

Supporting Information

for

Palladium-Catalyzed Addition of Acylsilanes across Alkynes via the Activation of a C–Si Bond

Tetsuya Inagaki,^a Takahiro Ando,^a Shun Sakurai,^a Masahiro Yamanaka*^c and Mamoru Tobisu*^{a,b}

^a*Department of Applied Chemistry, Graduate School of Engineering, Osaka University, Suita, Osaka 565-0871, Japan*

^b*Innovative Catalysis Science Division, Institute for Open and Transdisciplinary Research Initiatives (ICS-OTRI), Osaka University, Suita, Osaka 565-0871, Japan.*

^c*Department of Chemistry, Faculty of Science, Rikkyo University, 3-34-1 Nishi-Ikebukuro, Toshima-ku, Tokyo 171-8501, Japan*
myamanak@rikkyo.ac.jp; tobisu@chem.eng.osaka-u.ac.jp

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I. General Information

^1H NMR, ^{13}C NMR, ^{19}F NMR and ^{29}Si NMR spectra were recorded on a JEOL ECS-400 spectrometer in CDCl_3 or C_6D_6 . The chemical shifts in ^1H NMR spectra were recorded relative to CHCl_3 (δ 7.26) or C_6H_6 (δ 7.15). The chemical shifts in ^{13}C NMR spectra were recorded relative to CDCl_3 (δ 77.00) or C_6D_6 (δ 128.00). The chemical shifts in ^{19}F NMR spectra were recorded relative to perfluorobenzene (-163.0 ppm). ^{29}Si NMR spectra were recorded relative to tetramethylsilane (0.0 ppm). Data are reported as follows: chemical shift (δ) in ppm, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, m = multiplet), coupling constant (J) in Hz, and integration. The data is reported as follows: chemical shift (δ) in ppm, coupling constant (Hz), and integration. Infrared spectra (IR) were obtained using a JASCO FT/IR-4200 spectrometer. Absorption is reported in reciprocal centimeters (cm^{-1}) with the following relative intensities: s (strong), m (medium), or w (weak). Mass spectra and high-resolution mass spectra (HRMS) were obtained on a JEOL JMS-700 spectrometer or JMS-T100LP. Analytical gas chromatography (GC) was carried out on a Shimadzu GC-2014 gas chromatograph, equipped with a flame ionization detector. Column chromatography was performed with SiO_2 (Silica Gel 60 N (spherical, neutral) (40-50 μm), (KANTO CHEMICAL CO., INC.).

II. Materials

$\text{Pd}_2(\text{dba})_3$ (Aldrich), IPr (TCI), **2a** (TMO), **2b** (Wako), **2c** (Wako), **2f** (TCI), **2g** (TCI), **2j** (TCI) and toluene (Wako) were purchased from the commercial suppliers and used as received. Acylsilane **1a** [CAS: 5908-41-8] was prepared from benzyltrimethylsilane (TCI) according to the literature method.¹ Acylsilanes **1b** [CAS: 75748-09-3], **1c** [CAS: 75748-12-8], **1d** [CAS: 144968-85-4], **1e** [CAS: 107325-81-5], **1f** [CAS: 1354579-01-3] and **1g** [CAS: 22364-54-1] were prepared from the corresponding acyl chlorides according to the literature methods.² Alkyne **2d** [CAS: 1016981-17-1] was prepared from phenethylacetylene and ethyl chloroformate according to the literature method.³ Alkyne **2e** [CAS: 33547-94-3] was prepared from ethynylcyclohexane and ethyl chloroformate according to the literature method.⁴ Alkynes **2h** [CAS: 207225-49-8] and **2i** [CAS: 2464939-88-4] were prepared from but-2-ynoic acid and the corresponding alcohols according to the literature method.⁵ Alkynes **2k** [CAS: 51718-85-5], **2l** [CAS: 1736-31-8] and **2p** [CAS: 58686-71-8] were prepared from the corresponding ethynylarenes and ethyl chloroformate according to the literature method.⁶ Alkynes **2m** [CAS: 61354-73-2] and **2o** [CAS: 906820-21-1] were prepared from the corresponding aryl iodides and ethyl propiolate according to the literature method.⁷ Alkyne **2n** [CAS: 946420-91-3] was prepared from 4-phenyl-1-butyne and pivaloyl chloride according to the literature method.⁸ Alkyne **2q** [CAS: 124235-10-5] was prepared from 1-hexyne and dimethylcarbamic chloride according to the literature method.⁹

III. Typical Procedures

Method A: Procedure for the Palladium-Catalyzed Silylacylation of Alkyne **2a** Using Acylsilane **1a**.

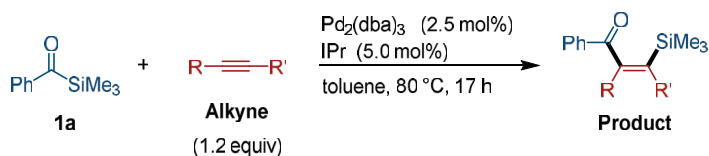
In a glovebox filled with nitrogen, Pd₂(dba)₃ (9.2 mg, 0.010 mmol), IPr (7.8 mg, 0.020 mmol), acylsilane **1a** (71 mg, 0.4 mmol), and alkyne **2a** (37 mg, 0.22 mmol) were added to a 10 mL-sample vial with a teflon-sealed screwcap. Toluene (0.6 mL) was then added, and the vial was sealed with the cap. The vial was stirred at 60 °C for 17 h. After allowing the mixture to cool to rt, the crude mixture was filtered through a pad of Celite, and the pad was washed with EtOAc. The filtrate was analyzed by GC using dodecane as an internal standard. The filtrate was concentrated in vacuo and purified by flash column chromatography over silica gel (elution with hexane/EtOAc = 10/1) to give **3aa** as a yellow oil (63 mg, 83% yield).

Method B: Procedure for the Palladium-Catalyzed Synthesis of Indanone Derivatives Using Acylsilane **1a** and alkyne **2j**.

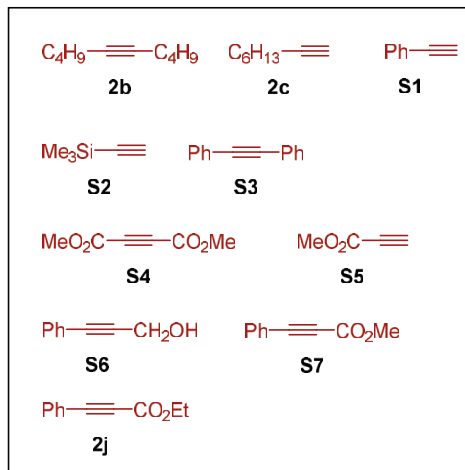
In a glovebox filled with nitrogen, Pd₂(dba)₃ (9.2 mg, 0.010 mmol), IPr (7.8 mg, 0.020 mmol), acylsilane **1a** (37 mg, 0.21 mmol), and alkyne **2j** (41.8 mg, 0.24 mmol) were added to a 10 mL-sample vial with a teflon-sealed screwcap. Toluene (0.6 mL) was then added, and the vial was sealed with the cap. The vial was stirred at 140 °C for 17 h. After allowing the mixture to cool to rt, the crude mixture was filtered through a pad of Celite, and the pad was washed with EtOAc. The filtrate was analyzed by GC using dodecane as an internal standard. The filtrate was concentrated in vacuo and purified by flash column chromatography over silica gel (elution with hexane/EtOAc = 10/1) to give **4aj** as a yellow oil (50 mg, 87% yield).

IV. Optimization Studies

IV-1. Screening of Alkynes

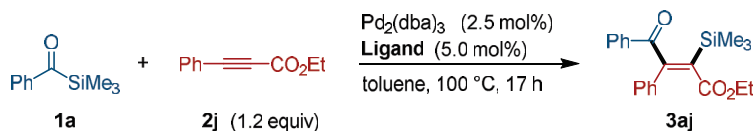


Entry	Alkyne	GC yield (%) ^a	
		1a	Product
1	2b	>99	0
2	2c	62	trace
3	S1	48	5
4	S2	78	2
5	S3	65	trace
6	S4	>99	0
7	S5	92	0
8	S6	57	0
9	S7	49	25 (4.7:1)
10	2j	15	46(1.4:1) ^b

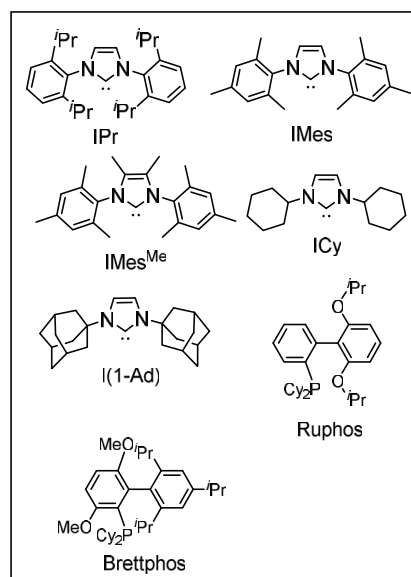


^aThe yield was estimated by GC analysis using dodecane as an internal standard unless otherwise noted. ^bRun at 100 °C.

IV-2. Effect of Ligands

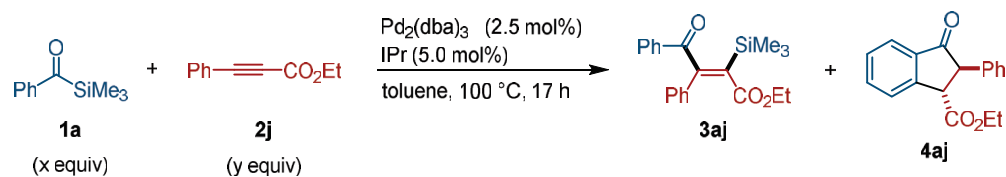


Entry	Ligand	GC yield (%) ^a	
		1a	3aj
1	IPr	15	46 (1.4:1)
2	IMes•HCl + ^t BuONa	31	31 (0.4:1)
3	IMes ^{Me} •HCl + ^t BuONa	18	27 (0.7:1)
4	ICy•HBF ₄ + ^t BuONa	61	0
5	I(1-Ad)•HBF ₄ + ^t BuONa	63	0
6	RuPhos	65	0
7	BrettPhos	64	0
8	PCy ₃	45	35 (0.6:1)
9	PPh ₃	0	2
10	P ^t Bu ₃	56	0
11	P ⁿ Bu ₃	42	35 (0.1:1)
12	2,2'-bipyridine	66	0
13	IPr, w/o Pd ₂ (dba) ₃	54	0



^aThe yield was estimated by GC analysis using dodecane as an internal standard unless otherwise noted.

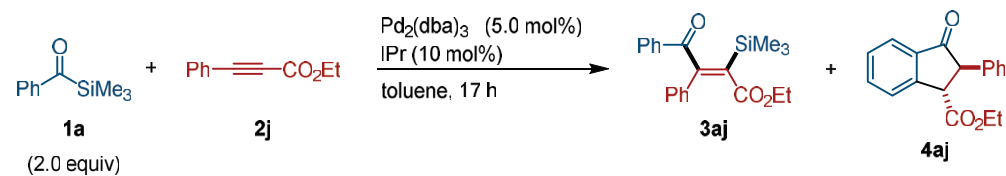
IV-3. Effect of Amounts of Substrates



Entry	Equiv		Yield (%)		
	x	y	1a or 2j	3aj	4aj
1	3	1	0	68 (2.0:1) ^a	25 ^a
2	2	1	0	67 (6.7:1) ^a	17 ^a
3	1.5	1	16 ^b	47 (>10:1) ^b	5 ^b
4	1.2	1	8 ^b	53 (9:1) ^b	6 ^b
5	1	1.2	15 ^b	46 (1.4:1) ^b	9 ^b
6	1	2	65 ^b	0	0
7	1	3	64 ^b	0	0

^aIsolated yield. ^bThe yield was estimated by GC analysis using dodecane as an internal standard unless otherwise noted.

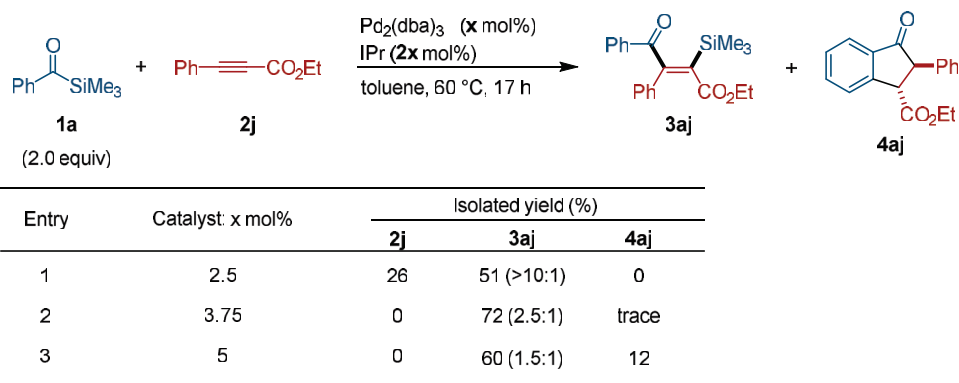
IV-4. Effect of Temperature



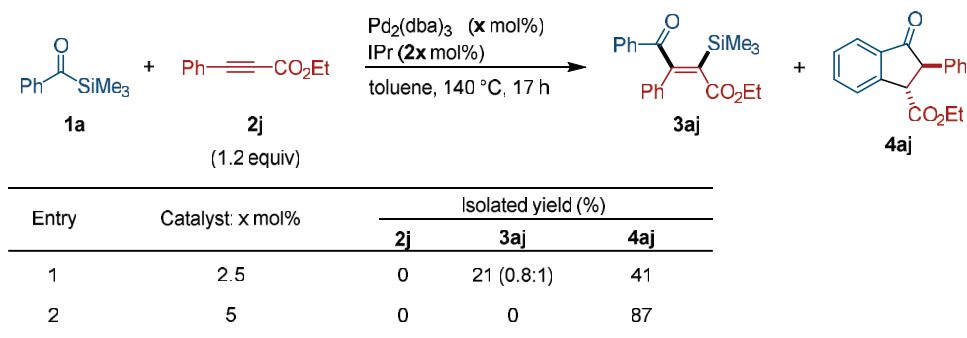
Entry	Temperature	Yield (%)		
		2j	3aj	4aj
1	RT	70 ^a	0	0
2	40 °C	74 ^a	13 ^a	0
3	60 °C	0	60 (1.5:1) ^b	12 ^b
4	80 °C ^c	0	63 (2.3:1) ^b	21 ^b
5	100 °C ^c	0	67 (6.7:1) ^b	17 ^b
6	140 °C ^c	0	40 ^b	19 ^b
7	140 °C ^d	0	0	87 ^b

^aThe yield was estimated by GC analysis using dodecane as an internal standard unless otherwise noted. ^bIsolated yield. ^cPd₂(dba)₃ (2.5 mol%) and IPr (5.0 mol%) were used. ^dAcylsilane **1a** (1.0 equiv) and alkyne **2j** (1.2 equiv) was used.

