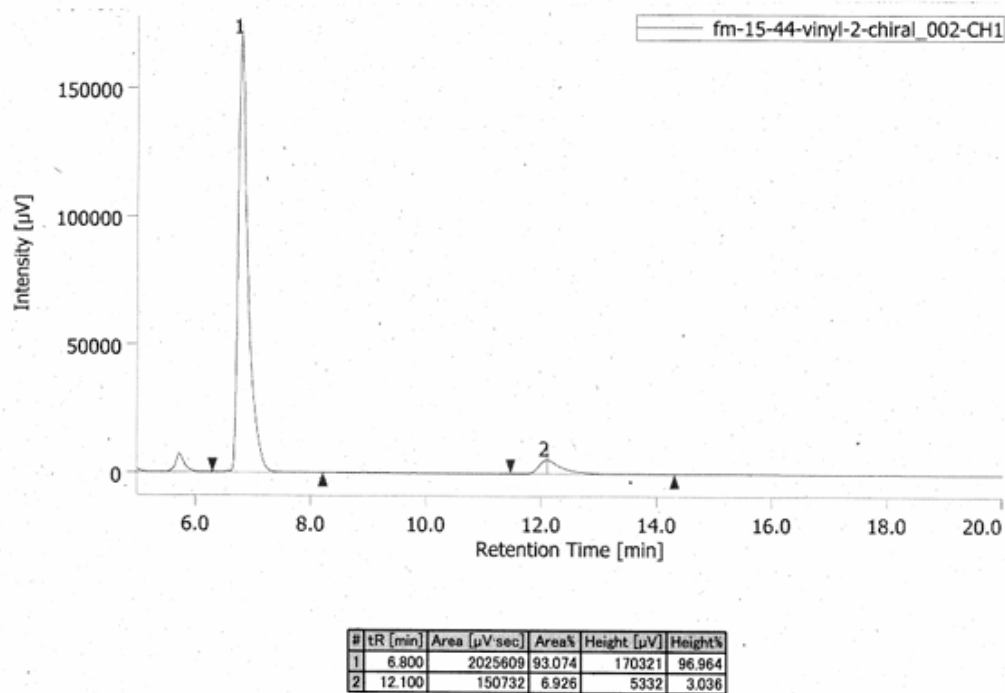
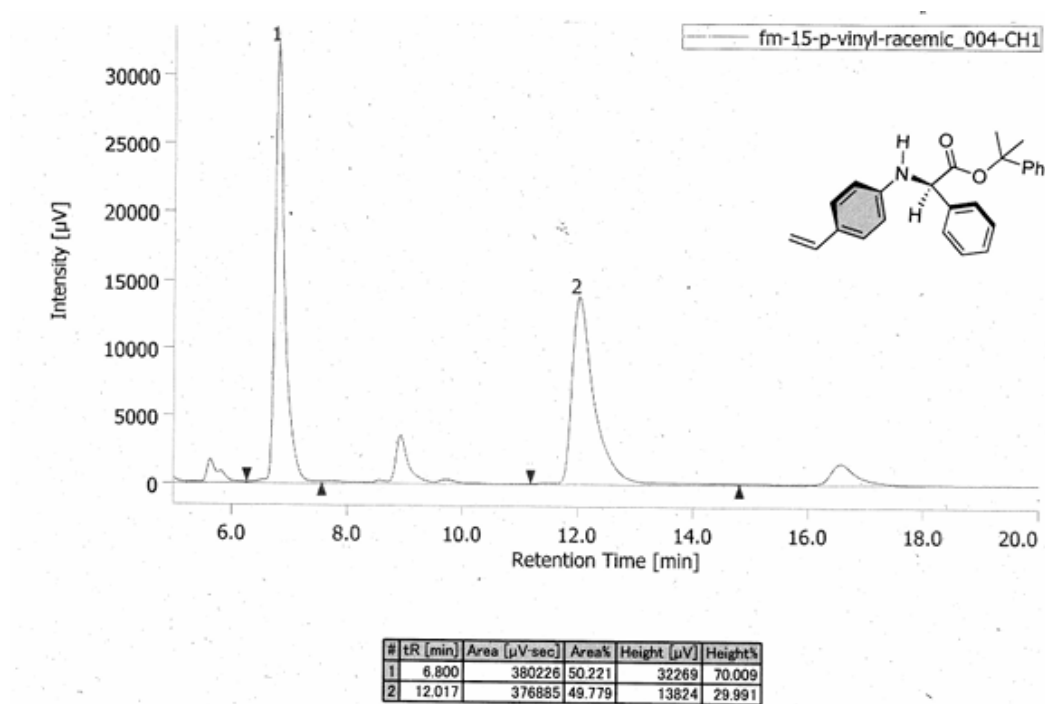


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3

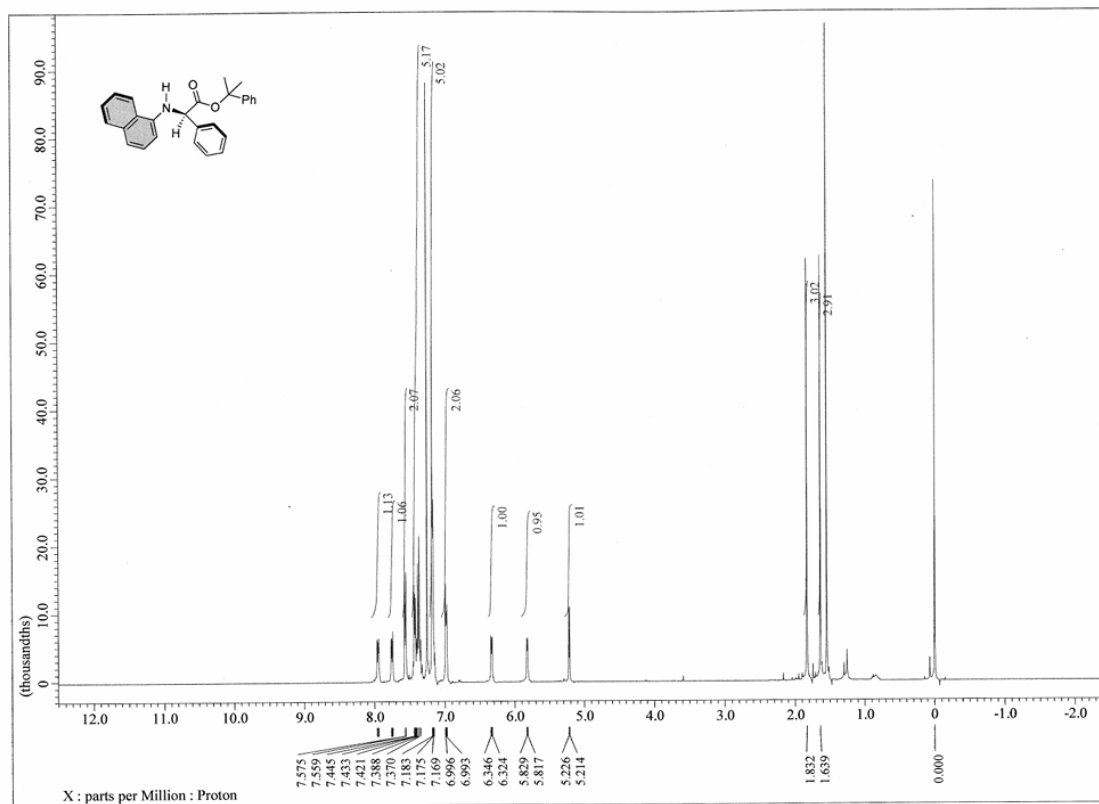
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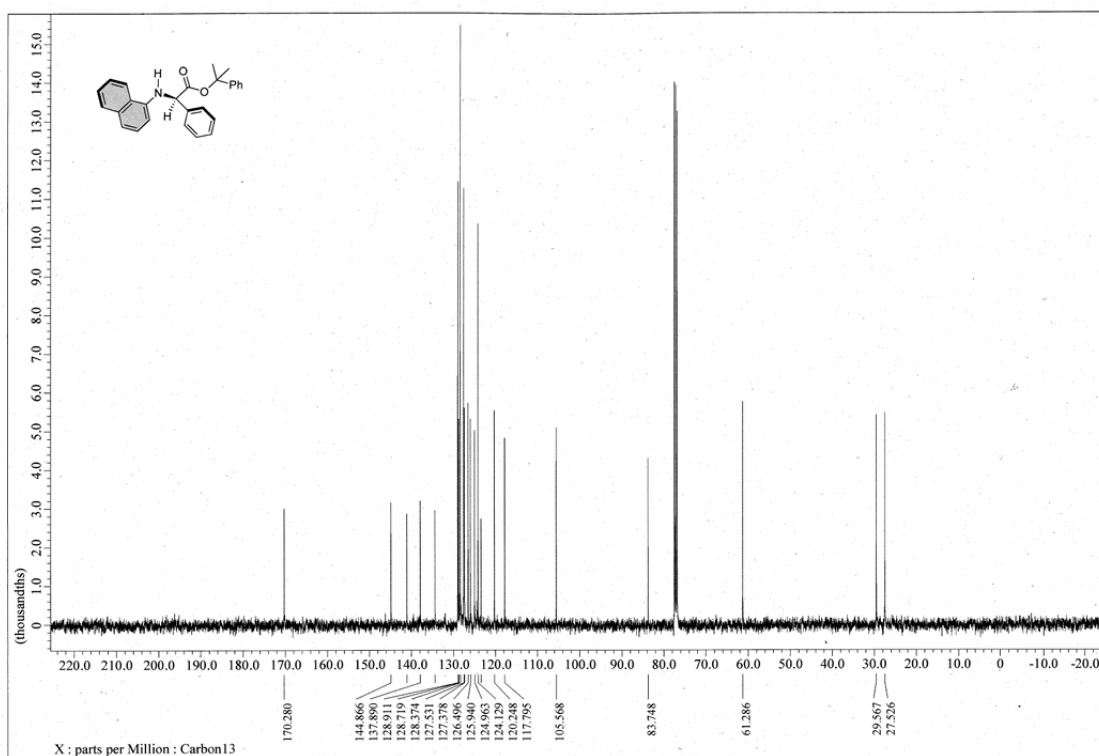
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1
2

3o

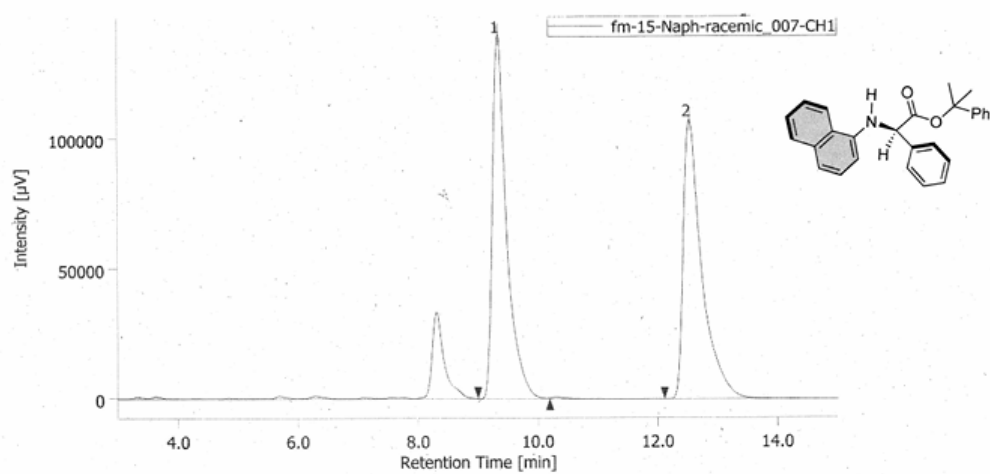


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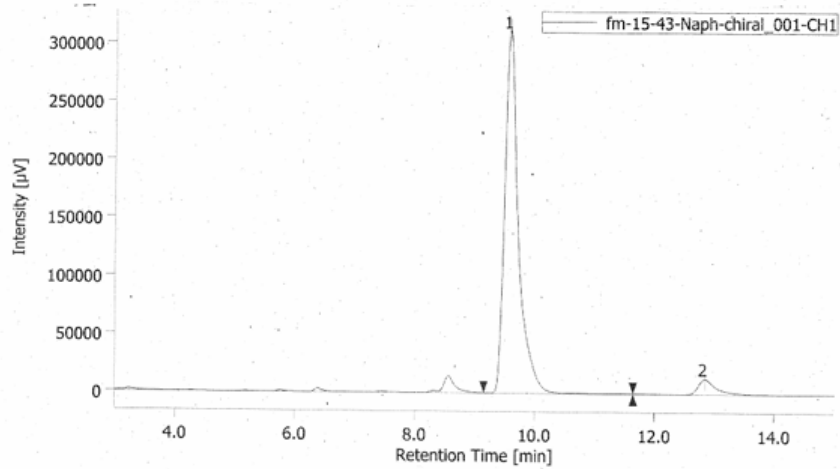


4

1



#	tR [min]	Area [µV.sec]	Area%	Height [µV]	Height%
1	9.342	2316307	49.925	140770	56.600
2	12.533	2323237	50.075	107941	43.400

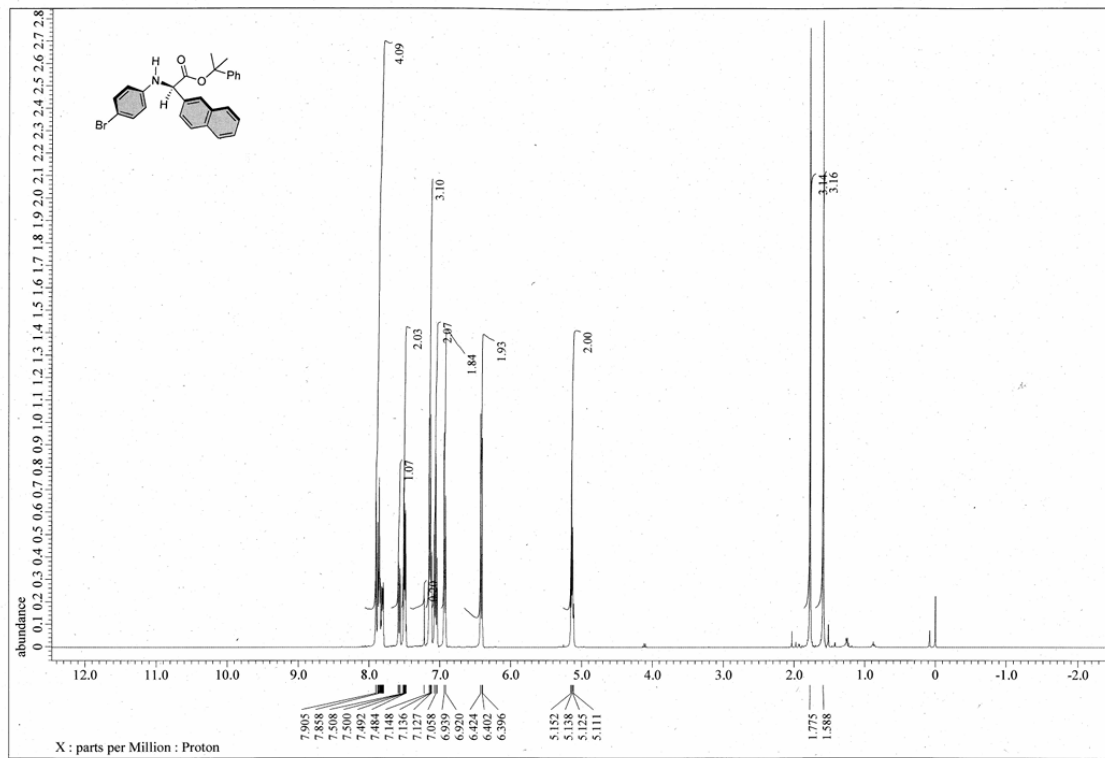


#	tR [min]	Area [µV.sec]	Area%	Height [µV]	Height%
1	9.567	4978078	94.789	312670	95.975
2	12.842	273694	5.211	13114	4.025

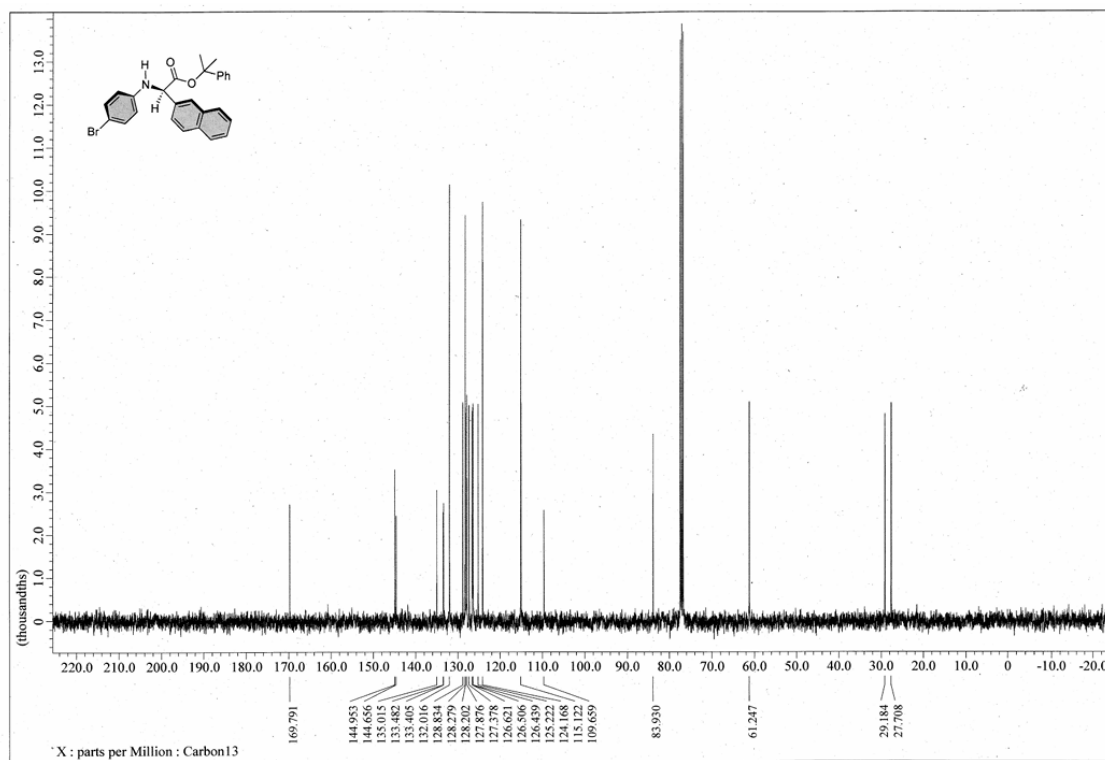
2
3
4
5
6

1
2

3p

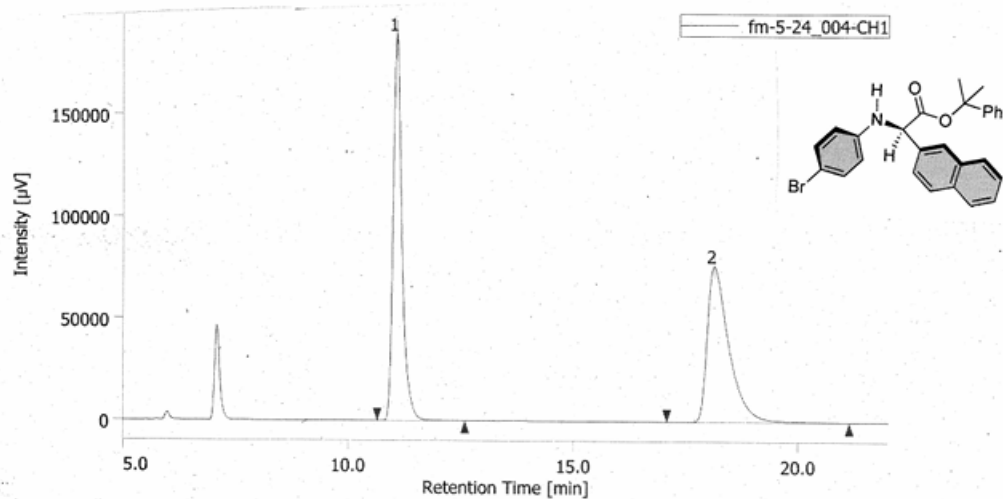


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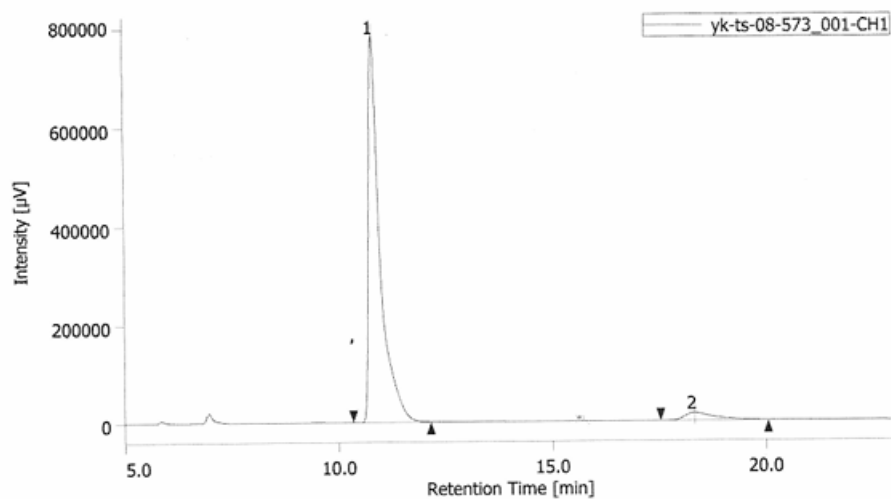
4

1



#	tR (min)	Area [$\mu\text{V}\cdot\text{sec}$]	Area%	Height [μV]	Height%
1	11.067	2578944	50.298	190152	71.361
2	18.133	2548352	49.702	76313	28.639

0612 yk-ts-08-573_001 2026/06/16 4:29:10



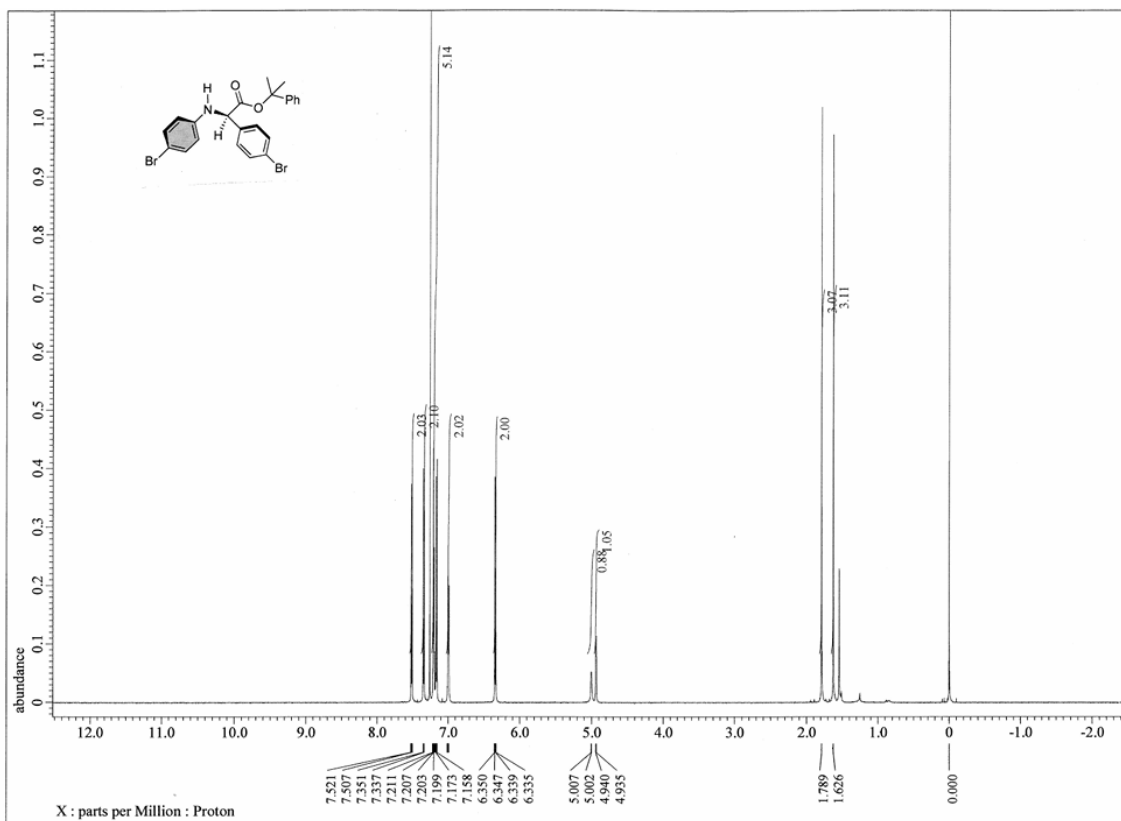
#	tR (min)	Area [$\mu\text{V}\cdot\text{sec}$]	Area%	Height [μV]	Height%
1	10.825	14617732	95.270	785010	98.061
2	18.317	725751	4.730	15524	1.939

2

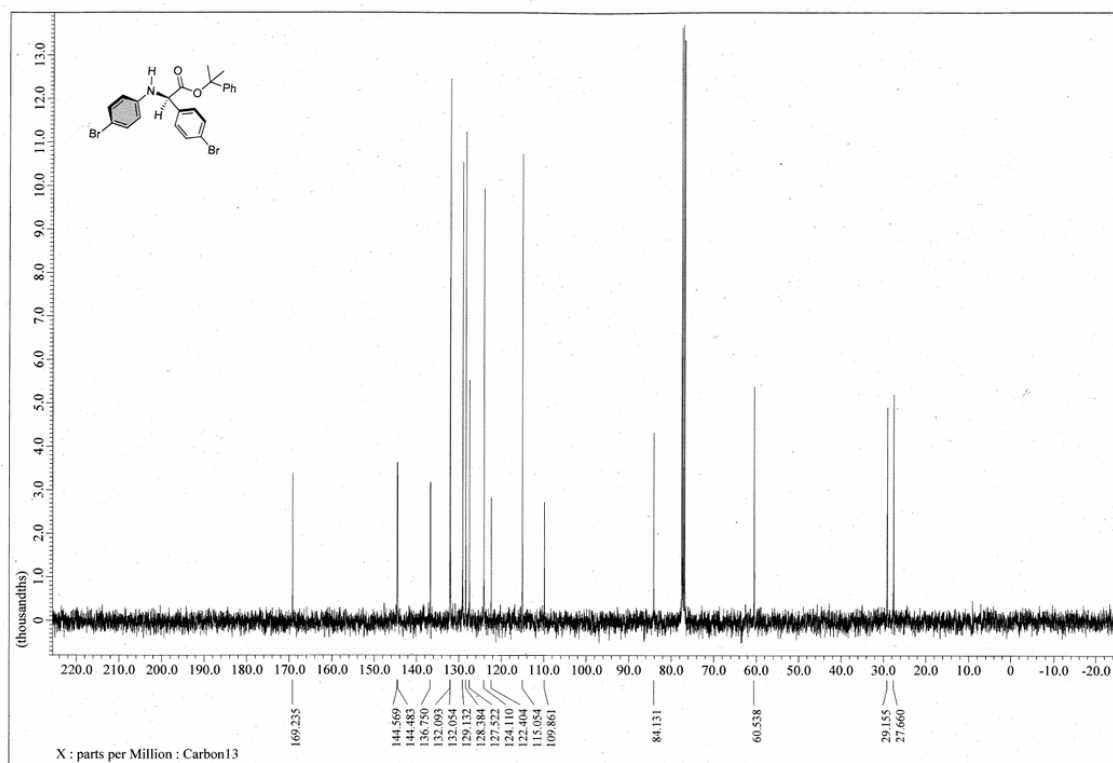
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1

3q

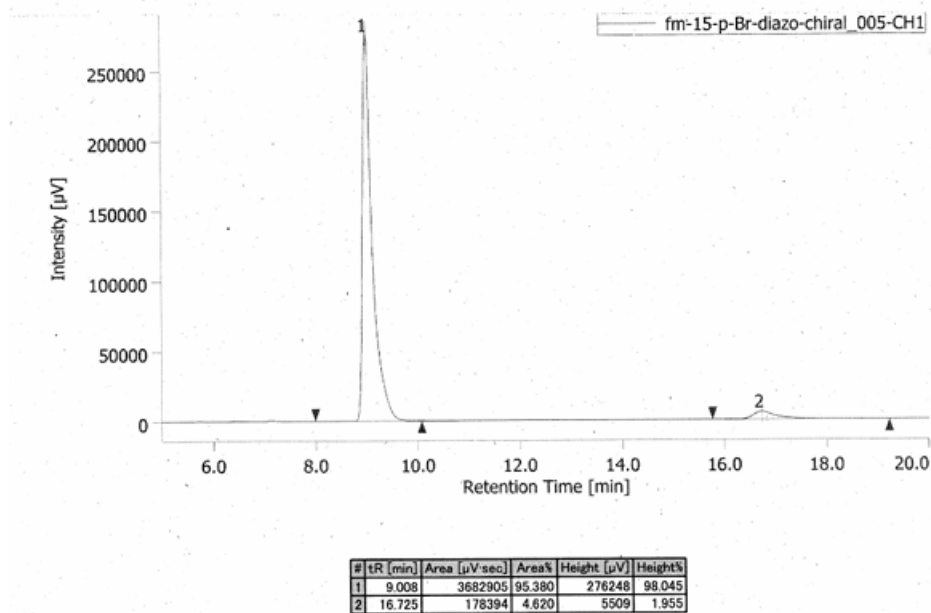
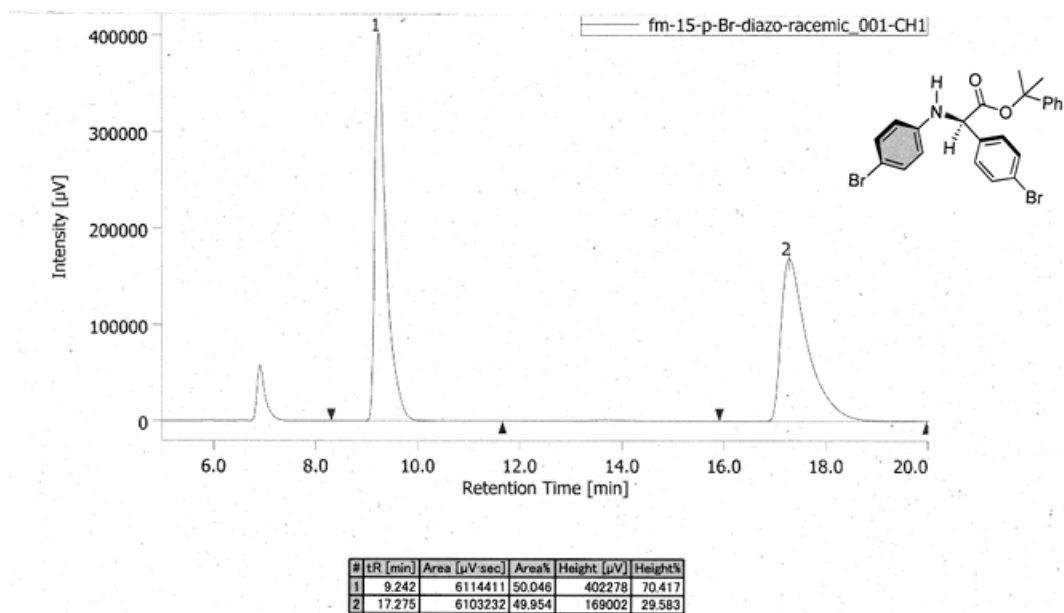


2



3

1

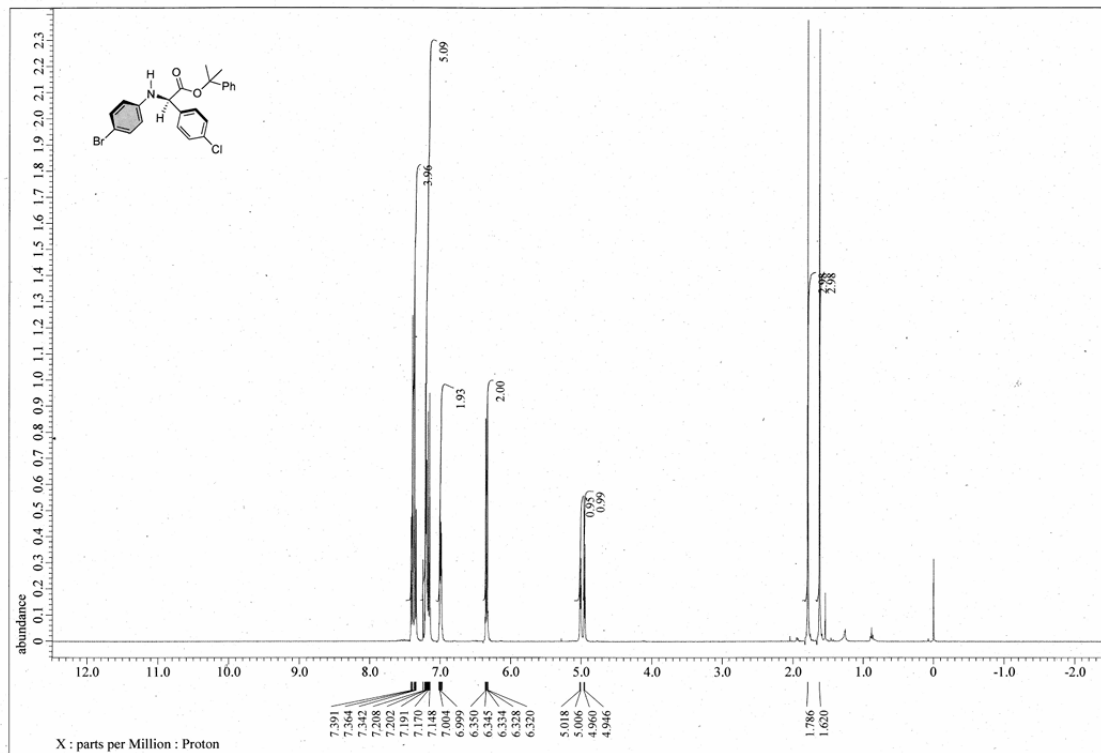


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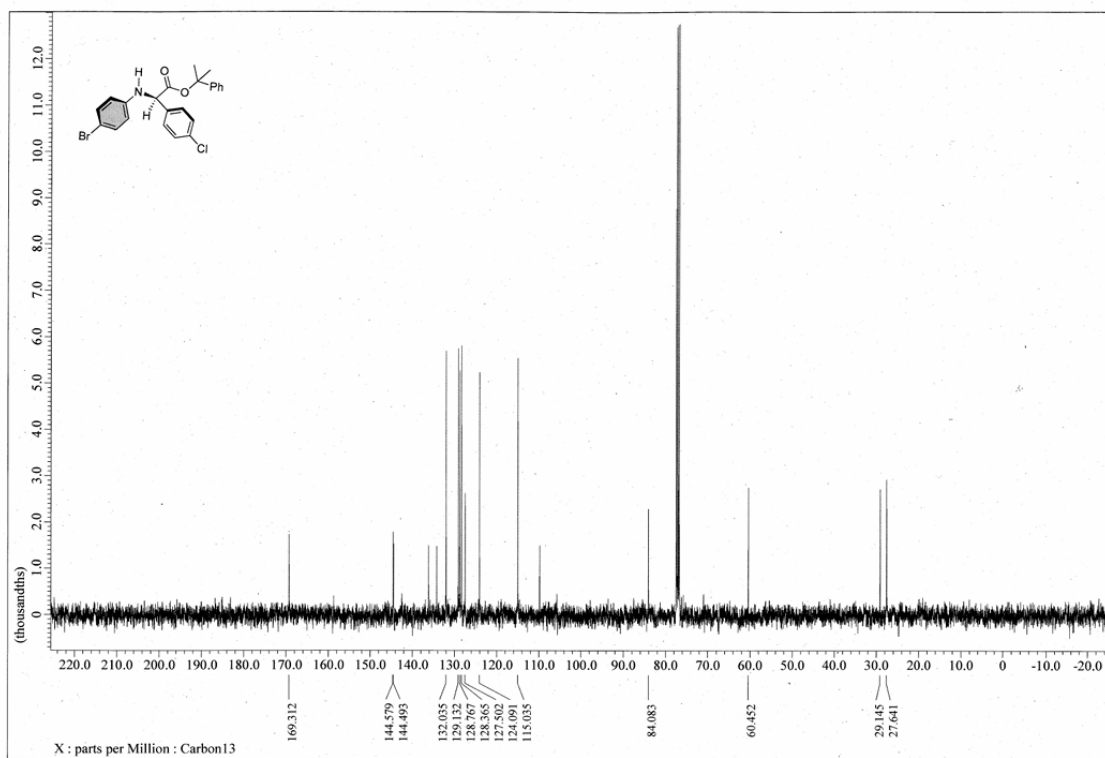
3

1
2

3r

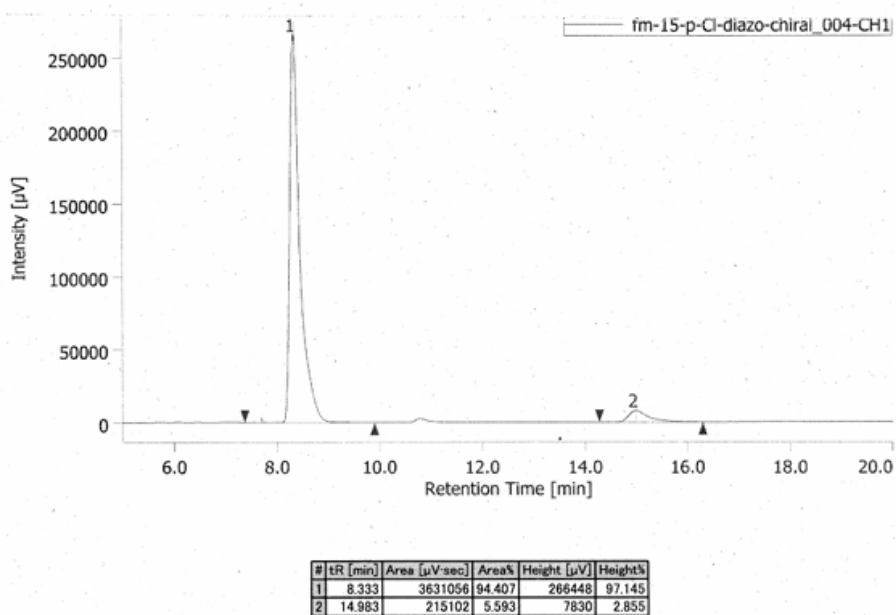
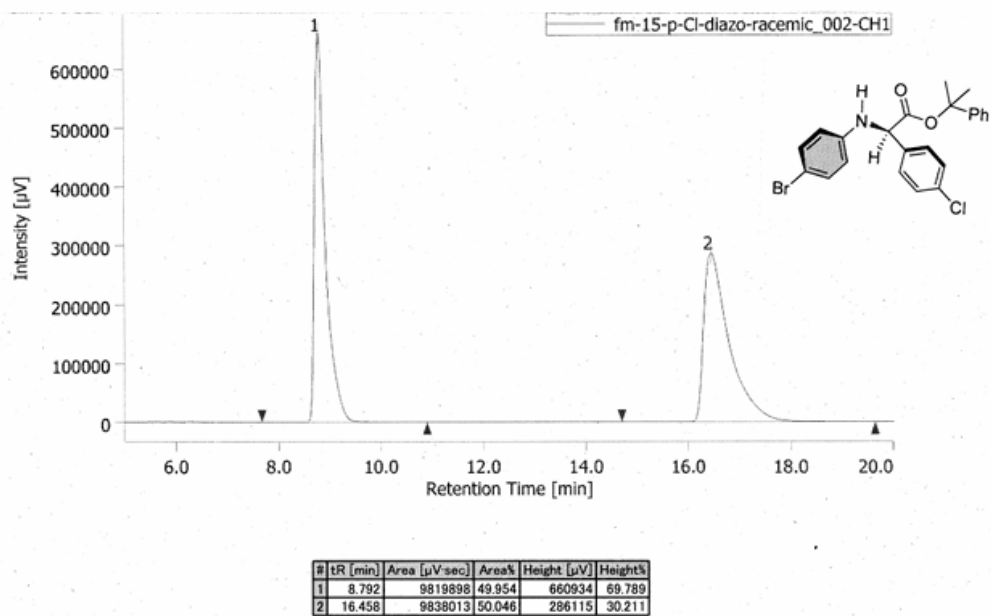