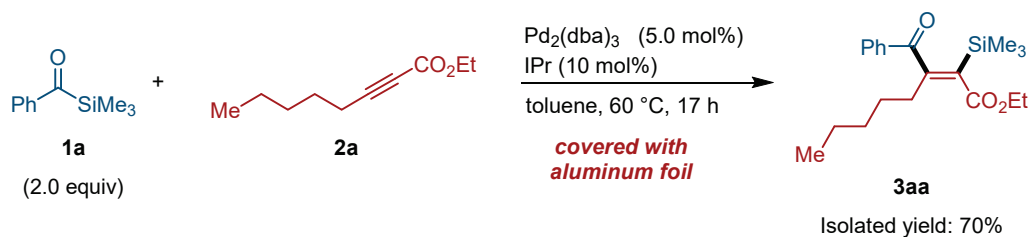
IV-5. Effect of Catalyst Loading for the Palladium-Catalyzed Silylacylation



IV-6. Effect of Catalyst Loading for the Palladium-Catalyzed Synthesis of Indanone Derivatives



IV-7. The Palladium-Catalyzed Silylacetylation under a Shading Condition^a



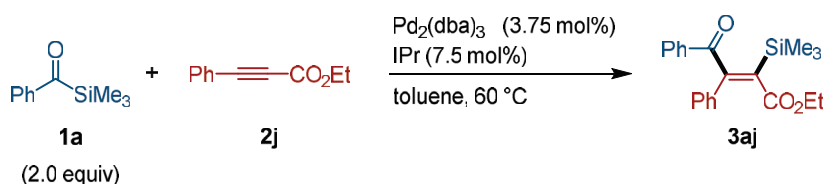
^aThe reaction was performed in the absence of any light by covering the reaction vessel with aluminum foil.

V. Mechanistic Studies

V-1. Dependence of *Z/E* ratio on the reaction time

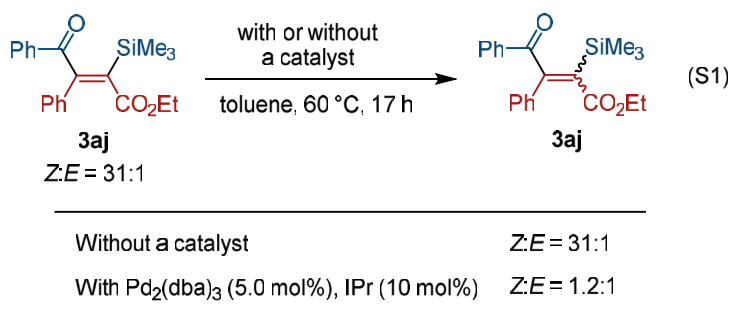
We investigated the *cis/trans* ratio as a function of reaction time and found that the *cis* addition product was produced selectively and that it then isomerized to the *trans* product as the reaction mixture was heated longer (Table S1). Isolated (*Z*)-**3aj**, in fact, isomerized to give a mixture of isomers when exposed to the palladium-catalyzed conditions, whereas (*Z*)-**3aj** did not isomerize in the absence of the catalyst (Eq. S1). Therefore, the isomerization process was promoted by a palladium catalyst, possibly via an addition/elimination mechanism.

Table S1. Dependence of *Z/E* ratio on the reaction time.

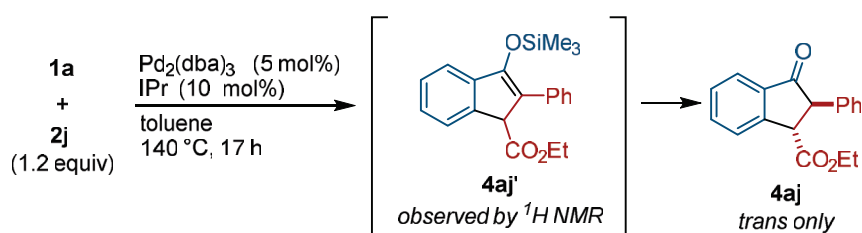


Entry	Reaction time	Yield (%)	
		2j	3aj (<i>Z/E</i> ratio)
1	4 h	19 ^a	53 (31:1) ^a
2	17 h	0	72 (2.5:1) ^b

^aThe yield was estimated by NMR analysis using mesitylene as an internal standard using Pd₂(dba)₃ (5.0 mol%) and IPr (10 mol%). ^bIsolated yield.

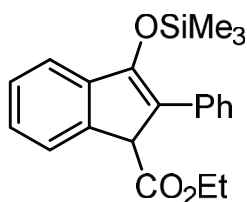


V-2. Observation of Silyl Enol Ether **4aj'** and Its Decomposition



In a glovebox filled with nitrogen, $\text{Pd}_2(\text{dba})_3$ (9.2 mg, 0.010 mmol), IPr (7.8 mg, 0.020 mmol), acylsilane **1a** (35 mg, 0.20 mmol), and alkyne **2j** (41.8 mg, 0.24 mmol) were added to a 10 mL-sample vial with a teflon-sealed screwcap. Toluene (0.6 mL) was then added, and the vial was sealed with the cap. The vial was stirred at 140 °C for 17 h. After allowing the mixture cool to rt, the crude mixture was concentrated in a glovebox. The residue was dissolved in C_6D_6 and analyzed by NMR using mesitylene as an internal standard, which revealed that the silyl enol ether **4aj'** was formed (NMR yield: 75%). The crude mixture was then filtered through a pad of Celite under an atmosphere of air, and the pad was washed with EtOAc. The filtrate was concentrated in vacuo and analyzed by NMR, which indicated that the indanone **4aj** was formed (NMR yield: 59%).

Ethyl 2-phenyl-3-((trimethylsilyl)oxy)-1H-indene-1-carboxylate (**4aj'**).



$^1\text{H NMR}$ (C_6D_6 , 399.78 MHz): δ 7.79–7.76 (m, 2H), 7.50–7.48 (m, 1H), 7.33–7.32 (m, 1H), 7.17–7.09 (m, 3H), 7.06–6.96 (m, 2H), 4.67 (s, 1H), 3.83–3.75 (m, 1H), 3.67–3.59 (m, 1H), 0.62 (t, $J = 6.9$ Hz, 3H), 0.05 (s, 9H).

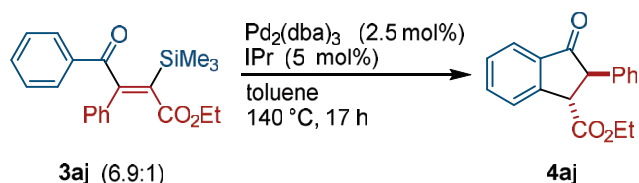
$^{13}\text{C NMR}$ (C_6D_6 , 100.53 MHz): δ 171.0, 152.0, 142.8, 139.6, 135.5, 129.3, 128.6, 127.7, 126.7, 126.6, 123.5, 122.5, 119.2, 60.9, 53.9, 13.9, 0.7.

IR (ATR): 3026 w, 2921 w, 1734 s, 1726 s, 1604 m, 1496 s, 1457 w, 1366 m, 1254 w, 1217 w, 1079 w, 1030 w, 850 m, 759 m, 729 s, 695 s, 465 w, 409 w.

MS m/z (% relative intensity): 352 (M^+ , 33), 280 (21), 279 (81), 73 (100), 45 (10).

HRMS (DART+, $[\text{M}+\text{H}]^+$): Calcd for $\text{C}_{21}\text{H}_{25}\text{O}_3\text{Si}$ 353.1568, Found 353.1564.

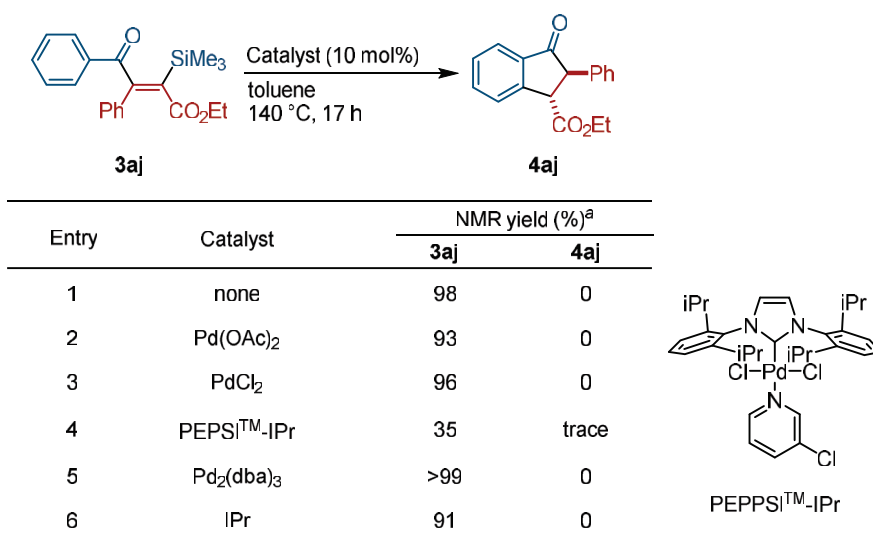
V-3. Pd-Catalyzed Conversion of **3aj** to **4aj**



In a glovebox filled with nitrogen, $\text{Pd}_2(\text{dba})_3$ (13.7 mg, 0.015 mmol), IPr (11.7 mg, 0.030 mmol),

silylacylation product **3aj** (118 mg, 0.34 mmol) were added to a 10 mL-sample vial with a teflon-sealed screwcap. Toluene (0.9 mL) was then added, and the vial was sealed with the cap. The vial was stirred at 140 °C for 17 h. After allowing the mixture to cool to rt, the crude mixture was filtered through a pad of Celite, and the pad was washed with EtOAc. The filtrate was analyzed by GC using dodecane as an internal standard. The filtrate was concentrated in vacuo and purified by flash column chromatography over silica gel (elution with hexane/EtOAc = 10/1) to give **4aj** as a yellow oil (49.1 mg, 52% yield).

V-4. Catalyst Screening for The Synthesis of Indanone Derivatives

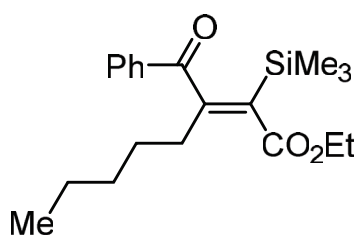


^aThe yield was estimated by NMR analysis using mesitylene as an internal standard.

VI. Spectroscopic Data

VI-1. Silylacylation Products

Ethyl (*Z*)-3-benzoyl-2-(trimethylsilyl)oct-2-enoate (**3aa**).



Method A was followed.

R_f 0.37 (hexane/EtOAc = 10/1). Yellow oil (63.1 mg, 83%).

The product was obtained as a mixture of the title compound and its isomers (7.0:1) determined by ¹H NMR.

¹H NMR (CDCl₃, 399.78 MHz): δ 7.93–7.91 (m, 2H), 7.60–7.56 (m, 1H), 7.50–7.46 (m, 2H), 4.26 (q, *J* = 7.2 Hz, 2H), 2.41–2.37 (m, 2H), 1.39–1.31 (m, 5H), 1.21–1.17 (m, 4H), 0.82–0.75 (m, 3H), -0.01 (s, 9H).

¹³C NMR (CDCl₃, 100.53 MHz): δ 198.8, 171.3, 154.9, 137.7, 135.9, 133.6, 129.6, 128.5, 60.5, 34.6, 31.5, 27.7, 22.2, 14.4, 13.8, -0.7.

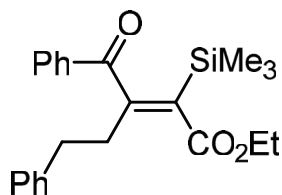
²⁹Si NMR (CDCl₃, 79.43 MHz): δ -5.1.

IR (ATR): 2955 m, 2932 m, 2871 w, 1715 s, 1671s, 1597 w, 1558 w, 1522 w, 1472 w, 1449 w, 1250 s, 1214 s, 1175 w, 1038 m, 956 w, 844 s, 717 w, 693 w.

MS *m/z* (% relative intensity): 346 (M⁺, 3), 331 (13), 301 (13), 300 (15), 289 (11), 285 (33), 258 (11), 217 (11), 135 (16), 123 (37), 105 (83), 103 (59), 77 (51), 75 (71), 73 (100), 67 (17), 59 (17), 55 (11), 45 (14).

HRMS (DART⁺, [M+H]⁺): Calcd for C₂₀H₃₁O₃Si 347.2037, Found 347.2039.

Ethyl (*Z*)-3-benzoyl-5-phenyl-2-(trimethylsilyl)pent-2-enoate (3ad**).**



Method A was followed using **2d** (38.6 mg, 0.19 mmol) and **1a** (71.2 mg, 0.40 mmol).

R_f 0.29 (hexane/EtOAc = 10/1). Pale yellow oil (49.5 mg, 70%).

The product was obtained as a mixture of the title compound and its isomers (8.8:1) determined by ¹H NMR.

¹H NMR (CDCl₃, 399.78 MHz): δ 7.96–7.94 (m, 2H), 7.63–7.58 (m, 1H), 7.52–7.47 (m, 2H), 7.24–7.19 (m, 2H), 7.17–7.12 (m, 1H), 7.09–7.07 (m, 2H), 4.21 (q, *J* = 7.1 Hz, 2H), 2.70 (s, 4H), 1.32 (t, *J* = 7.1 Hz, 3H), 0.02 (s, 9H).

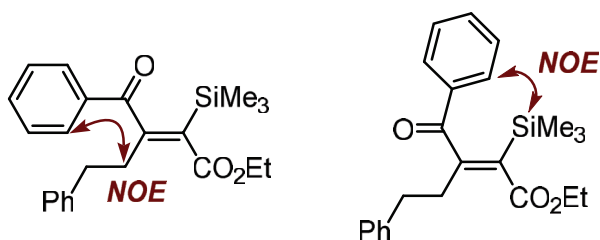
¹³C NMR (CDCl₃, 100.53 MHz): δ 198.7, 171.1, 153.8, 140.8, 138.7, 135.8, 133.8, 129.6, 128.8, 128.4, 128.3, 126.0, 60.6, 36.4, 34.4, 14.4, -0.7.