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4

1



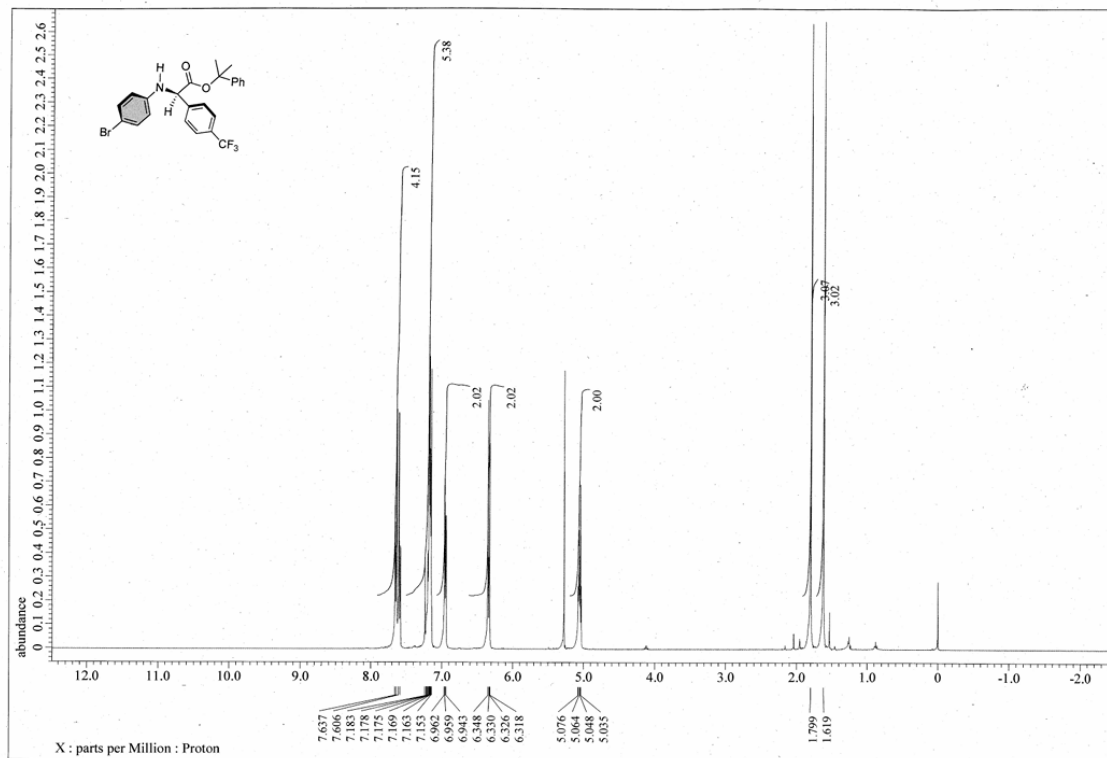
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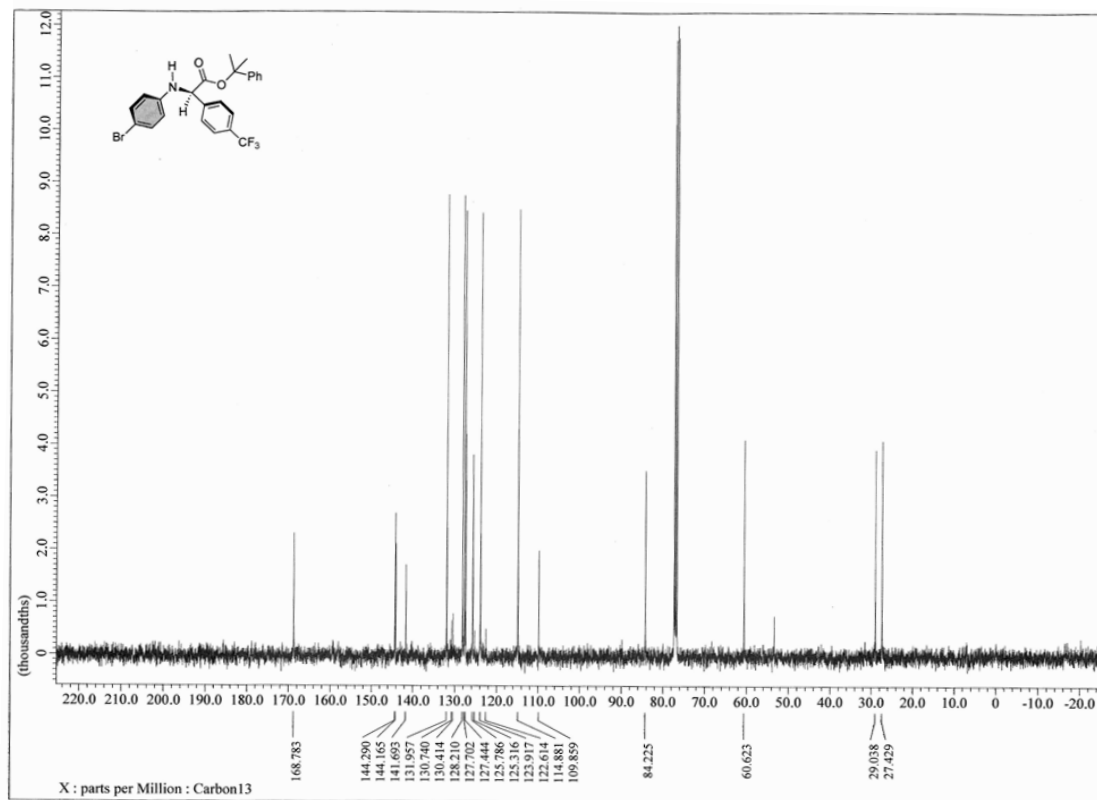
4

1
2

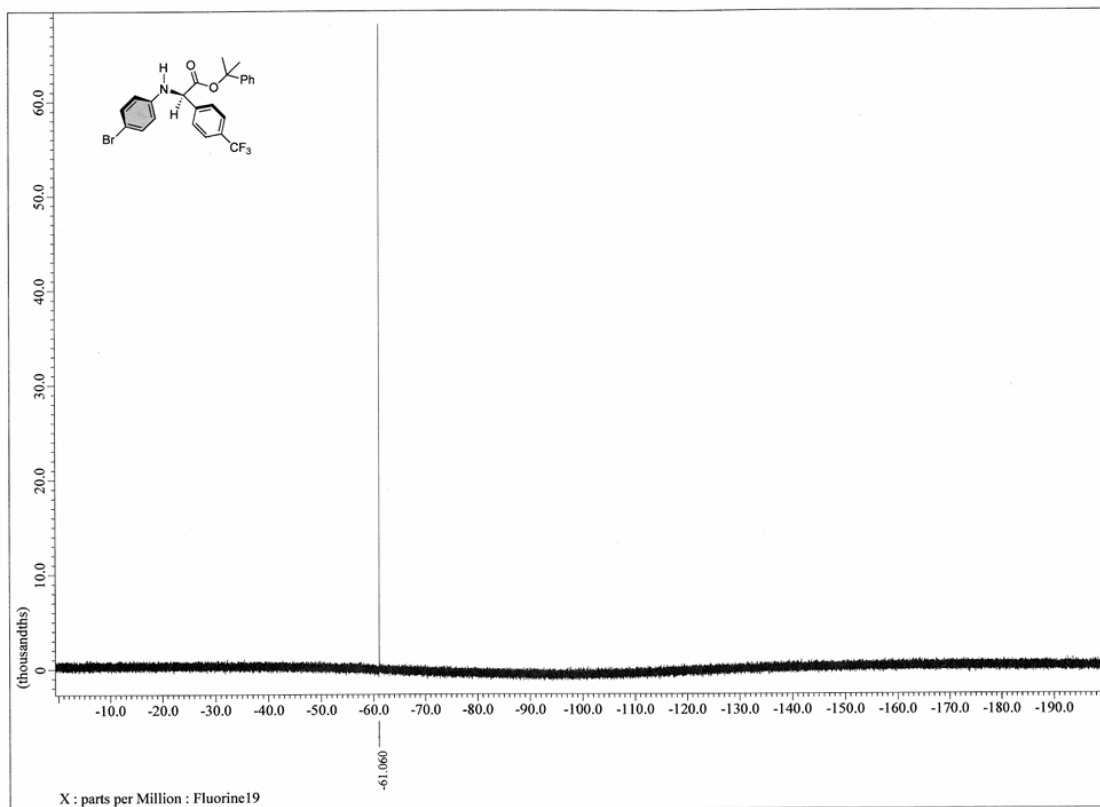
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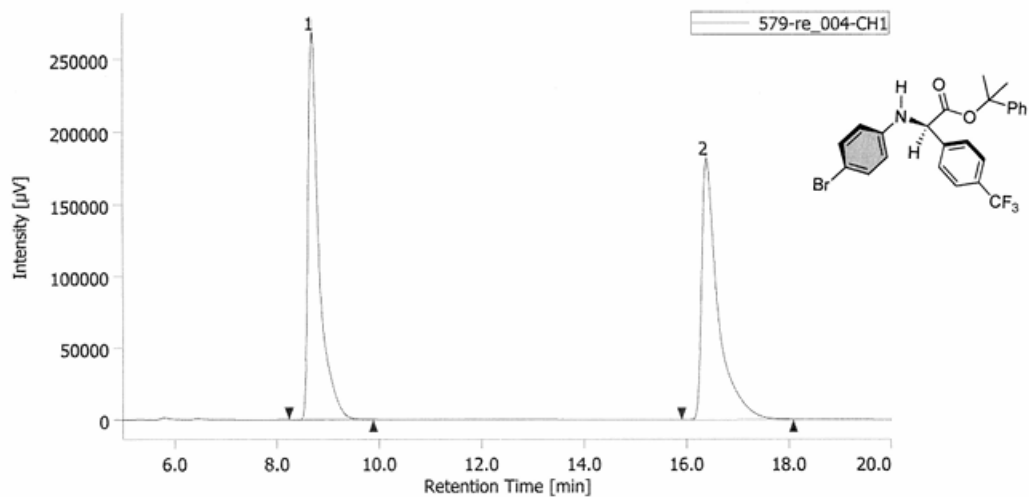
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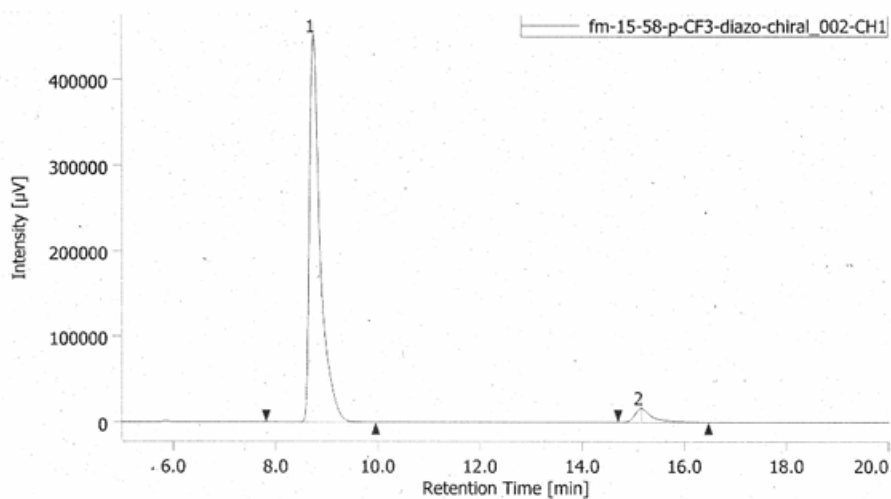
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2



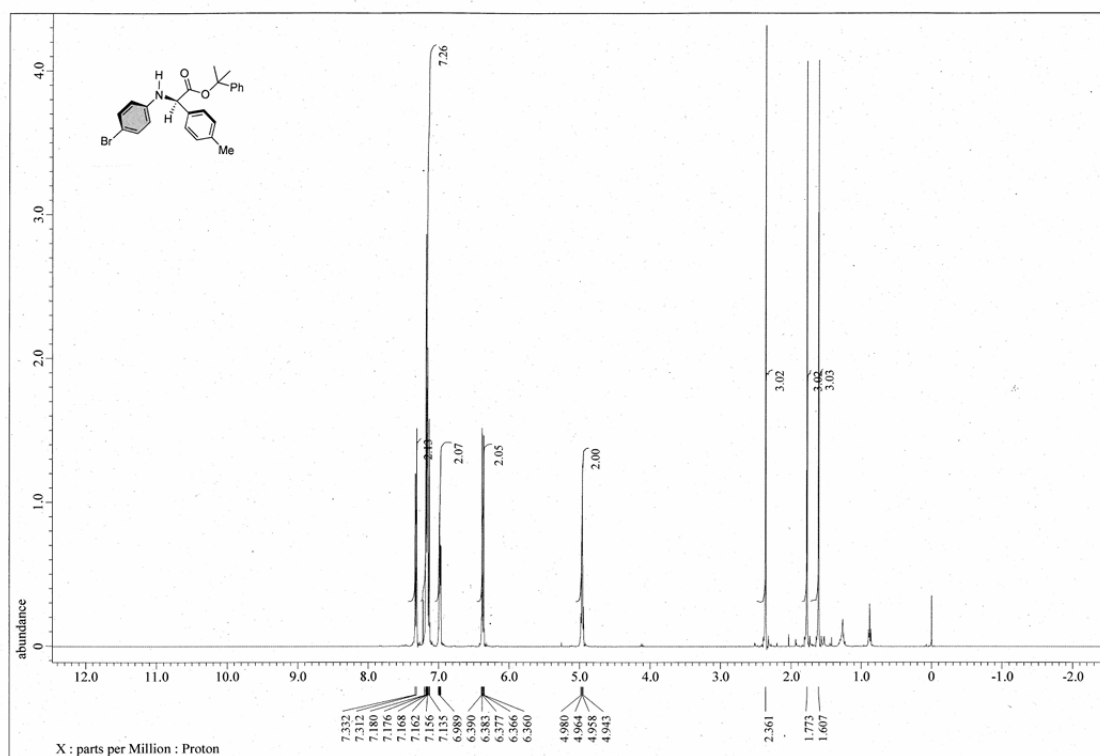
#	tR [min]	Area [$\mu\text{V}\cdot\text{sec}$]	Area%	Height [μV] [μV]	Height%
1	8.700	4007836	49.947	268938	59.655
2	16.408	4016386	50.053	181881	40.345



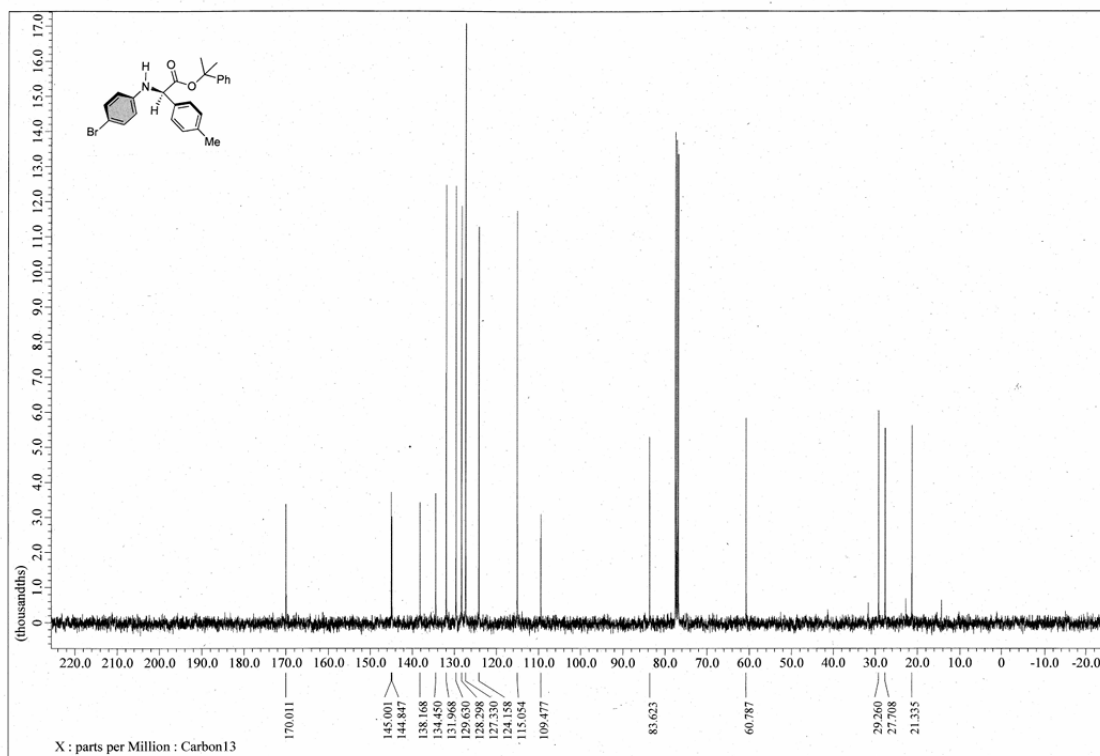
#	tR [min]	Area [$\mu\text{V}\cdot\text{sec}$]	Area%	Height [μV] [μV]	Height%
1	8.742	6589508	94.611	452937	96.580
2	15.150	375321	5.389	16039	3.420

1

3t

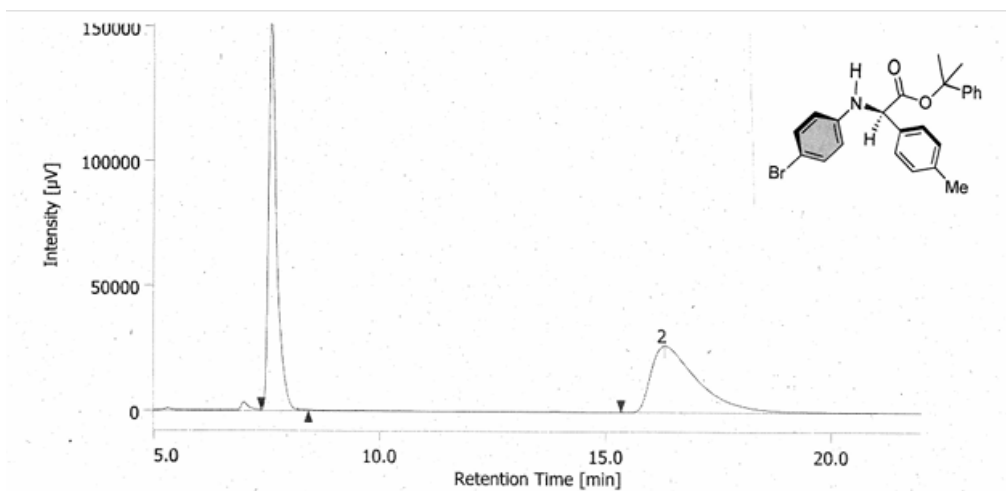


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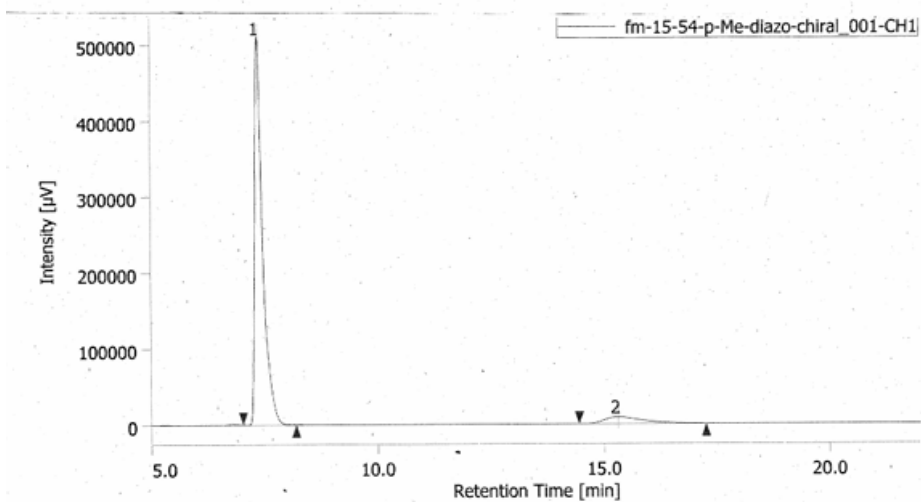


3

4



#	tR [min]	Area [μV·sec]	Area%	Height [μV]	Height%
1	7.600	1960584	50.237	155787	85.402
2	16.317	1942091	49.763	26629	14.598

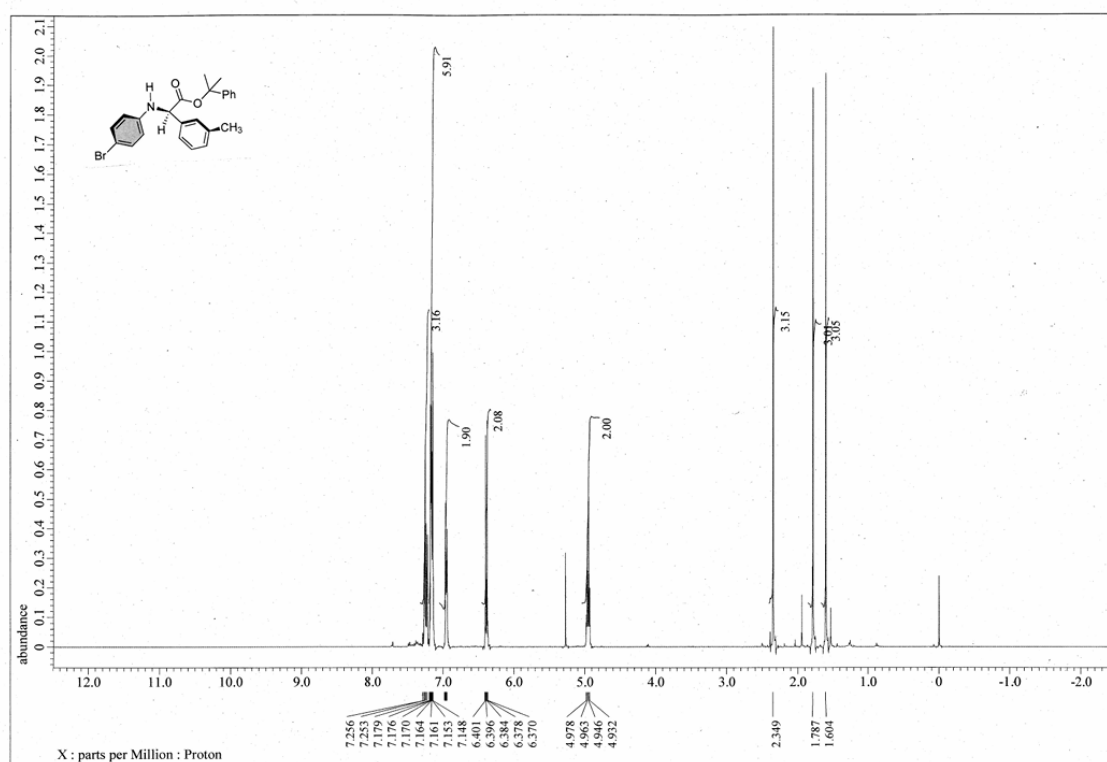


#	tR [min]	Area [μV·sec]	Area%	Height [μV]	Height%
1	7.367	6260759	92.298	510568	98.311
2	15.308	522479	7.702	8771	1.689

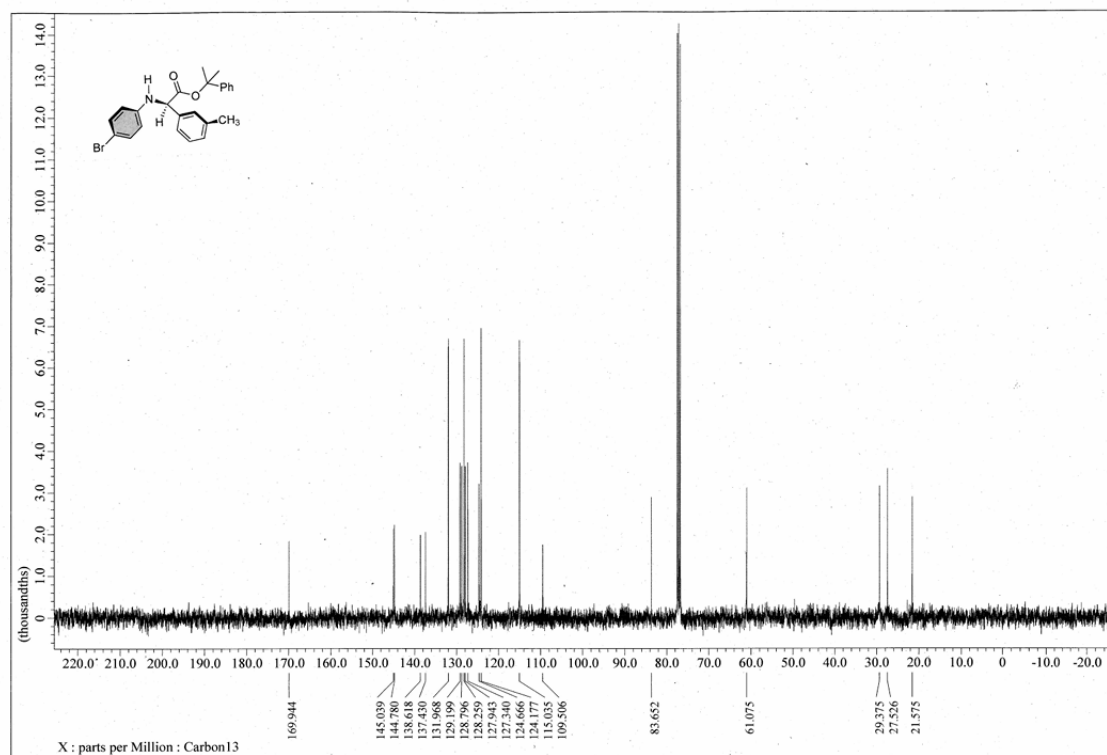
- 1
- 2
- 3
- 4

1

3u

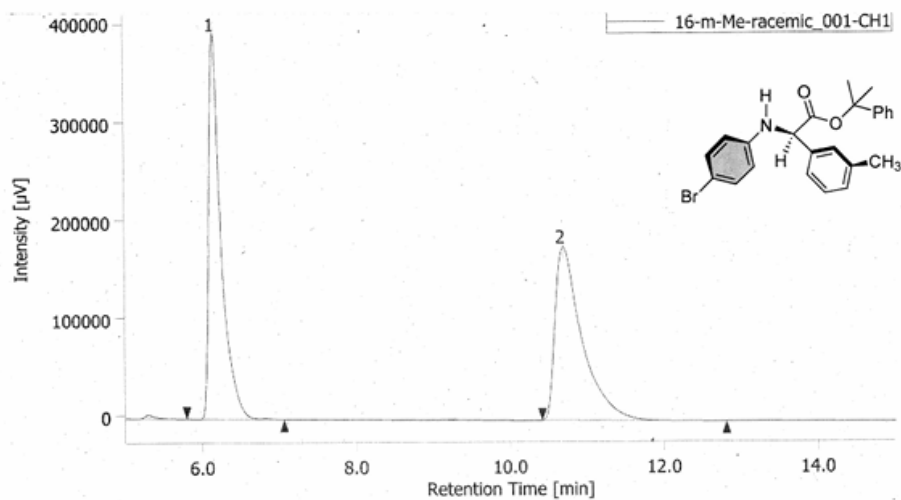


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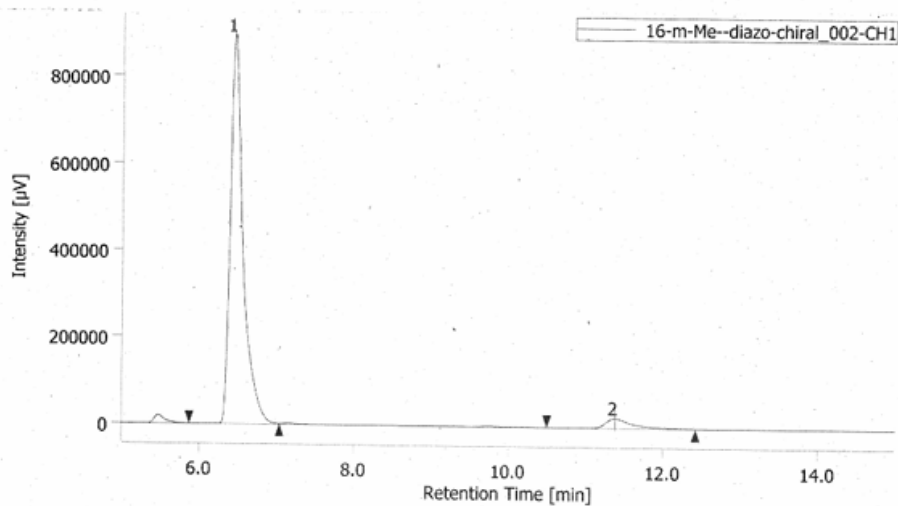


3

4



#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	6.158	4323987	50.194	394745	68.998
2	10.700	4290580	49.806	177370	31.002

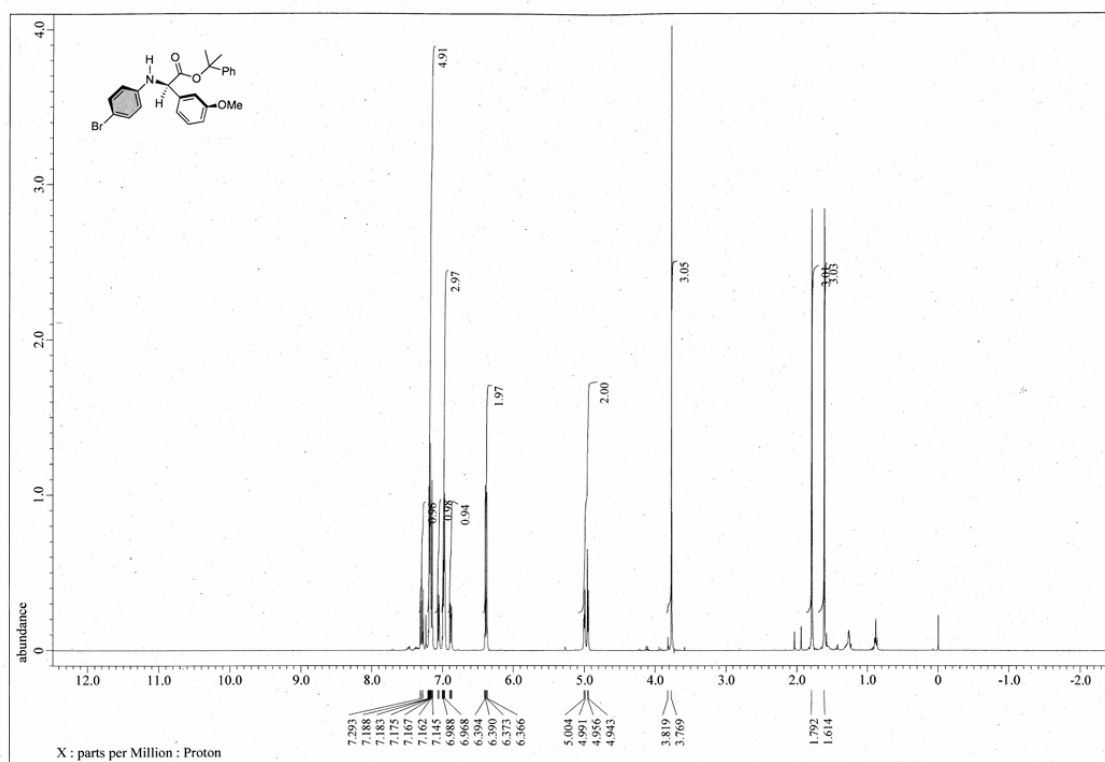


#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	6.442	10286464	95.098	898660	97.588
2	11.383	530239	4.902	22212	2.412

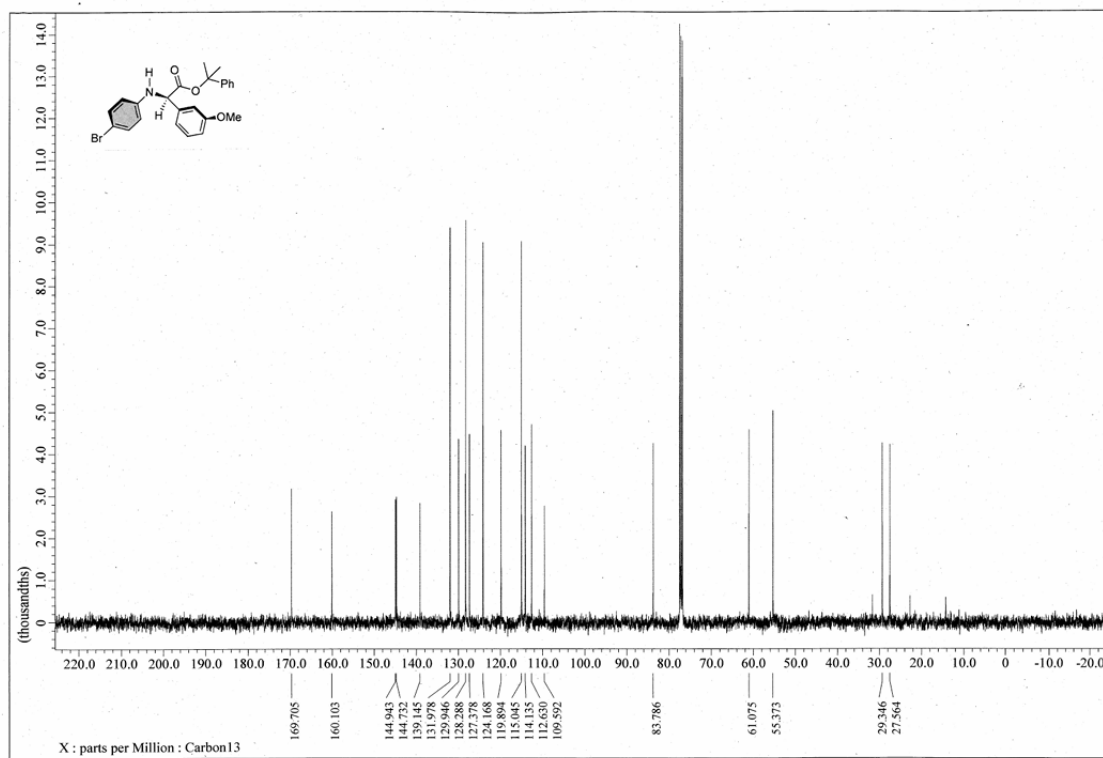
1
2
3

1

3v

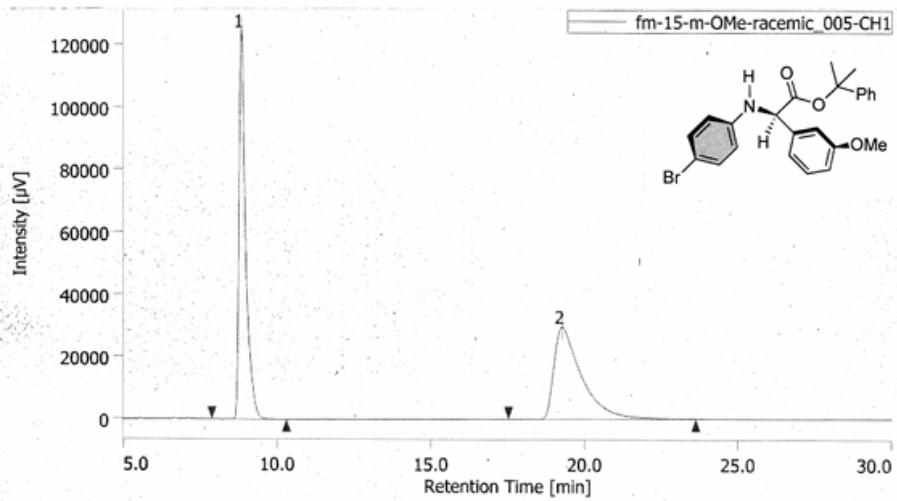


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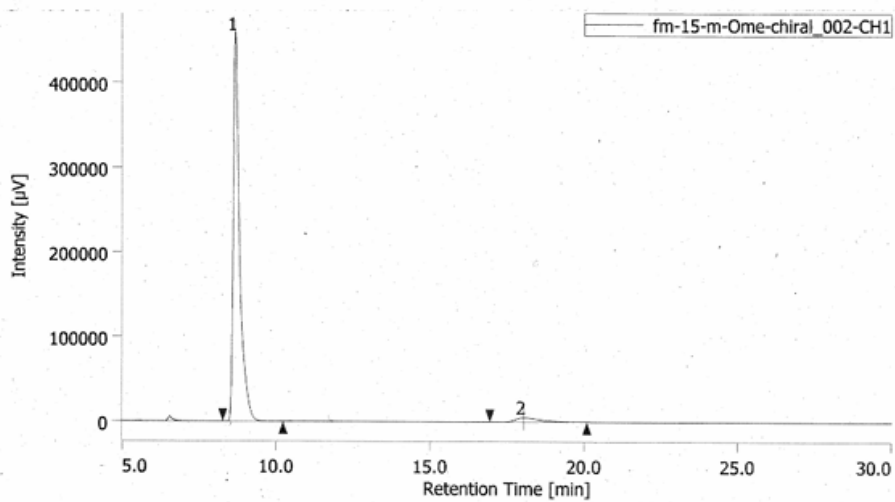


3

4



#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	8.842	1870275	50.401	125093	80.854
2	19.275	1840500	49.599	29821	19.146

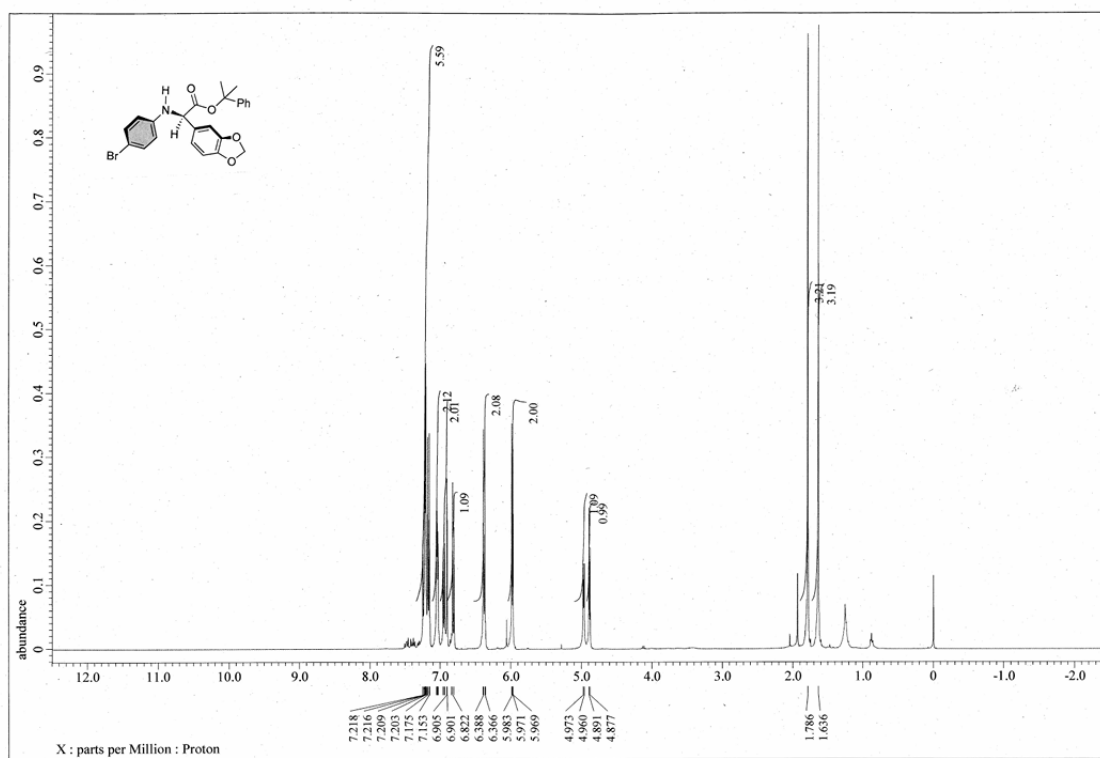


#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	8.675	6727676	96.004	459302	98.936
2	18.050	279993	3.996	4941	1.064