IR (ATR): 3031 w, 2961 w, 2903 w, 1713 s, 1669s, 1597 w, 1579 w, 1496 w, 1449 m, 1315 w, 1250 s, 1212 s, 1174 w, 1036 m, 980 w, 842 s, 737 m, 699 s, 451 m, 436 m.

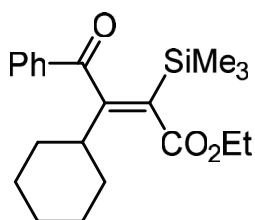
MS *m/z* (% relative intensity): 380 (M⁺, 3), 335 (11), 334 (28), 290 (11), 289 (48), 217 (14), 143 (16), 129 (15), 105 (62), 103 (29), 91 (65), 77 (36), 75 (43), 73 (100), 59 (10), 45 (14).

HRMS (DART⁺, [M+H]⁺): Calcd for C₂₃H₂₉O₃Si 381.1881, Found 381.1800.

The regio- and stereochemistry of the major isomer was determined by NOESY spectroscopy.



Ethyl (Z)-3-cyclohexyl-4-oxo-4-phenyl-2-(trimethylsilyl)but-2-enoate (3ae).



Method A was followed using **2e** (36.5 mg, 0.20 mmol) and **1a** (71.2 mg, 0.40 mmol).

R_f 0.43 (hexane/EtOAc = 10/1). Pale yellow oil (56.0 mg, 77%).

^1H NMR (CDCl_3 , 399.78 MHz): δ 8.00–7.97 (m, 2H), 7.58 (tt, J = 1.5, 7.3 Hz, 1H), 7.49–7.45 (m, 2H), 4.27 (q, J = 7.2 Hz, 2H), 2.52–2.45 (m, 1H), 1.83–1.80 (m, 2H), 1.67–1.61 (m, 2H), 1.56–1.54 (m, 1H), 1.35 (t, J = 7.2 Hz, 3H), 1.22–1.06 (m, 4H), 1.02–0.92 (m, 1H), -0.09 (s, 9H)

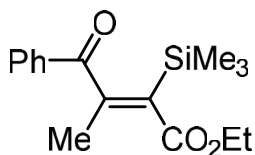
^{13}C NMR (CDCl_3 , 100.53 MHz): δ 198.4, 171.5, 157.6, 137.3, 134.7, 133.7, 130.2, 128.4, 60.4, 44.9, 31.8, 26.3, 25.5, 14.5, -0.7.

IR (ATR): 2930 s, 2853 m, 1714 s, 1669 s, 1595 s, 1542 w, 1521 w, 1449 s, 1317 s, 1251 m, 1215 s, 1036 w, 1010 w, 862 w, 843 s, 733 w, 693 w.

MS m/z (% relative intensity): 358 (M^+ , 9), 312 (22), 297(16), 285 (12), 135 (21), 105 (70), 103 (16), 79 (10), 77 (35), 75 (34), 73 (100), 45 (13).

HRMS (DART+, $[\text{M}+\text{H}]^+$): Calcd for $\text{C}_{21}\text{H}_{31}\text{O}_3\text{Si}$ 359.2037, Found 359.2034.

Ethyl (Z)-3-methyl-4-oxo-4-phenyl-2-(trimethylsilyl)but-2-enoate (3af).



Method A was followed using **2f** (21.1 mg, 0.19 mmol) and **1a** (71.2 mg, 0.40 mmol).

R_f 0.34 (hexane/EtOAc = 10/1). Yellow oil (43.7 mg, 80%).

The product was obtained as a mixture of the title compound and its isomers (7.3:1) determined by ^1H NMR.

^1H NMR (CDCl_3 , 399.78 MHz): δ 7.92–7.90 (m, 2H), 7.61–7.57 (m, 1H), 7.50–7.46 (m, 2H), 4.27 (q, J = 7.3 Hz, 2H), 2.04 (s, 3H), 1.34 (t, J = 7.3 Hz, 3H), 0.01 (s, 9H).

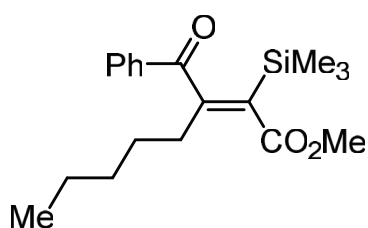
^{13}C NMR (CDCl_3 , 100.53 MHz): δ 199.0, 171.2, 150.5, 138.5, 135.2, 133.7, 129.6, 128.7, 60.6, 20.3, 14.4, -0.7.

IR (ATR): 2971 w, 2958 w, 1715 s, 1671 s, 1598 w, 1449 m, 1365 w, 1268 m, 1217 s, 1040 m, 948 m, 843 s, 726 m, 705 m, 631 w, 418 w.

MS m/z (% relative intensity): 290 (M^+ , 2), 276 (17), 275 (73), 247 (11), 245 (14), 105 (66), 104 (11), 103 (100), 97 (24), 77 (49), 75 (70), 73 (65), 67 (44), 59 (13), 45 (14).

HRMS (DART+, $[\text{M}+\text{H}]^+$): Calcd for $\text{C}_{16}\text{H}_{23}\text{O}_3\text{Si}$ 291.1411, Found 291.1415.

Methyl (*Z*)-3-benzoyl-2-(trimethylsilyl)oct-2-enoate (3ag**).**



Method A was followed using **2g** (28.9 mg, 0.19 mmol) and **1a** (71.2 mg, 0.40 mmol).

R_f 0.37(hexane/EtOAc = 10/1). Pale yellow oil (39.7 mg, 64%).

The product was obtained as a mixture of the title compound and its isomers (8.3:1) determined by ^1H NMR.

^1H NMR (CDCl_3 , 399.78 MHz): δ 7.92-7.89 (m, 2H), 7.60-7.56 (m, 1H), 7.50-7.44 (m, 2H), 3.79 (s, 3H), 2.40-2.36 (m, 2H), 1.37-1.30 (m, 2H), 1.22-1.12 (m, 4H), 0.80 (t, J = 6.9 Hz, 3H), -0.01 (s, 9H).

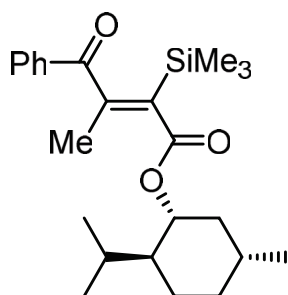
^{13}C NMR (CDCl_3 , 100.53 MHz): δ 198.7, 171.8, 155.3, 137.6, 135.9, 133.6, 129.6, 128.7, 51.4, 34.7, 31.4, 27.7, 22.1, 13.8, -0.7.

IR (ATR): 2953 m, 2931 w, 2872 w, 2155 w, 1717 s, 1671 s, 1597 w, 1580 w, 1449 m, 1433 w, 1315 w, 1250 m, 1219 s, 1176 w, 962 w, 844 s, 732 w, 692 w.

MS m/z (% relative intensity): 333 ($\text{M}+\text{H}^+$, 2), 317 (27), 301 (12), 300 (21), 285 (37), 275 (24), 258 (12), 233 (12), 123 (34), 105 (73), 89 (100), 77 (36), 75 (16), 73 (73), 67 (13), 59 (31), 45 (11).

HRMS (DART+, $[\text{M}+\text{H}]^+$): Calcd for $\text{C}_{19}\text{H}_{29}\text{O}_3\text{Si}$ 333.1881, Found 333.1878.

(1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl (*Z*)-3-methyl-4-oxo-4-phenyl-2-(trimethylsilyl)but-2-enoate (3ah**).**



Method A was followed using **2h** (42.7 mg, 0.19 mmol) and **1a** (71.2 mg, 0.40 mmol).

R_f 0.43(hexane/EtOAc = 10/1). Yellow solid (63.0 mg, 82%). Mp 101.1–101.3 °C.

The product was obtained as a mixture of the title compound and its isomers (11:1) determined by ^1H NMR.

^1H NMR (CDCl_3 , 399.78 MHz): δ 7.92–7.90 (m, 2H), 7.61–7.56 (m, 1H), 7.49 (t, $J = 7.6$ Hz, 2H), 4.80 (dt, $J = 4.3, 10.9$ Hz, 1H), 2.16–2.13 (m, 1H), 2.07–1.98 (m, 4H), 1.73–1.68 (m, 2H), 1.58–1.43 (m, 2H), 1.13–1.01 (m, 2H), 0.94–0.86 (m, 7H), 0.81–0.78 (m, 3H), 0.02 (s, 9H).

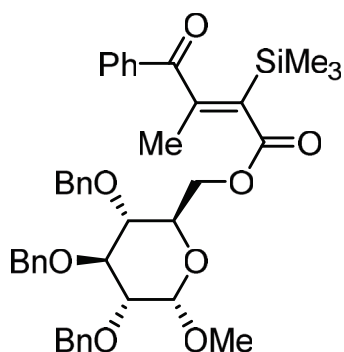
^{13}C NMR (CDCl_3 , 100.53 MHz): δ 199.1, 171.0, 149.5, 138.8, 135.3, 133.7, 129.6, 128.8, 75.1, 46.9, 41.0, 34.2, 31.5, 25.8, 22.9, 22.1, 20.8, 20.2, 15.8, -0.6

IR (ATR): 2954 m, 2930 w, 2870 w, 1709 s, 1672 s, 1597 w, 1580 w, 1456 m, 1449 m, 1371 w, 1223 s, 1022 w, 953 w, 845 s, 727 w, 706 w.

MS m/z (% relative intensity): 400 (M^+ , 10), 262 (23), 261 (23), 247 (23), 245 (31), 219 (15), 218 (19), 217 (49), 138 (14), 105 (45), 97 (26), 95 (20), 83 (77), 81 (22), 77 (17), 75 (35), 73 (100), 69 (30), 67 (14), 57 (22), 55 (47), 43 (19), 41 (20).

HRMS (DART+, $[\text{M}+\text{H}]^+$): Calcd for $\text{C}_{24}\text{H}_{37}\text{O}_3\text{Si}$ 401.2507, Found 401.2506.

((2R,3R,4S,5R,6S)-3,4,5-Tris(benzyloxy)-6-methoxytetrahydro-2H-pyran-2-yl)methyl (Z)-3-methyl-4-oxo-4-phenyl-2-(trimethylsilyl)but-2-enoate (3ai).



Method A was followed using **2i** (97.8 mg, 0.18 mmol) and **1a** (71.2 mg, 0.40 mmol).

R_f 0.46(hexane/EtOAc = 2/1). Pale yellow oil (85.7 mg, 66%).

The product was obtained as a mixture of the title compound and its isomers (30:1) determined by ^1H

NMR.

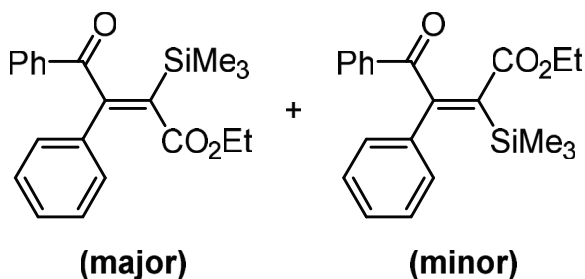
^1H NMR (CDCl_3 , 399.78 MHz): δ 7.91–7.89 (m, 2H), 7.60 (tt, $J = 1.5, 7.3$ Hz, 1H), 7.51–7.47 (m, 2H), 7.38–7.27 (m, 15H), 5.01 (d, $J = 11.0$ Hz, 1H), 4.94 (d, $J = 10.5$ Hz, 1H), 4.82 (t, $J = 11.7$ Hz, 2H), 4.67 (d, $J = 11.9$ Hz, 1H), 4.62 (d, $J = 11.0$ Hz, 1H), 4.56 (d, $J = 3.2$ Hz, 1H), 4.53 (dd, $J = 11.7, 2.1$ Hz, 1H), 4.27 (dd, $J = 5.8$ Hz, 11.9 Hz, 1H), 4.05 (t, $J = 9.2$ Hz, 1H), 3.93–3.88 (m, 1H), 3.53–3.46 (m, 2H), 3.40 (s, 3H), 2.02 (s, 3H), 0.01 (s, 9H).

^{13}C NMR (CDCl_3 , 100.53 MHz): δ 198.8, 171.0, 151.1, 138.5, 138.1, 137.9, 137.8, 135.2, 133.8, 129.6, 128.8, 128.5, 128.5, 128.4, 128.1, 128.0, 128.0, 127.9, 127.8, 127.7, 98.0, 81.8, 79.8, 78.1, 75.8, 75.2, 73.4, 68.8, 63.4, 55.3, 20.6, -0.7.

IR (ATR): 3030 w, 2948 w, 2908 w, 1716 s, 1671 s, 1648 w, 1540 w, 1455 m, 1362 w, 1211 s, 1089 s, 1046 s, 951 w, 844 s, 738 s, 697 s, 419 m.

HRMS (ESI+, $[\text{M}+\text{Na}]^+$): Calcd for $\text{C}_{42}\text{H}_{48}\text{O}_8\text{NaSi}$ 731.3011, Found 731.3025.

Ethyl 4-oxo-3,4-diphenyl-2-(trimethylsilyl)but-2-enoate (3aj).



Method A was followed using **2j** (32.5 mg, 0.19 mmol) and **1a** (71.2 mg, 0.40 mmol), except that $\text{Pd}_2(\text{dba})_3$ (0.0075 mmol) and IPr (0.015 mmol) were used.

R_f 0.29 (hexane/EtOAc = 10/1). Pale yellowish oil (47.1 mg, 72%).

The product was obtained as a mixture of stereoisomers (2.5:1) determined by ^1H NMR.

^1H NMR (CDCl_3 , 399.78 MHz): δ 7.97–7.93 (m, 4H (2H (major) + 2H (minor))), 7.52–7.21 (m, 16H (8H (major) + 8H (minor))), 4.01 (q, $J = 7.2$ Hz, 2H, major), 3.83 (q, $J = 7.2$ Hz, 2H, minor), 1.02–0.96 (m, 6H (3H (major) + 3H (minor))), 0.08 (s, 9H, major), -0.02 (s, 9H, minor).