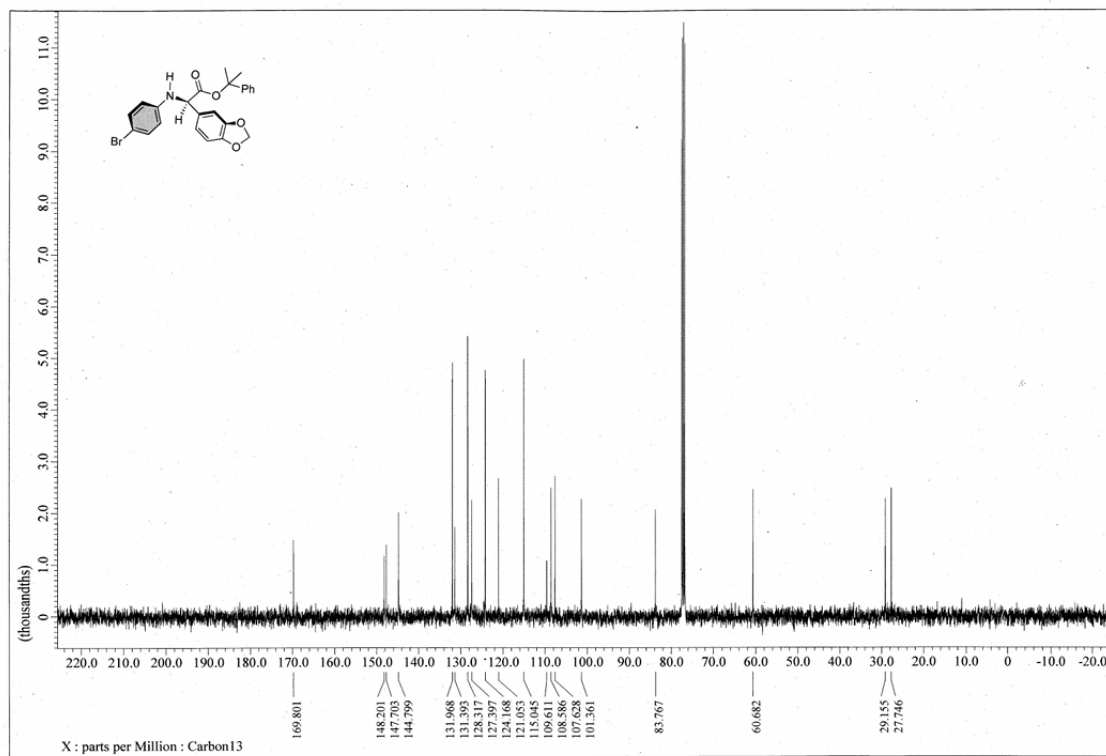
- 1
- 2
- 3

1

3w

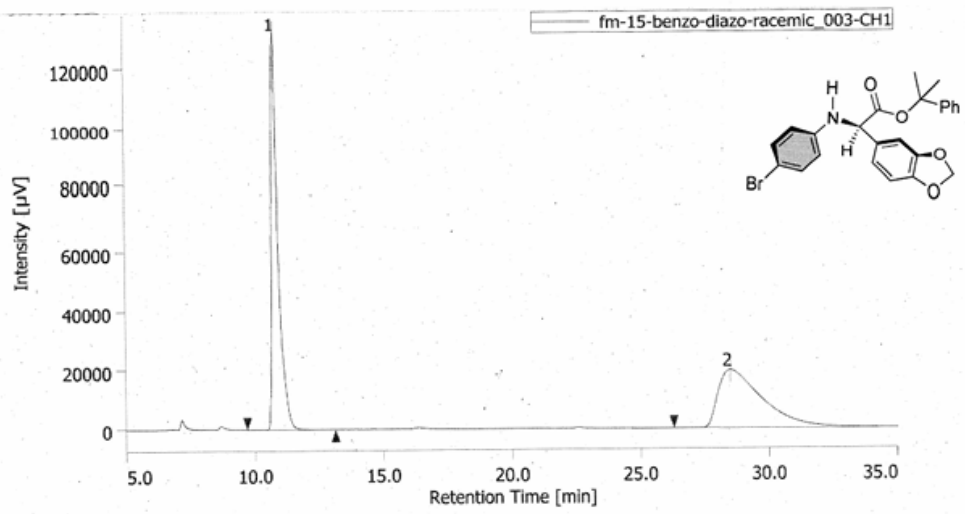


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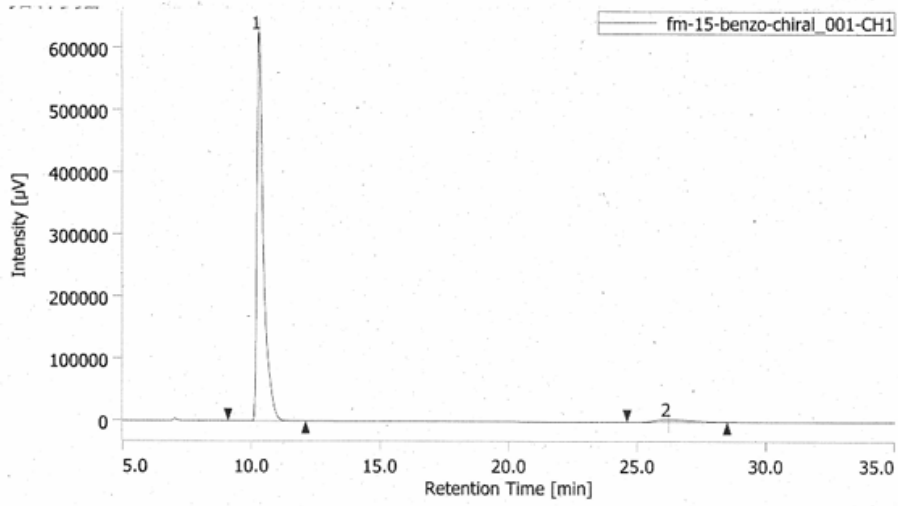


3

4



#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	10.800	2360433	50.099	131915	87.032
2	28.483	2351073	49.901	19655	12.968

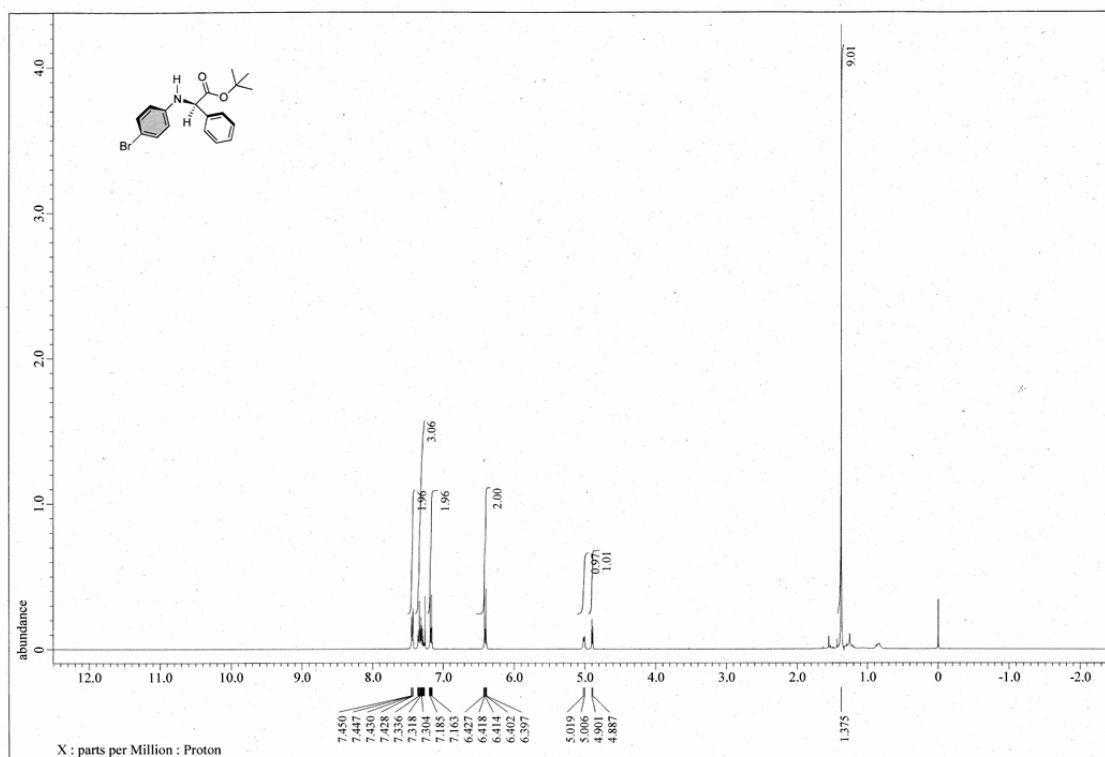


#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	10.308	11073607	96.557	628530	99.335
2	26.217	394847	3.443	4205	0.665

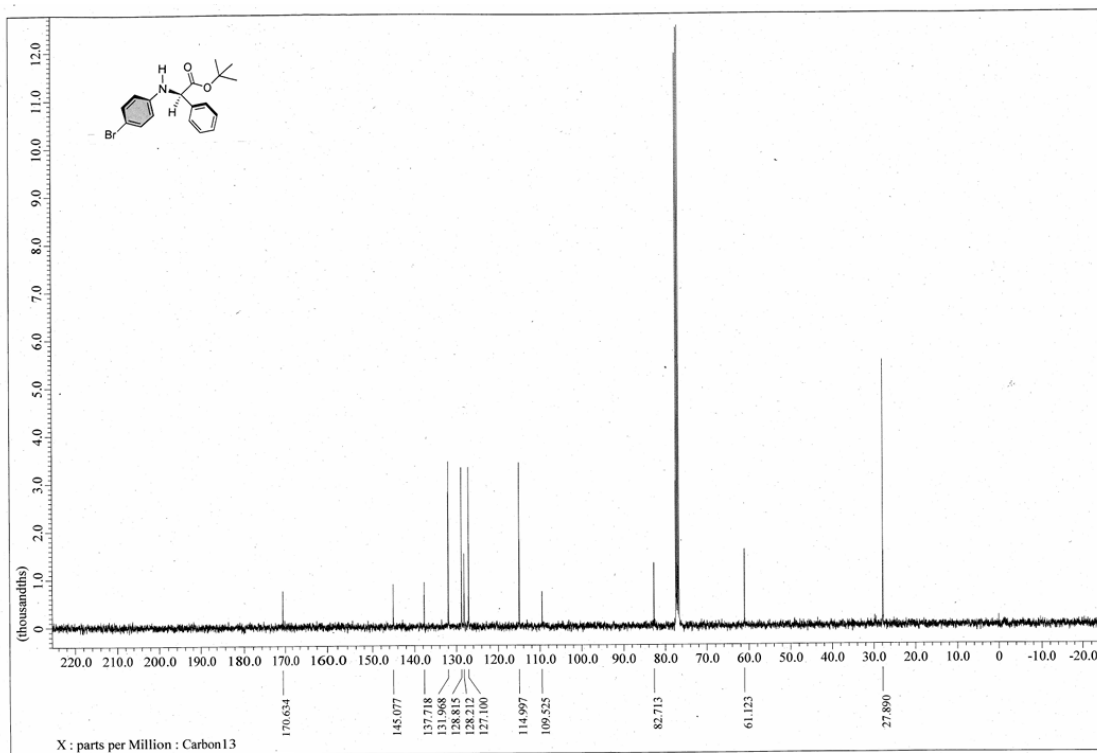
- 1
- 2
- 3

1

3x



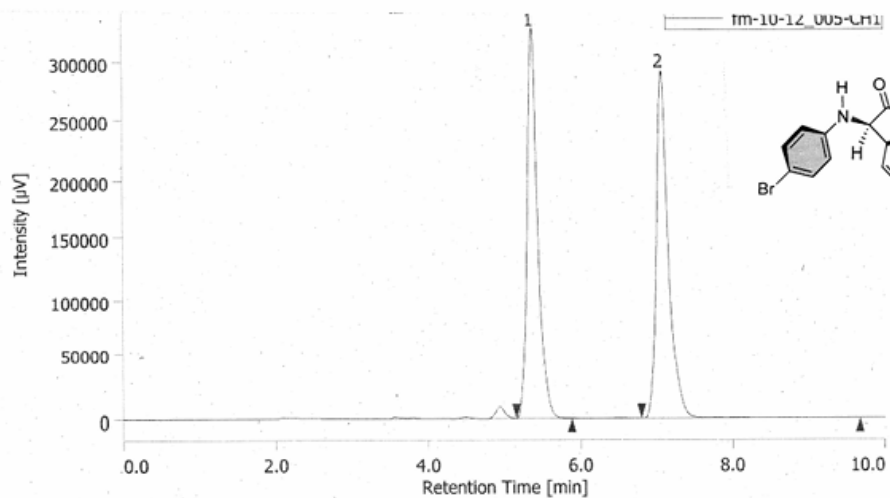
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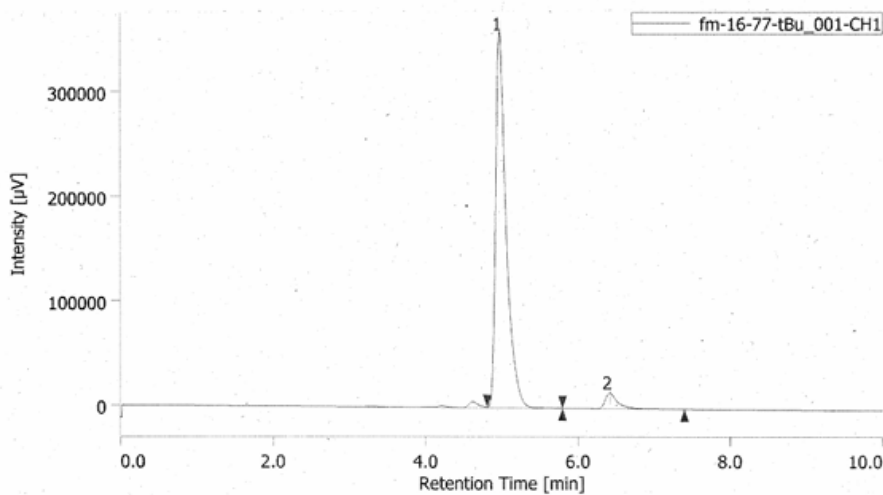
3

4

5



#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	5.375	3101856	49.870	328067	52.930
2	7.075	3117991	50.130	291745	47.070

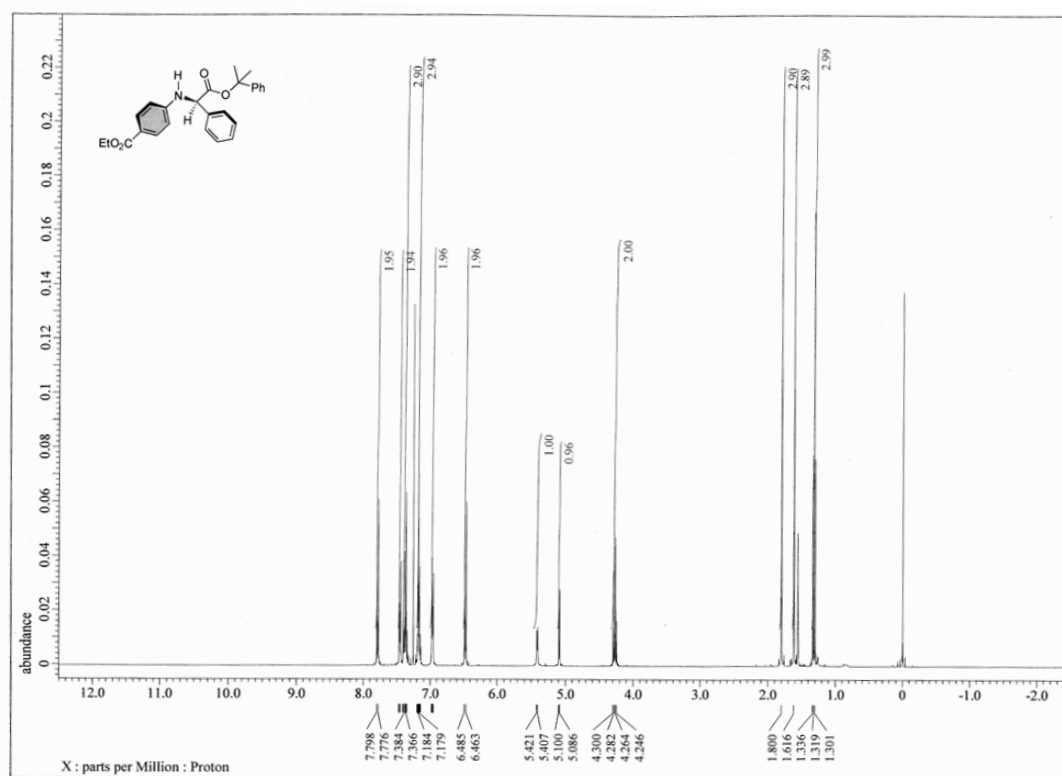


#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	4.975	3453041	95.355	360200	95.997
2	6.417	168216	4.645	15018	4.003

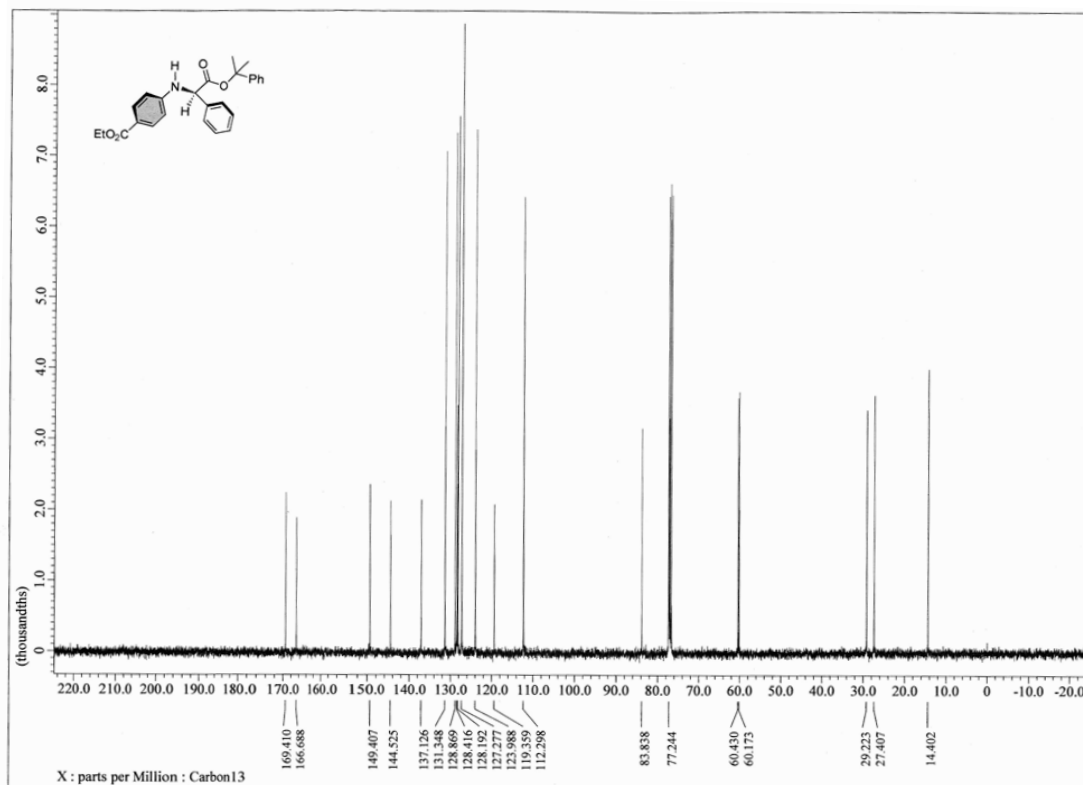
- 1
- 2
- 3
- 4

1

3y

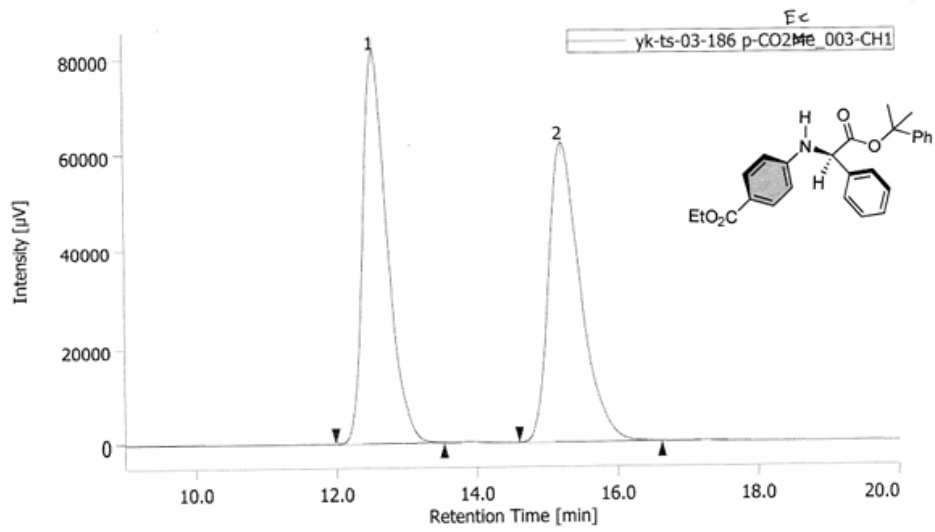


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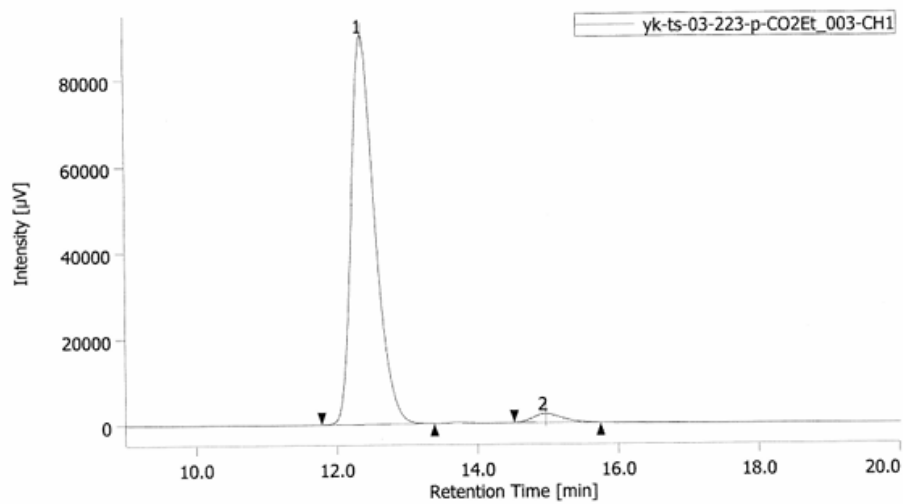
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0529 yk-ts-03-186 p-CO₂Me_003 2026/05/07 16:09:56



#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	12.558	1954277	50.163	81608	56.683
2	15.225	1941578	49.837	62363	43.317

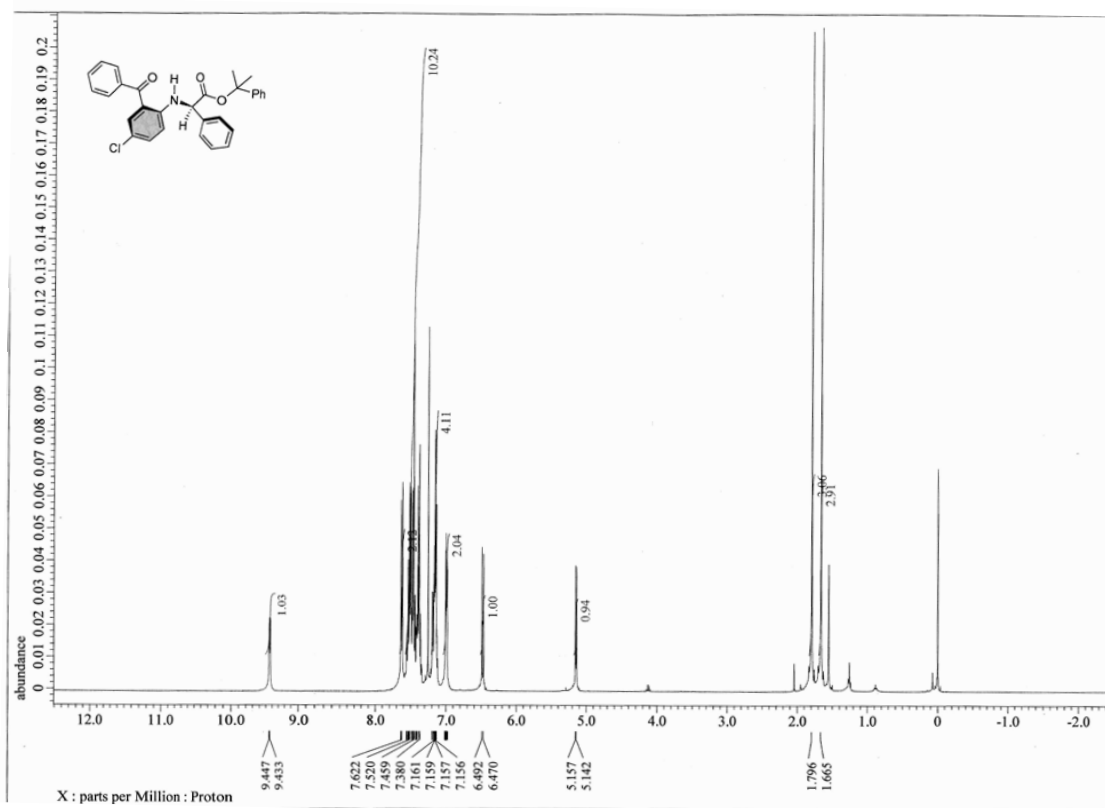
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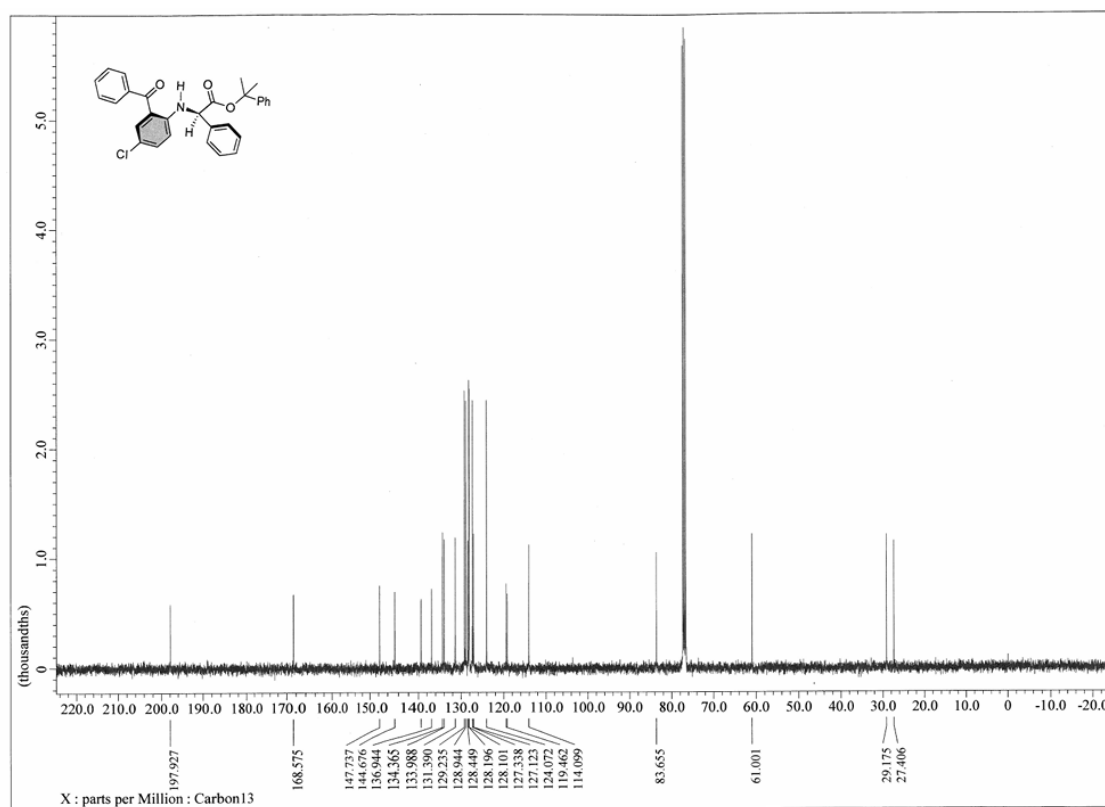
#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	12.375	2090641	97.208	90324	97.788
2	14.967	60058	2.792	2043	2.212

1

3z

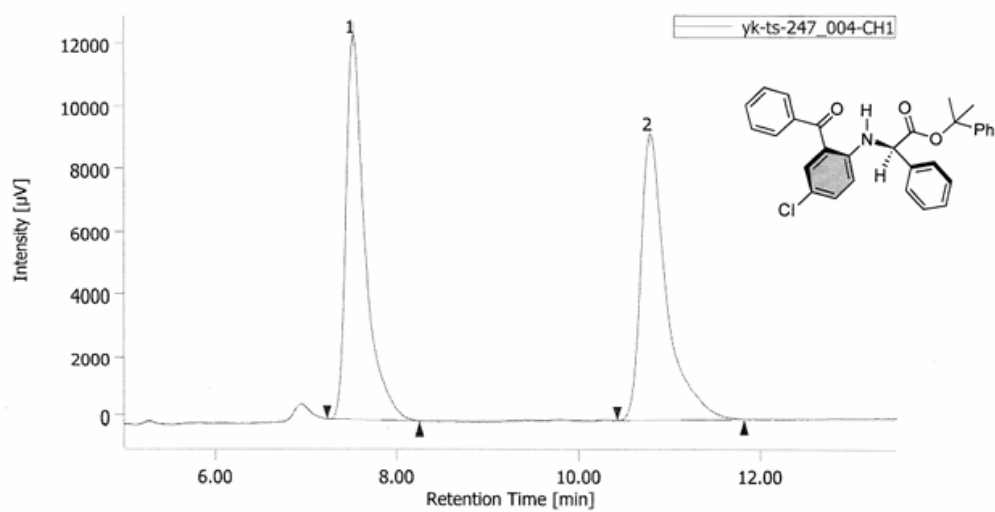


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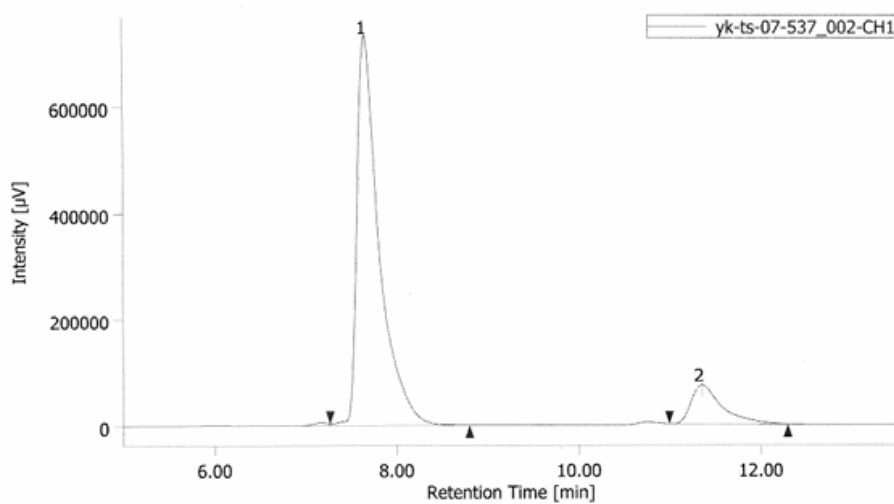
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0714 yk-ts-247_004 2026/05/16 9:42:09



#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	7.525	182099	49.994	12419	57.327
2	10.792	182142	50.006	9245	42.673

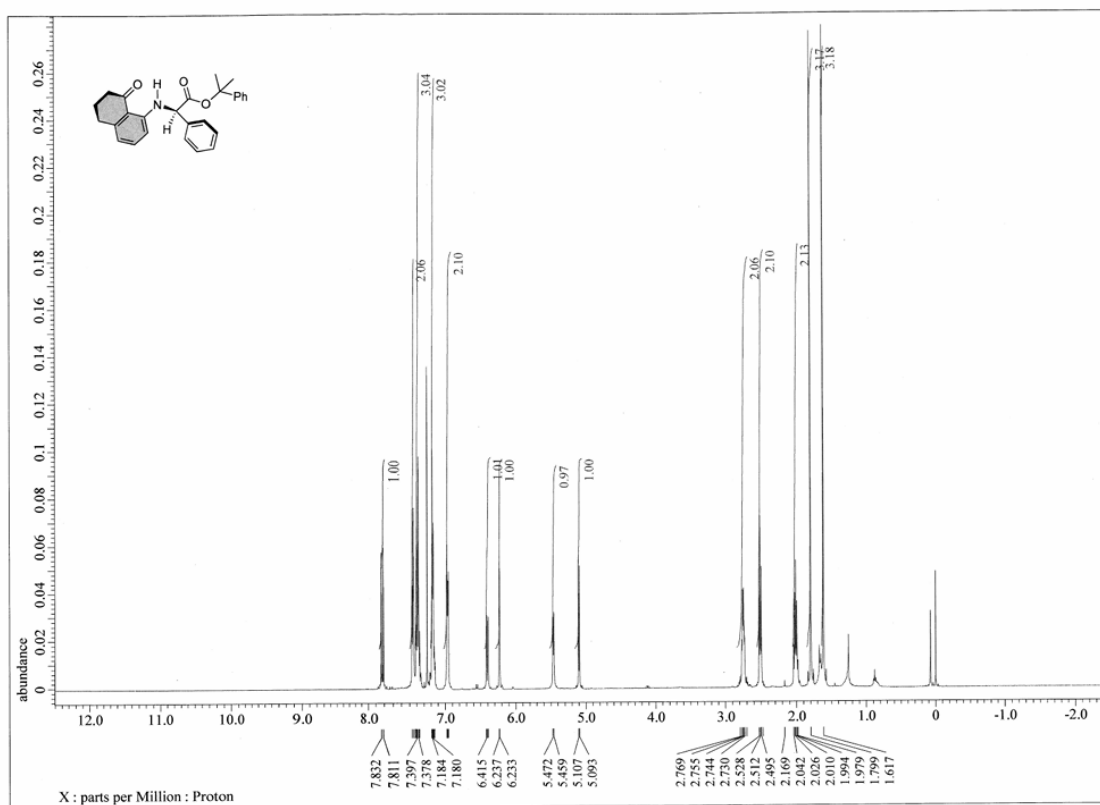
0516 yk-ts-07-537_002 2026/05/16 14:48:18



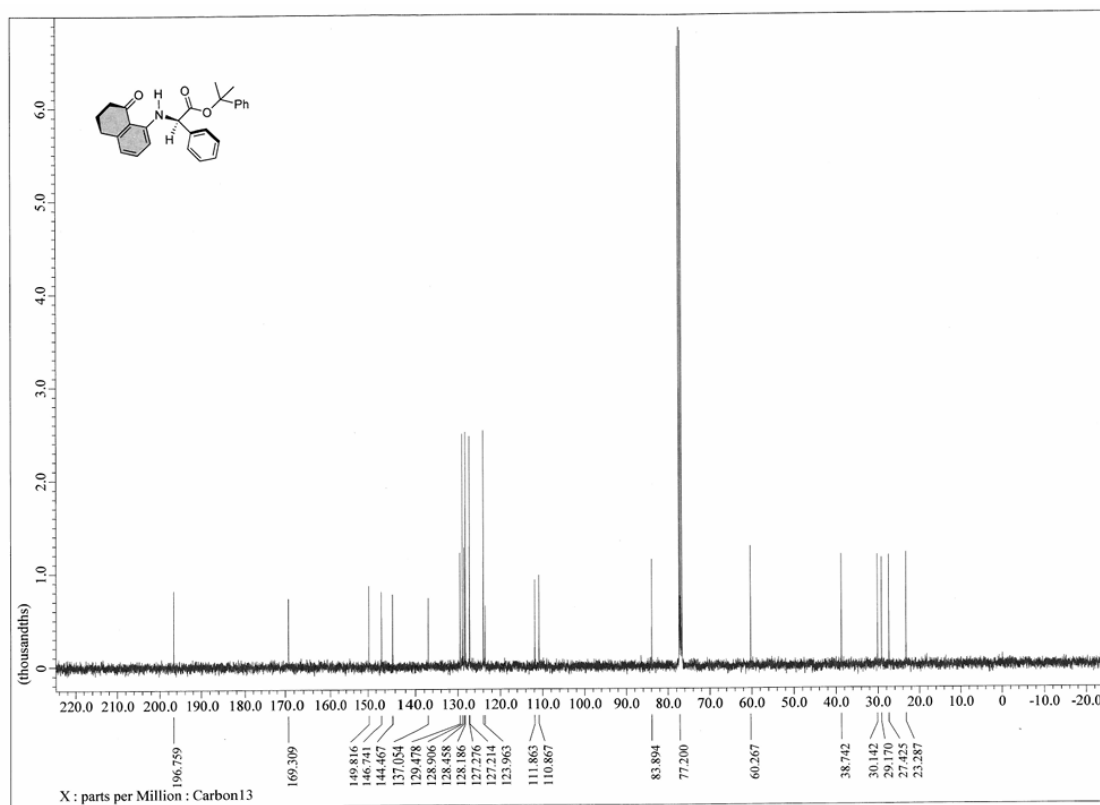
#	tR [min]	Area [µV·sec]	Area%	Height [µV]	Height%
1	7.658	12329185	88.012	730246	90.994
2	11.350	1679330	11.988	72279	9.006

1

3aa

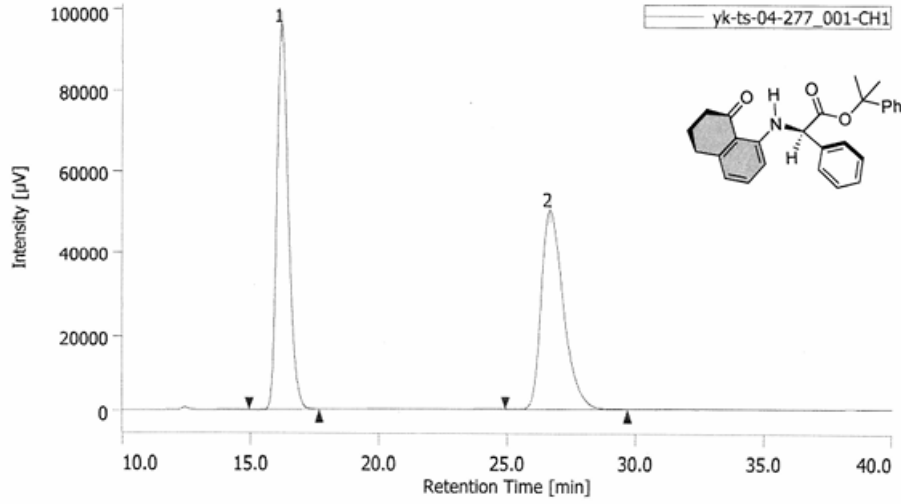


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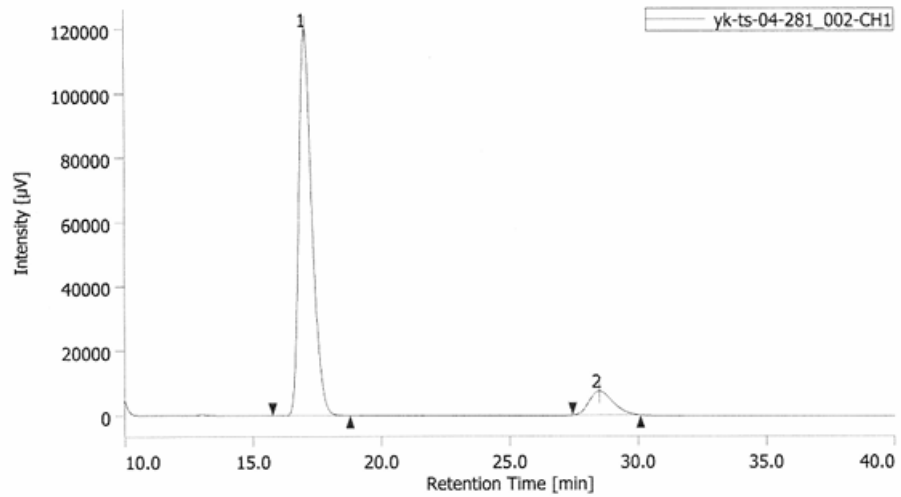
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0911 yk-ts-04-277_001 2026/06/16 6:04:57



#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	16.217	3059059	49.988	96005	65.591
2	26.692	3060530	50.012	50364	34.409

0929 yk-ts-04-281_002 2026/06/16 6:06:21



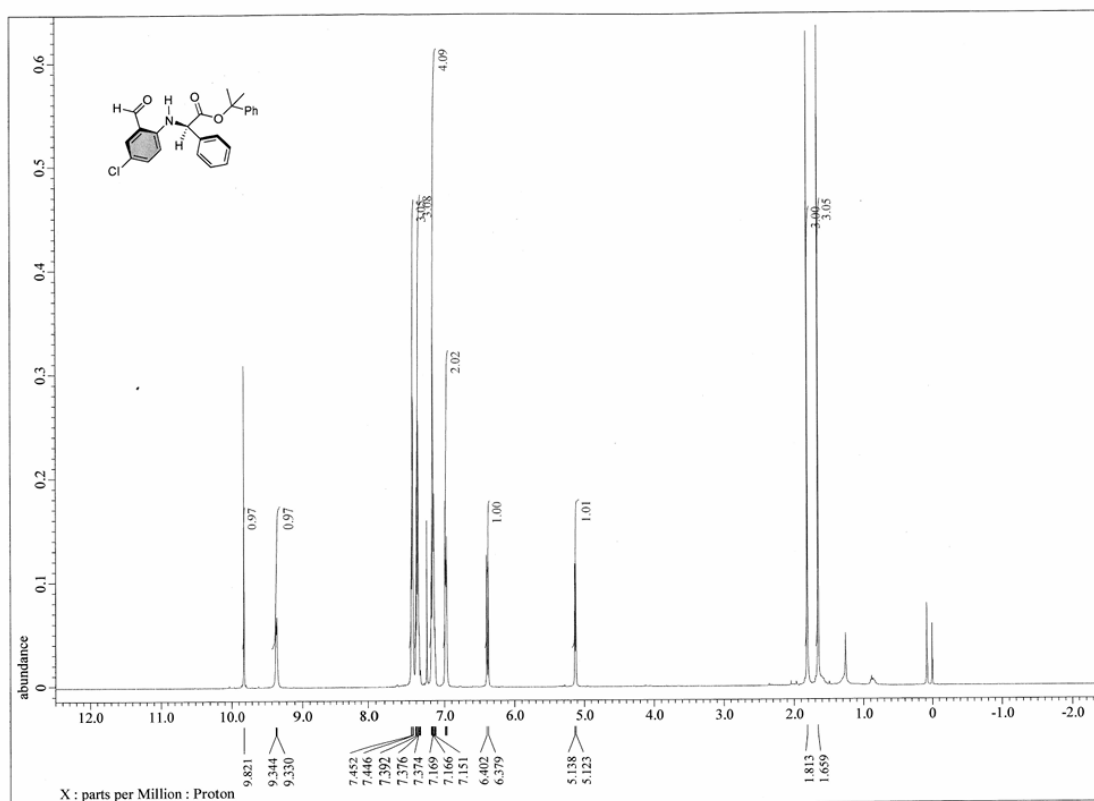
#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	17.025	4234773	89.971	120237	94.277
2	28.483	472035	10.029	7299	5.723

1

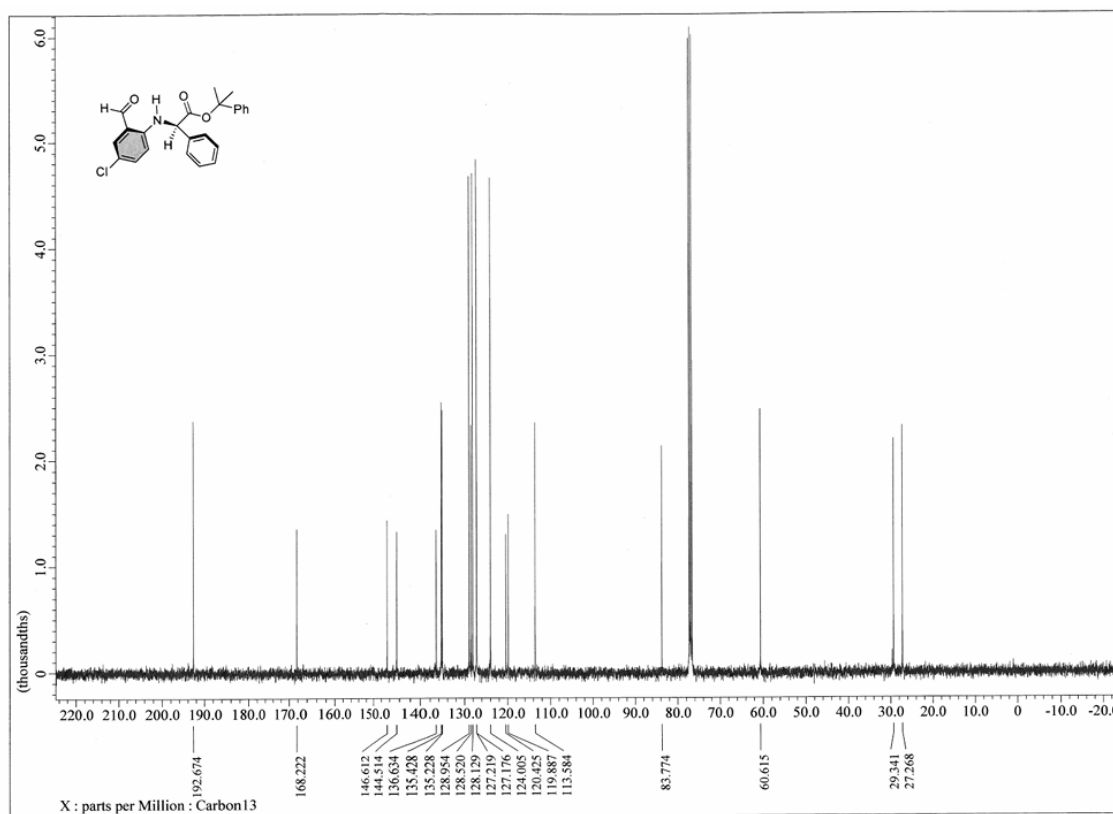
2

1

3ab

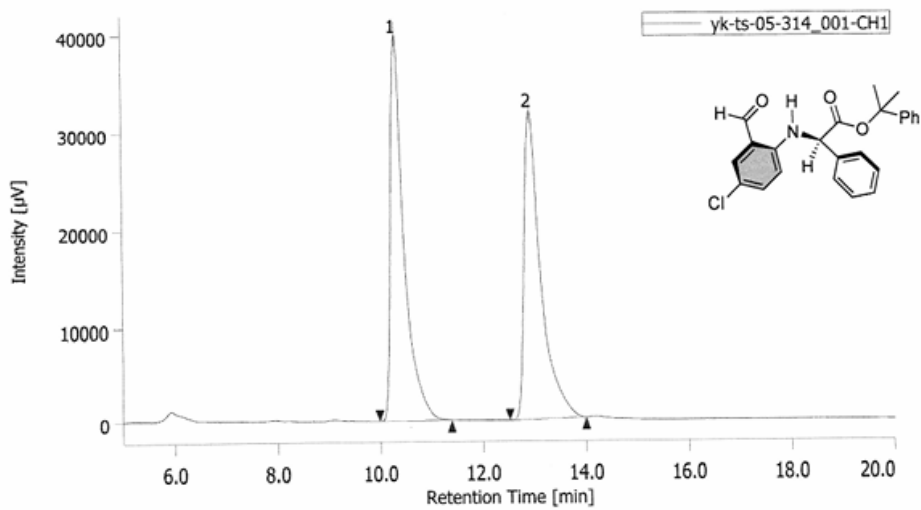


2



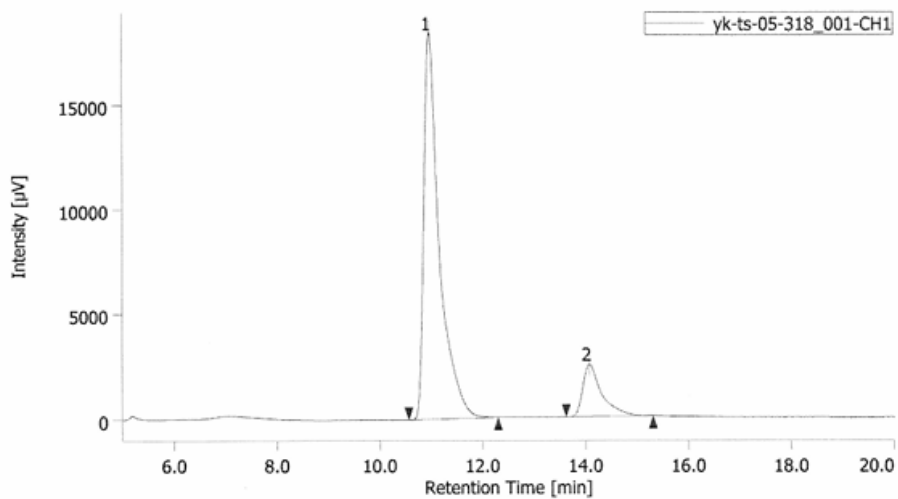
3

1015 yk-ts-05-314_001 2026/06/16 6:15:59



#	tR [min]	Area [µV·sec]	Area%	Height (µV) [µV]	Height%
1	10.325	740271	50.408	39973	55.577
2	12.942	728286	49.592	31950	44.423

1031 yk-ts-05-318_001 2026/06/16 6:16:09

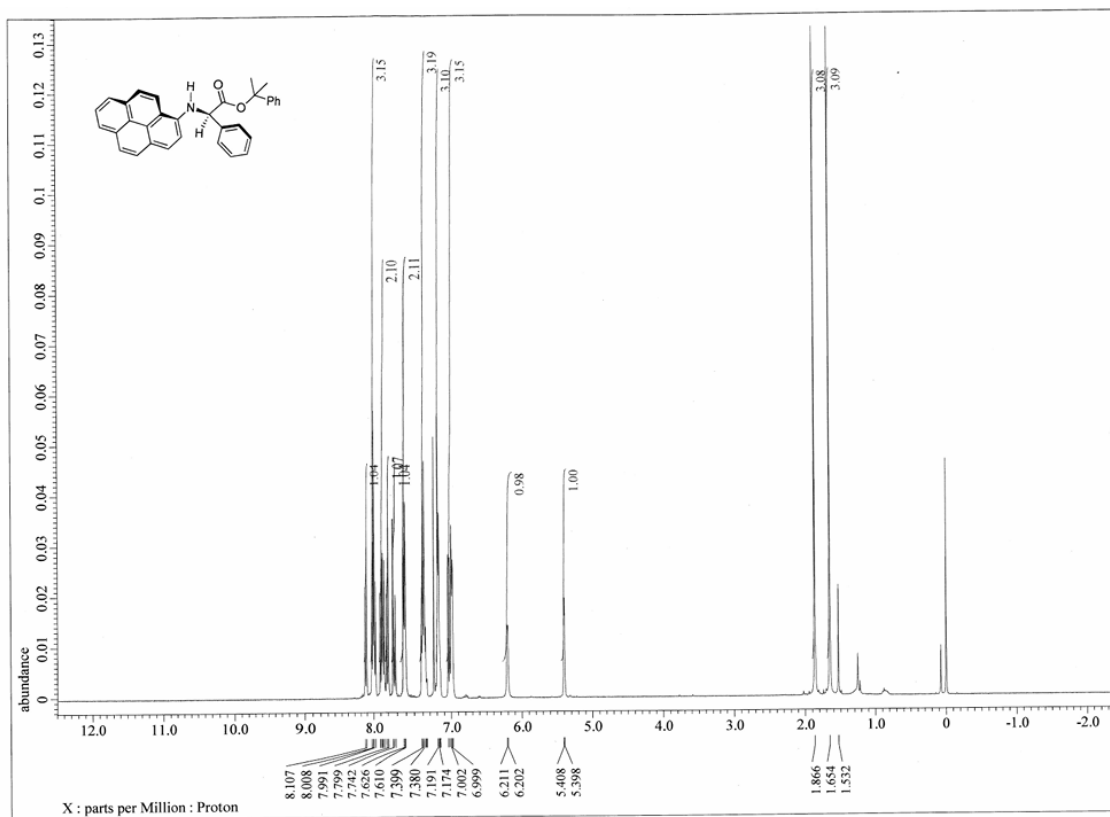


#	tR [min]	Area [µV·sec]	Area%	Height (µV) [µV]	Height%
1	10.975	383395	86.035	18462	68.170
2	14.075	62234	13.965	2477	11.830

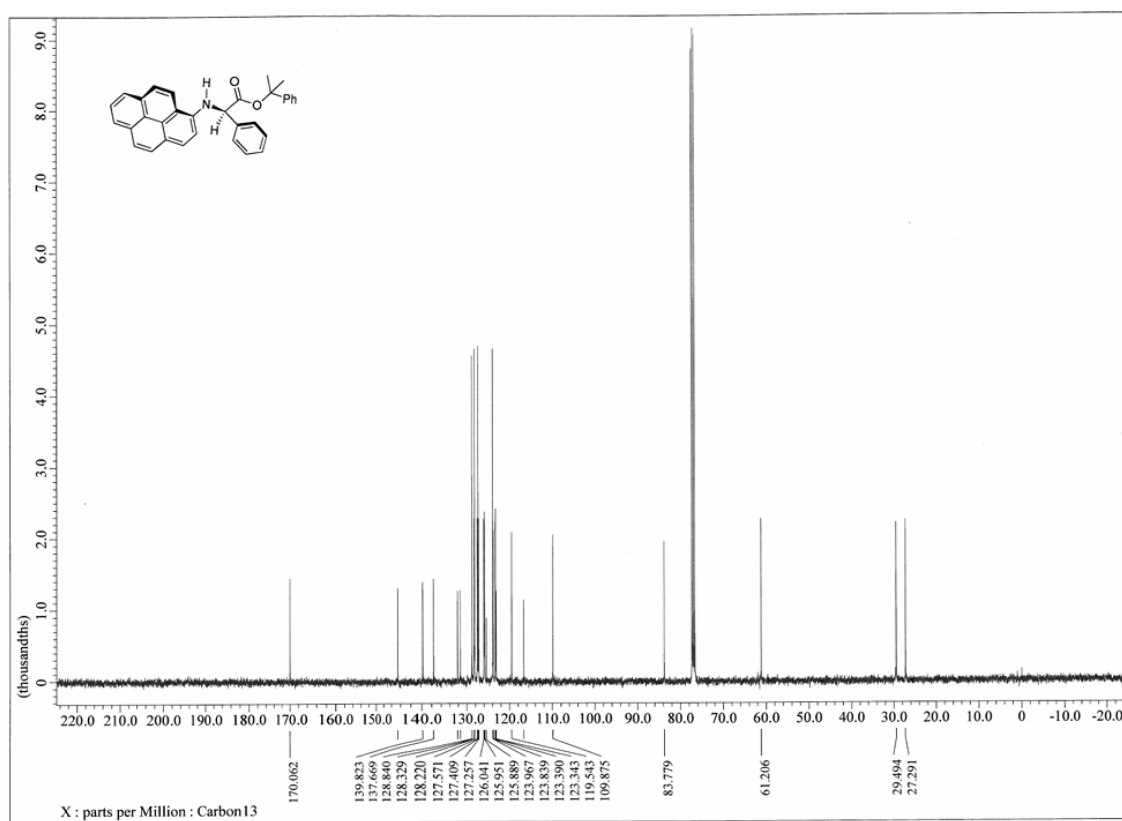
1
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1

3ac

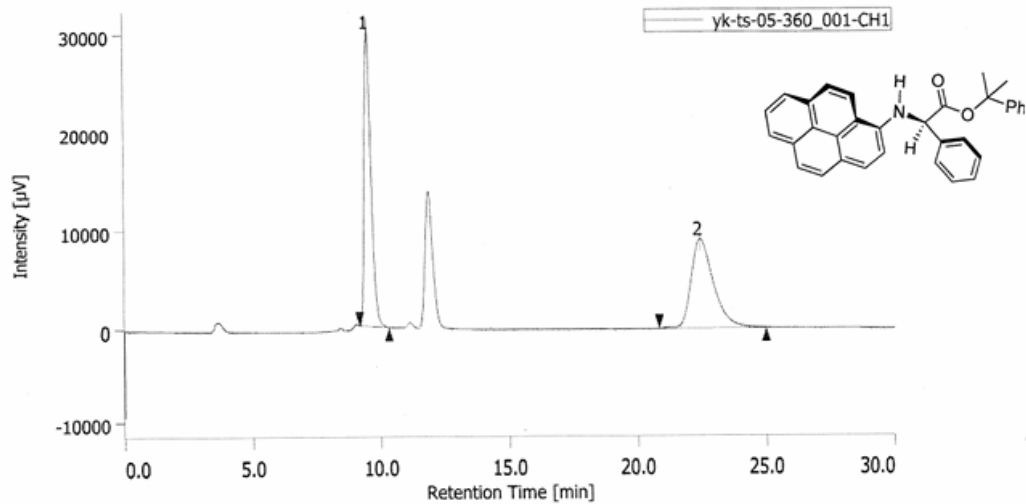


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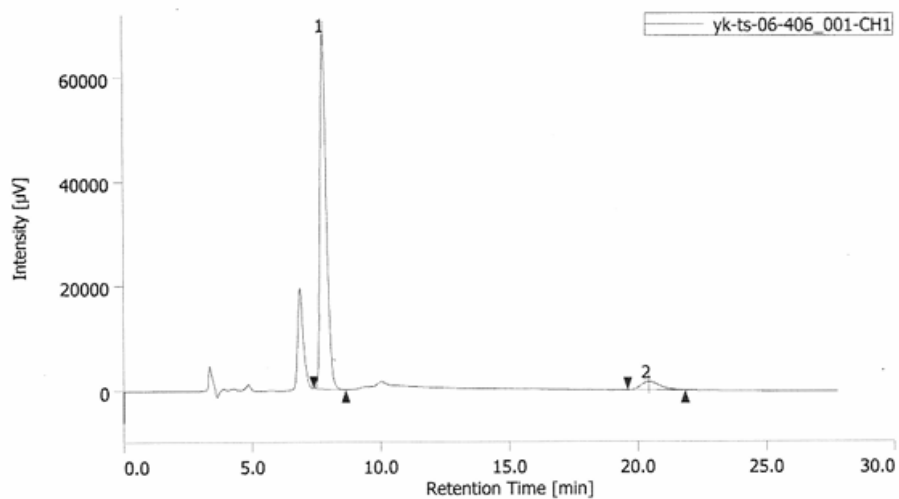
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1118 yk-ts-05-360_001 2026/06/16 6:27:28



#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	9.517	546020	50.953	30156	76.866
2	22.458	525603	49.047	9076	23.134

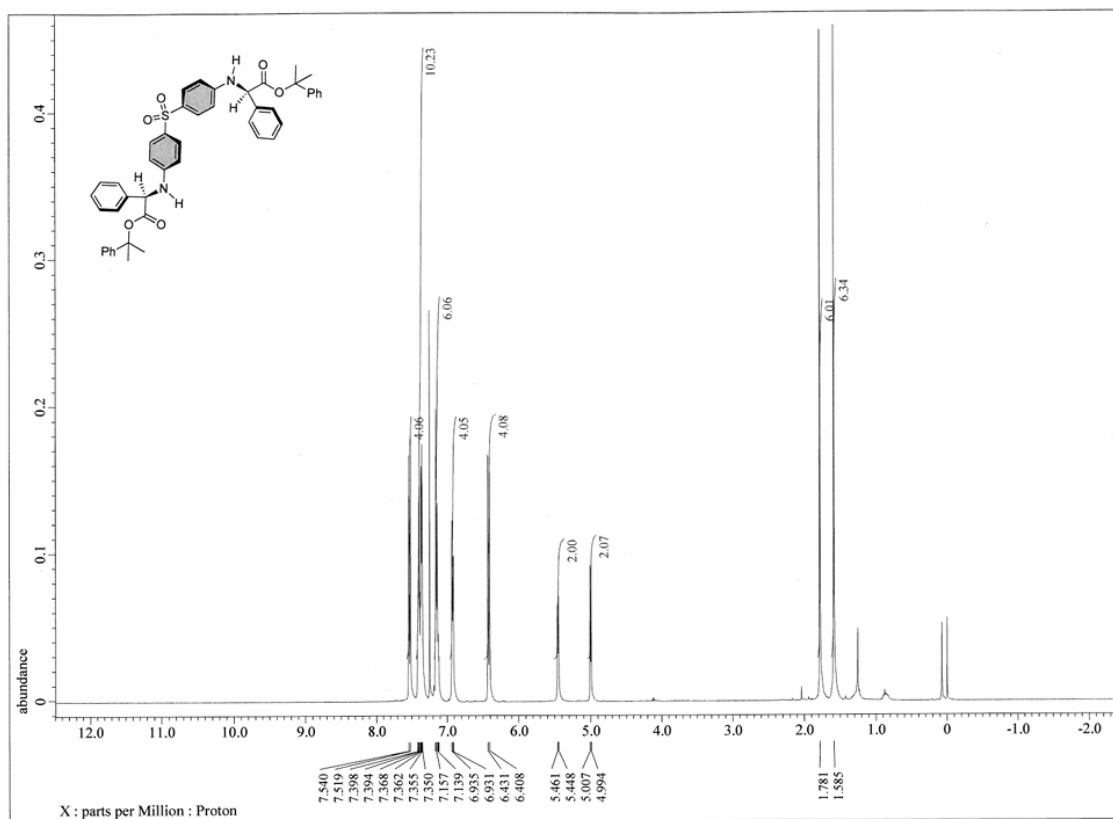
1219 yk-ts-06-406_001 2026/06/16 6:27:09



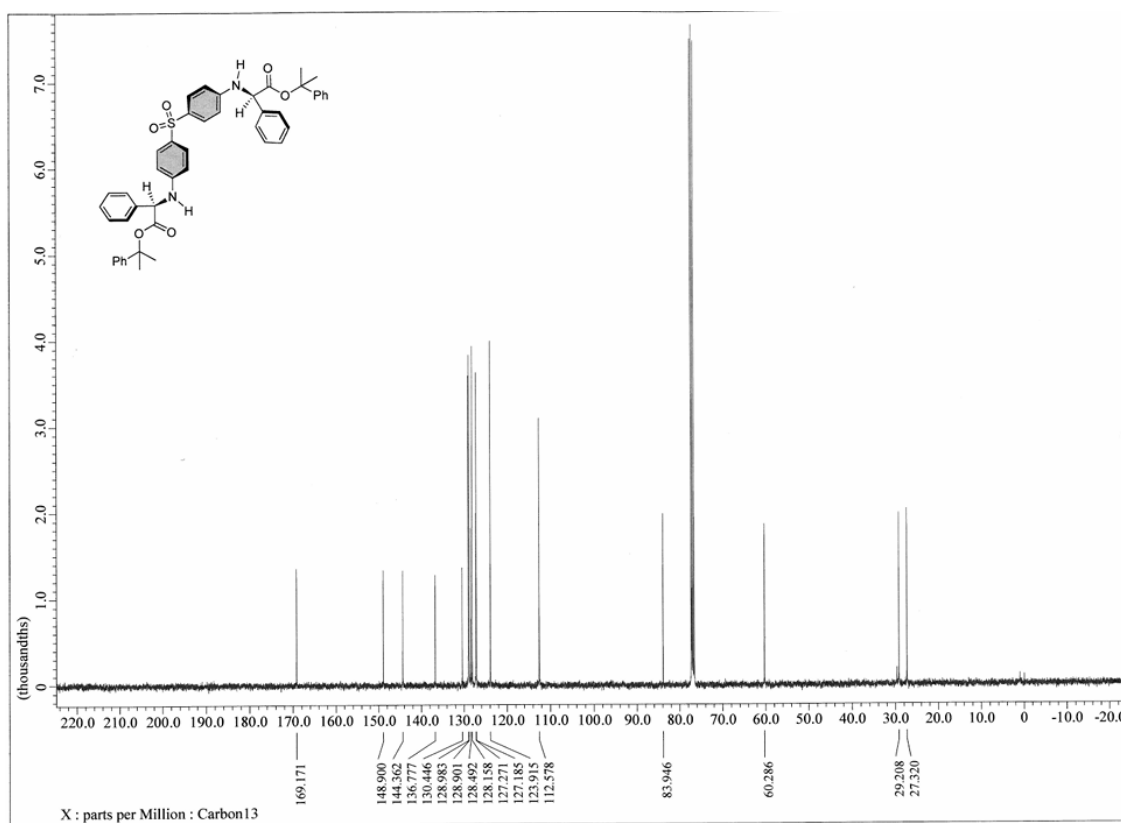
#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	7.783	1161198	93.588	67993	97.750
2	20.425	79558	6.412	1565	2.250

1

3ad

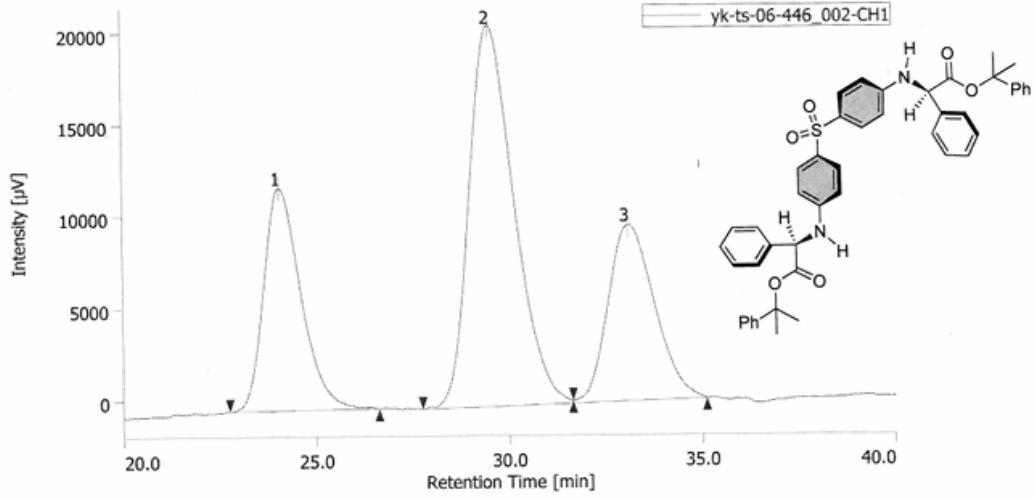


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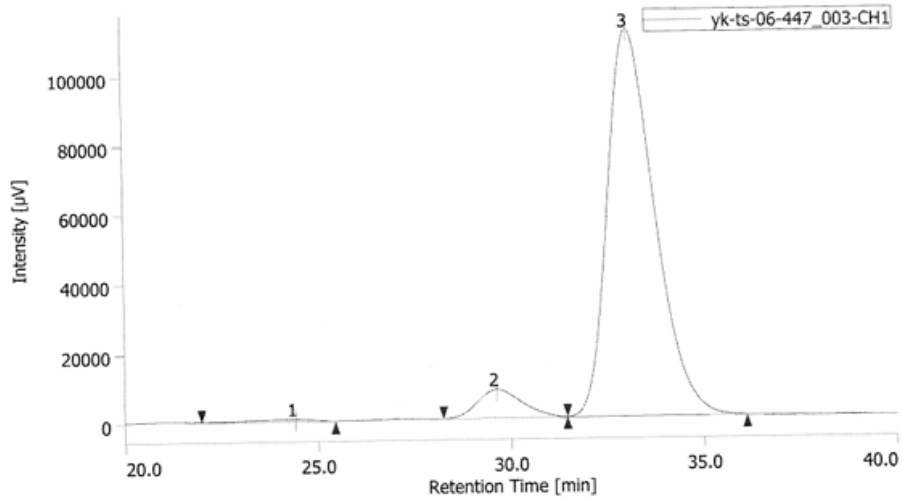
3

0206 yk-ts-06-446_002 2026/05/26 17:31:37



#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	24.058	807544	24.674	12061	28.494
2	29.525	1668981	50.995	20741	49.000
3	33.092	796328	24.331	9527	22.507

0206 yk-ts-06-447_003 2026/05/26 17:31:48



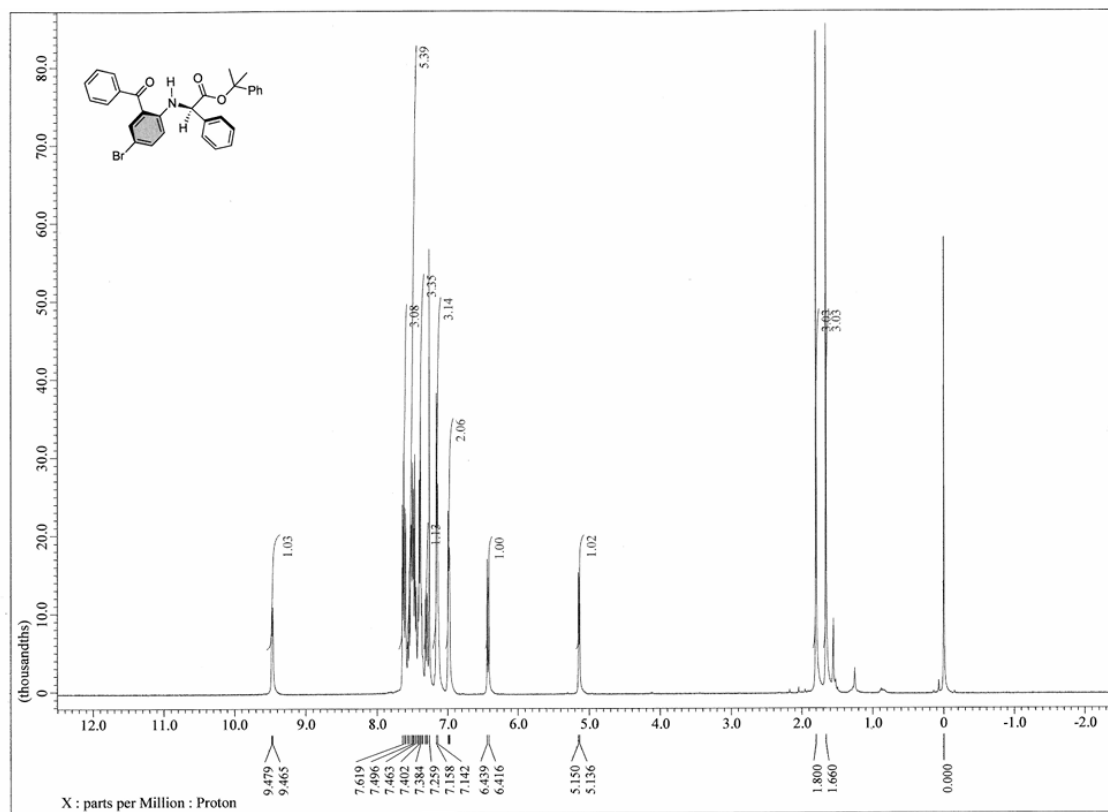
#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	24.400	72874	0.715	732	0.607
2	29.633	667413	6.550	8285	6.864
3	33.092	9449768	92.735	111679	92.529

1

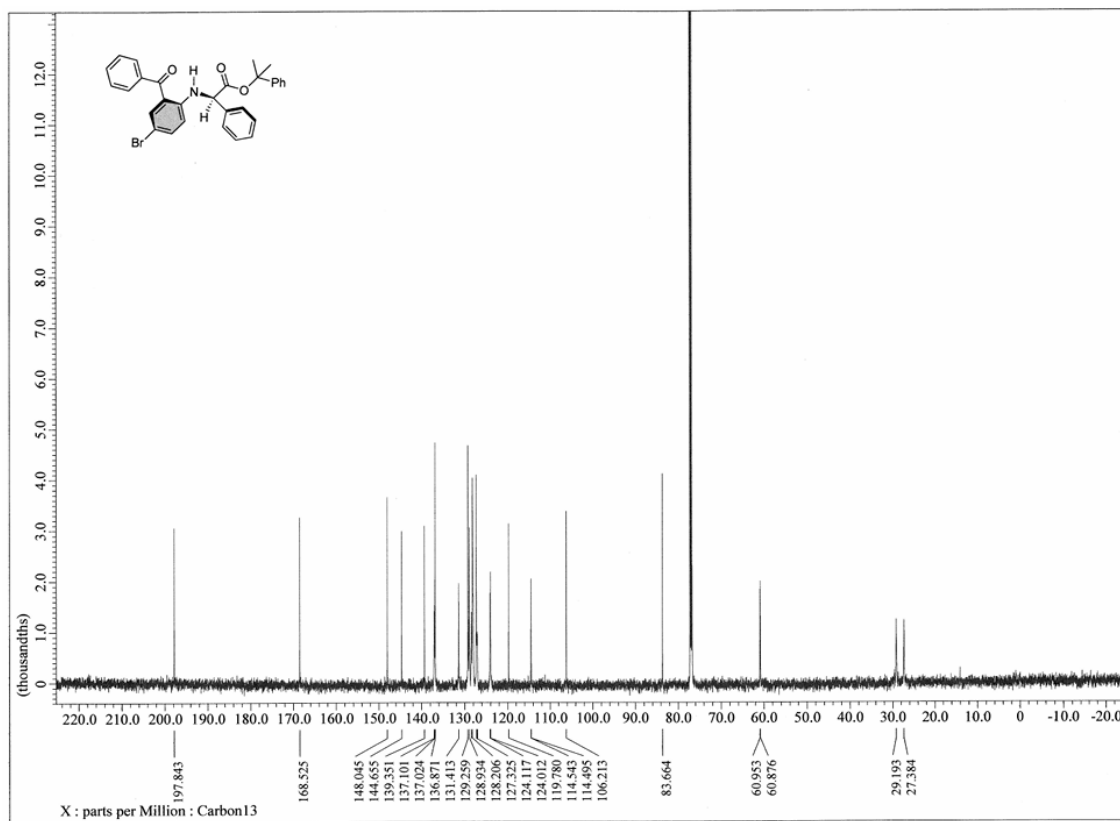
2

1

3ae

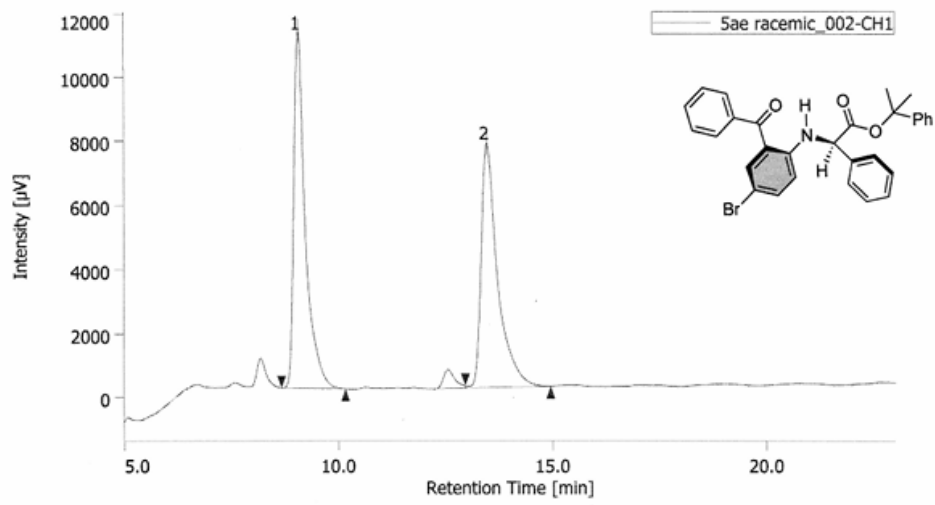


2



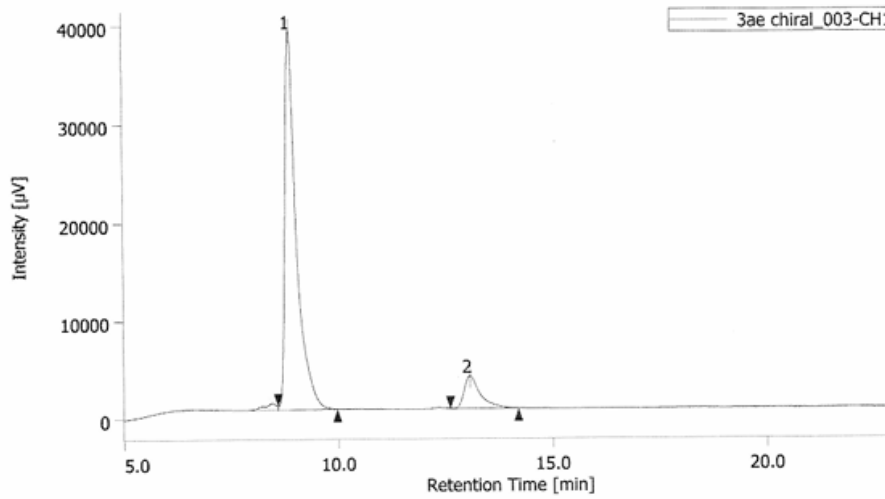
3

0616 5ae racemic_002 2026/06/16 6:55:34



#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	9.075	208178	50.610	11171	59.435
2	13.483	203162	49.390	7624	40.565

0616 3ae chiral_003 2026/06/16 4:47:43

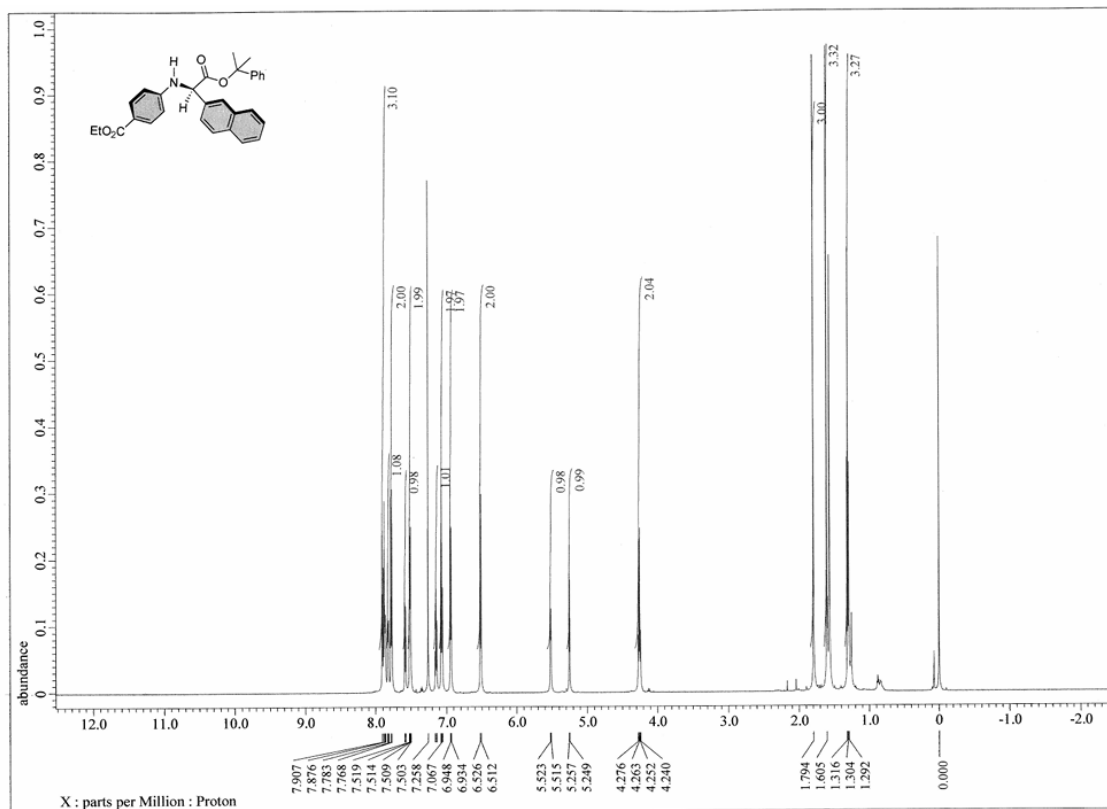


#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	8.883	714660	89.404	38635	92.100
2	13.067	84697	10.596	3314	7.900