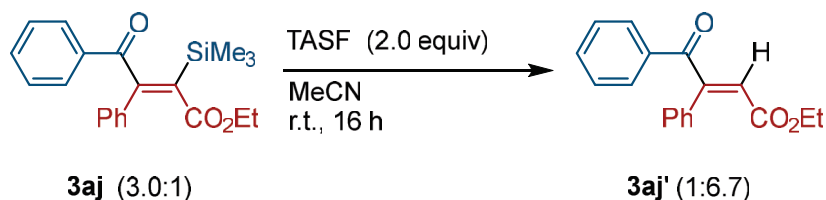
^{13}C NMR (CDCl_3 , 100.53 MHz): δ 196.7 (minor), 196.1 (major), 171.1 (major), 169.7 (minor), 158.0 (minor), 152.6 (major), 139.8 (major), 137.6 (minor), 136.9 (major), 136.4 (minor), 135.9 (major), 134.9 (minor), 133.7 (major), 133.3 (minor), 130.0 (major), 129.4 (minor), 128.60 (major), 128.55 (minor), 128.5 (minor), 128.4 (major), 128.3 (minor), 127.6 (major), 60.8 (minor), 60.6 (major), 13.9 (major), 13.6 (minor), -0.0 (minor), -0.7 (major).

IR (ATR): 3063 s, 2980 s, 2960 s, 2901 s, 1709 m, 1670 m, 1596 w, 1579 w, 1491 w, 1448 w, 1365 w, 1390 w, 1315 w, 1250 w, 1229 s, 1175 w, 1033 w, 871 w, 842 m, 633 w, 445 w.

MS m/z (% relative intensity): 352 (M^+ , 8), 337 (29), 279 (16), 130 (10), 129 (100), 105 (37), 103 (13), 77 (21), 75 (18), 73 (46).

HRMS (DART+, [M+H]⁺): Calcd for C₂₁H₂₅O₃Si 353.1568, Found 353.1572.

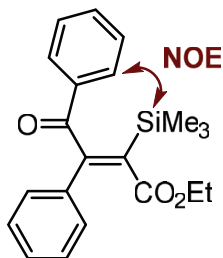
The regiochemistry of the major isomer of **3aj** was determined to be the compound with the silyl group incorporated into the carbon α to the ester group by converting **3aj** into known desilylated product **3aj'**.¹⁰



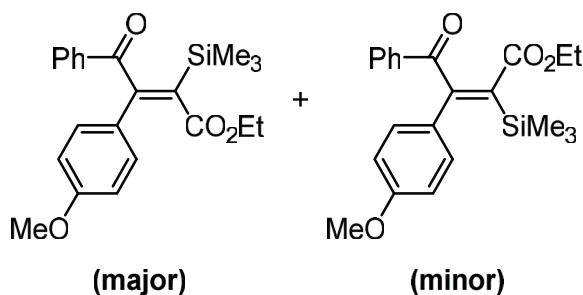
Deprotection of silylacetylated products was performed according to the literature.¹¹ A solution of TASF (40 mg, 0.144 mmol) in MeCN (4.5 mL) was added to a solution of **3aj** (25 mg, 0.072 mmol) in wet MeCN (1.5 mL). After stirring for 16 h, the mixture was filtered through a pad of silica, which was carefully rinsed with EtOAc, the combined filtrates were evaporated, and the residue purified by flash chromatography (hexane/EtOAc, 10/1) to afford **3aj'** (13.7 mg, 68%). The product was obtained as a mixture of *E/Z* isomers (1:6.7) determined by ¹H NMR.

¹H NMR (CDCl₃, 399.78 MHz): δ 7.98–7.91 (m, 4H (2H (*E*) + 2H (*Z*))), 7.57–7.33 (m, 16H (8H (*E*) + 8H (*Z*))), 6.51 (s, 1H, *Z*), 6.27 (s, 1H, *E*), 4.14–4.04 (m, 4H (2H (*E*) + 2H (*Z*))), 1.19–1.09 (m, 6H (3H (*E*) + 3H (*Z*))).

The stereochemistry of the major isomer **3aj** was determined to be *Z* configuration by NOESY spectroscopy.



Ethyl 3-(4-methoxyphenyl)-4-oxo-4-phenyl-2-(trimethylsilyl)but-2-enoate (**3ak**).



Method A was followed using **2k** (61.6 mg, 0.30 mmol) and **1a** (107.0 mg, 0.60 mmol).

R_f 0.20 (hexane/EtOAc = 10/1). Yellow oil (84.3mg, 73%).

The product was obtained as a mixture of stereoisomers (1.9:1) determined by ¹H NMR.

¹H NMR (CDCl₃, 399.78 MHz): δ 7.96–7.92 (m, 4H (2H (major) + 2H (minor))), 7.53–7.48 (m, 2H (1H (major) + 1H (minor))), 7.44–7.32 (m, 8H (4H (major) + 4H (minor))), 6.87–6.83 (m, 2H, minor), 6.81–6.77 (m, 2H, major), 4.06 (q, *J* = 7.2 Hz, 2H, major), 3.84 (q, *J* = 7.2 Hz, 2H, minor), 3.78 (s, 3H, minor), 3.74 (s, 3H, major), 1.09 (t, *J* = 7.2 Hz, 3H, major), 0.98 (t, *J* = 7.2 Hz, 3H, minor), 0.08 (s, 9H, major), 0.03 (s, 9H, minor).

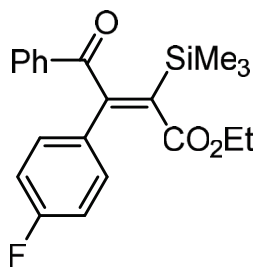
¹³C NMR (CDCl₃, 100.53 MHz): δ 197.0 (minor), 196.3 (major), 171.4 (major), 169.8 (minor), 160.2 (minor), 159.8 (major), 158.1 (minor), 152.1 (major), 138.5 (major), 136.7 (minor), 135.9 (major), 135.0 (minor), 133.6 (major), 133.2 (minor), 130.03 (major), 129.95 (minor), 129.3 (major), 129.2 (minor), 129.0 (major), 128.63 (minor), 128.57 (major), 128.52 (minor), 113.9 (major), 113.7 (minor), 60.7 (minor), 60.6 (major), 55.2 (minor), 55.1 (major), 14.1 (major), 13.6 (minor), 0.1 (minor), -0.6 (major).

IR (ATR): 2956 w, 2838 w, 1707 s, 1668 s, 1605 m, 1508 s, 1449 m, 1297 w, 1250 s, 1229 s, 1176 m, 1069 w, 1031 m, 843 s, 693 m, 609 w.

MS *m/z* (% relative intensity): 382 (M⁺, 25), 367 (23), 310 (14), 309 (49), 159 (60), 105 (23), 77 (18), 75 (17), 73 (100), 45 (11).

HRMS (DART⁺, [M+H]⁺): Calcd for C₂₂H₂₇O₄Si 383.1673, Found 383.1674.

Ethyl (*Z*)-3-(4-fluorophenyl)-4-oxo-4-phenyl-2-(trimethylsilyl)but-2-enoate (**3al**).



Method A was followed using **2l** (38.4mg, 0.20 mmol) and **1a** (71.2 mg, 0.40 mmol), except that Pd₂(dba)₃ (0.005 mmol) and IPr (0.010 mmol) were used.

R_f 0.14 (hexane/EtOAc = 10/1). Yellowish oil (45.2 mg, 61%).

The product was obtained as a mixture of the title compound and its isomers (14:1) determined by ¹H NMR.

¹H NMR (CDCl₃, 399.78 MHz): δ 7.96–7.92 (m, 2H), 7.55–7.52 (m, 1H), 7.47–7.38 (m, 4H), 6.99–6.94 (m, 2H), 4.04 (q, *J* = 7.1 Hz, 2H), 1.06 (t, *J* = 7.1 Hz, 3H), 0.07 (s, 9H).

¹³C NMR (CDCl₃, 100.53 MHz): δ 196.1, 171.0, 162.7 (d, *J* = 248.2 Hz), 151.2, 140.3, 135.7, 133.8, 132.9 (d, *J* = 2.9 Hz), 130.0, 129.5 (d, *J* = 8.6 Hz), 128.7, 115.5 (d, *J* = 21.1 Hz), 60.7, 14.0, -0.7.

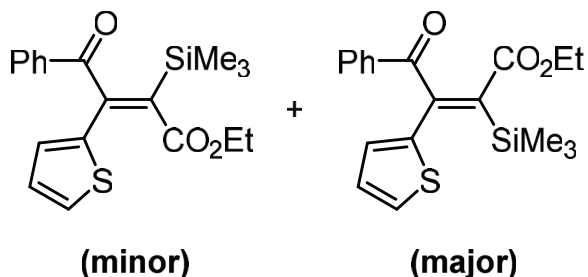
¹⁹F NMR (CDCl₃, 376.17 MHz): δ -114.0.

IR (ATR): 2976 w, 1961 w, 1707 s, 1668 s, 1597 m, 1505 s, 1449 w, 1228 s, 1161 w, 1001 w, 840 s, 734 w, 613 w, 523 w, 461 w.

MS m/z (% relative intensity): 370 (M^+ , 11), 356 (12), 355 (45), 297 (22), 177 (11), 147 (100), 105 (57), 103 (23), 77 (31), 75 (24), 73 (71), 45 (11).

HRMS (DART+, $[M+H]^+$): Calcd for $C_{21}H_{24}O_3FSi$ 371.1473, Found 371.1476.

Ethyl 4-oxo-4-phenyl-3-(thiophen-2-yl)-2-(trimethylsilyl)but-2-enoate (3am).



Method A was followed using **2m** (38.1 mg, 0.21 mmol) and **1a** (71.2 mg, 0.40 mmol), except that $Pd_2(dba)_3$ (0.0075 mmol) and IPr (0.015 mmol) were used.

R_f 0.20 (hexane/EtOAc = 10/1). Yellow oil (40.3 mg, 53%).

The product was obtained as a mixture of stereoisomers (0.4:1) determined by 1H NMR.

1H NMR ($CDCl_3$, 399.78 MHz): δ 8.00–7.98 (m, 2H, major), 7.95–7.93 (m, 2H, minor), 7.57–7.52 (m, 3H, minor), 7.47–7.42 (m, 3H, major), 7.35 (dd, $J = 5.0, 1.4$ Hz, 1H, minor), 7.28 (dd, $J = 5.0, 1.4$ Hz, 1H, major), 7.15–7.14 (m, 1H, minor), 7.00–6.98 (m, 2H (1H(major) + 1H(minor))), 6.90 (dd, $J = 5.0, 3.7$ Hz, 1H, major), 4.23 (q, $J = 7.2$ Hz, 2H, major), 3.81 (q, $J = 7.2$ Hz, 2H, minor), 1.26 (t, $J = 7.2$ Hz, 3H, major), 0.98 (t, $J = 7.2$ Hz, 3H, minor), 0.12 (s, 9H, minor), 0.06 (s, 9H, major).

^{13}C NMR ($CDCl_3$, 100.53 MHz): δ 196.0 (minor), 195.3 (major), 171.2 (major), 169.6 (minor), 150.4 (minor), 144.3 (major), 139.4 (minor), 138.1 (major), 137.7 (major), 137.0 (minor), 135.9 (major), 134.7 (minor), 133.9 (major), 133.6 (minor), 130.1 (major), 129.4 (minor), 128.8 (minor), 128.7 (major), 128.62 (major), 128.59 (minor), 128.4 (minor), 127.8 (major), 127.2 (major), 127.1 (minor), 61.1 (major), 60.9 (minor), 14.1 (major), 13.6 (minor), -0.2 (minor), -0.7 (major).

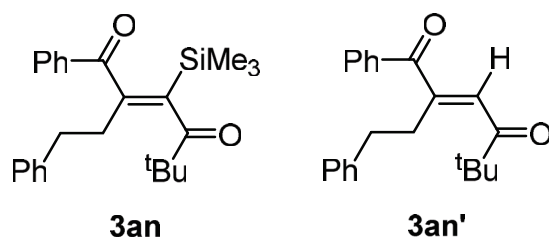
IR (ATR): 2977 w, 2957 w, 1708 s, 1671 s, 1595 m, 1578 m, 1508 w, 1449 m, 1388 w, 1315 w, 1250 m, 1233 s, 1223 s, 1177 w, 1036 m, 984 w, 843 s, 744 w, 700 w, 633 m.

MS m/z (% relative intensity): 358 (22), 343 (25), 286 (14), 285 (49), 135 (100), 105 (59), 103 (13), 77 (38), 75 (26), 73 (90), 45 (16).

HRMS (DART+, $[M+H]^+$): Calcd for $C_{19}H_{23}O_3SiS$ 359.1132, Found 359.1139.

(Z)-5,5-Dimethyl-2-phenethyl-1-phenyl-3-(trimethylsilyl)hex-2-ene-1,4-dione (3an).

(E)-5,5-Dimethyl-2-phenethyl-1-phenylhex-2-ene-1,4-dione (3an').



Method A was followed using **2n** (45.0 mg, 0.21 mmol) and **1a** (71.2 mg, 0.40 mmol), except that Pd₂(dba)₃ (0.0075 mmol) and IPr (0.015 mmol) was used.

Silylacylation product **3an** and its desilylated product **3an'** were obtained and could be separated by column chromatography.

3an

R_f 0.46(hexane/EtOAc = 10/1). Pale yellow oil (16.7 mg, 20%).

The product was obtained as a mixture of the title compound and its isomers (12:1) determined by ¹H NMR.

¹H NMR (CDCl₃, 399.78 MHz): δ 8.02–8.00 (m, 2H), 7.58–7.54 (m, 1H), 7.49–7.44 (m, 2H), 7.30 (t, *J* = 7.3 Hz, 2H), 7.23–7.19 (m, 3H), 2.82–2.78 (m, 2H), 2.39–2.35 (m, 2H), 1.06 (s, 9H), 0.14 (s, 9H).

¹³C NMR (CDCl₃, 100.53 MHz): δ 213.0, 195.7, 154.7, 150.3, 141.8, 137.2, 133.6, 130.2, 128.6, 128.5, 128.2, 126.1, 45.6, 37.7, 36.8, 26.9, 0.1.