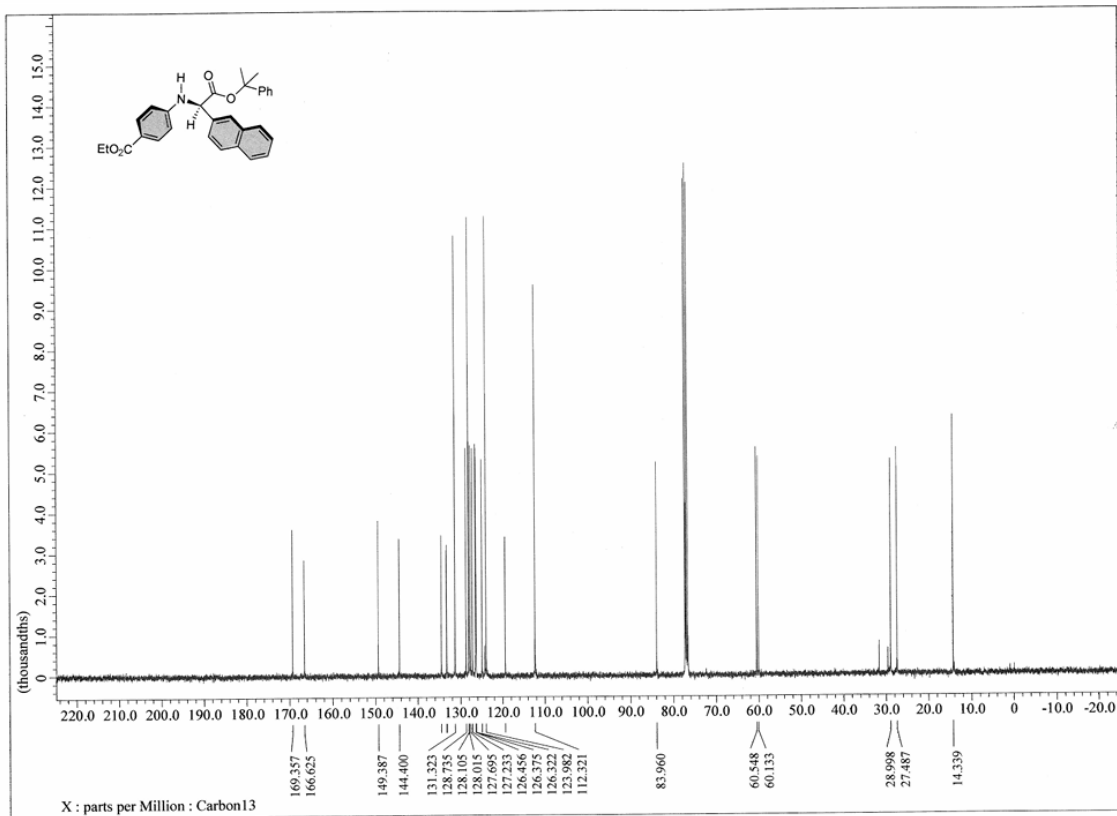
1
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3af



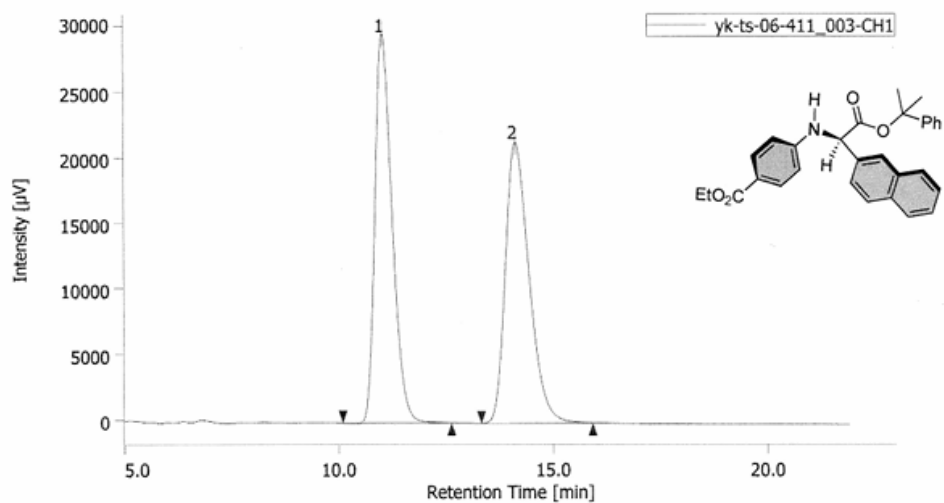
2



3

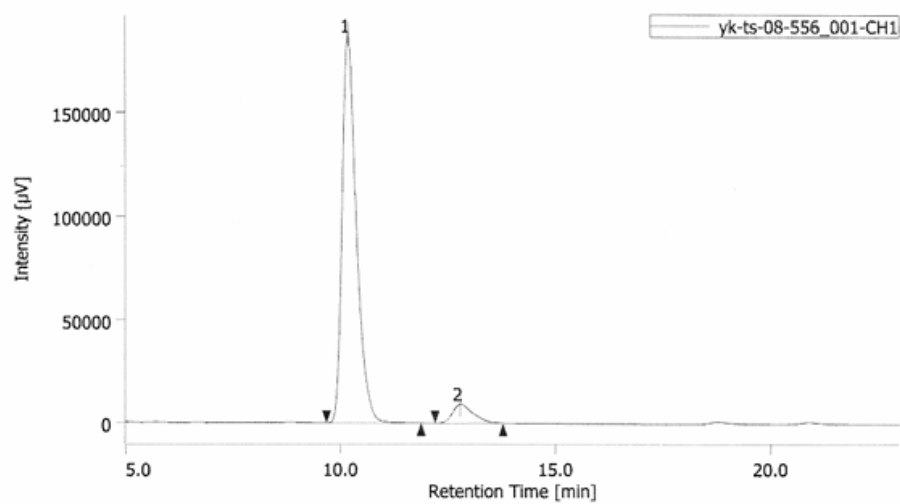
4

1219 yk-ts-06-411_003 2026/06/03 19:03:13



#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	11.042	825909	50.085	29620	58.052
2	14.133	823091	49.915	21404	41.948

0603 yk-ts-08-556_001 2026/06/16 7:16:43

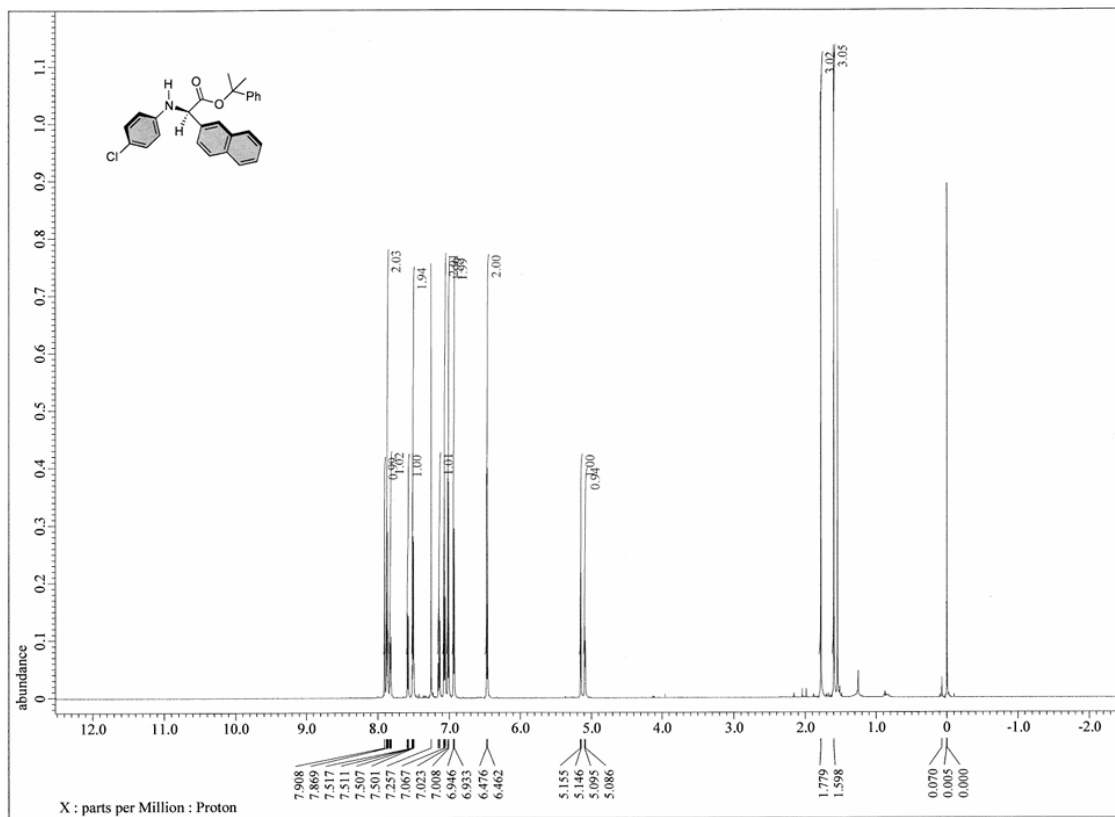


#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	10.183	4330639	93.500	188438	95.400
2	12.792	301046	6.500	9085	4.600

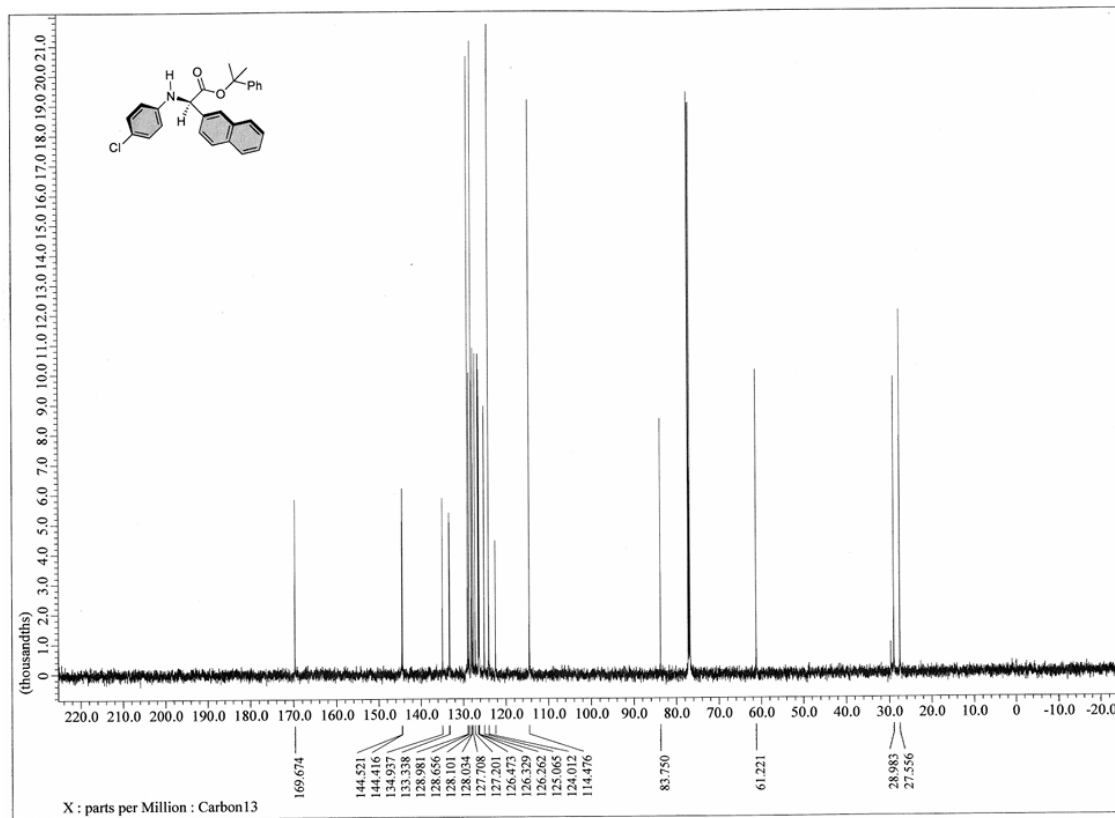
1
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1

3ag

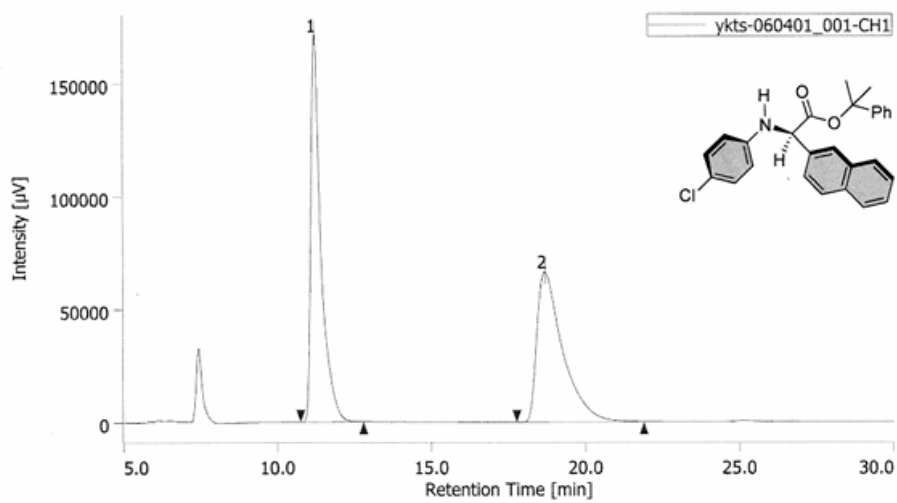


2



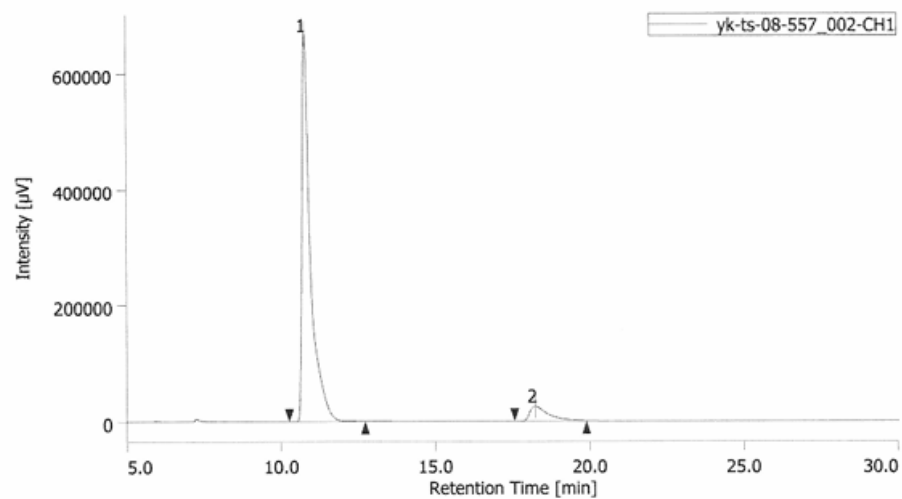
3

1218 ykts-060401_001 2026/06/03 19:11:21



#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	11.233	3887927	50.217	172252	72.224
2	18.692	3854292	49.783	66245	27.776

0603 yk-ts-08-557_002 2026/06/04 1:45:08

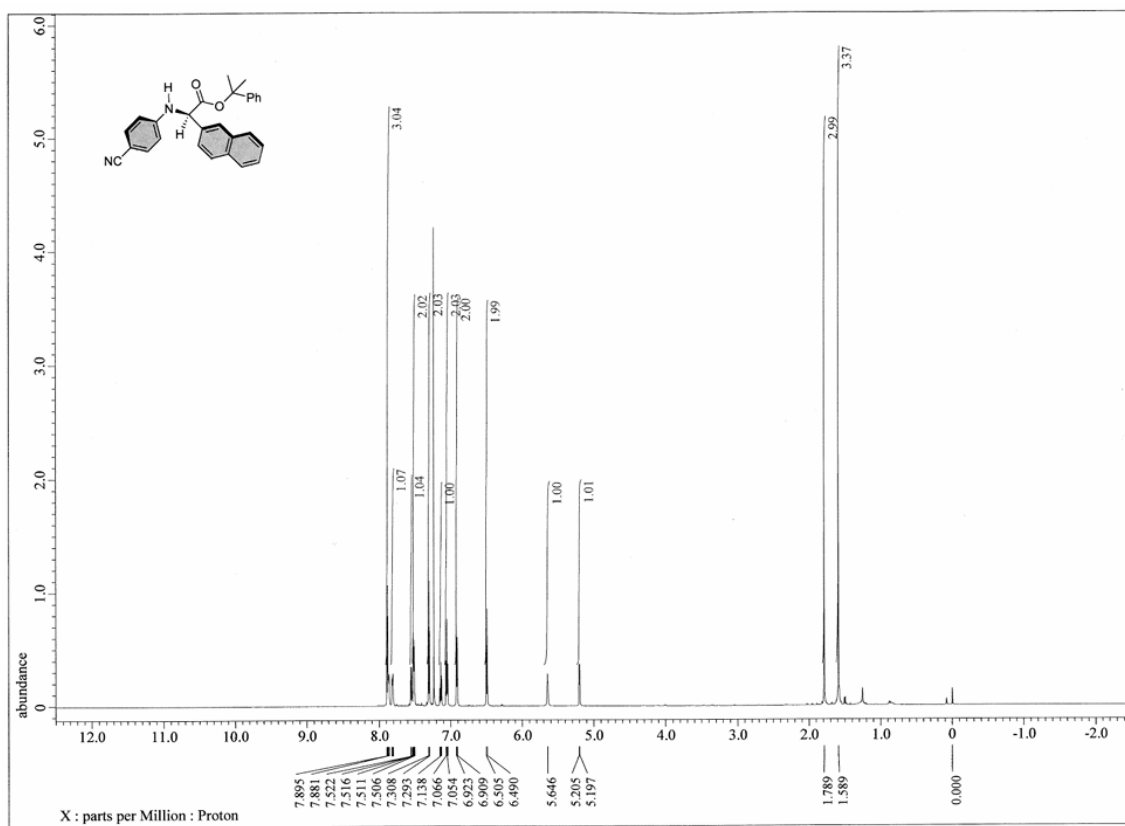


#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	10.783	12829912	92.693	669146	96.422
2	18.233	1011449	7.307	24828	3.578

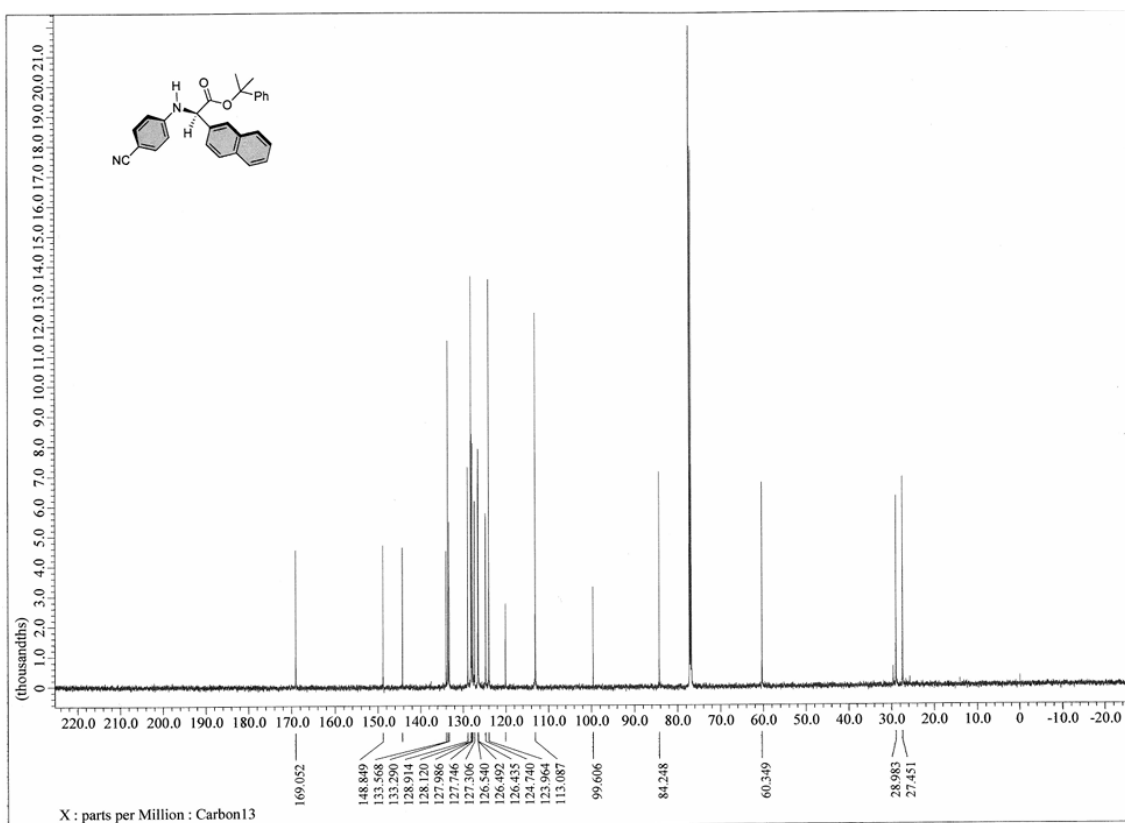
- 1
- 2
- 3

1

3ah

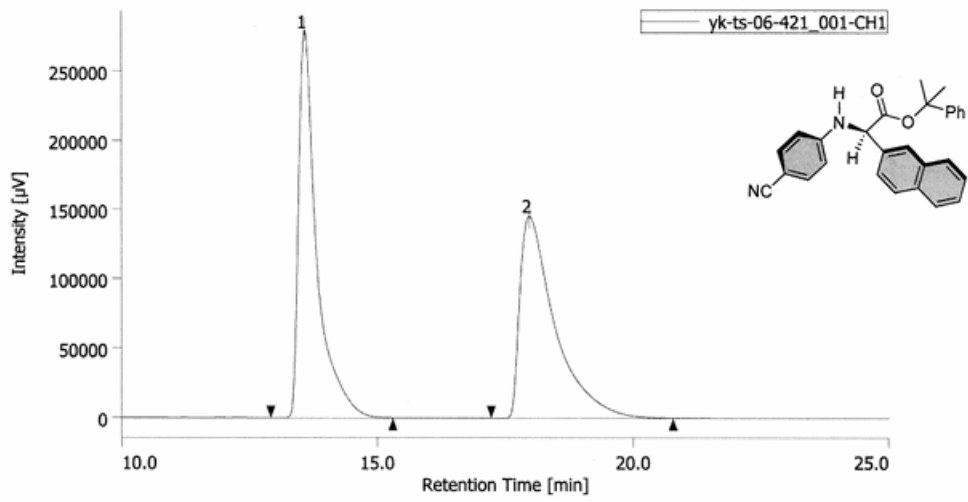


2



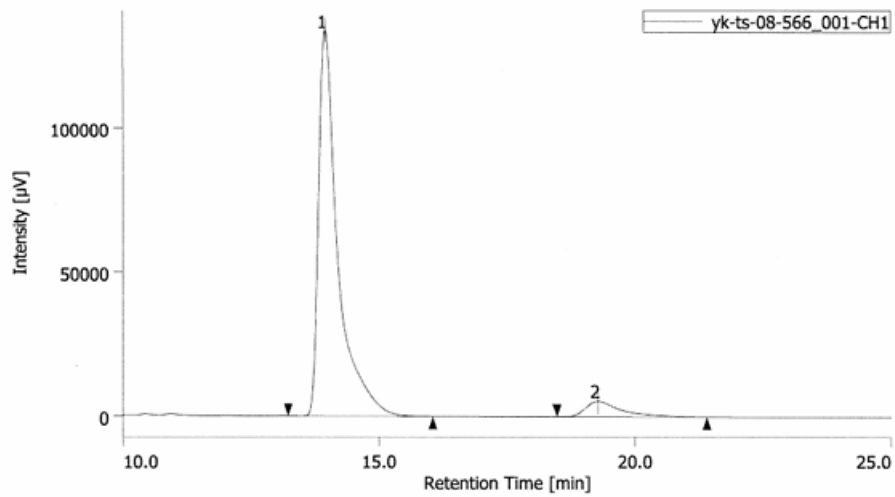
3

0115 yk-ts-06-421_001 2026/06/08 12:36:01



#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	13.583	6893121	49.992	279655	65.850
2	17.983	6895237	50.008	145032	34.150

0607 yk-ts-08-566_001 2026/06/08 12:36:08

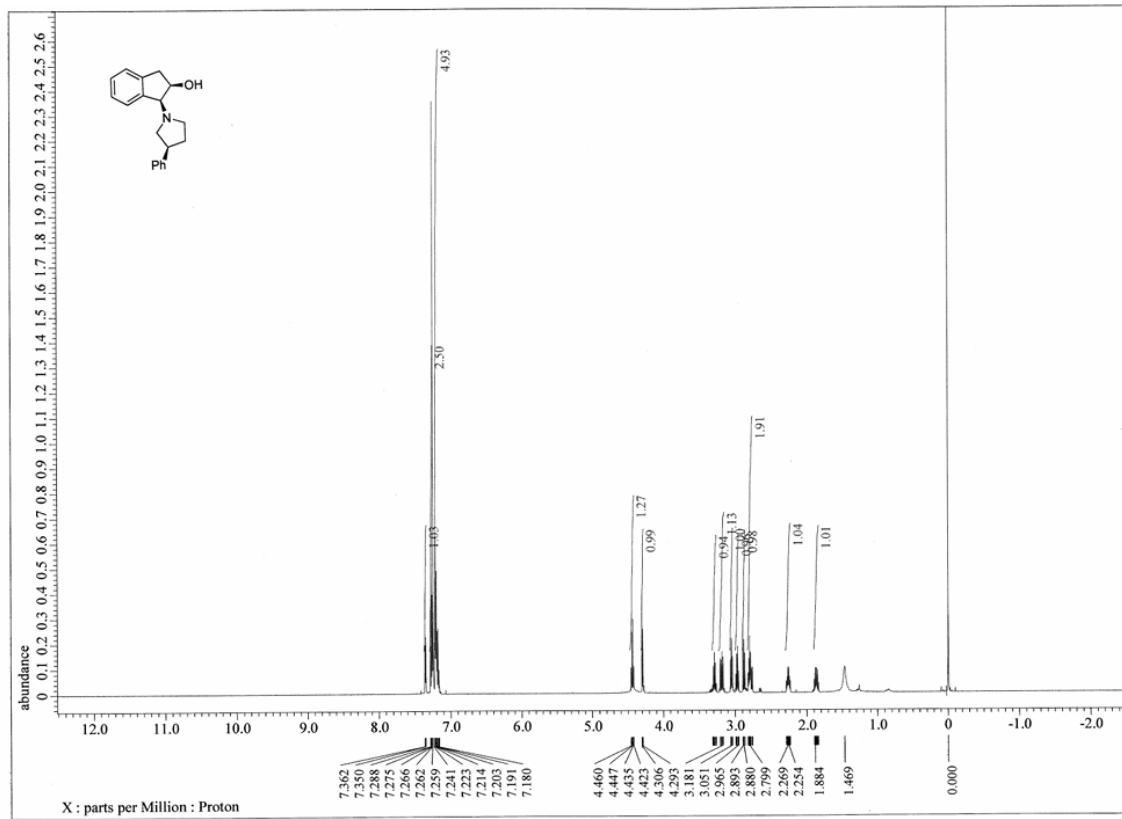


#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	13.950	3506807	93.075	134397	96.211
2	19.267	260906	6.925	5293	3.789

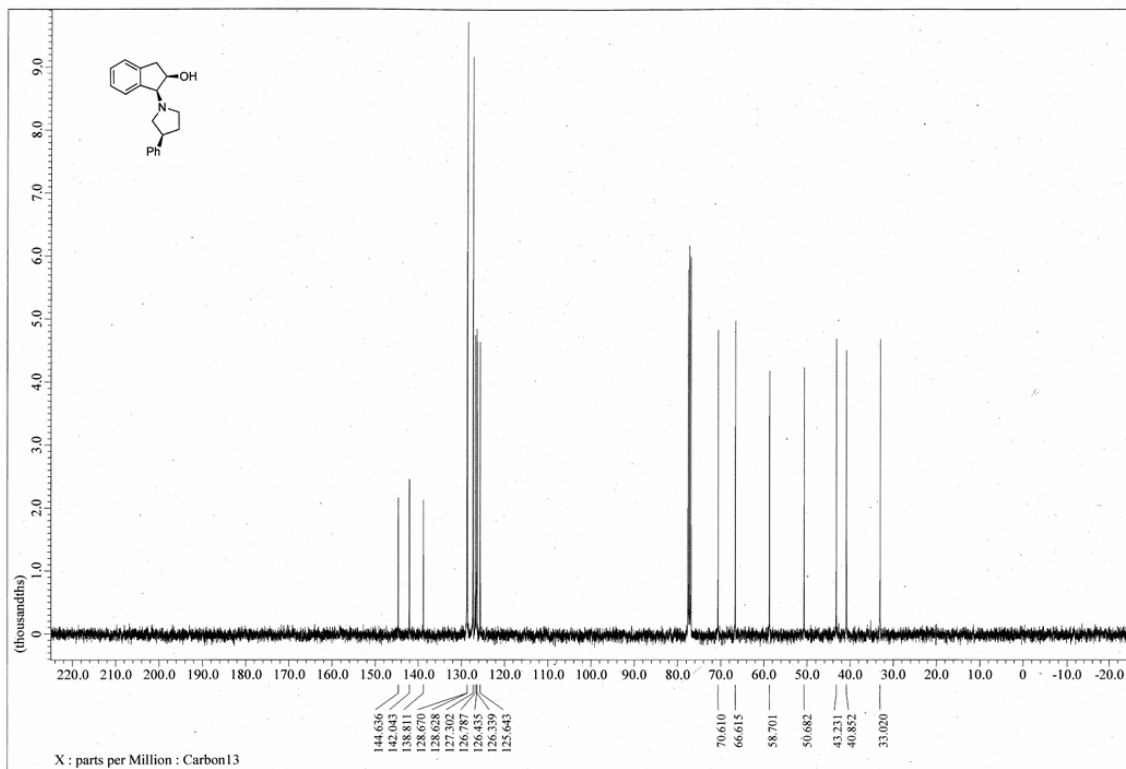
1
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7



2

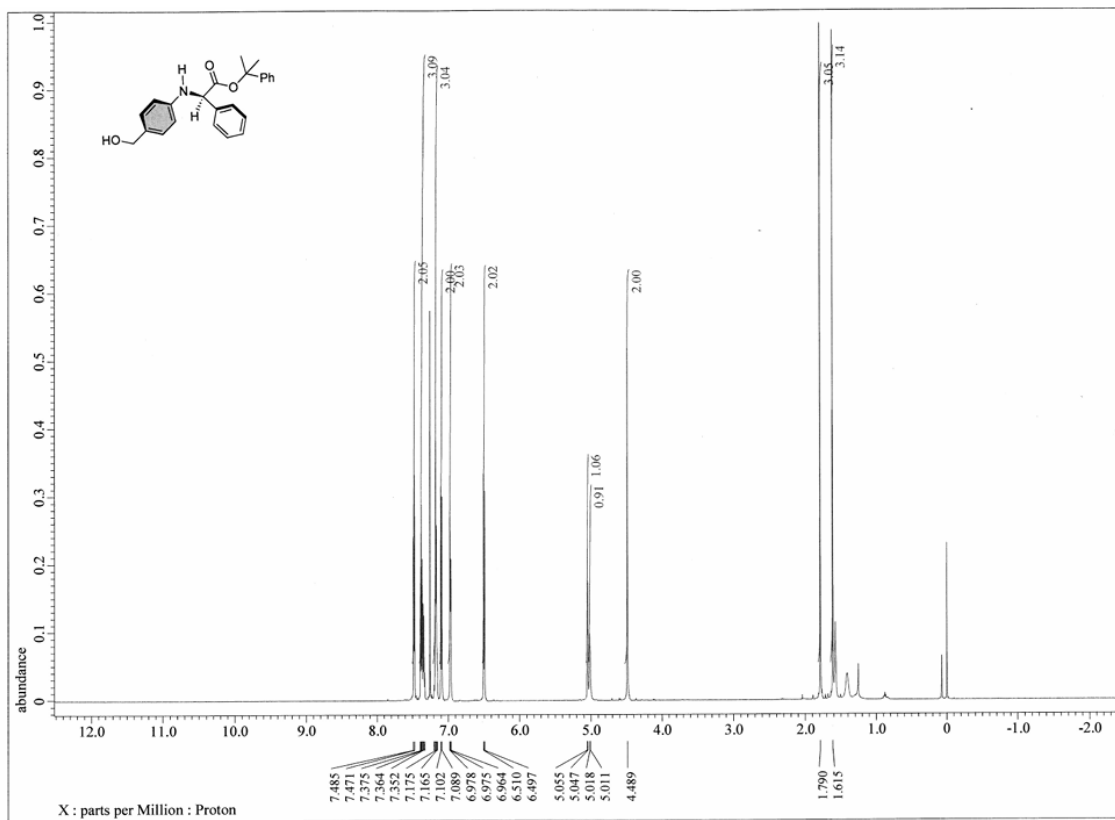


3

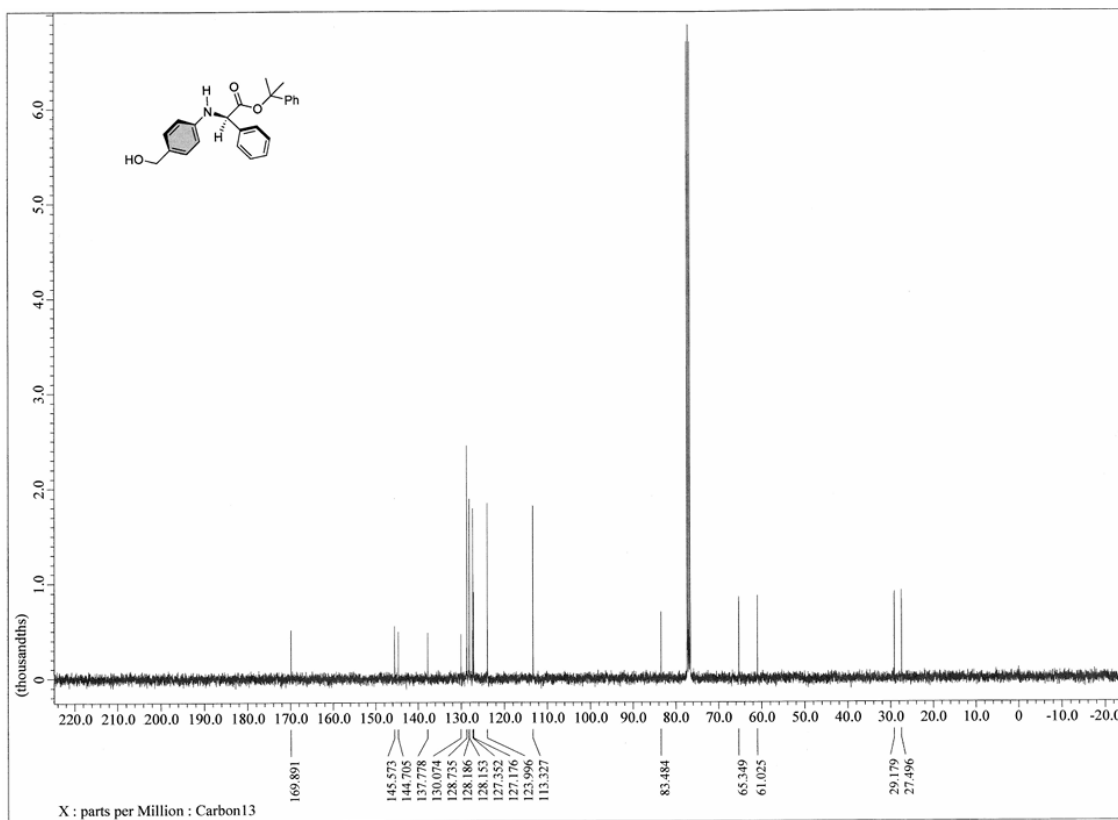
4

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9a

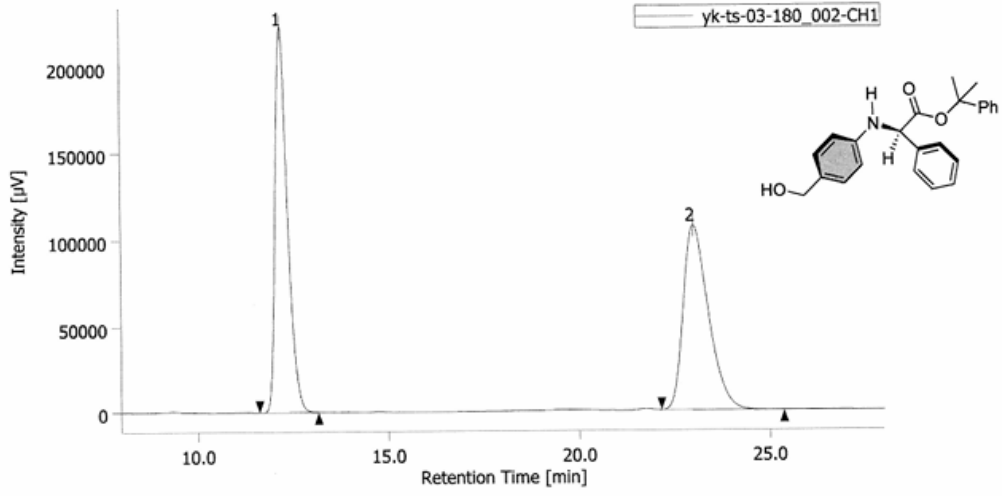


2



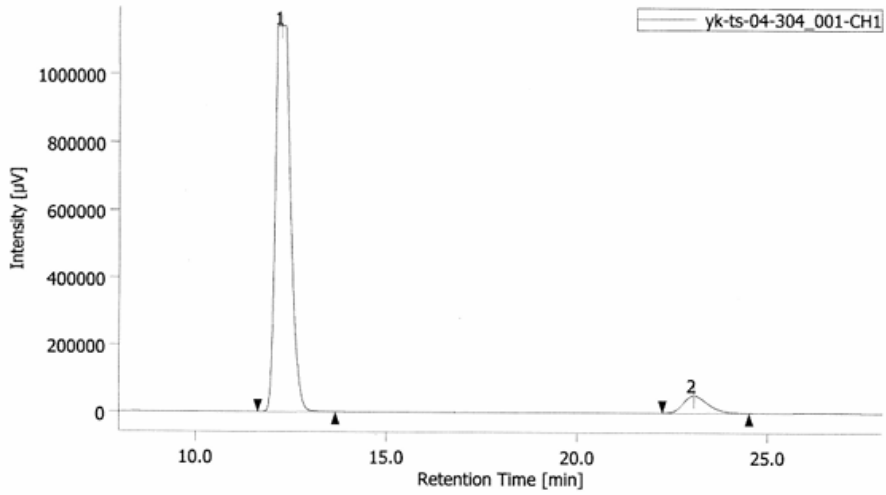
3

0528 yk-ts-03-180_002 2026/05/28 18:53:27



#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	12.208	5019375	50.407	223612	67.575
2	23.017	4938260	49.593	107296	32.425

1008 yk-ts-04-304_001 2026/05/28 18:53:45



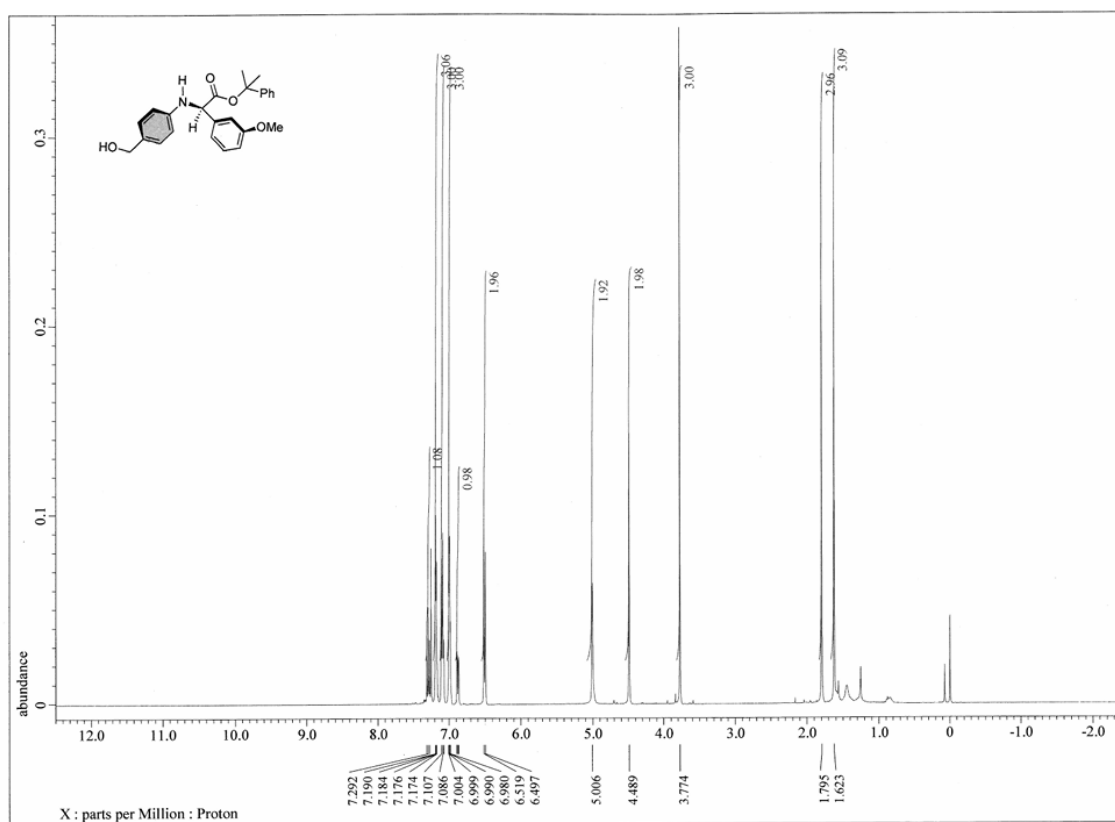
#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	12.267	31979450	93.256	1140739	95.717
2	23.058	2312829	6.744	51045	4.283

1

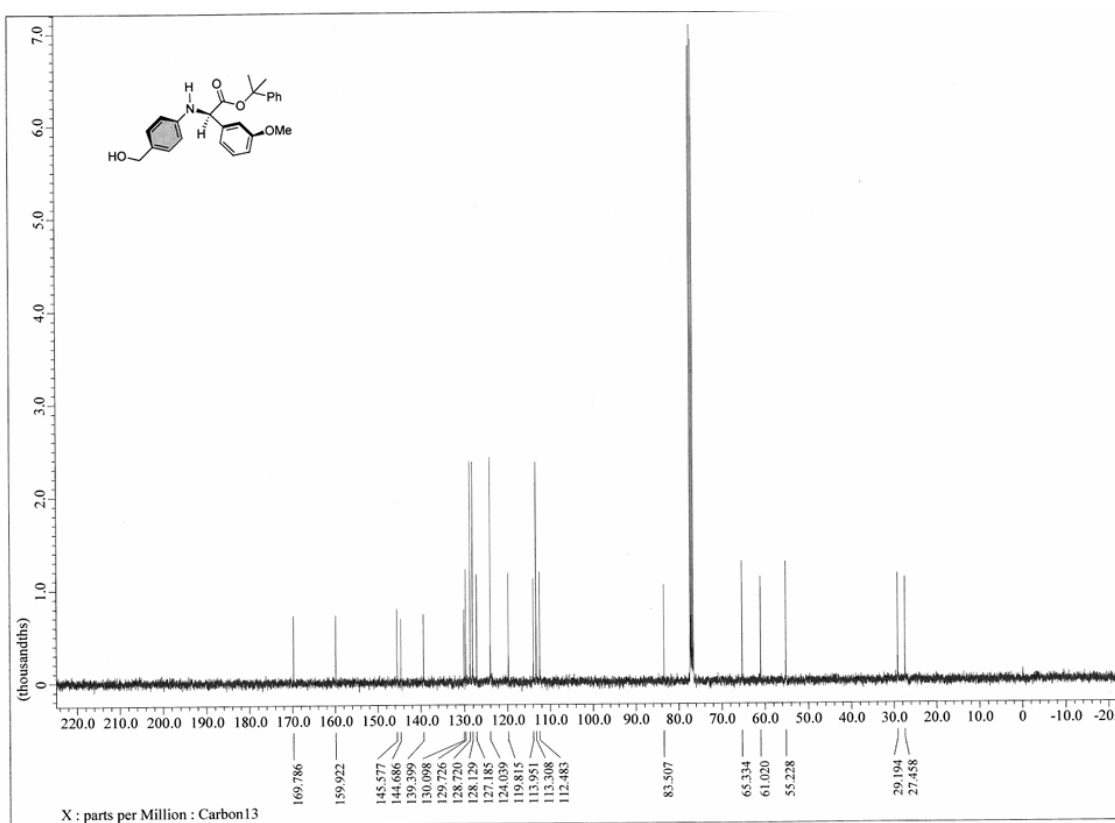
2

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9b



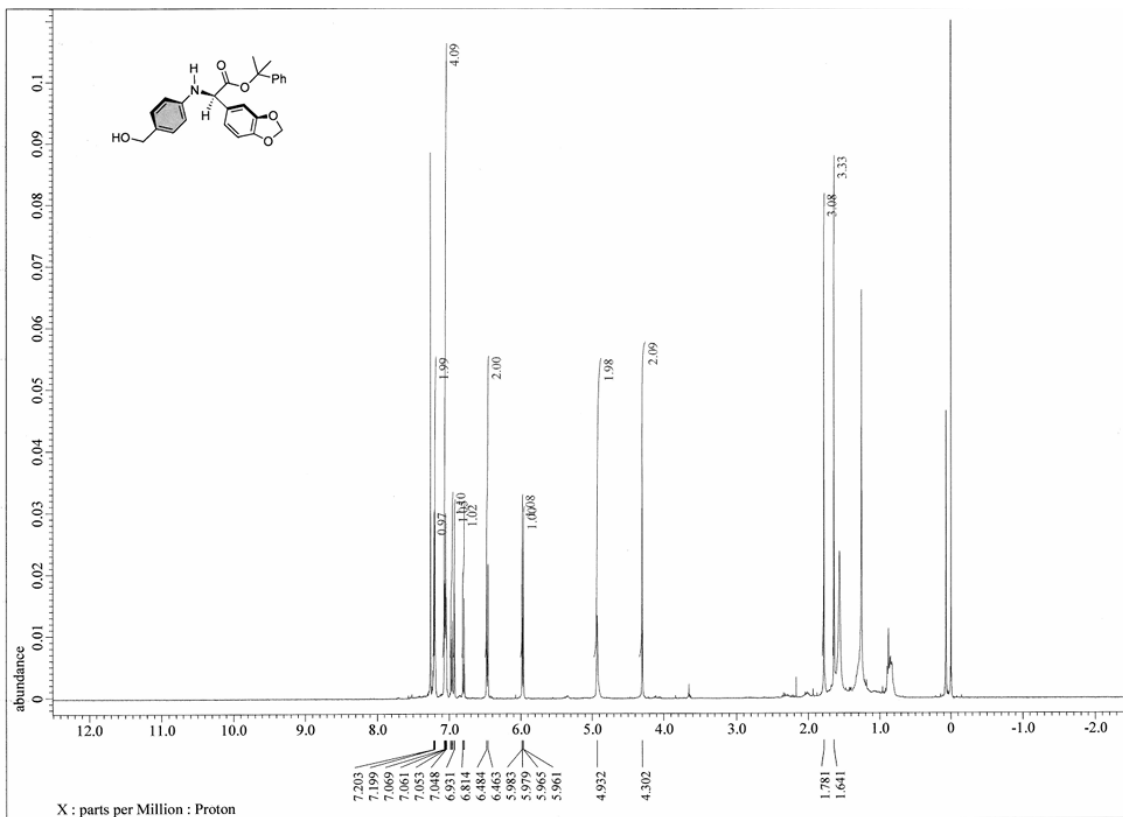
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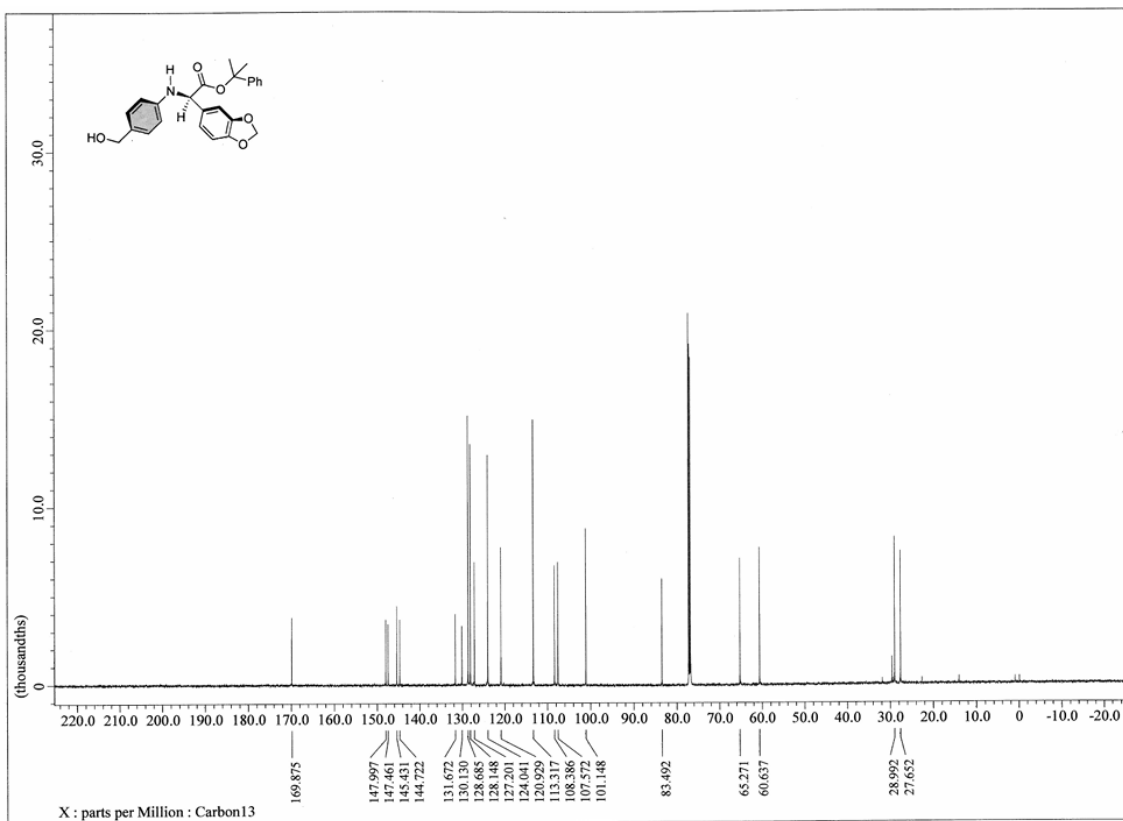
3

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9c

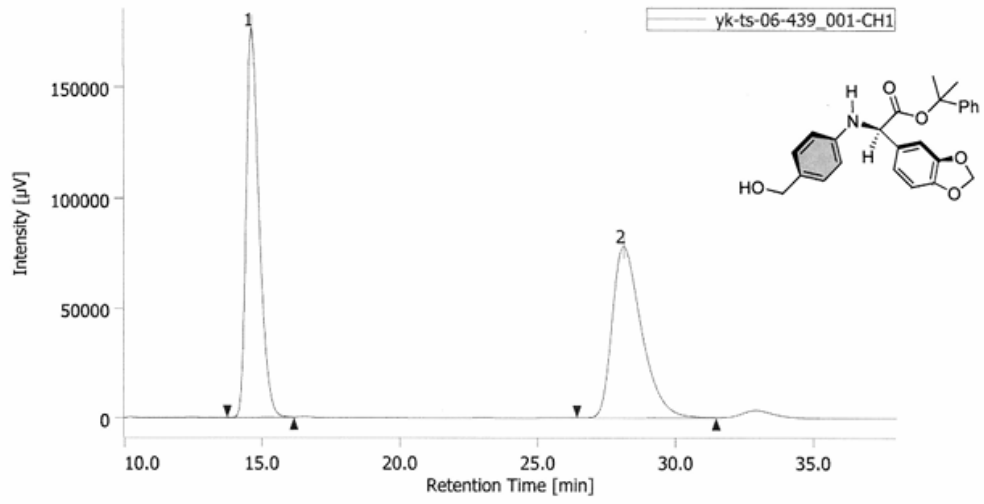


2



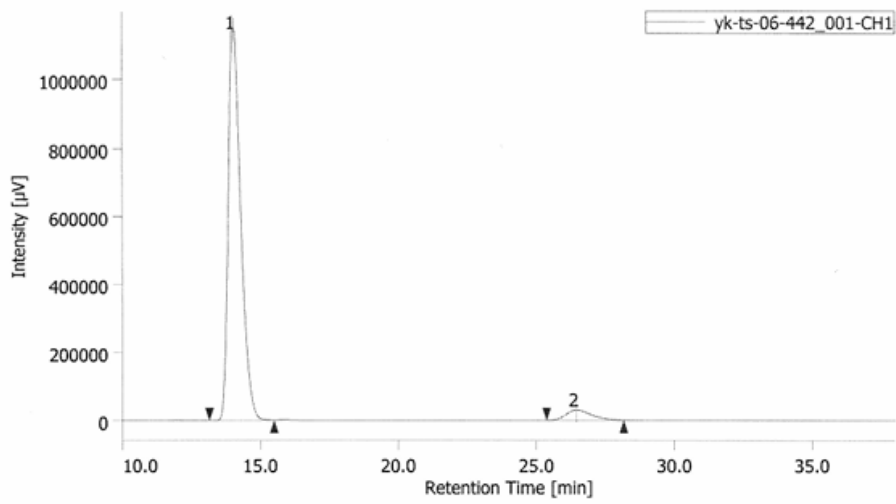
3

0123 yk-ts-06-439_001 2026/05/23 1:50:09



#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	14.650	5819183	50.174	176553	69.345
2	28.125	5778881	49.826	78049	30.655

0201 yk-ts-06-442_001 2026/05/23 1:50:44



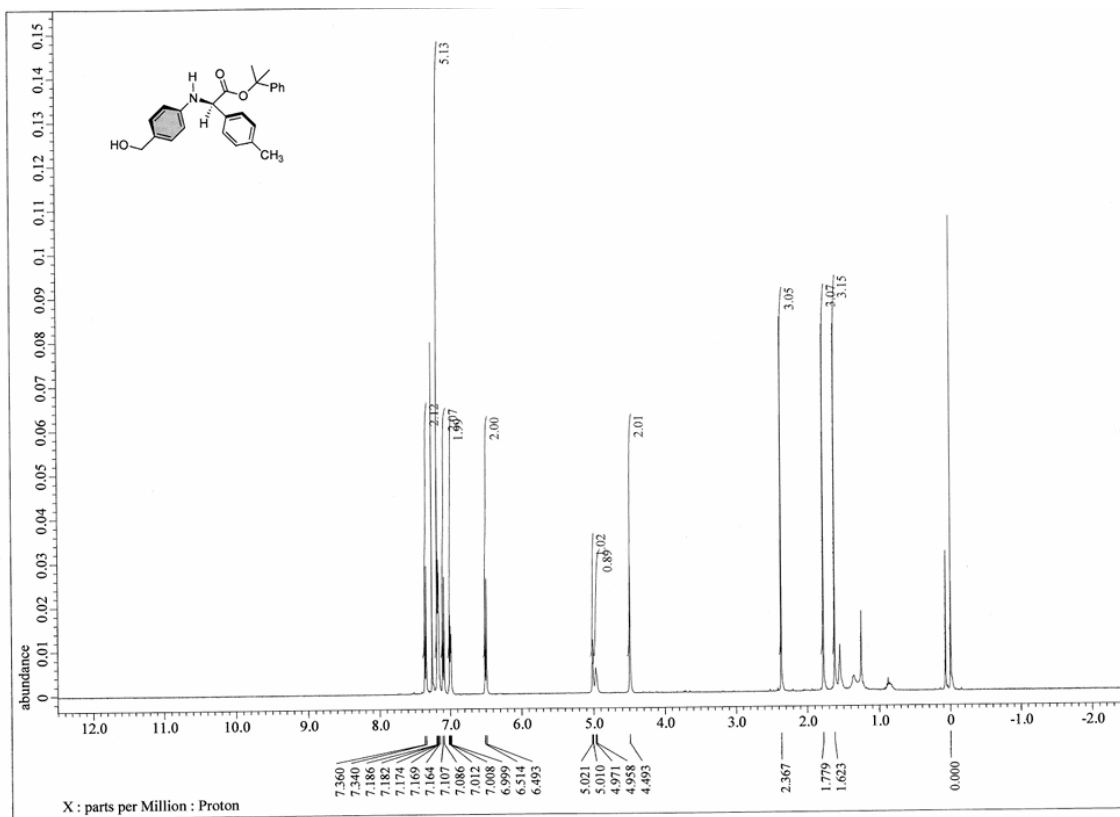
#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	14.033	36429982	95.033	1141565	97.487
2	26.450	1904016	4.967	29427	2.513

1

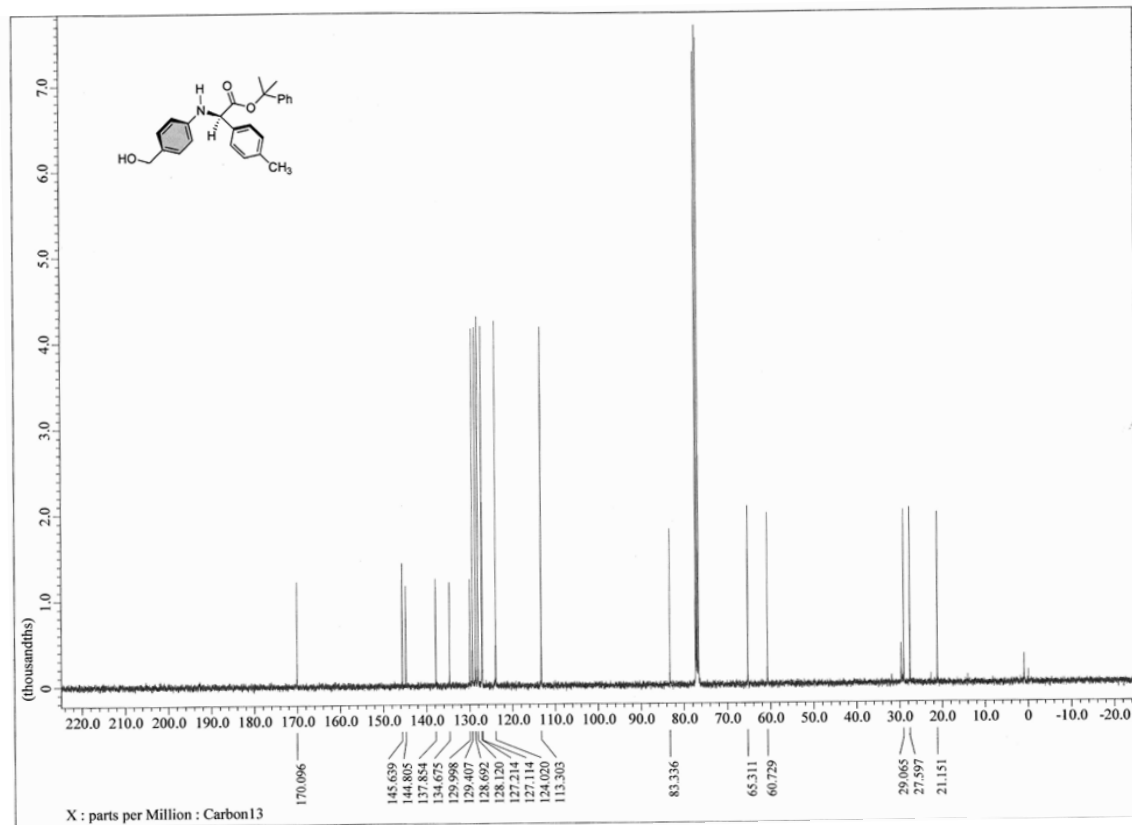
2

1

9d

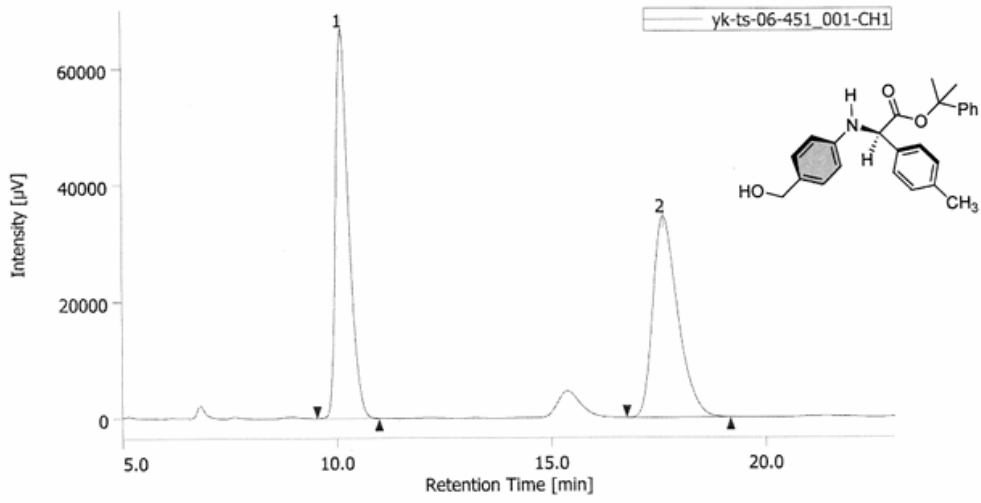


2



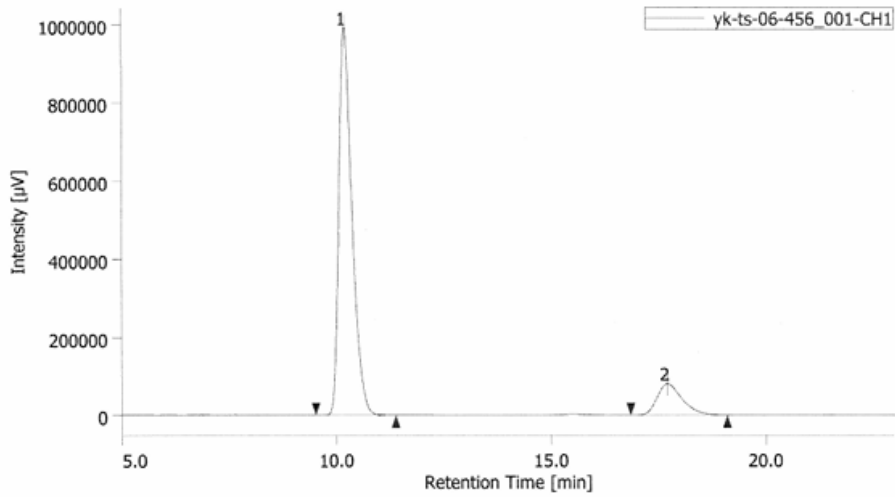
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0206 yk-ts-06-451_001 2026/05/26 17:44:49



#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	10.125	1416688	50.217	67027	66.018
2	17.617	1404423	49.783	34501	33.982

0209 yk-ts-06-456_001 2026/05/26 17:45:02

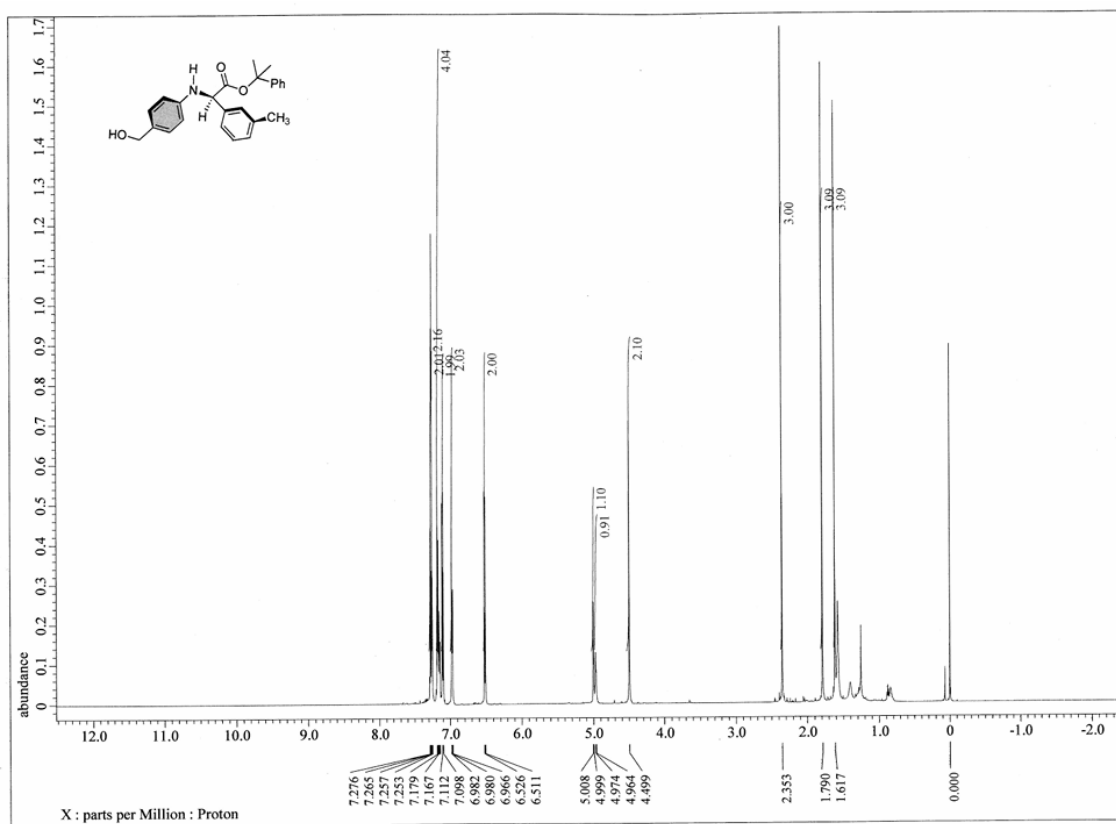


#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	10.192	21212244	86.677	995072	92.520
2	17.708	3260449	13.323	80443	7.480

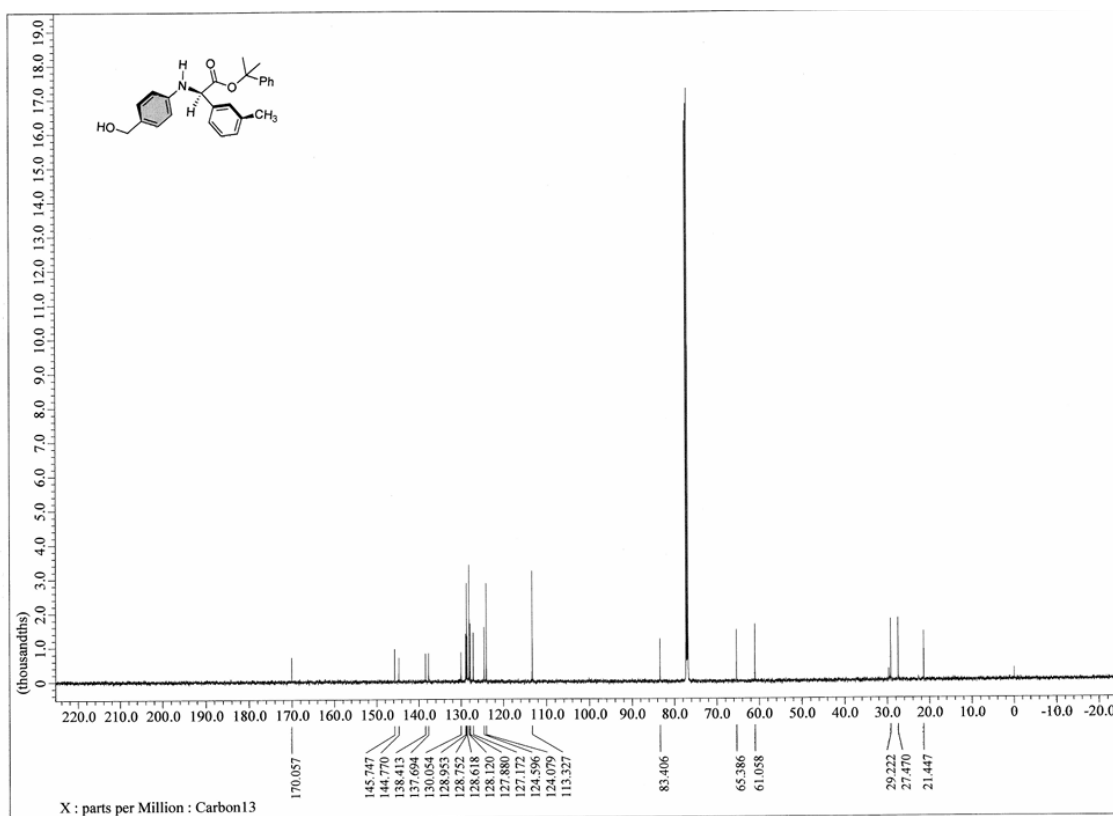
1
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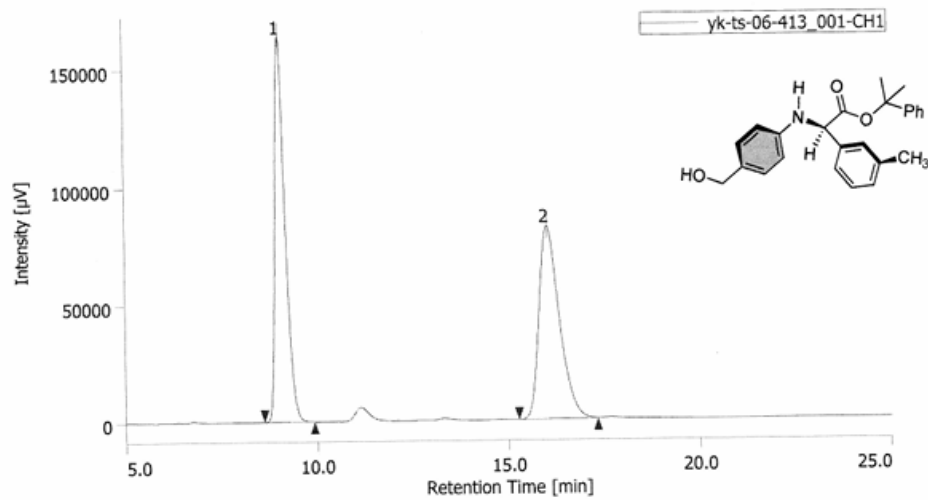


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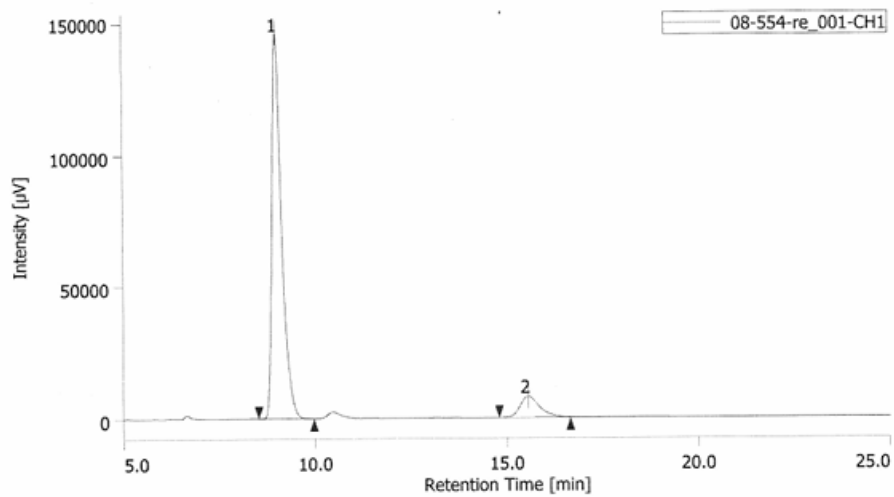
3

0107 yk-ts-06-413_001 2026/06/13 13:32:14



#	tR [min]	Area [$\mu\text{V}\cdot\text{sec}$]	Area%	Height [μV] [μV]	Height%
1	9.058	3049977	50.258	164121	66.619
2	16.042	3018617	49.742	82238	33.381

0613 08-554-re_001 2026/06/13 13:32:21

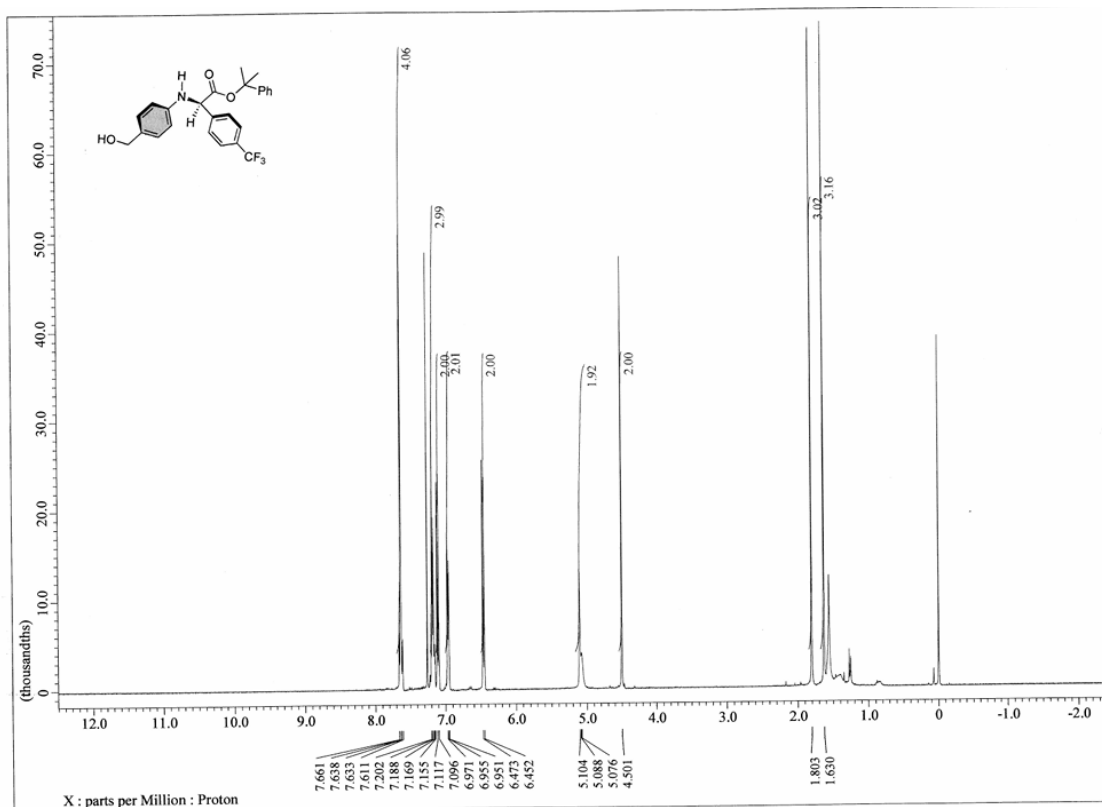


#	tR [min]	Area [$\mu\text{V}\cdot\text{sec}$]	Area%	Height [μV] [μV]	Height%
1	9.008	2557548	90.022	146463	94.820
2	15.558	283488	9.978	8001	5.180

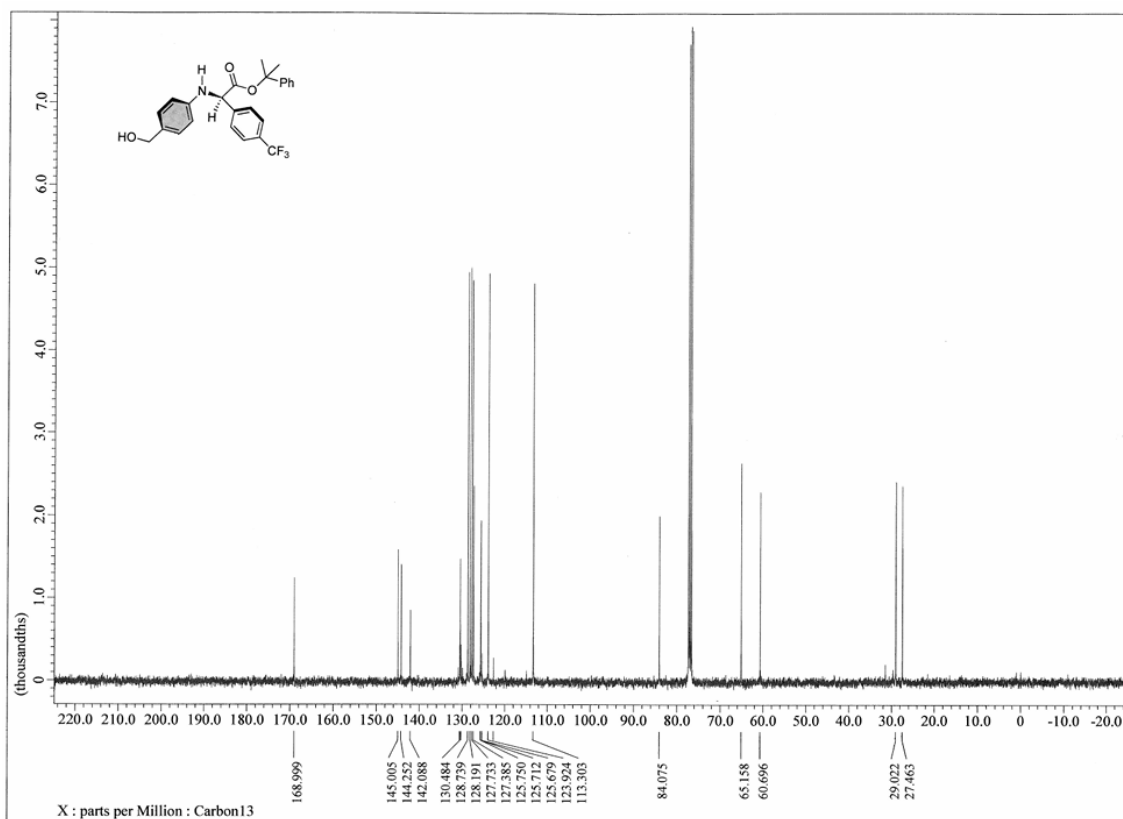
- 1
- 2
- 3

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9f

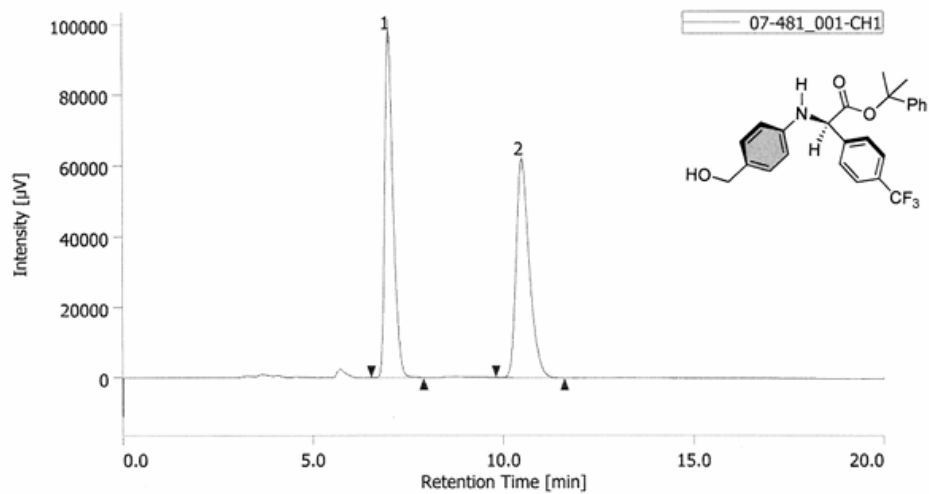


2



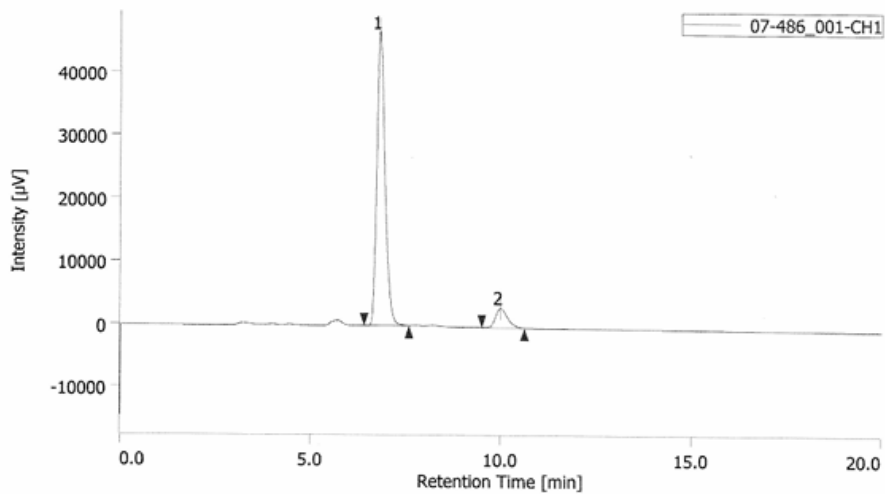
3

0227 07-481_001 2026/06/16 12:56:28



#	tR [min]	Area [$\mu\text{V}\cdot\text{sec}$]	Area%	Height [μV] [μV]	Height%
1	6.992	1498794	50.104	98258	61.331
2	10.492	1492545	49.896	61951	38.669