IR (ATR): 3062 w, 2962 m, 2870 w, 2155 w, 1685 s, 1657 s, 1598 m, 1496 w, 1449 m, 1317 w, 1243 s, 1177 w, 1082 m, 964 m, 887 w, 842 s, 698 s, 555 w, 478 w, 404 w.

MS *m/z* (% relative intensity): 392 (M⁺, 0.2), 335 (24), 287 (25), 218 (23), 217 (12), 155 (11), 105 (16), 91 (19), 77 (14), 75 (14), 73 (100), 57 (48), 45 (11).

HRMS (DART⁺, [M+H]⁺): Calcd for C₂₅H₃₃O₂Si 393.2244, Found 393.2247.

3an'

R_f 0.20 (hexane/EtOAc = 10/1). Pale yellow oil (51.1 mg, 76%).

The product was obtained as a mixture of the title compound and its isomers (53:1) determined by ¹H NMR.

¹H NMR (CDCl₃, 399.78 MHz): δ 7.85–7.83 (m, 2H), 7.57–7.53 (m, 1H), 7.46–7.42 (m, 2H), 7.31–7.27 (m, 2H), 7.22–7.18 (m, 3H), 6.51 (s, 1H), 2.90–2.87 (m, 2H), 2.73–2.69 (m, 2H), 1.07 (s, 9H).

¹³C NMR (CDCl₃, 100.53 MHz): δ 203.0, 199.2, 157.1, 140.1, 134.8, 133.2, 128.6, 128.49, 128.46, 128.29, 126.3, 122.3, 42.9, 36.6, 33.2, 25.9.

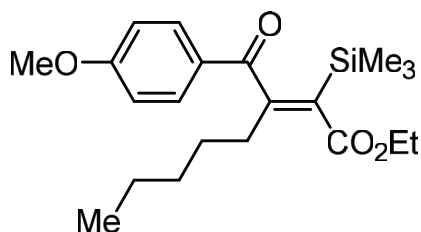
IR (ATR): 2966 w, 2930 w, 1700 s, 1684 s, 1610 s, 1497 w, 1449 s, 1367 m, 1232 s, 1131 w, 1084 m, 1001 w, 888 w, 752 w, 700 s, 492 w.

MS *m/z* (% relative intensity): 320 (M⁺, 20), 264 (44), 263 (16), 235 (12), 173 (49), 145 (19), 117

(12), 105 (86), 91 (100), 77 (39), 57 (64), 41 (15).

HRMS (DART+, [M+H]⁺): Calcd for C₂₂H₂₅O₂ 321.1849, Found 321.1857.

Ethyl (Z)-3-(4-methoxybenzoyl)-2-(trimethylsilyl)oct-2-enoate (3ba).



Method A was followed using **2a** (34.6 mg, 0.21 mmol) and **1b** (83.3 mg, 0.40 mmol).

R_f 0.40 (hexane/EtOAc = 10/1). Yellow oil (62.2 mg, 80%).

The product was obtained as a mixture of the title compound and its isomers (3.7:1) determined by ¹H NMR.

¹H NMR (CDCl₃, 399.78 MHz): δ 7.91–7.89 (m, 2H), 6.96–6.95 (m, 2H), 4.25 (q, *J* = 7.2 Hz, 2H), 3.88 (s, 3H), 2.40–2.36 (m, 2H), 1.38–1.32 (m, 5H), 1.21–1.18 (m, 4H), 0.82–0.77 (m, 3H), -0.02 (s, 9H).

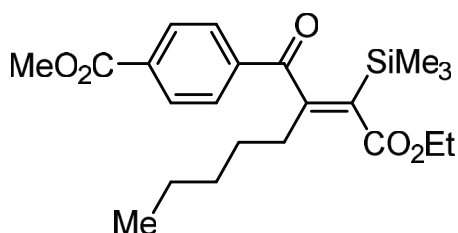
¹³C NMR (CDCl₃, 100.53 MHz): δ 197.4, 171.4, 163.9, 155.2, 136.7, 132.0, 129.1, 113.9, 60.4, 55.5, 34.9, 31.6, 27.8, 22.2, 14.4, 13.9, -0.7.

IR (ATR): 2953 m, 2933 m, 1715 s, 1663 m, 1599 s, 1542 w, 1508 m, 1419 w, 1254 s, 1169 m, 1034 m, 847 s.

MS *m/z* (% relative intensity): 376 (M⁺, 7), 361 (27), 331 (11), 330 (14), 319 (23), 315 (16), 135 (100), 123 (13), 103 (20), 77 (13), 75 (21), 73 (46).

HRMS (DART+, [M+H]⁺): Calcd for C₂₁H₃₃O₄Si 377.2143, Found 377.2144.

Methyl (Z)-4-(2-(2-ethoxy-2-oxo-1-(trimethylsilyl)ethylidene)heptanoyl)benzoate (3ca).



Method A was followed using **2a** (34.5 mg, 0.21 mmol) and **1c** (94.6 mg, 0.40 mmol).

R_f 0.29 (hexane/EtOAc = 10/1). Pale yellow oil (61.0 mg, 73%).

The product was obtained as a mixture of the title compound and its isomers (10:1) determined by ¹H NMR.

¹H NMR (CDCl₃, 399.78 MHz): δ 8.14 (d, *J* = 8.8 Hz, 2H), 7.97 (d, *J* = 8.8 Hz, 2H), 4.27 (q, *J* = 7.2 Hz, 2H), 3.95 (s, 3H), 2.38 (t, *J* = 8.0 Hz, 2H), 1.37–1.30 (m, 5H), 1.20–1.16 (m, 4H), 0.80 (t, *J* = 7.2

Hz, 3H), 0.00 (s, 9H).

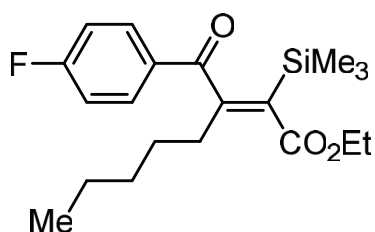
^{13}C NMR (CDCl_3 , 100.53 MHz): δ 198.3, 171.1, 166.1, 154.2, 139.2, 138.8, 134.4, 129.9, 129.4, 60.6, 52.5, 34.3, 31.4, 27.7, 22.2, 14.4, 13.8, -0.7.

IR (ATR): 2954 m, 2933 w, 2871 w, 1723 s, 1672 w, 1558 w, 1521 w, 1472 w, 1437 w, 1406 w, 1279 s, 1250 m, 1219 m, 1107 m, 845 m, 745 m.

MS m/z (% relative intensity): 404 (M^+ , 9), 389 (11), 347 (30), 343 (22), 299 (19), 275 (13), 262 (33), 227 (19), 201 (11), 189 (20), 188 (12), 163 (43), 135 (17), 123 (39), 115 (12), 104 (14), 103 (38), 77 (11), 75 (41), 73 (100), 69 (10), 67 (14), 59 (20), 55 (18), 45 (15), 44 (20), 43 (17), 41 (17).

HRMS (DART+, $[\text{M}+\text{H}]^+$): Calcd for $\text{C}_{22}\text{H}_{33}\text{O}_5\text{Si}$ 405.2092, Found 405.2085.

Ethyl (Z)-3-(4-fluorobenzoyl)-2-(trimethylsilyl)oct-2-enoate (3da).



Method A was followed using **2a** (36.7 mg, 0.22 mmol) and **1d** (78.4 mg, 0.40 mmol).

R_f 0.50 (hexane/EtOAc = 10/1). Yellow oil (65.5 mg, 82%).

The product was obtained as a mixture of the title compound and its isomers (7.4:1) determined by ^1H NMR.

^1H NMR (CDCl_3 , 399.78 MHz): δ 7.98–7.92 (m, 2H), 7.18–7.13 (m, 2H), 4.26 (q, $J = 7.2$ Hz, 2H), 2.39–2.35 (m, 2H), 1.36–1.29 (m, 5H), 1.27–1.12 (m, 4H), 0.82–0.77 (m, 3H), -0.01 (s, 9H).

^{13}C NMR (CDCl_3 , 100.53 MHz): δ 197.2, 171.2, 166.0 (d, $J = 255.9$ Hz), 154.4, 137.8, 132.2 (d, $J = 8.6$ Hz), 131.6 (d, $J = 9.6$ Hz), 115.9 (d, $J = 22.0$ Hz), 60.6, 34.6, 31.5, 27.8, 22.2, 14.4, 13.8, -0.7.

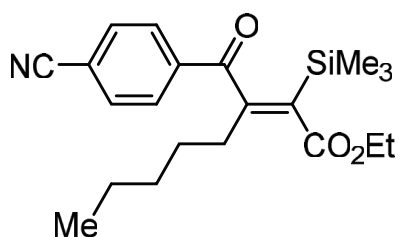
^{19}F NMR (CDCl_3 , 376.17 MHz): δ -105.1.

IR (ATR): 2957 m, 2932 m, 2861 w, 1715 s, 1671 s, 1597 s, 1506 m, 1449 w, 1365 w, 1249 w, 1227 s, 1152 m, 1037 w, 957 w, 844 s, 692w.

MS m/z (% relative intensity): 364 (M^+ , 4), 349 (20), 321 (13), 319 (17), 318 (22), 307 (14), 304 (10), 303 (42), 276 (15), 235 (10), 123 (100), 103 (66), 95 (27), 75 (52), 73 (78), 67 (11), 59 (13).

HRMS (DART+, $[\text{M}+\text{H}]^+$): Calcd for $\text{C}_{20}\text{H}_{30}\text{O}_3\text{FSi}$ 365.1943, Found 365.1946.

Ethyl (Z)-3-(4-cyanobenzoyl)-2-(trimethylsilyl)oct-2-enoate (3ea).



Method A was followed using **2a** (36.4 mg, 0.22 mmol) and **1e** (81.3 mg, 0.40 mmol).

R_f 0.29 (hexane/EtOAc = 10/1). Yellow oil (44.4 mg, 56%).

The product was obtained as a mixture of the title compound and its isomers (22:1) determined by ^1H NMR.

^1H NMR (CDCl_3 , 399.78 MHz): δ 8.01 (d, $J = 8.7$ Hz, 2H), 7.79 (d, $J = 8.7$ Hz, 2H), 4.27 (q, $J = 7.2$ Hz, 2H), 2.38–2.34 (m, 2H), 1.37–1.27 (m, 5H), 1.22–1.16 (m, 4H), 0.80 (t, $J = 6.9$ Hz, 3H), 0.00 (s, 9H).

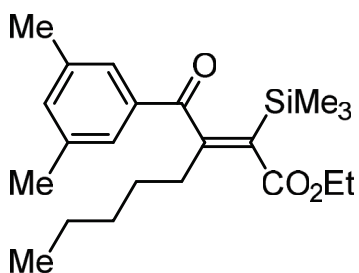
^{13}C NMR (CDCl_3 , 100.53 MHz): δ 197.4, 170.9, 153.4, 139.8, 138.9, 132.6, 129.8, 117.8, 116.8, 60.7, 34.1, 31.3, 27.7, 22.1, 14.4, 13.8, -0.7.

IR (ATR): 2957 m, 2933 m, 2232 w, 1715 s, 1679 s, 1604 w, 1465 w, 1405 w, 1251 s, 1220 s, 1037 w, 955 w, 846 s, 418 m.

MS m/z (% relative intensity): 371 (M^+ , 5), 356 (11), 314 (14), 310 (20), 242 (13), 130 (30), 123 (36), 103 (58), 102 (20), 75 (61), 73 (100), 67 (13), 59 (13), 45 (13).

HRMS (DART+, $[\text{M}+\text{H}]^+$): Calcd for $\text{C}_{21}\text{H}_{30}\text{NO}_3\text{Si}$ 372.1990, Found 372.1982.

Ethyl (Z)-3-(3,5-dimethylbenzoyl)-2-(trimethylsilyl)oct-2-enoate (3fa).



Method A was followed using **2a** (32.7 mg, 0.19 mmol) and **1f** (82.5 mg, 0.40 mmol).

R_f 0.40 (hexane/EtOAc = 10/1). Colorless oil (55.5 mg, 76%).

The product was obtained as a mixture of the title compound and its isomers (7.0:1) determined by ^1H NMR.

^1H NMR (CDCl_3 , 399.78 MHz): δ 7.52 (s, 2H), 7.21 (s, 1H), 4.26 (q, $J = 7.1$ Hz, 2H), 2.40–2.34 (m, 8H), 1.36–1.30 (m, 5H), 1.21–1.17 (m, 4H), 0.81 (t, $J = 7.1$ Hz, 3H), 0.00 (s, 9H).

^{13}C NMR (CDCl_3 , 100.53 MHz): δ 199.2, 171.5, 155.3, 138.3, 137.4, 136.0, 135.4, 127.3, 60.5, 34.7, 31.5, 27.8, 22.2, 21.2, 14.4, 13.9, -0.6.

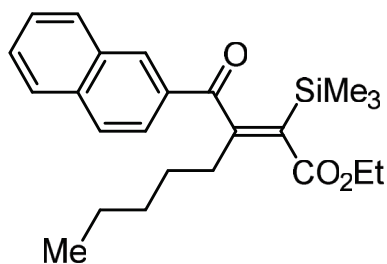
IR (ATR): 2956 m, 2929 m, 1715 s, 1670 s, 1605 w, 1508 w, 1457 w, 1379 w, 1305 m, 1210 s, 1092

w, 966 w, 845 s, 694 w.

MS m/z (% relative intensity): 374 (M^+ , 13), 359 (20), 329 (21), 328 (30), 318 (14), 317 (45), 314 (13), 313 (45), 301 (15), 245 (20), 134 (10), 133 (100), 123 (37), 105 (42), 103 (50), 79 (15), 77 (12), 75 (46), 73 (86), 67 (11), 59 (13).

HRMS (DART+, $[M+H]^+$): Calcd for $C_{22}H_{35}O_3Si$ 375.2350, Found 375.2350.

Ethyl (Z)-3-(2-naphthoyl)-2-(trimethylsilyl)oct-2-enoate (3ga).



Method A was followed using **2a** (34.4 mg, 0.20 mmol) and **1g** (91.3 mg, 0.40 mmol).

R_f 0.34 (hexane/EtOAc = 10/1). Pale yellow oil (60.1 mg, 74%).

The product was obtained as a mixture of the title compound and its isomers (9.4:1) determined by 1H NMR.