0303 07-486_001 2026/06/16 12:56:20

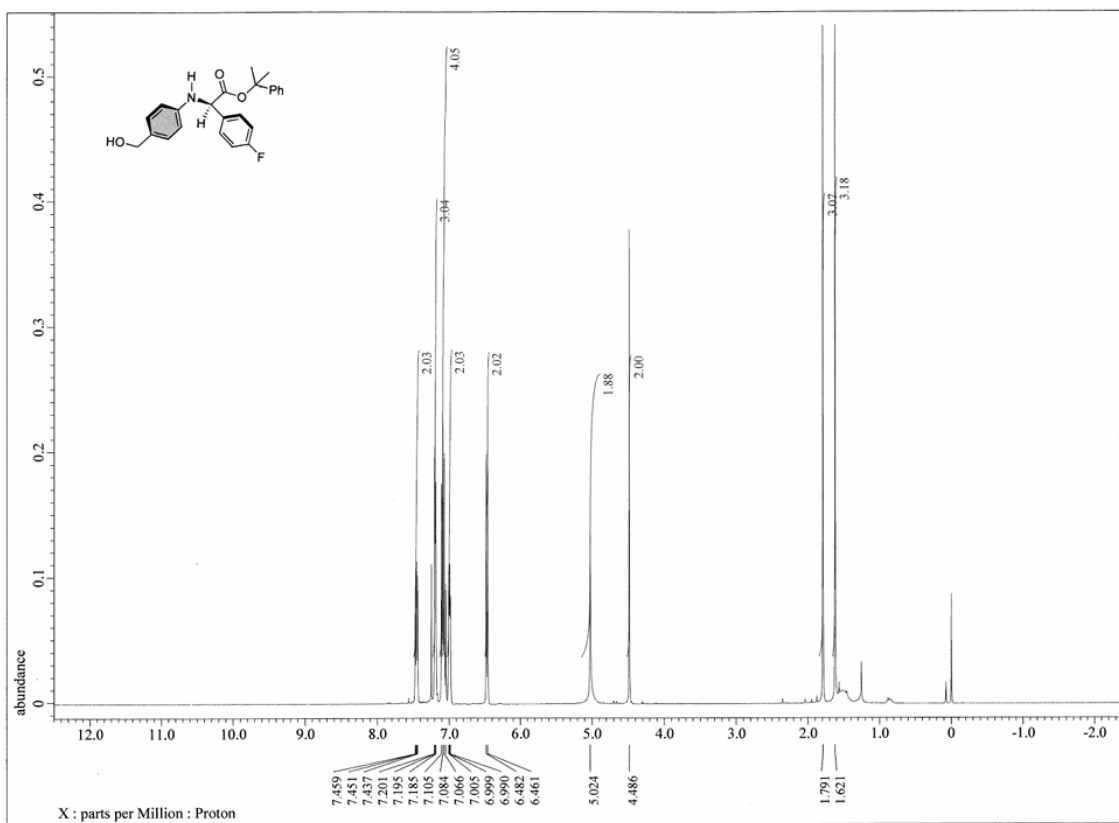


#	tR [min]	Area [$\mu\text{V}\cdot\text{sec}$]	Area%	Height [μV] [μV]	Height%
1	6.817	697810	91.097	46922	93.781
2	10.000	68194	8.903	3112	6.219

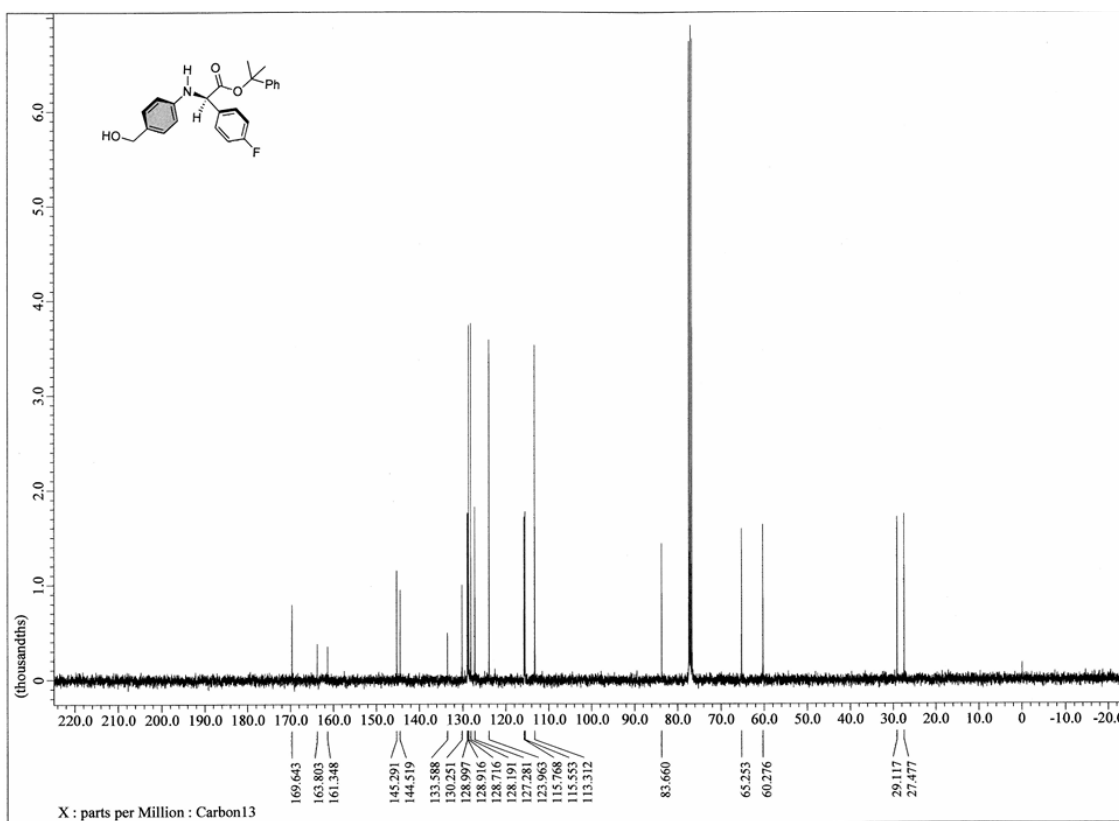
- 1
- 2
- 3

1

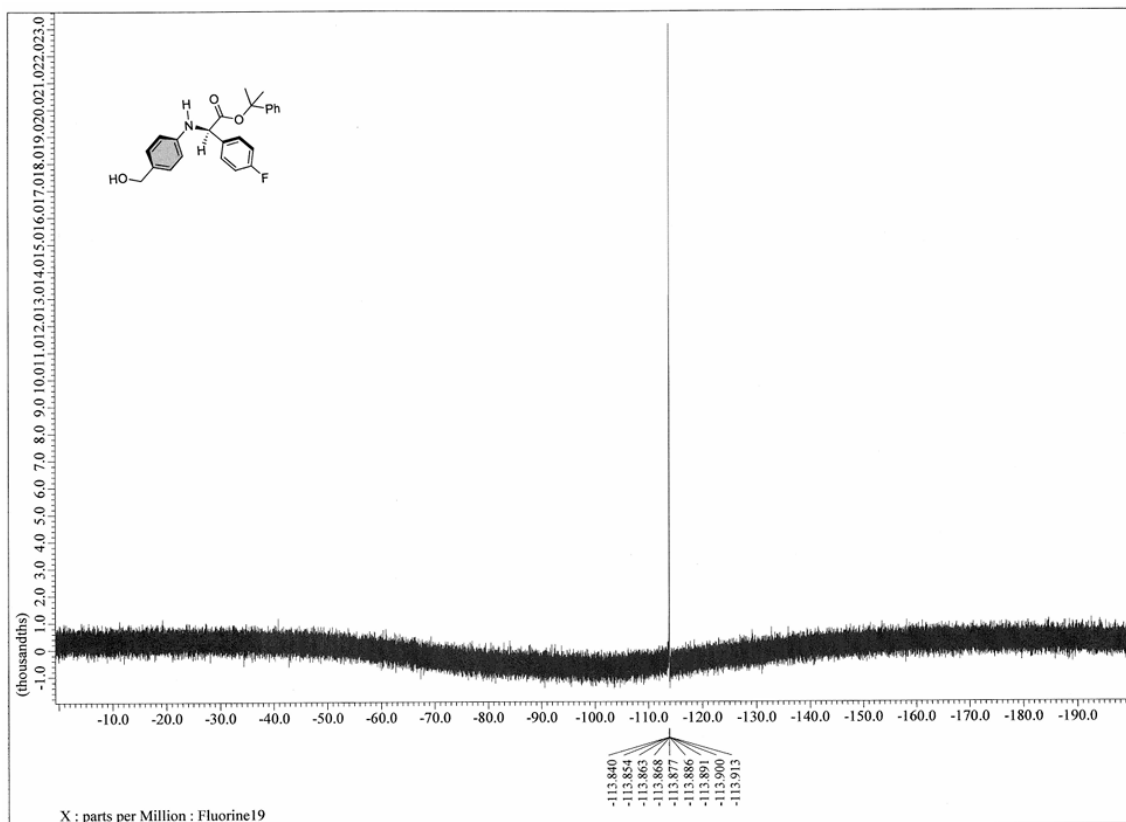
9g



2

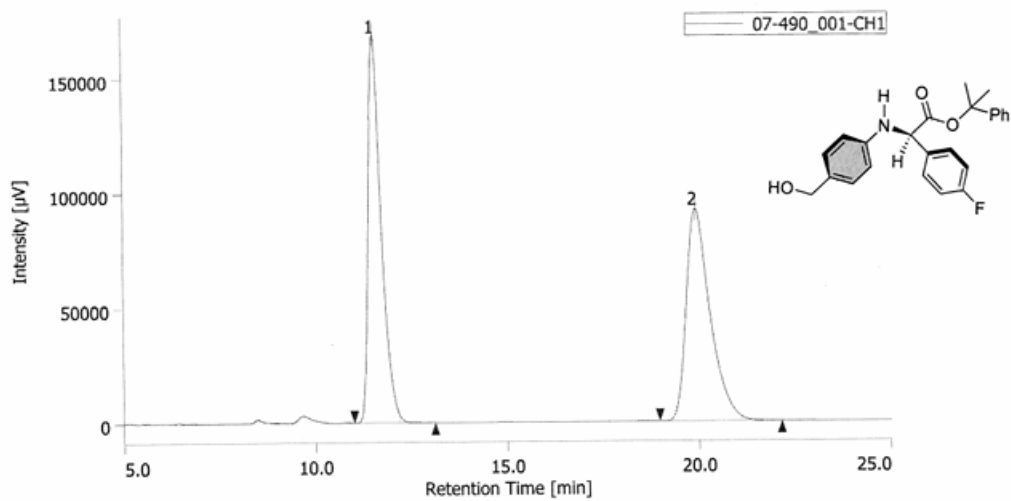


3



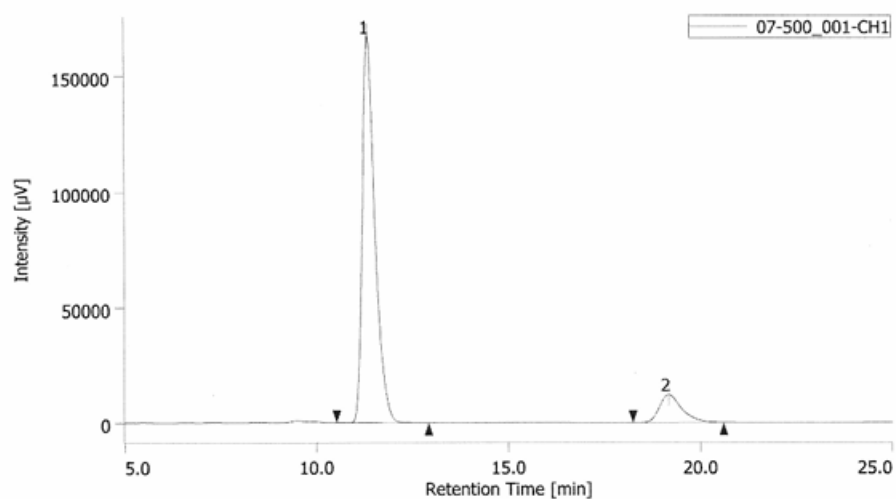
1
2

0304 07-490_001 2026/06/05 17:43:34



#	tR [min]	Area [$\mu\text{V}\cdot\text{sec}$]	Area%	Height [μV]	Height%
1	11.558	3986093	50.025	169238	64.712
2	19.933	3982175	49.975	92287	35.288

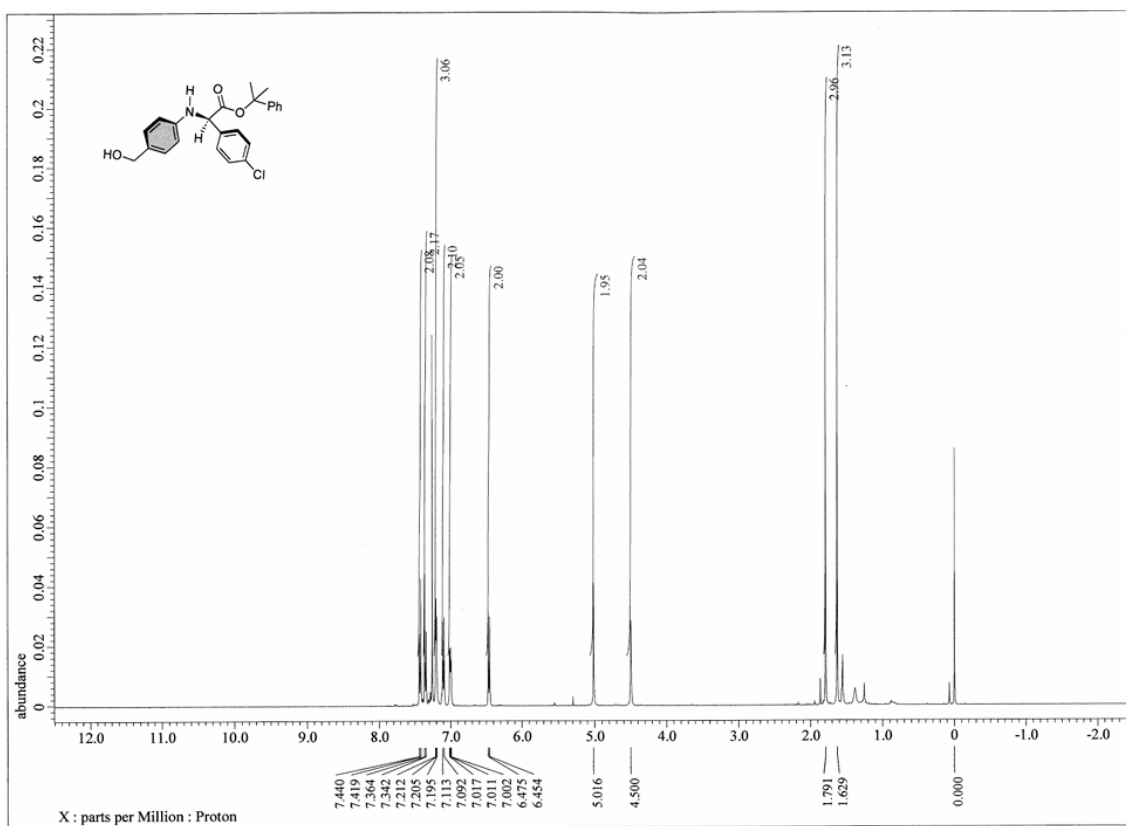
0310 07-500_001 2026/06/05 17:43:42



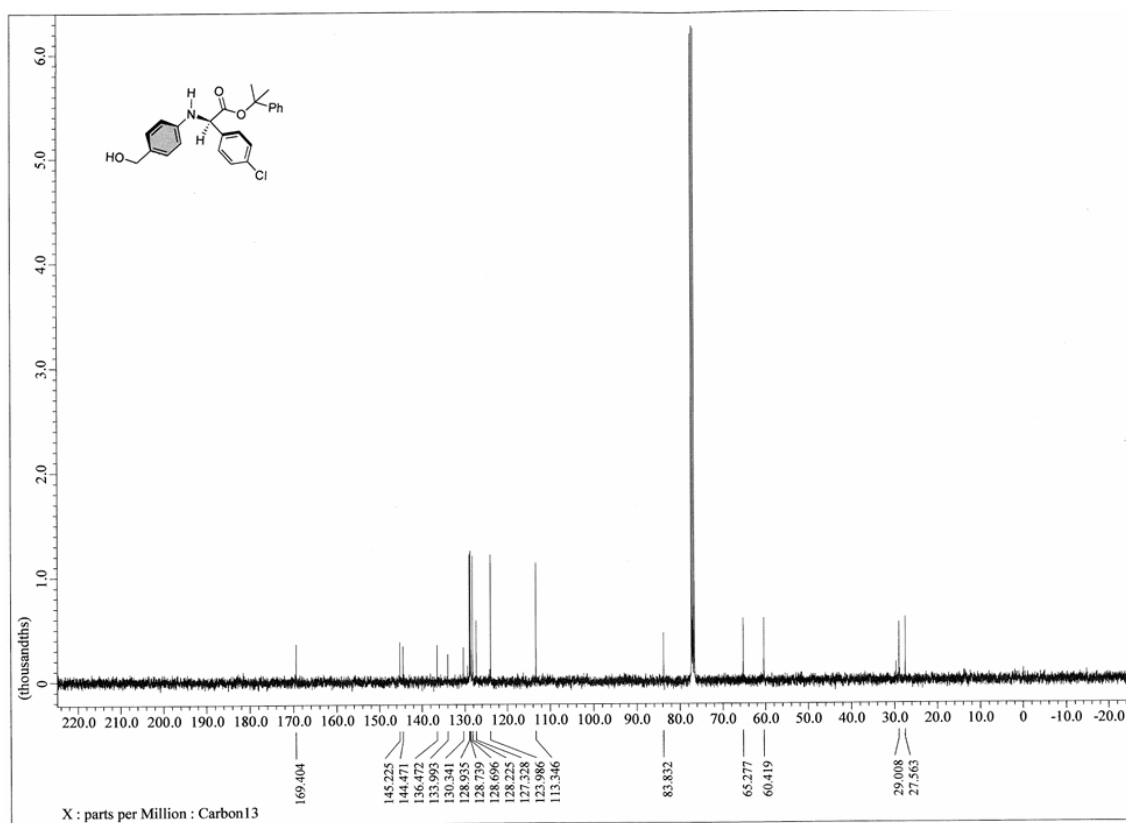
#	tR [min]	Area [$\mu\text{V}\cdot\text{sec}$]	Area%	Height [μV]	Height%
1	11.342	3817234	88.675	167863	93.263
2	19.167	487524	11.325	12126	6.737

1

9h

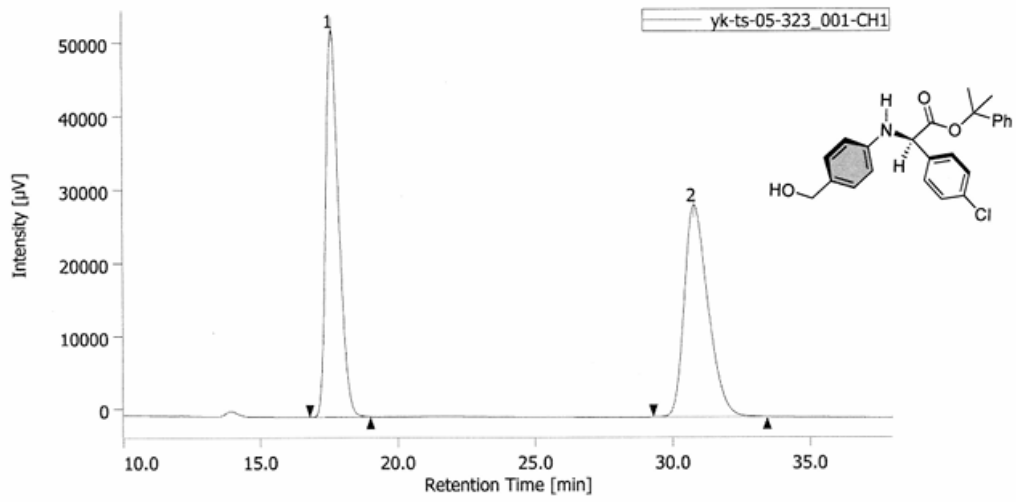


2



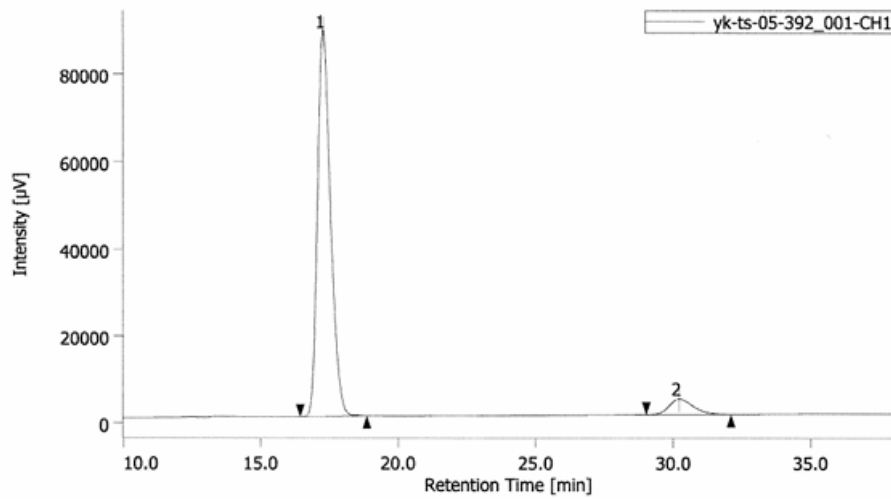
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1022 yk-ts-05-323_001 2026/05/28 13:49:02



#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	17.825	1743998	49.967	53023	84.627
2	30.808	1746328	50.033	29021	35.373

1210 yk-ts-05-392_001 2026/05/28 13:49:13

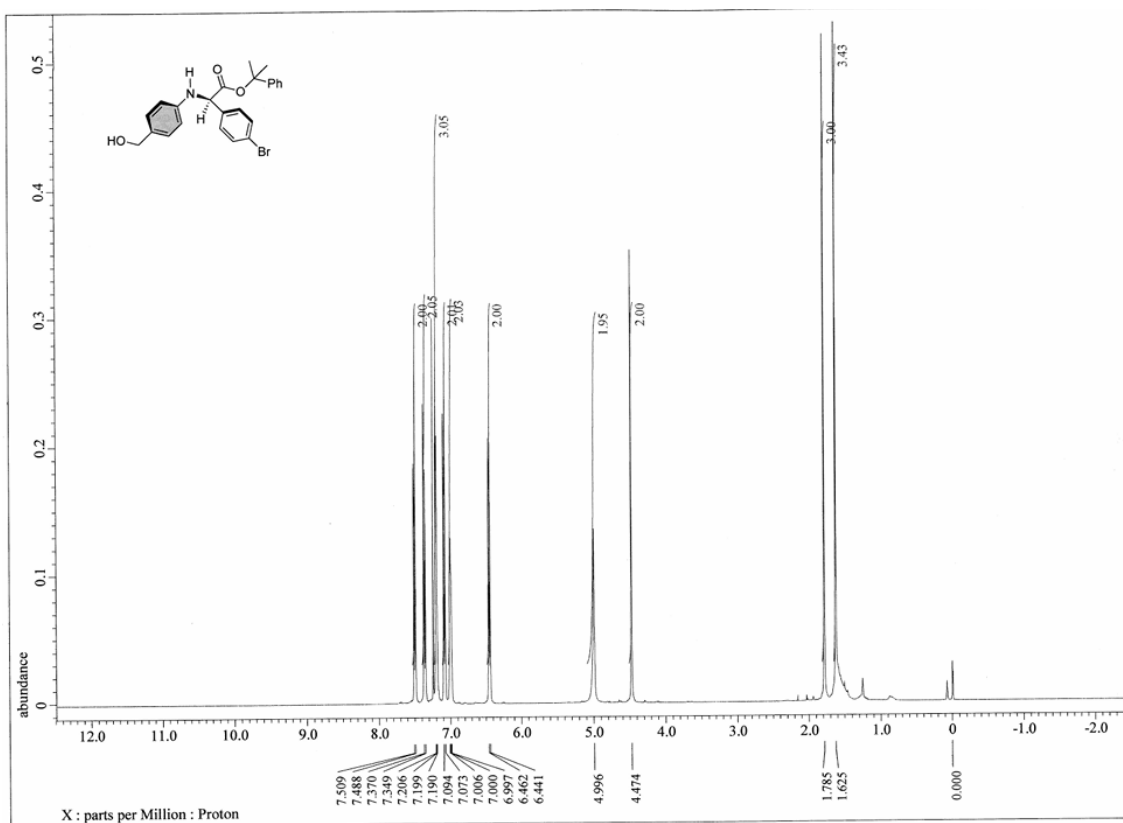


#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	17.283	2918186	93.216	88709	96.188
2	30.208	212361	6.784	3516	3.812

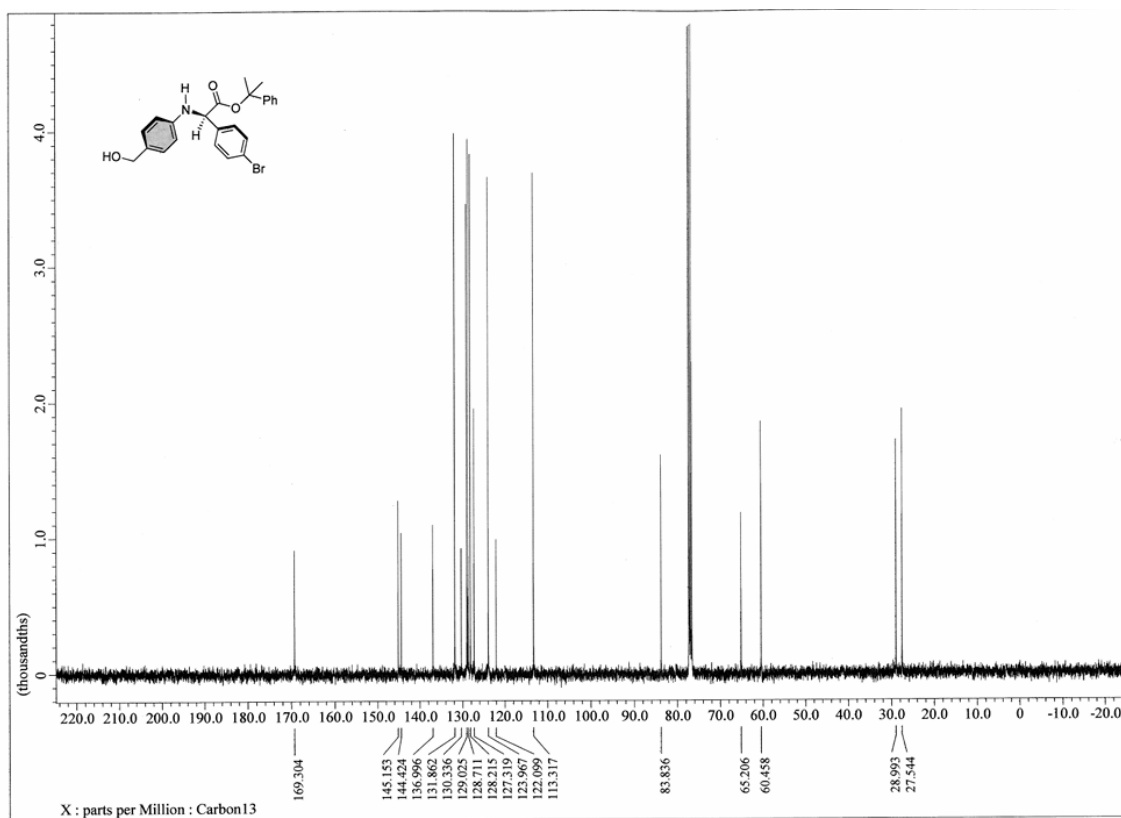
- 1
- 2
- 3

1

9i

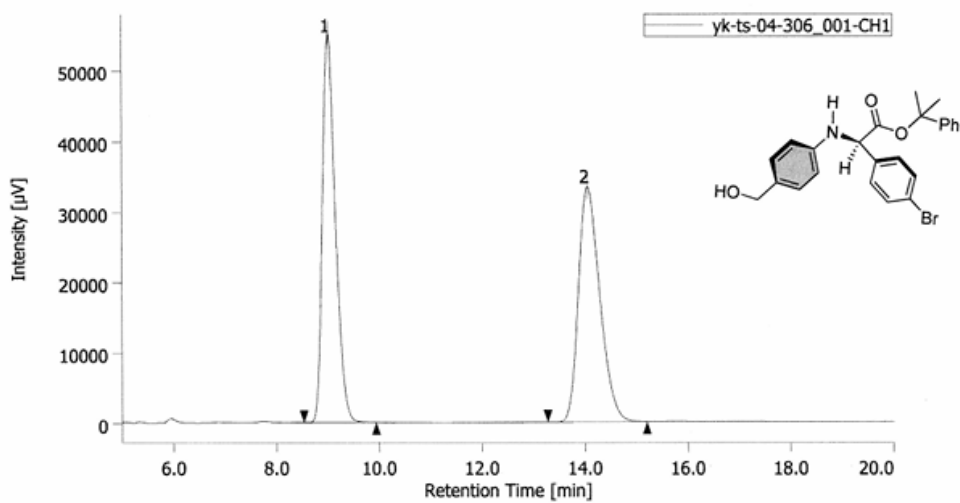


2



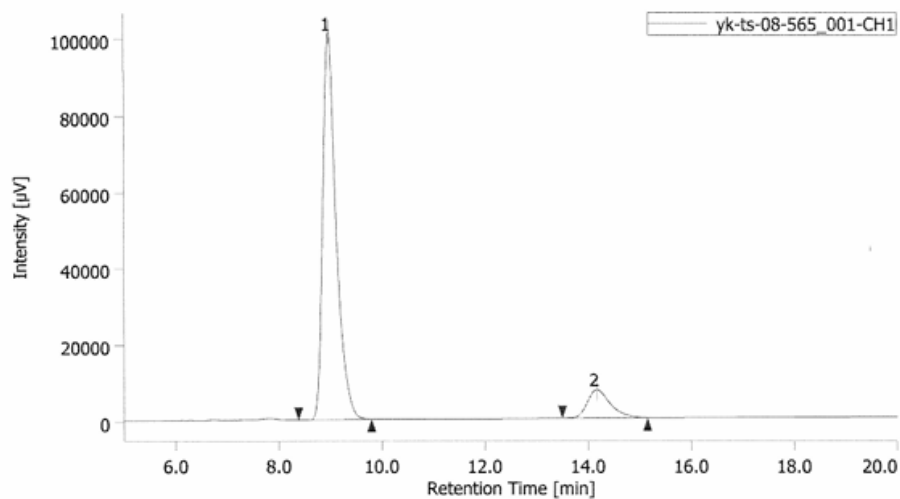
3

1007 yk-ts-04-306_001 2026/05/28 13:52:41



#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	9.017	965418	50.085	55068	62.208
2	14.058	962152	49.915	33454	37.792

0605 yk-ts-08-565_001 2026/06/05 17:23:01

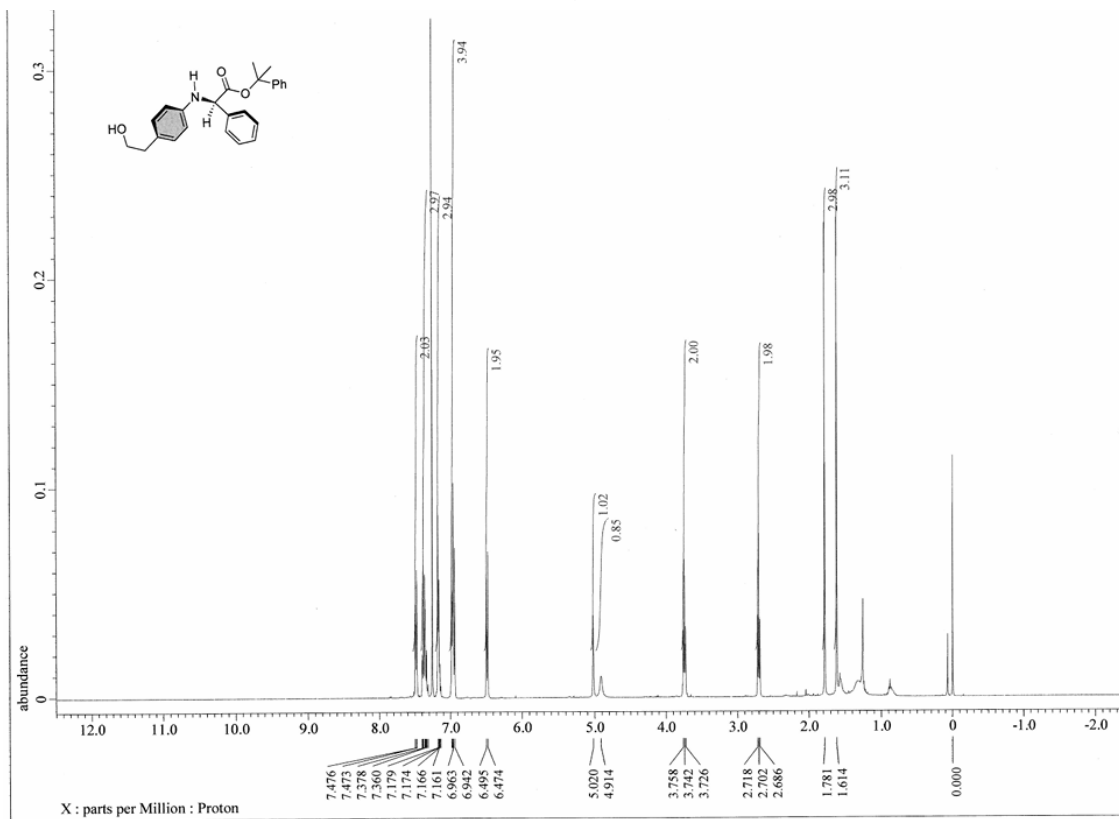


#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	8.975	1815018	89.064	101211	93.273
2	14.175	222868	10.936	7300	6.727

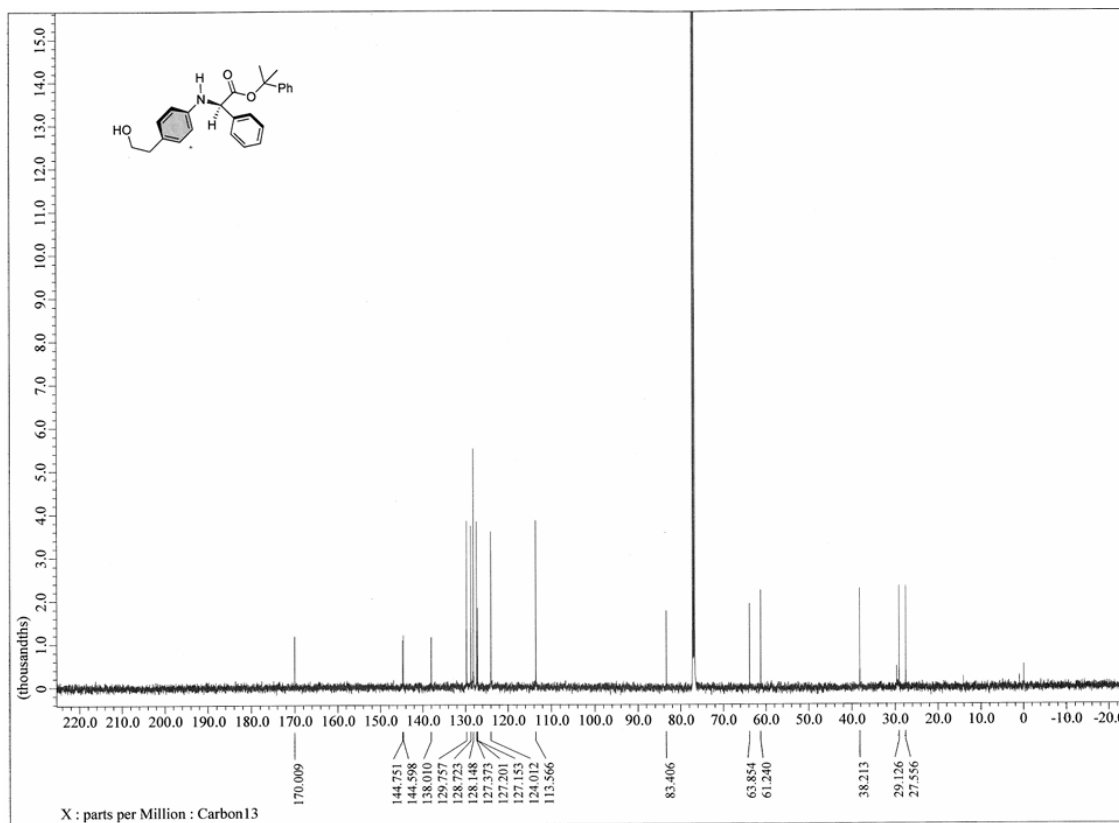
1
2
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1

9j

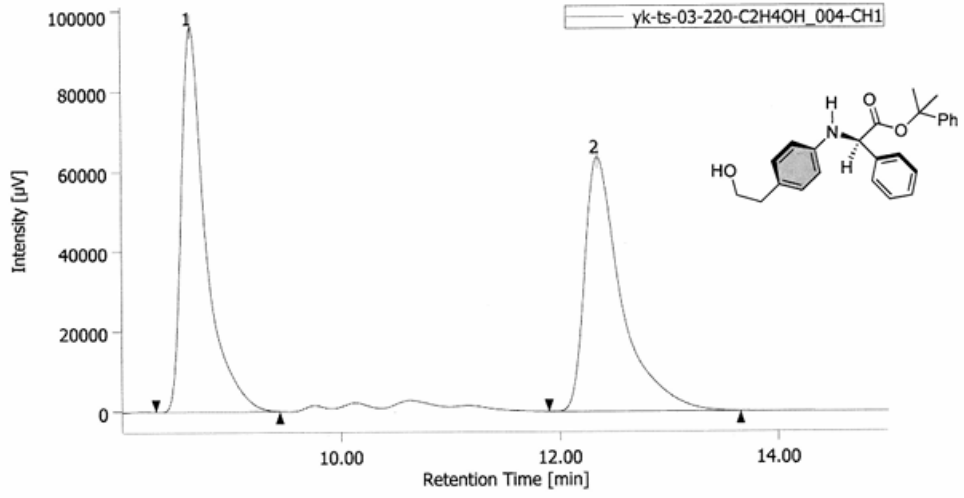


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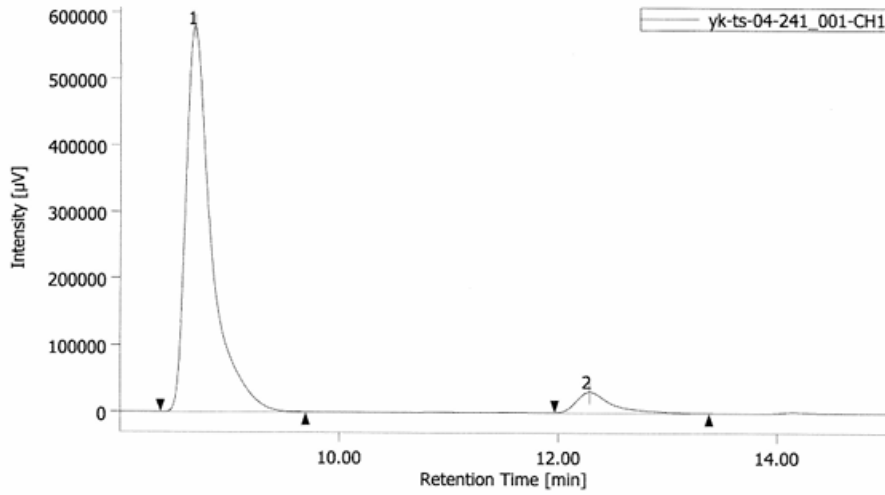
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0624 yk-ts-03-220-C2H4OH_004 2026/05/28 19:14:53



#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	8.633	1487838	50.162	96308	60.189
2	12.358	1478201	49.838	63702	39.811

0701 yk-ts-04-241_001 2026/05/28 19:24:51

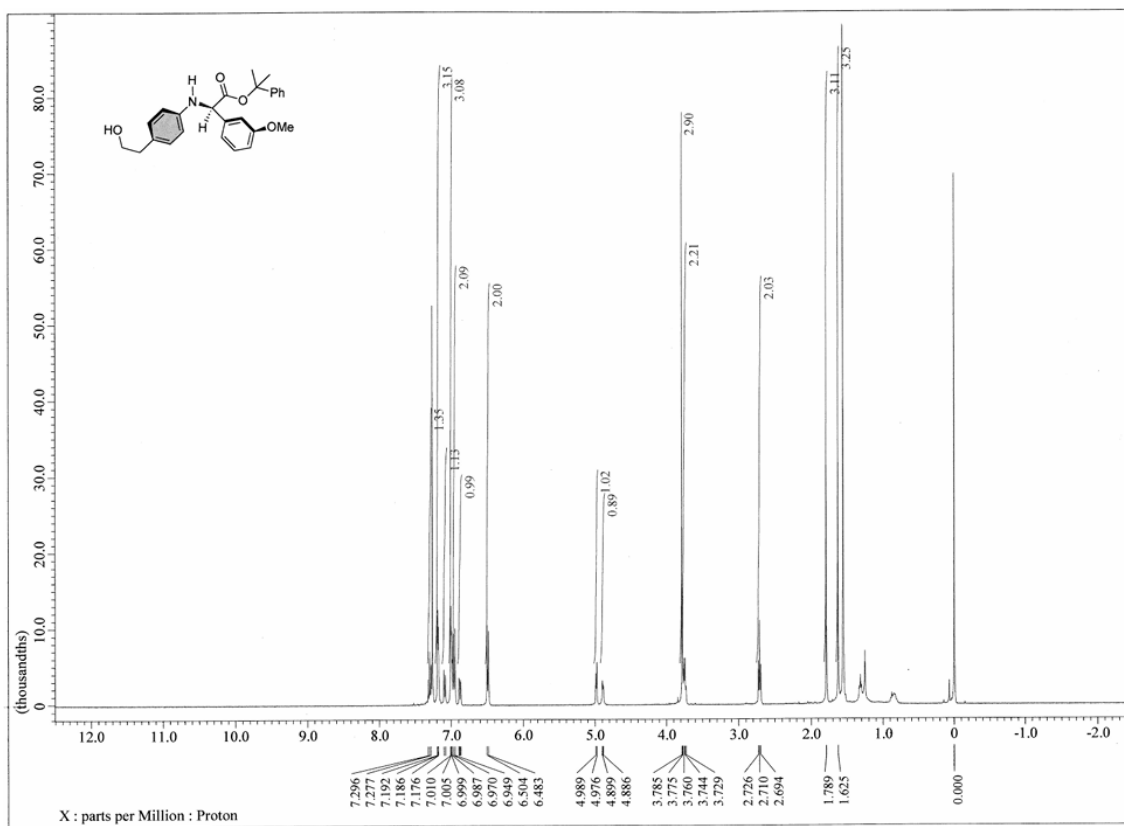


#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	8.683	9422366	93.101	579618	94.944
2	12.283	698211	6.899	30867	5.056

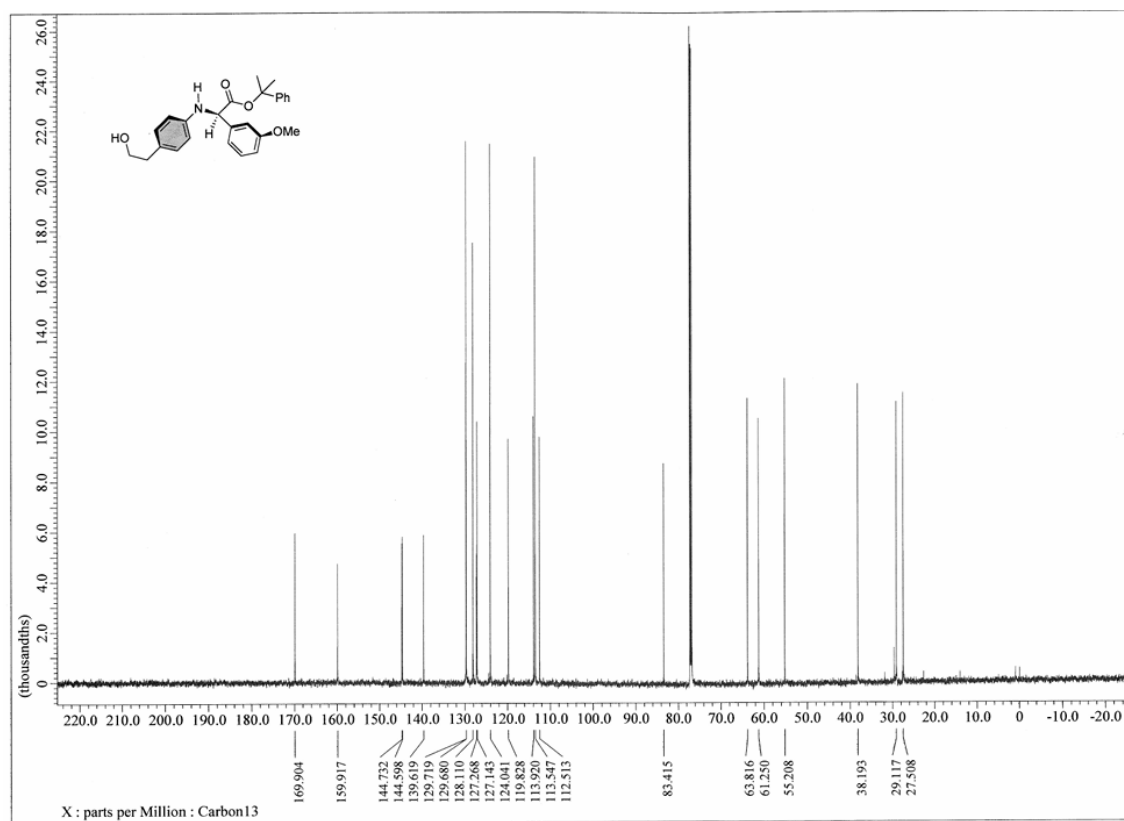
1
2
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1

9k

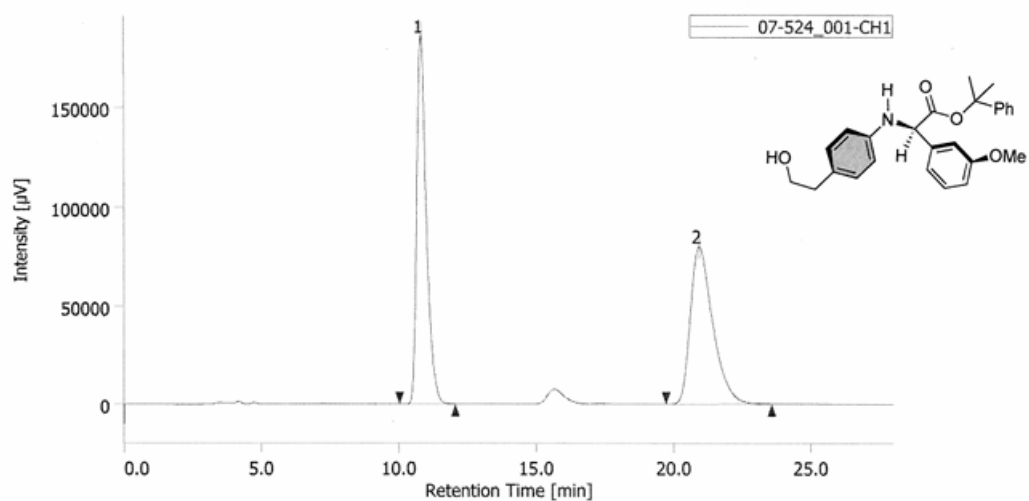


2



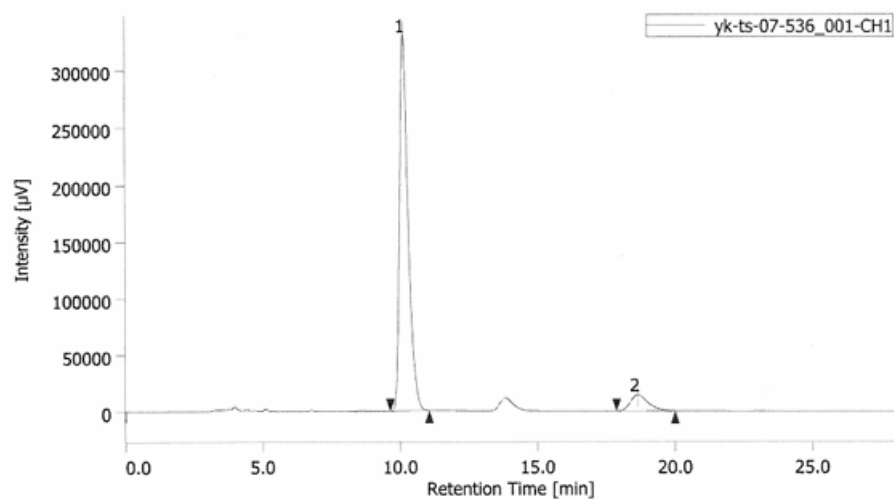
3

0425 07-524_001 2026/06/16 16:16:04



#	tR [min]	Area [$\mu\text{V}\cdot\text{sec}$]	Area%	Height [μV] [μV]	Height%
1	10.817	4541280	50.090	186643	69.982
2	20.942	4524925	49.910	80058	30.018

0513 yk-ts-07-536_001 2026/06/16 16:14:23

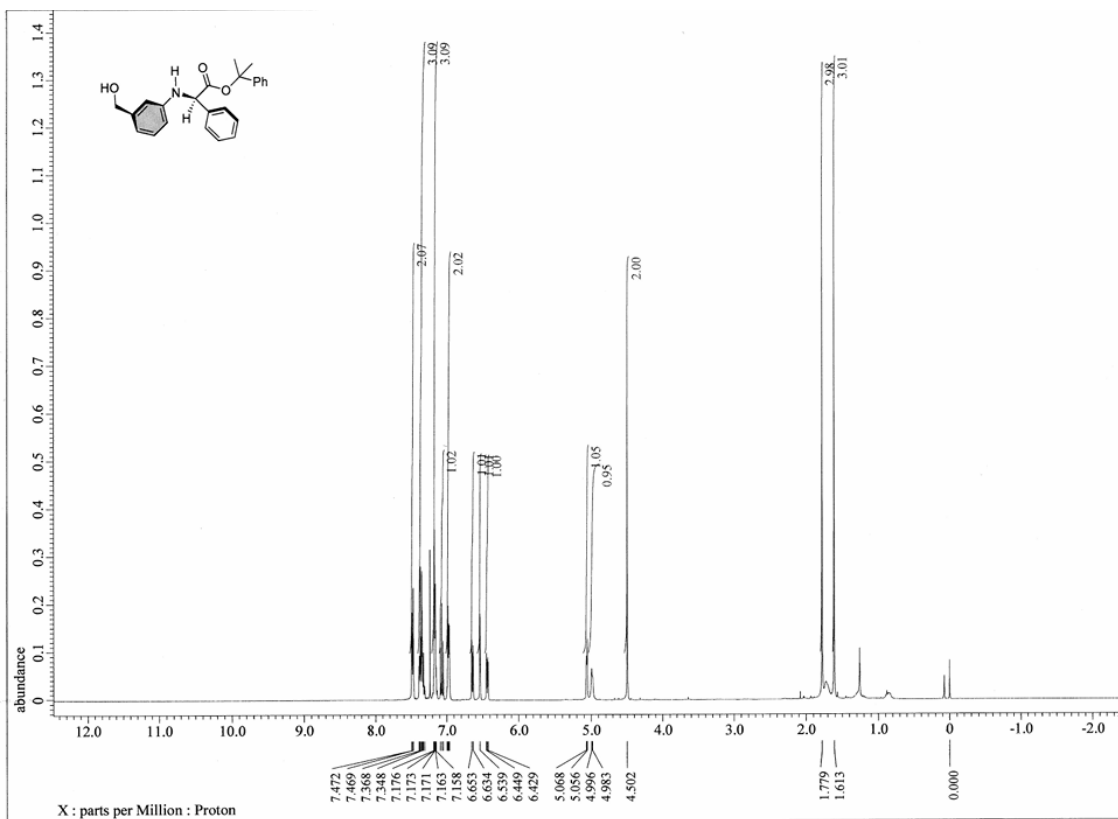


#	tR [min]	Area [$\mu\text{V}\cdot\text{sec}$]	Area%	Height [μV] [μV]	Height%
1	10.125	7228213	91.854	330941	95.876
2	18.633	641033	8.146	14234	4.124

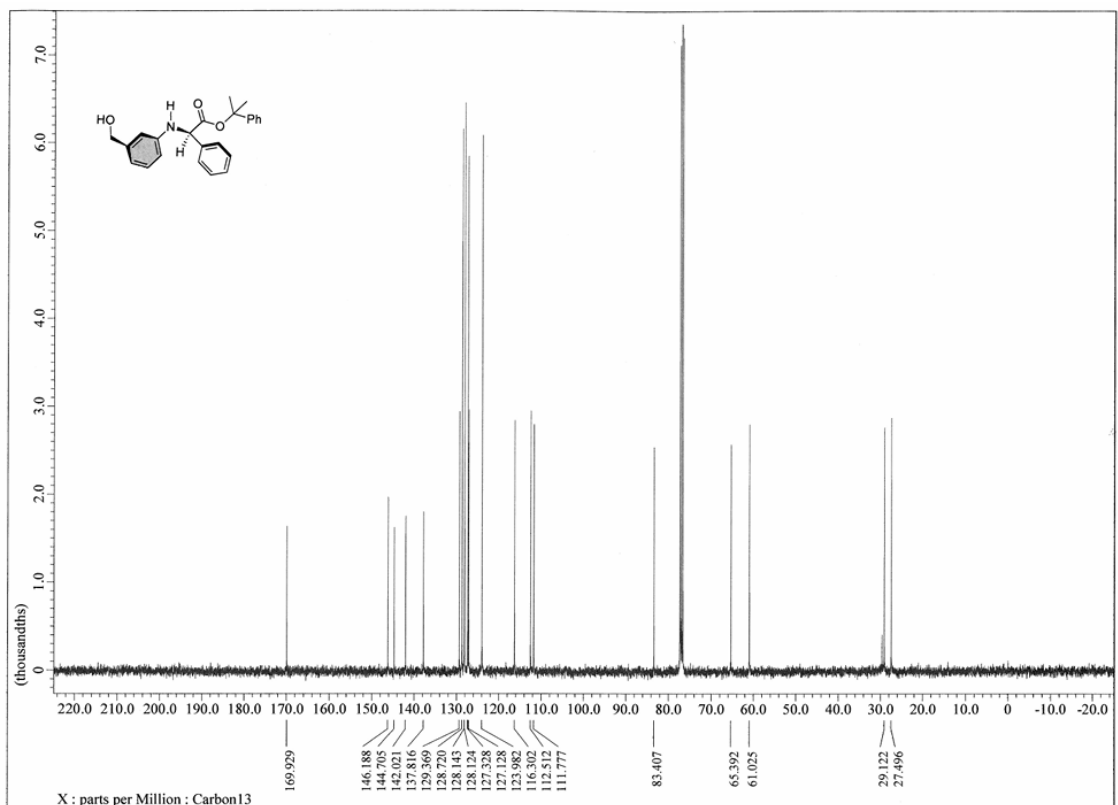
1
2
3

1

91



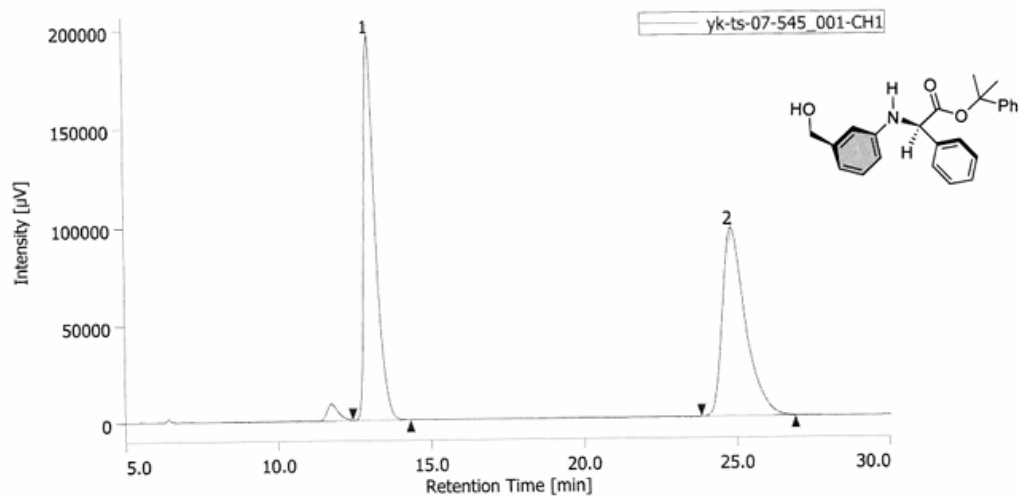
2



3

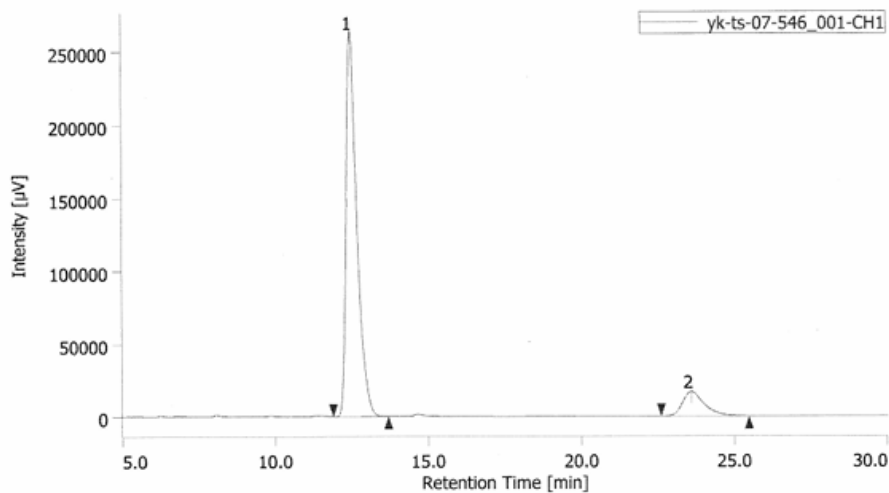
4

0522 yk-ts-07-545_001 2026/05/26 18:03:39



#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	13.017	5060966	50.050	196412	67.087
2	24.842	5050767	49.950	96359	32.913

0526 yk-ts-07-546_001 2026/05/26 18:54:16

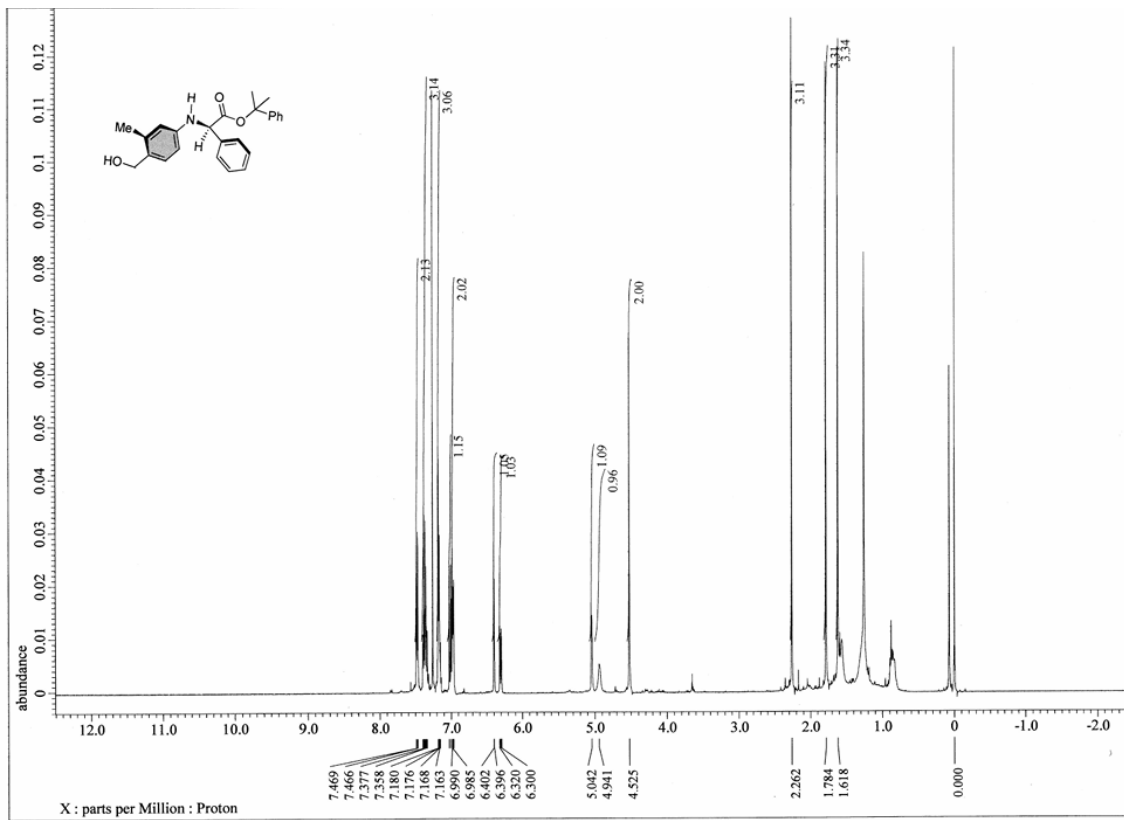


#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	12.483	6415270	88.918	263879	94.103
2	23.575	799548	11.082	16535	5.897

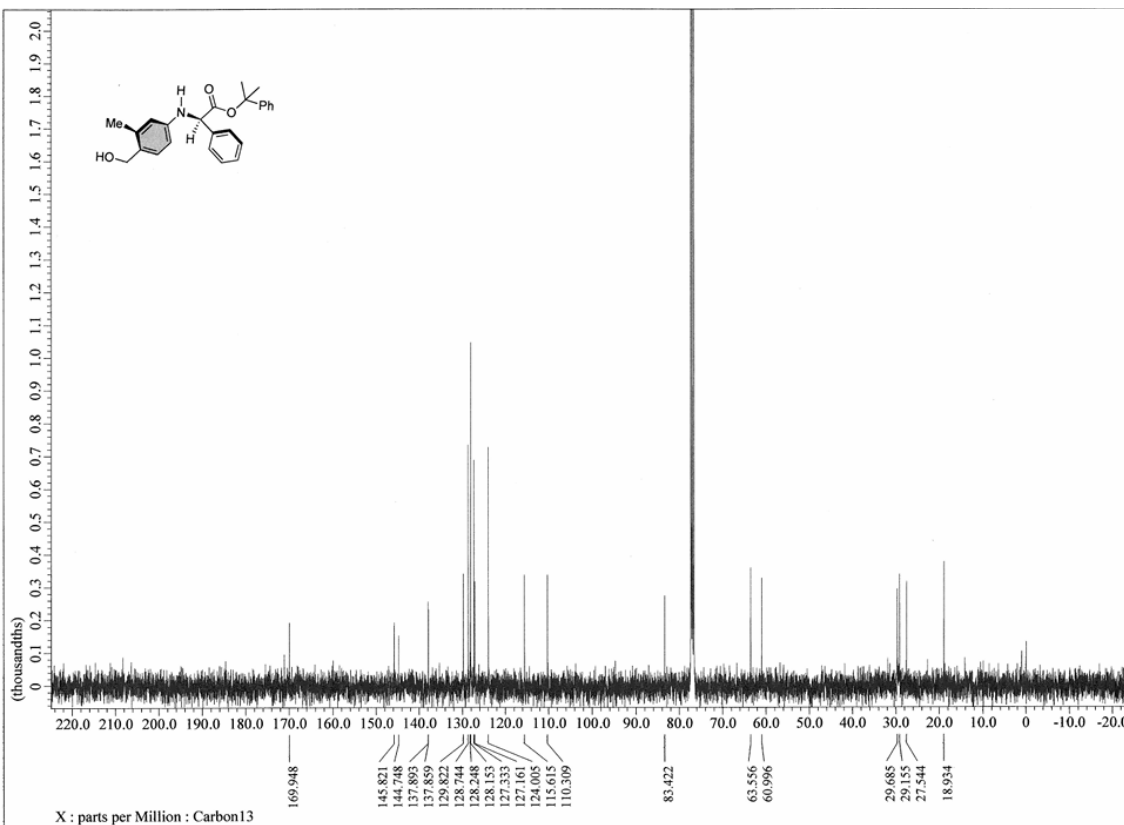
1
2

1

9m

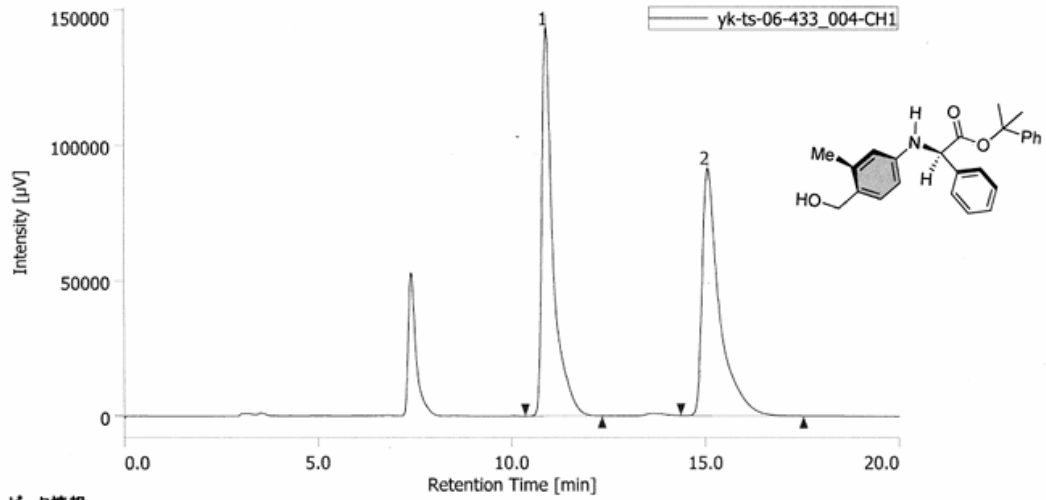


2



3

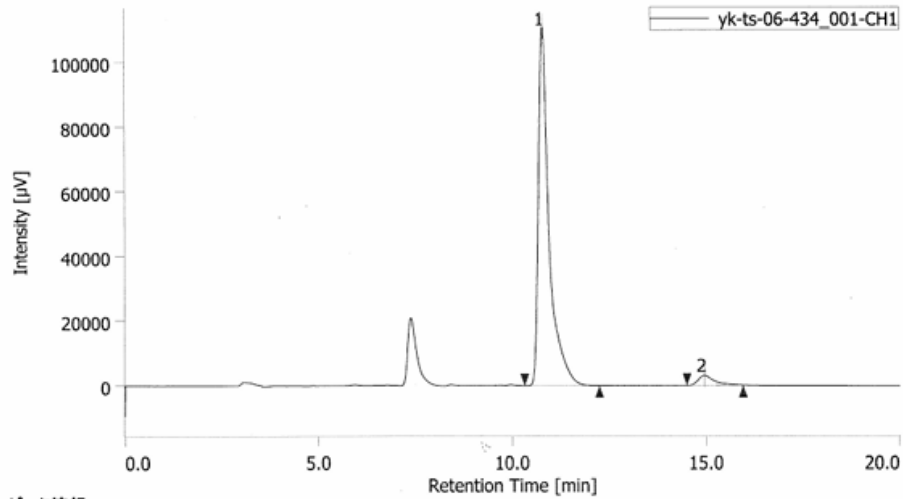
0120 yk-ts-06-433_004 2026/04/09 17:39:47



ピーク情報

#	ピーク名	CH	tR [min]	面積 [μV·sec]	高さ [μV]	面積%	高さ%	定量値	NTP	分離度	シメトリー係数	警告
1	Unknown	1	10.900	2880324	143876	50.514	61.160	N/A	9674	7.382	2.008	
2	Unknown	1	15.067	2821680	91368	49.486	38.840	N/A	7661	N/A	2.187	

0121 yk-ts-06-434_001 2026/04/09 17:38:48



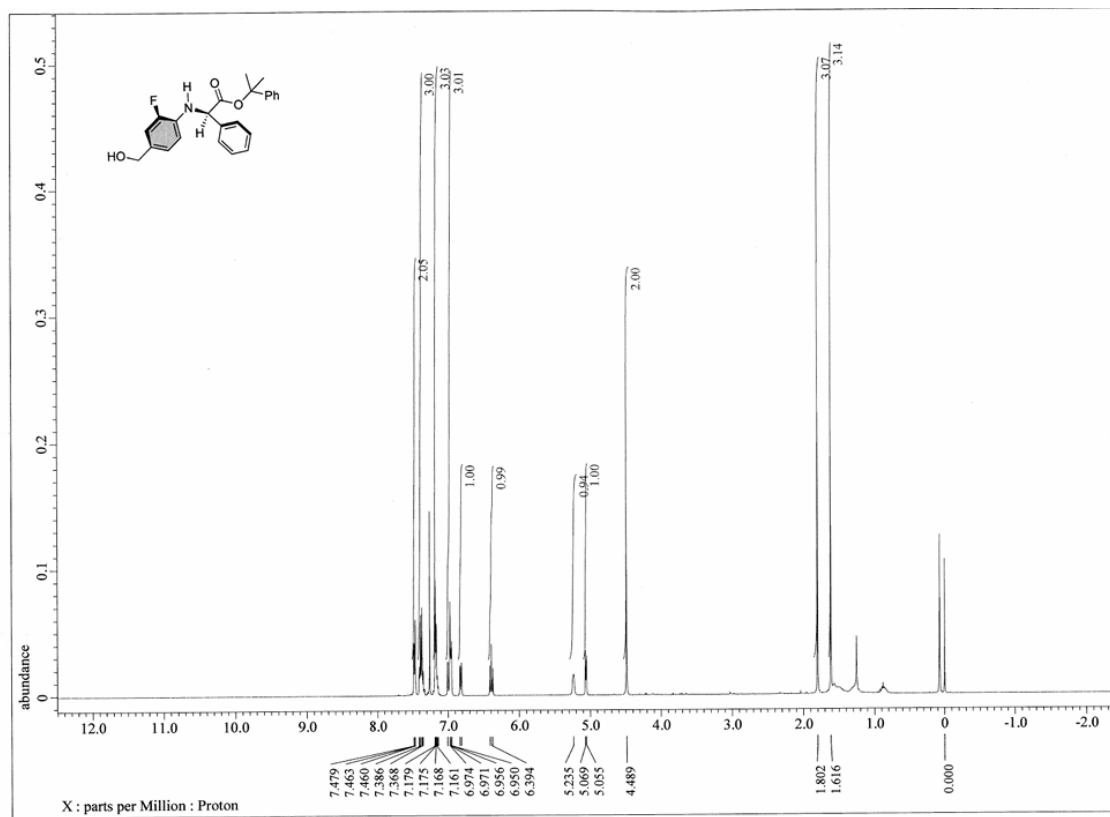
ピーク情報

#	ピーク名	CH	tR [min]	面積 [μV·sec]	高さ [μV]	面積%	高さ%	定量値	NTP	分離度	シメトリー係数	警告
1	Unknown	1	10.783	2133586	110670	95.918	97.248	N/A	9988	7.442	2.031	
2	Unknown	1	14.950	90807	3131	4.082	2.752	N/A	7487	N/A	1.722	

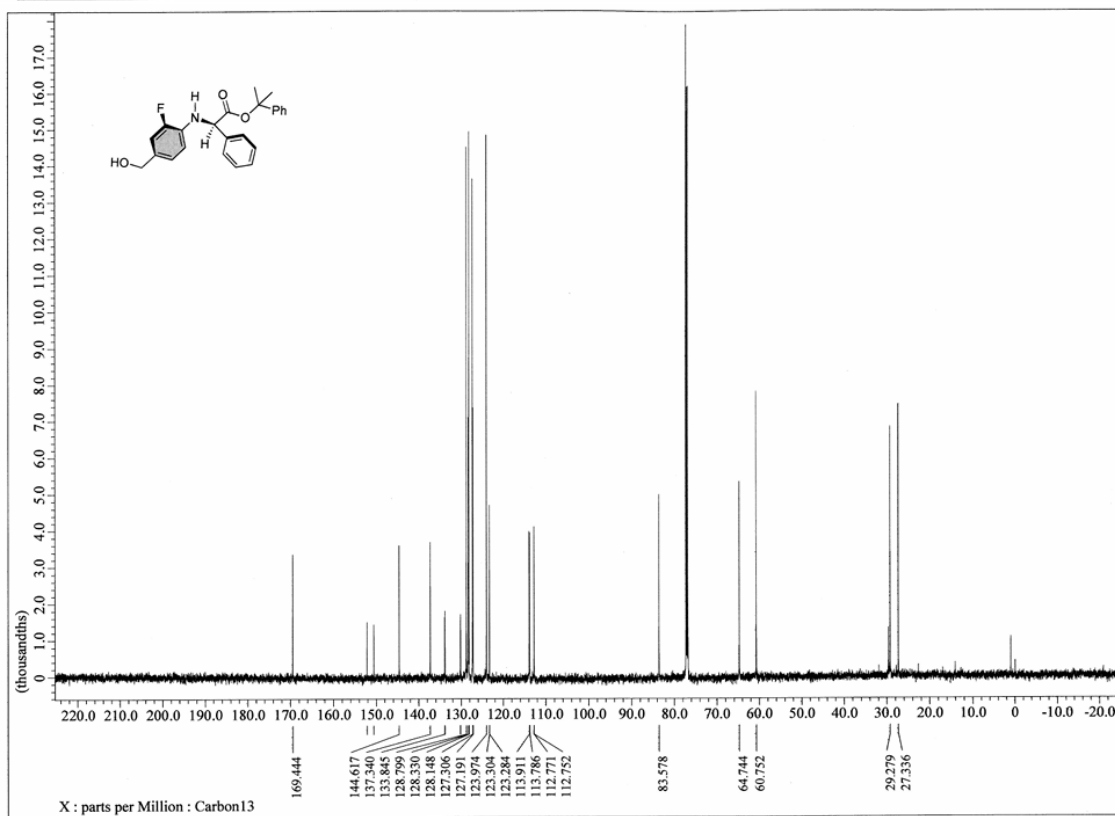
1
2

1

9n

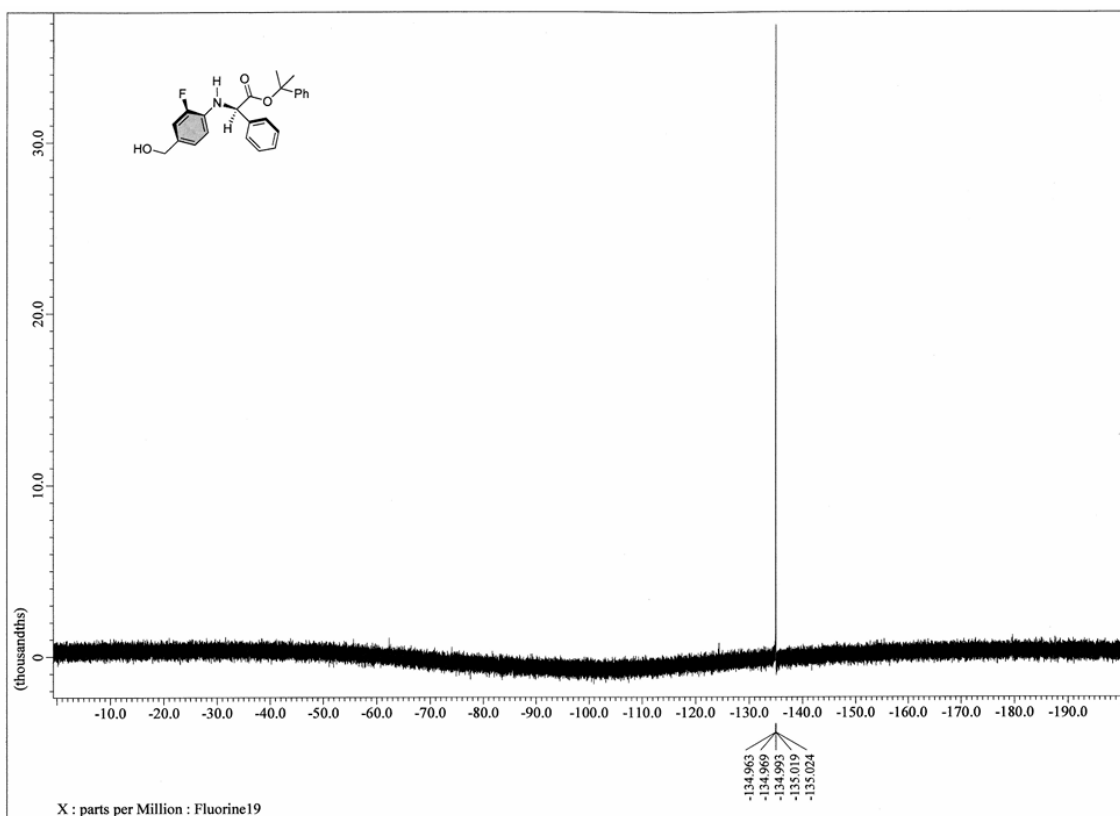


2



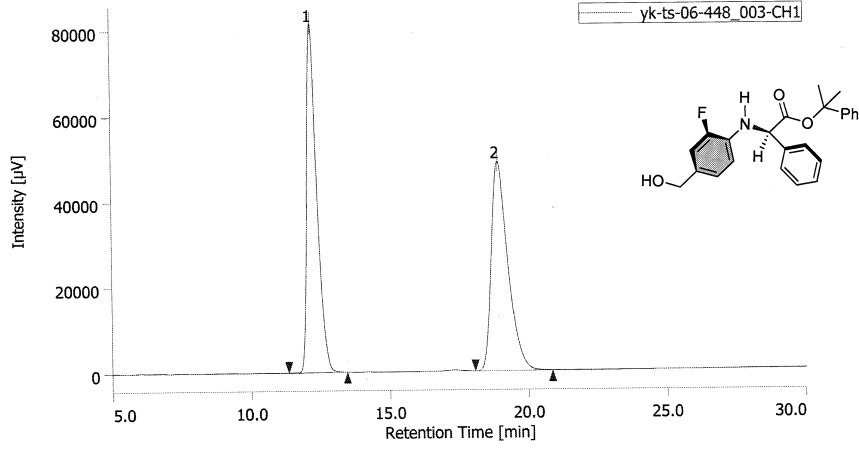
3

4



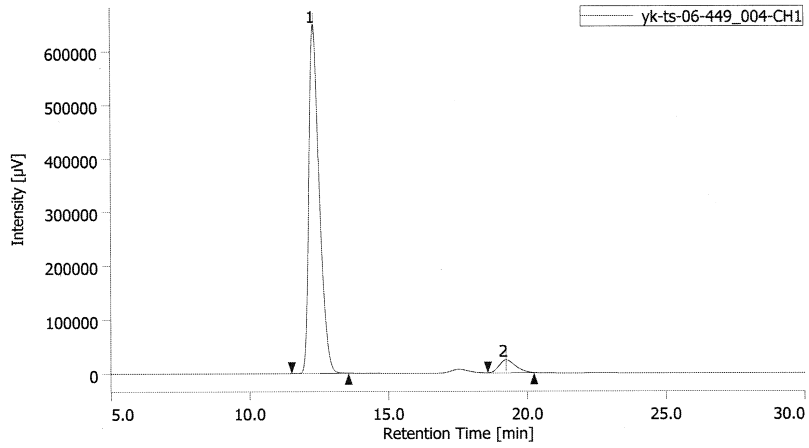
1
2
3

0207 yk-ts-06-448_003 2026/06/05 17:35:19



#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	12.225	2030847	50.039	81540	62.517
2	18.933	2027703	49.961	48889	37.483

0207 yk-ts-06-449_004 2026/06/19 0:58:47



#	tR [min]	Area [µV·sec]	Area%	Height [µV] [µV]	Height%
1	12.317	16756793	94.598	649994	96.496
2	19.225	956944	5.402	23603	3.504

1
2

1

2 **10. References**

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(10) The Avogadro software is available free of charge from the following website:

<https://avogadro.cc/install/>