1H NMR ($CDCl_3$, 399.78 MHz): δ 8.43 (s, 1H), 8.03–8.00 (m, 2H), 7.94–7.89 (m, 2H), 7.65–7.55 (m, 2H), 4.30 (q, $J = 7.0$ Hz, 2H), 2.50–2.46 (m, 2H), 1.42–1.36 (m, 5H), 1.23–1.18 (m, 4H), 0.82–0.79 (m, 3H), 0.01 (s, 9H).

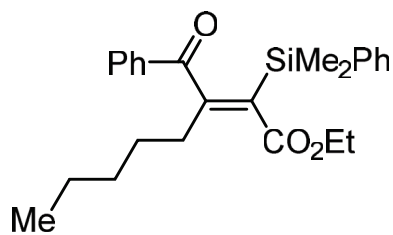
^{13}C NMR ($CDCl_3$, 100.53 MHz): δ 198.8, 171.4, 155.0, 137.8, 135.9, 133.3, 132.4, 132.1, 129.8, 128.8, 128.7, 127.9, 126.9, 124.4, 60.6, 34.8, 31.5, 27.8, 22.2, 14.4, 13.9, -0.6.

IR (ATR): 2955 m, 2929 m, 2870 w, 2860 w, 1714 s, 1667 m, 1626 w, 1508 w, 1458 w, 1387 w, 1353 w, 1248 m, 1218 s, 1185 m, 1122 w, 1037 w, 844 s, 781 w, 452 m.

MS m/z (% relative intensity): 396 (M^+ , 15), 381 (11), 340 (16), 339 (53), 293 (11), 267 (13), 207 (11), 193 (11), 155 (26), 127 (29), 123 (12), 103 (17), 75 (24), 73 (100), 45 (11).

HRMS (DART+, $[M+H]^+$): Calcd for $C_{24}H_{33}O_3Si$ 397.2194, Found 397.2199.

Ethyl (Z)-3-benzoyl-2-(dimethyl(phenyl)silyl)oct-2-enoate (3ha).



Method A was followed using **2a** (32.4 mg, 0.19 mmol) and **1h** (96.2 mg, 0.40 mmol).

R_f 0.43 (hexane/EtOAc = 10/1). Light brown oil (72.9 mg, 92%).

The product was obtained as a mixture of the title compound and its isomers (5.7:1) determined by ¹H NMR.

¹H NMR (CDCl₃, 399.78 MHz): δ 7.75–7.72 (m, 2H), 7.52–7.47 (m, 1H), 7.38–7.33 (m, 4H), 7.21–7.13 (m, 3H), 4.10 (q, *J* = 7.3 Hz, 2H), 2.44–2.40 (m, 2H), 1.38–1.30 (m, 2H), 1.25–1.17 (m, 7H), 0.82–0.78 (m, 3H), 0.31 (s, 6H).

¹³C NMR (CDCl₃, 100.53 MHz): δ 198.3, 171.0, 156.7, 136.4, 136.0, 135.5, 134.2, 133.3, 129.5, 129.1, 128.3, 127.3, 60.5, 34.7, 31.5, 27.8, 22.2, 14.2, 13.9, -1.9.

IR (ATR): 3068 w, 2956 m, 2931 m, 1713 s, 1670 s, 1597 w, 1449 w, 1315 w, 1218 s, 1112 w, 1038 w, 986 w, 838 m, 729m, 701 m, 654 w, 481 w.

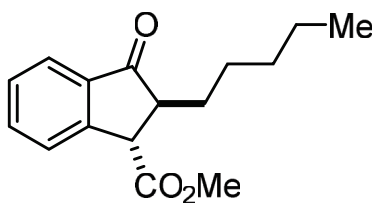
MS *m/z* (% relative intensity): 408 (M⁺, 18), 394 (10), 393 (33), 351 (1), 331 (25), 305 (17), 203 (19), 165 (10), 137 (26), 136 (14), 135 (100), 123 (19), 121 (20), 107 (13), 105 (61), 103 (16), 91 (11), 77 (31), 75 (28), 43 (14).

HRMS (DART⁺, [M+H]⁺): Calcd for C₂₅H₃₃O₃Si 409.2194, Found 409.2190.

VI-2. Indanone Products

The relative stereochemistries of the following indanone derivatives were determined to be *trans* based on the coupling constants of the ring methine protons (*trans*: ~5 Hz; *cis*: ~8 Hz).¹²

Methyl *trans*-3-oxo-2-pentyl-2,3-dihydro-1*H*-indene-1-carboxylate (**4ag**).



Method B was followed using **1a** (35.6 mg, 0.20 mmol) and **2g** (37.0mg, 0.24 mmol).

R_f 0.29 (hexane/EtOAc = 10/1). Yellow oil (44.0 mg, 85%).

¹H NMR (CDCl₃, 399.78 MHz): δ 7.77 (d, *J* = 7.8 Hz, 1H), 7.66–7.61 (m, 2H), 7.48–7.43 (m, 1H), 3.96 (d, *J* = 4.1 Hz, 1H), 3.80 (s, 3H), 3.14–3.10 (m, 1H), 2.01–1.92 (m, 1H), 1.61–1.52 (m, 2H), 1.43–1.27 (m, 5H), 0.90–0.86 (m, 3H).

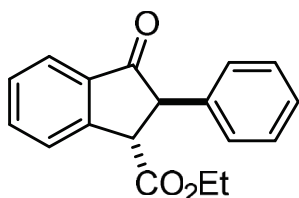
¹³C NMR (CDCl₃, 100.53 MHz): δ 206.3, 172.6, 150.0, 136.1, 135.0, 128.8, 126.1, 124.1, 52.6, 51.1, 50.4, 31.7, 30.7, 26.7, 22.4, 14.0.

IR (ATR): 2953 m, 2931 m, 2936 w, 1739 s, 1717 s, 1670 w, 1647 w, 1541 w, 1507 w, 1457 w, 1418 w, 1364 w, 1216 m, 1168 w, 758 w, 458 w, 419 w.

MS *m/z* (% relative intensity): 260 (M⁺, 4), 203 (12), 191 (10), 190 (86), 158 (24), 131 (63), 130 (100), 129 (12), 128 (10), 116 (12), 115 (31), 103 (10), 91 (11), 41 (13).

HRMS (DART+, [M+H]⁺): Calcd for C₁₆H₂₁O₃ 261.1485, Found 261.1485.

Ethyl *trans*-3-oxo-2-phenyl-2,3-dihydro-1*H*-indene-1-carboxylate (4aj). [CAS: 79379-67-2]



Method B was followed using **1a** (36.7 mg, 0.21 mmol) and **2j** (41.8mg, 0.24 mmol).

R_f 0.14 (hexane/EtOAc = 10/1). Yellow oil (50.4 mg, 87%).

¹H NMR (CDCl₃, 399.78 MHz): δ 7.85 (d, *J* = 7.8 Hz, 1H), 7.77–7.68 (m, 2H), 7.52 (t, *J* = 7.6 Hz, 1H), 7.36–7.27 (m, 3H), 7.20–7.17 (m, 2H), 4.40 (d, *J* = 4.6 Hz, 1H), 4.35 (d, *J* = 4.6 Hz, 1H), 4.32–4.23 (m, 2H), 1.33 (t, *J* = 7.1 Hz, 3H).

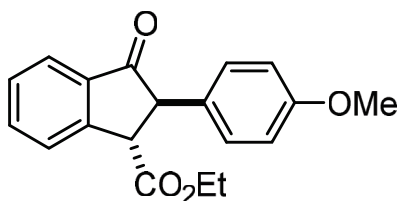
¹³C NMR (CDCl₃, 100.53 MHz): δ 203.8, 171.3, 149.9, 138.2, 135.6, 135.3, 129.1, 128.9, 128.2, 127.4, 126.0, 124.6, 61.8, 56.5, 53.4, 14.2.

IR (ATR): 3062 w, 2981 w, 2936 w, 2871 w, 1719 s, 1671 w, 1601 m, 1464 w, 1393 w, 1317 w, 1216 s, 1192 s, 1178 s, 1034 m, 1015 m, 848 m, 760 m, 699 s, 447 w.

MS *m/z* (% relative intensity): 281 (M+H⁺, 21), 280 (M⁺, 100), 253 (11), 252 (61), 208 (21), 207 (92), 206 (81), 205 (17), 180 (10), 179 (68), 178 (99), 177 (19), 176 (21), 152 (21), 151 (11), 133 (12), 89 (31), 88 (12), 77 (12), 76 (24).

HRMS (DART+, [M+H]⁺): Calcd for C₁₈H₁₇O₃ 281.1172, Found 281.1175.

Ethyl *trans*-2-(4-methoxyphenyl)-3-oxo-2,3-dihydro-1*H*-indene-1-carboxylate (4ak).



Method B was followed using **1a** (44.4 mg, 0.25 mmol) and **2k** (56.1mg, 0.29 mmol).

R_f 0.11 (hexane/EtOAc = 10/1). Red oil (46.7 mg, 61%).

¹H NMR (CDCl₃, 399.78 MHz): δ 7.84 (d, *J* = 7.3 Hz, 1H), 7.75–7.67 (m, 2H), 7.53–7.49 (m, 1H), 7.11 (dt, *J* = 9.3, 2.5 Hz, 2H), 6.87 (dt, *J* = 9.3, 2.5 Hz, 2H), 4.34 (d, *J* = 4.6 Hz, 1H), 4.32–4.22 (m, 3H), 3.79 (s, 3H), 1.33 (t, *J* = 7.1 Hz, 3H).

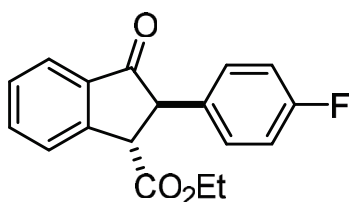
¹³C NMR (CDCl₃, 100.53 MHz): δ 204.1, 171.3, 158.9, 149.8, 135.5, 135.3, 130.2, 129.3, 129.0, 126.0, 124.6, 114.4, 61.8, 55.9, 55.3, 53.5, 14.3.

IR (ATR): 2970 m, 2936 m, 1719 s, 1647 w, 1609 m, 1514 s, 1463 m, 1368 m, 1318 w, 1288 w, 1251 s, 1229 m, 1179 m, 1035 m, 1016 w, 830 w, 759 m, 527 w, 419 w.

MS m/z (% relative intensity): 311 (M+H⁺, 16), 310 (M⁺, 69), 282 (41), 238 (13), 237 (65), 236 (100), 235 (11), 209 (12), 194 (15), 166 (13), 165 (43), 108 (17).

HRMS (DART+, [M+H]⁺): Calcd for C₁₉H₁₉O₄ 311.1278, Found 311.1277.

Ethyl *trans*-2-(4-fluorophenyl)-3-oxo-2,3-dihydro-1*H*-indene-1-carboxylate (4al).



Method B was followed using **1a** (36.4 mg, 0.20 mmol) and **2l** (46.1 mg, 0.24 mmol).

R_f 0.14 (hexane/EtOAc = 10/1). Pale yellowish oil (51.7 mg, 85%).

¹H NMR (CDCl₃, 399.78 MHz): δ 7.84 (d, *J* = 7.8 Hz, 1H), 7.77–7.69 (m, 2H), 7.52 (t, *J* = 7.3 Hz, 1H), 7.19–7.14 (m, 2H), 7.02 (tt, *J* = 8.9, 2.4 Hz, 2H), 4.38 (d, *J* = 5.0 Hz, 1H), 4.33–4.23 (m, 3H), 1.34 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (CDCl₃, 100.53 MHz): δ 203.5, 171.1, 162.1 (d, *J* = 245.3 Hz), 149.6, 135.5, 135.4, 133.8 (d, *J* = 3.8 Hz), 129.9 (d, *J* = 8.6 Hz), 129.2, 126.0, 124.6, 115.8 (d, *J* = 22.0 Hz), 61.9, 55.7, 53.4, 14.2.

¹⁹F NMR (CDCl₃, 376.17 MHz): δ -116.3.

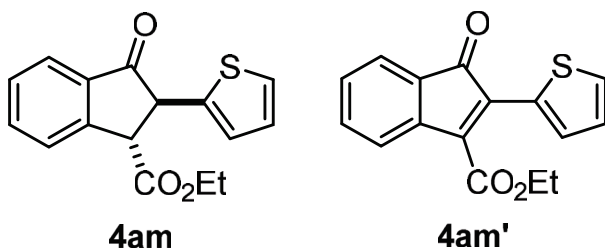
IR (ATR): 2982 w, 2908 w, 1718 s, 1604 m, 1509 s, 1463 m, 1369 w, 1319 w, 1287 w, 1226 s, 1161 m, 1097 m, 1034 m, 1014 m, 833 w, 758 s, 550 w, 518 w, 433 w, 407 w.

MS m/z (% relative intensity): 299 (M+H⁺, 20), 298 (M⁺, 100), 271 (14), 270 (76), 242 (11), 241 (12), 226 (23), 225 (96), 224 (85), 223 (19), 197 (43), 196 (79), 195 (13), 194 (13), 177 (19), 176 (18), 170 (13), 133 (24), 98 (23), 85 (11).

HRMS (DART+, [M+H]⁺): Calcd for C₁₈H₁₆O₃F 299.1078, Found 299.1081.

Ethyl *trans*-3-oxo-2-(thiophen-2-yl)-2,3-dihydro-1*H*-indene-1-carboxylate (4am).

Ethyl 1-oxo-2-(thiophen-2-yl)-1*H*-indene-3-carboxylate (4am').



Method B was followed using **1a** (33.6 mg, 0.19 mmol) and **2m** (43.2 mg, 0.24 mmol).

Indanone **4am** and indenone **4am'** were obtained and these compounds could be separated by GPC.

4am

R_f 0.14 (hexane/EtOAc = 10/1) Pale purple oil (31.0 mg, 57%).

¹H NMR (CDCl₃, 399.78 MHz): δ 7.85 (d, *J* = 7.8 Hz, 1H), 7.74–7.68 (m, 2H), 7.53–7.49 (m, 1H), 7.24 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.01–6.98 (m, 2H), 4.67 (d, *J* = 4.6 Hz, 1H), 4.42 (d, *J* = 4.6 Hz, 1H), 4.37–4.24 (m, 2H), 1.35 (t, *J* = 7.3 Hz, 3H).

¹³C NMR (CDCl₃, 100.53 MHz): δ 201.5, 170.9, 149.1, 139.0, 135.5, 134.7, 129.2, 127.0, 125.9, 125.8, 124.9, 124.8, 62.0, 53.5, 51.5, 14.3.

IR (ATR): 3027 w, 2970 w, 2934 w, 1731 s, 1685 w, 1604 m, 1542 w, 1473 w, 1457 w, 1319 w, 1216 m, 1199 m, 1176 m, 1011 w, 702 m, 407 w.

MS *m/z* (% relative intensity): 287 (M+H⁺, 17), 286 (M⁺, 90), 258 (30), 229 (10), 214 (21), 213 (100), 212 (79), 186 (10), 185 (51), 184 (61), 152 (31), 141 (19), 139 (23), 133 (12), 115 (22), 97 (21), 92 (29).

HRMS (DART⁺, [M+H]⁺): Calcd for C₁₆H₁₅O₃S 287.0736, Found 287.0736.

4am'

R_f 0.29 (hexane/EtOAc = 10/1) Purple oil (14.3 mg, 27%).

¹H NMR (CDCl₃, 399.78 MHz): δ 7.93 (dd, *J* = 3.9, 1.1 Hz, 1H), 7.56–7.53 (m, 2H), 7.43–7.42 (m, 2H), 7.25–7.21 (m, 1H), 7.15–7.12 (m, 1H), 4.48 (q, *J* = 7.2 Hz, 2H), 1.44 (t, *J* = 7.2 Hz, 3H).

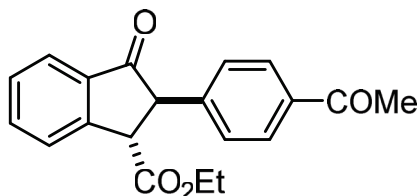
¹³C NMR (CDCl₃, 100.53 MHz): δ 195.4, 164.7, 143.5, 137.7, 134.8, 132.0, 130.8, 130.6, 129.0, 128.7, 128.4, 127.3, 124.0, 122.6, 61.7, 14.2.

IR (ATR): 2995 w, 2935 w, 1771 s, 1757 s, 1718 w, 1653 w, 1636 s, 1559 m, 1457 w, 1387 m, 1246 s, 1060 m, 846 w, 741 w, 514 w.

MS *m/z* (% relative intensity): 285 (M+H⁺, 20), 284 (M⁺, 100), 256 (14), 239 (14), 228 (28), 227 (30), 212 (25), 211 (18), 184 (14), 183 (10), 172 (10), 171 (16), 139 (58), 91 (12).

HRMS (DART⁺, [M+H]⁺): Calcd for C₁₆H₁₃O₃S 285.0580, Found 285.0582.

Ethyl *trans*-2-(4-acetylphenyl)-3-oxo-2,3-dihydro-1*H*-indene-1-carboxylate (4ao**).**



Method B was followed using **1a** (35.4 mg, 0.20 mmol) and **2o** (51.8 mg, 0.24 mmol).

R_f 0.71 (EtOAc). Yellow oil (49.7 mg, 78%).

¹H NMR (CDCl₃, 399.78 MHz): δ 7.92 (dt, *J* = 8.2, 1.8 Hz, 2H), 7.84 (d, *J* = 7.8 Hz, 1H), 7.78–7.69 (m, 2H), 7.55–7.51 (m, 1H), 7.32–7.29 (m, 2H), 4.46 (d, *J* = 4.6 Hz, 1H), 4.35 (d, *J* = 4.6 Hz, 1H), 4.33–4.23 (m, 2H), 2.58 (s, 3H), 1.33 (t, *J* = 7.1 Hz, 3H).

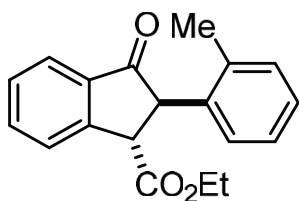
¹³C NMR (CDCl₃, 100.53 MHz): δ 202.7, 197.6, 170.9, 149.6, 143.4, 136.2, 135.6, 135.3, 129.3, 128.9, 128.5, 126.1, 124.7, 62.0, 56.3, 52.9, 26.6, 14.2.

IR (ATR): 2983 w, 1780 w, 1718 s, 1684 s, 1604 m, 1576 w, 1465 w, 1361 w, 1265 s, 1195 w, 1147 w, 1095 w, 1018 w, 959 w, 1250 w, 800 w, 758 w, 709 w, 606 m.

MS *m/z* (% relative intensity): 322 (M⁺, 6), 321 (16), 320 (71), 306 (22), 305 (100), 277 (33), 249 (27), 176 (19), 165 (15), 43 (31).

HRMS (DART⁺, [M+H]⁺): Calcd for C₂₀H₁₉O₄ 323.1278, Found 323.1279.

Ethyl *trans*-3-oxo-2-(*o*-tolyl)-2,3-dihydro-1*H*-indene-1-carboxylate (4ap).



Method B was followed using **1a** (34.7 mg, 0.19 mmol) and **2p** (45.1 mg, 0.24 mmol).

R_f 0.14 (hexane/EtOAc = 10/1). Yellow oil (56.2 mg, 98%).

¹H NMR (CDCl₃, 399.78 MHz): δ 7.86 (d, *J* = 7.3 Hz, 1H), 7.76–7.68 (m, 2H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.23–7.11 (m, 3H), 6.94 (d, *J* = 7.3 Hz, 1H), 4.64 (d, *J* = 4.6 Hz, 1H), 4.35–4.20 (m, 3H), 2.34 (s, 3H), 1.33 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (CDCl₃, 100.53 MHz): δ 204.4, 171.4, 149.9, 137.1, 137.0, 135.7, 135.2, 130.8, 129.1, 128.2, 127.5, 126.4, 125.9, 124.5, 61.8, 54.1, 53.2, 20.1, 14.2.

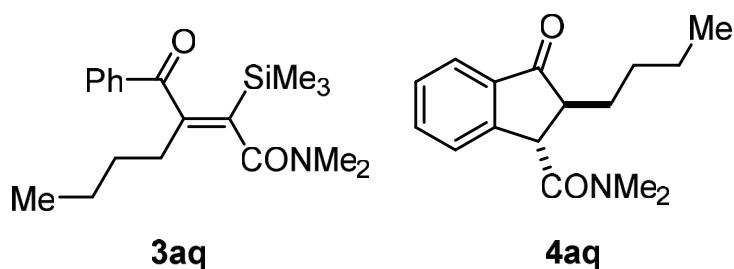
IR (ATR): 3014 w, 2971 w, 2936 w, 1718 s, 1602 m, 1541 w, 1507 w, 1462 m, 1368 m, 1319 w, 1228 m, 1191 m, 1096 w, 1033 w, 900 w, 753 m, 731 w, 507 w, 453 w, 419 w.

MS *m/z* (% relative intensity): 294 (M⁺, 26), 277 (20), 276 (100), 248 (14), 222 (14), 221 (76), 220 (36), 219 (34), 203 (29), 202 (19), 193 (32), 192 (33), 191 (27), 189 (14), 179 (14), 178 (50), 165 (14), 115 (38), 92 (19), 91 (25), 89 (12).

HRMS (DART⁺, [M+H]⁺): Calcd for C₁₉H₁₉O₃ 295.1329, Found 295.1331.

(*Z*)-3-Benzoyl-*N,N*-dimethyl-2-(trimethylsilyl)hept-2-enamide (3aq).

***trans*-2-Butyl-*N,N*-dimethyl-3-oxo-2,3-dihydro-1*H*-indene-1-carboxamide (4aq).**



Method A was followed using **2q** (30.7mg, 0.20 mmol) and **1a** (71.2 mg, 0.40 mmol), except that Pd₂(dba)₃ (0.0075 mmol) and IPr (0.015 mmol) were used.

Silylacylation product **3aq** and indanone **4aq** were obtained and these compounds could be separated by column chromatography.

3aq

R_f 0.40 (hexane/EtOAc = 3/2). Pale yellow oil (17.2 mg, 26%).

¹H NMR (CDCl₃, 399.78 MHz): δ 8.11–8.09 (m, 2H), 7.57–7.52 (m, 1H), 7.46–7.42 (m, 2H), 3.03 (s, 3H), 2.88 (s, 3H), 2.32–2.30 (m, 2H), 1.45–1.31 (m, 4H), 0.92 (t, *J* = 7.3 Hz, 3H), 0.05 (s, 9H).

¹³C NMR (CDCl₃, 100.53 MHz): δ 195.8, 167.6, 152.0, 147.7, 136.9, 133.5, 130.3, 128.3, 38.3, 34.5, 34.1, 31.7, 23.2, 13.9, 0.1.

IR (ATR): 2988 w, 2943 w, 1734 s, 1719 s, 1603 w, 1559 w, 1507 w, 1472 w, 1419 w, 1230 m, 1200 m, 1079 w, 1021 w, 842 w, 710 m, 625 w, 507 w, 409 w.

MS *m/z* (% relative intensity): 331 (M⁺, 26), 316 (15), 288 (34), 287 (39), 275 (29), 274 (100), 229 (41), 129 (11), 105 (24), 77 (14), 75 (33), 73 (14), 72 (56).

HRMS (DART+, [M+H]⁺): Calcd for C₁₉H₃₀NO₂Si 332.2040, Found 332.2041.

4aq

R_f 0.20 (hexane/EtOAc = 3/2). Pale yellow oil (35.9 mg, 70%).

¹H NMR (CDCl₃, 399.78 MHz): δ 7.68 (d, *J* = 7.8 Hz, 1H), 7.63–7.59 (m, 1H), 7.53–7.51 (m, 1H), 7.35 (t, *J* = 7.3 Hz, 1H), 4.03–3.99 (m, 1H), 3.73 (d, *J* = 3.5 Hz, 1H), 3.32 (s, 3H), 3.04 (s, 3H), 2.01–1.97 (m, 1H), 1.61–1.52 (m, 1H), 1.44–1.22 (m, 4H), 0.90 (t, *J* = 7.1 Hz, 3H).

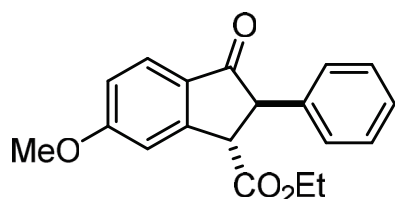
¹³C NMR (CDCl₃, 100.53 MHz): δ 201.4, 168.1, 158.5, 135.2, 135.0, 127.6, 125.4, 124.0, 57.9, 42.8, 38.1, 36.2, 34.8, 29.7, 22.7, 13.9.

IR (ATR): 2954 m, 2928 m, 2858 w, 1711 s, 1643 s, 1539 w, 1464 m, 1396 m, 1285 w, 1216 w, 1012 w, 762 w, 516 w, 402 w.

MS *m/z* (% relative intensity): 259 (M⁺, 27), 216 (11), 202 (14), 187 (37), 145 (26), 144 (13), 131 (18), 115 (13), 72 (100), 46 (10), 45 (11), 44 (21).

HRMS (DART+, [M+H]⁺): Calcd for C₁₆H₂₂NO₂ 260.1645, Found 260.1642.

Ethyl *trans*-6-methoxy-3-oxo-2-phenyl-2,3-dihydro-1*H*-indene-1-carboxylate (4bj).



Method B was followed using **1b** (44.6 mg, 0.21 mmol) and **2j** (41.8 mg, 0.24 mmol), except that the reaction was run at 160 °C, instead of 140 °C.

R_f 0.14 (hexane/EtOAc = 10/1). Pale yellow oil (22.2 mg, 34%).

¹H NMR (CDCl₃, 399.78 MHz): δ 7.83–7.81 (m, 1H), 7.28–7.22 (m, 3H), 7.13–7.10 (m, 2H), 7.06–7.03 (m, 2H), 4.62 (d, *J* = 8.7 Hz, 1H), 4.27 (d, *J* = 8.7 Hz, 1H), 3.92 (s, 3H), 3.77–3.61 (m, 2H), 0.80 (t, *J* = 7.1 Hz, 3H).

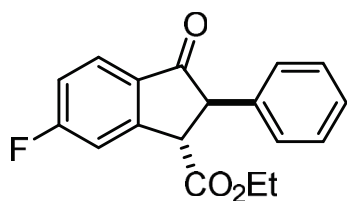
¹³C NMR (CDCl₃, 100.53 MHz): δ 201.7, 170.3, 165.7, 153.3, 136.5, 130.3, 129.2, 128.4, 127.5, 126.0, 117.0, 110.4, 60.9, 56.8, 55.8, 51.0, 13.5.

IR (ATR): 2970 w, 2944 w, 1735 s, 1716 s, 1521 w, 1507 w, 1490 w, 1367 m, 1254 m, 1217 m, 1093 w, 1037 w, 700 m, 505 w, 470 w, 418 w.

MS *m/z* (% relative intensity): 311 (M+H⁺, 20), 310 (100), 282 (34), 238 (21), 237 (88), 236 (74), 209 (45), 208 (18), 194 (25), 178 (14), 177 (11), 166 (16), 165 (53).

HRMS (DART+, [M+H]⁺): Calcd for C₁₉H₁₉O₄ 311.1278, Found 311.1277.

Ethyl *trans*-6-fluoro-3-oxo-2-phenyl-2,3-dihydro-1*H*-indene-1-carboxylate (4dj).



Method B was followed using **1d** (39.3mg, 0.20 mmol) and **2j** (41.8mg, 0.24 mmol), except that the reaction was run at 160 °C, instead of 140 °C.

R_f 0.23 (hexane/EtOAc = 10/1). Pale yellow oil (37.7 mg, 63%).

¹H NMR (CDCl₃, 399.78 MHz): δ 7.85 (dd, *J* = 5.5, 8.2 Hz, 1H), 7.44–7.42 (m, 1H), 7.36–7.27 (m, 3H), 7.24–7.17 (m, 3H), 4.41 (d, *J* = 4.6 Hz, 1H), 4.35–4.22 (m, 3H), 1.34 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (CDCl₃, 100.53 MHz): δ 201.8, 170.6, 167.3 (d, *J* = 257.8 Hz), 152.6 (d, *J* = 10.5 Hz), 137.9, 132.0, 129.0, 128.2, 127.6, 126.9 (d, *J* = 10.5 Hz), 117.4 (d, *J* = 23.0 Hz), 113.2 (d, *J* = 23.0 Hz), 62.1, 56.6, 53.1, 14.2.

¹⁹F NMR (CDCl₃, 376.17 MHz) δ -102.2.

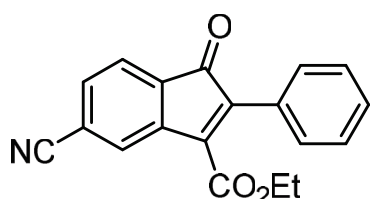
IR (ATR): 2985 w, 2971 w, 1724 s, 1611 m, 1593 m, 1507 w, 1474 w, 1436 w, 1371 m, 1243 s, 1217

s, 1089 m, 1038 m, 746 w, 700 m, 519 w, 434 w, 418 w.

MS m/z (% relative intensity): 299 (M+H⁺, 22), 298 (M⁺, 100), 270 (48), 226 (23), 225 (97), 224 (85), 223 (18), 197 (58), 196 (75), 195 (12), 194 (12), 177 (19), 176 (17), 170 (12), 151 (10), 98 (17), 85 (11).

HRMS (DART+, [M+H]⁺): Calcd for C₁₈H₁₆O₃F 299.1078, Found 299.1077.

Ethyl 5-cyano-1-oxo-2-phenyl-1*H*-indene-3-carboxylate (**4ej**).



Method B was followed using **1e** (44.7mg, 0.22 mmol) and **2j** (41.8mg, 0.24 mmol), except that the reaction was run at 160 °C, instead of 140 °C.

R_f 0.14 (hexane/EtOAc = 10/1). Yellow oil (39.9 mg, 60%).

¹H NMR (CDCl₃, 399.78 MHz): δ 7.90 (s, 1H), 7.68–7.62 (m, 2H), 7.44–7.41 (m, 5H), 4.34 (q, *J* = 7.3 Hz, 2H), 1.24 (t, *J* = 7.3 Hz, 3H).

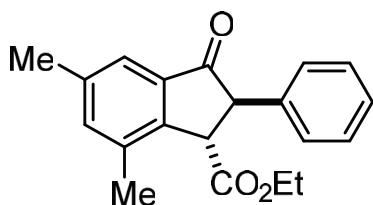
¹³C NMR (CDCl₃, 100.53 MHz): δ 194.4, 163.6, 143.4, 141.1, 140.3, 133.8, 132.1, 129.84, 129.81, 128.8, 128.0, 125.6, 123.7, 117.9, 117.6, 61.9, 13.8.

IR (ATR): 2982 w, 1723 s, 1670 w, 1636 w, 1607 m, 1541 w, 1507 w, 1457 w, 1419 w, 1215 s, 1183 m, 1137 w, 1065 m, 847 w, 792 w, 695 m, 546 w, 459 w, 419 w.

MS m/z (% relative intensity): 305 (M+2H⁺, 13), 304 (M+H⁺, 21), 303 (M⁺, 100), 276 (11), 275 (62), 274 (71), 258 (21), 247 (40), 246 (19), 232 (22), 231 (37), 230 (64), 219 (11), 207 (12), 204 (11), 203 (25), 202 (23), 201 (42), 190 (24), 176 (18), 175 (25), 174 (10), 87 (17), 77 (10).

HRMS (DART+, [M+H]⁺): Calcd for C₁₉H₁₄NO₃ 304.0968, Found 304.0978.

Ethyl *trans*-5,7-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-indene-1-carboxylate (**4fj**).



Method B was followed using **1f** (42.2mg, 0.20 mmol) and **2j** (41.8mg, 0.24 mmol), except that the reaction was run at 160 °C, instead of 140 °C.

R_f 0.14 (hexane/EtOAc = 10/1). Pale yellow oil (43.2 mg, 68%).

¹H NMR (CDCl₃, 399.78 MHz): δ 7.50 (s, 1H), 7.33–7.27 (m, 4H), 7.14–7.11 (m, 2H), 4.25–4.17 (m,

3H), 4.06 (d, $J = 3.2$ Hz, 1H), 2.41 (s, 3H), 2.35 (s, 3H), 1.26 (t, $J = 7.4$ Hz, 3H).

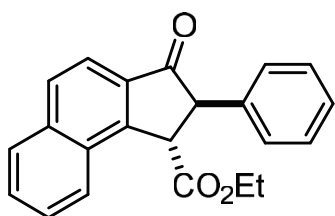
^{13}C NMR (CDCl_3 , 100.53 MHz): δ 204.0, 172.5, 146.9, 139.5, 138.4, 137.9, 136.4, 135.9, 128.9, 127.7, 127.4, 122.3, 61.5, 58.7, 52.6, 21.1, 18.0, 14.1.

IR (ATR): 2971 w, 1737 s, 1713 s, 1647 w, 1521 w, 1507 w, 1489 w, 1369 m, 1306 m, 1232 m, 1173 m, 1036 w, 701 m, 519 w, 460 w, 403 w.

MS m/z (% relative intensity): 309 ($\text{M}^+ \text{H}^+$, 22), 308 (98), 280 (20), 236 (21), 235 (100), 234 (87), 207 (30), 193 (11), 192 (34), 191 (35), 190 (11), 189 (15), 165 (11), 129 (16), 115 (25), 105 (11), 91 (11).

HRMS (DART+, $[\text{M}+\text{H}]^+$): Calcd for $\text{C}_{20}\text{H}_{21}\text{O}_3$ 309.1485, Found 309.1482.

Ethyl *trans*-1-oxo-2-phenyl-2,3-dihydro-1*H*-cyclopenta[*a*]naphthalene-3-carboxylate (**4gj**).



Method B was followed using **1g** (42.4mg, 0.19 mmol) and **2j** (41.8mg, 0.24 mmol).

R_f 0.20 (hexane/EtOAc = 10/1). yellowish oil (32.0mg, 52%).

^1H NMR (CDCl_3 , 399.78 MHz): δ 8.19 (d, $J = 7.8$ Hz, 1H), 8.01 (d, $J = 7.8$, 1H), 7.96 (d, $J = 8.2$, 1H), 7.83 (d, $J = 8.2$ Hz, 1H), 7.74-7.64 (m, 2H), 7.33-7.25 (m, 3H), 7.18-7.15 (m, 2H), 4.75 (d, $J = 2.7$ Hz, 1H), 4.29-4.15 (m, 3H), 1.23 (t, $J = 7.1$ Hz, 3H).

^{13}C NMR (CDCl_3 , 100.53 MHz): δ 203.6, 172.4, 151.5, 138.2, 137.2, 134.2, 130.5, 130.0, 129.5, 129.2, 129.0, 127.7, 127.63, 127.56, 124.8, 120.1, 61.8, 58.3, 53.0, 14.1.

IR (ATR): 3026 w, 3003 w, 2970 w, 1734 s, 1716 s, 1670 w, 1625 w, 1507 w, 1457 m, 1367 m, 1229 m, 1217 m, 1036 w, 757 w, 697 w, 536 w, 414 w.

MS m/z (% relative intensity): 330 (M^+ , 12), 258 (13), 257 (60), 256 (16), 229 (11), 207 (12), 156 (12), 155 (100), 128 (13), 127 (94), 126 (11), 77 (10).

HRMS (DART+, $[\text{M}+\text{H}]^+$): Calcd for $\text{C}_{22}\text{H}_{19}\text{O}_3$ 331.1329, Found 331.1327.

VII. DFT Calculations

VII -1. Computational details

Calculations were performed with the Gaussian 09 (G09RevD.01) program.¹³ Geometry optimizations and frequency calculations for all reported structures were performed using the ωB97XD functional¹⁴ with a basis set consisting of the LANL2DZ basis set for Pd and 6-31G* for the rest. Single-point energy calculations of the optimized structures were separately calculated using the ωB97XD

functional with a basis set consisting of the SDD basis set for metallic atoms (Pd) and 6-311+G* for the rest. Gibbs free energies were estimated by sum of the electronic energies at the higher-level single point energy calculations and the thermal corrections at the lower-level calculations. Each reported minimum has zero imaginary frequency and each transition state (TS) structure has only one imaginary frequency. From TSs, reaction paths were traced by the intrinsic reaction coordinate (IRC) method¹⁵ followed by geometry optimization to obtain the energy-minimum geometries. Energy changes were shown by the use of Gibbs free energies (T = 298.15 K and P = 1 atm).

VII -2. Computed energy profiles

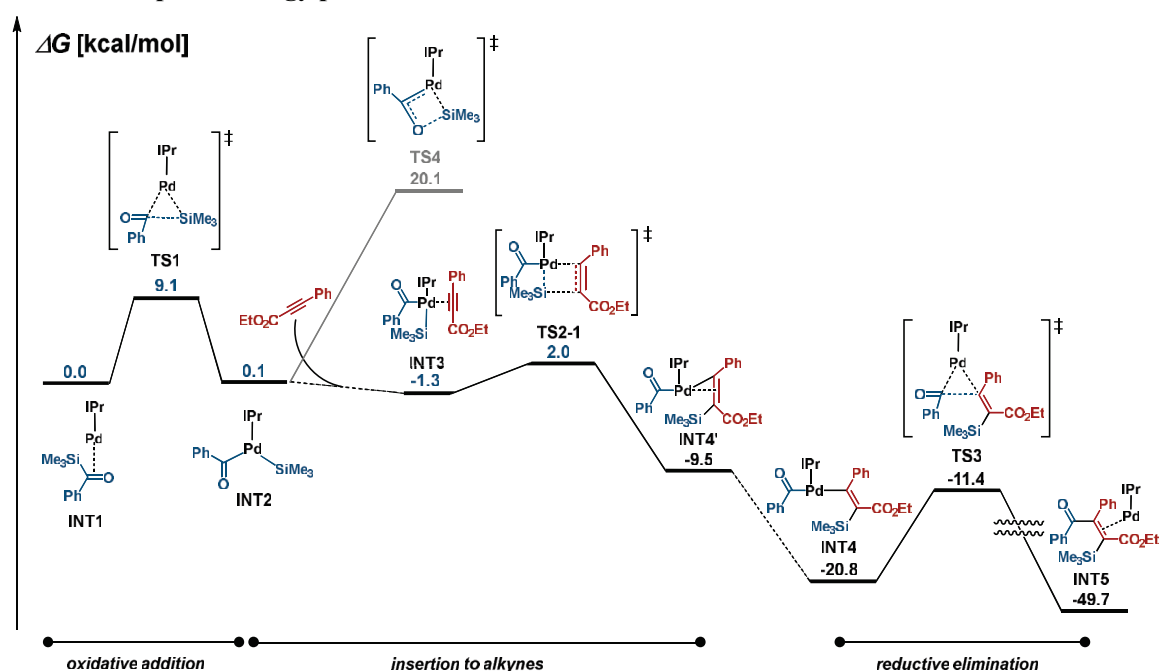


Figure S1. Computed energy profiles of the Pd-catalyzed silylacylation pathways of acylsilane **1a** with alkyne **2j** at the ω B97XD/SDD-6-311+G*// ω B97XD/LANL2DZ-6-31G* level of theory.

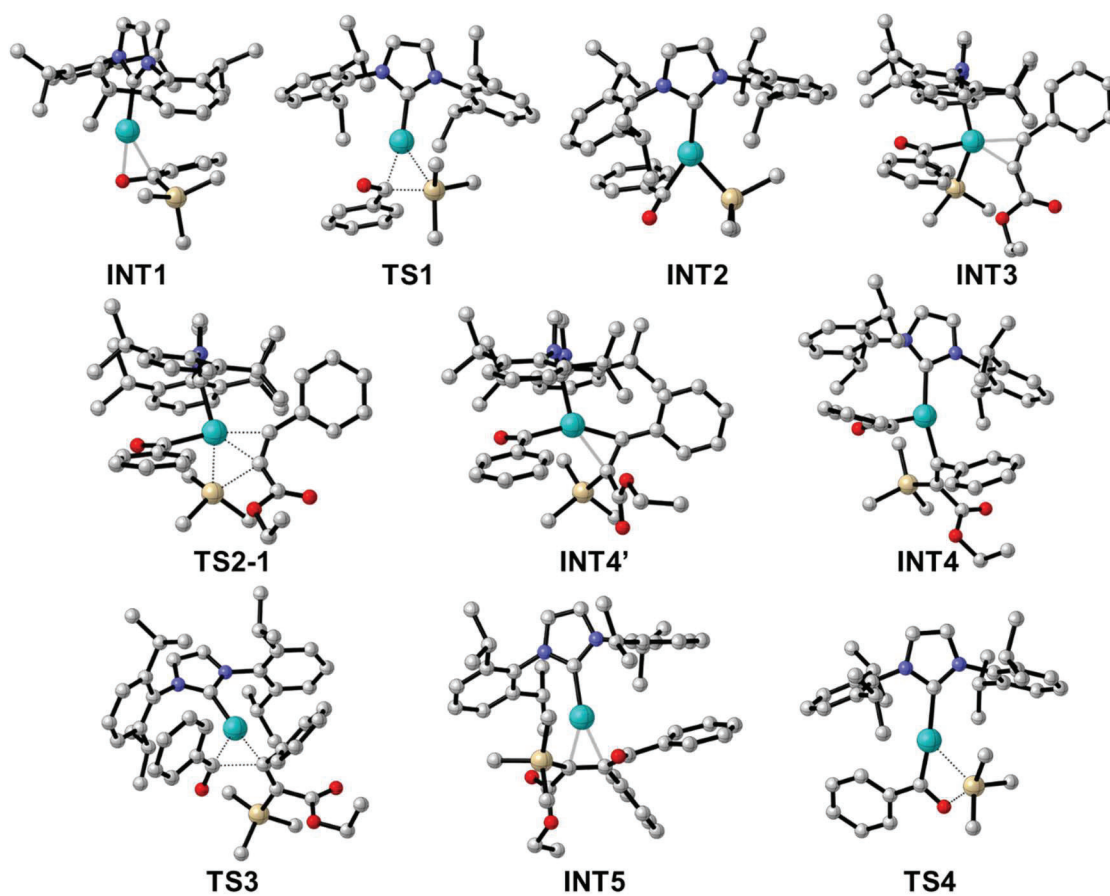


Figure S2. Structures of the intermediates and transition states shown in **Figure S1**.

Eight different transition states were investigated for the addition of a silyl group or an acyl group in **INT2** across an alkyne moiety (**Figure S3**). These transition states are distinguished by which silyl or benzoyl groups are inserted into the alkyne, the orientation of the alkyne, and whether the silyl and benzoyl groups are located in a *cis* or *trans* configuration. Among the eight transition states, **TS2-1** and **TS2-2** turned out to be the energetically most favored transition state ($\Delta G^\ddagger = 2.0$ kcal/mol).

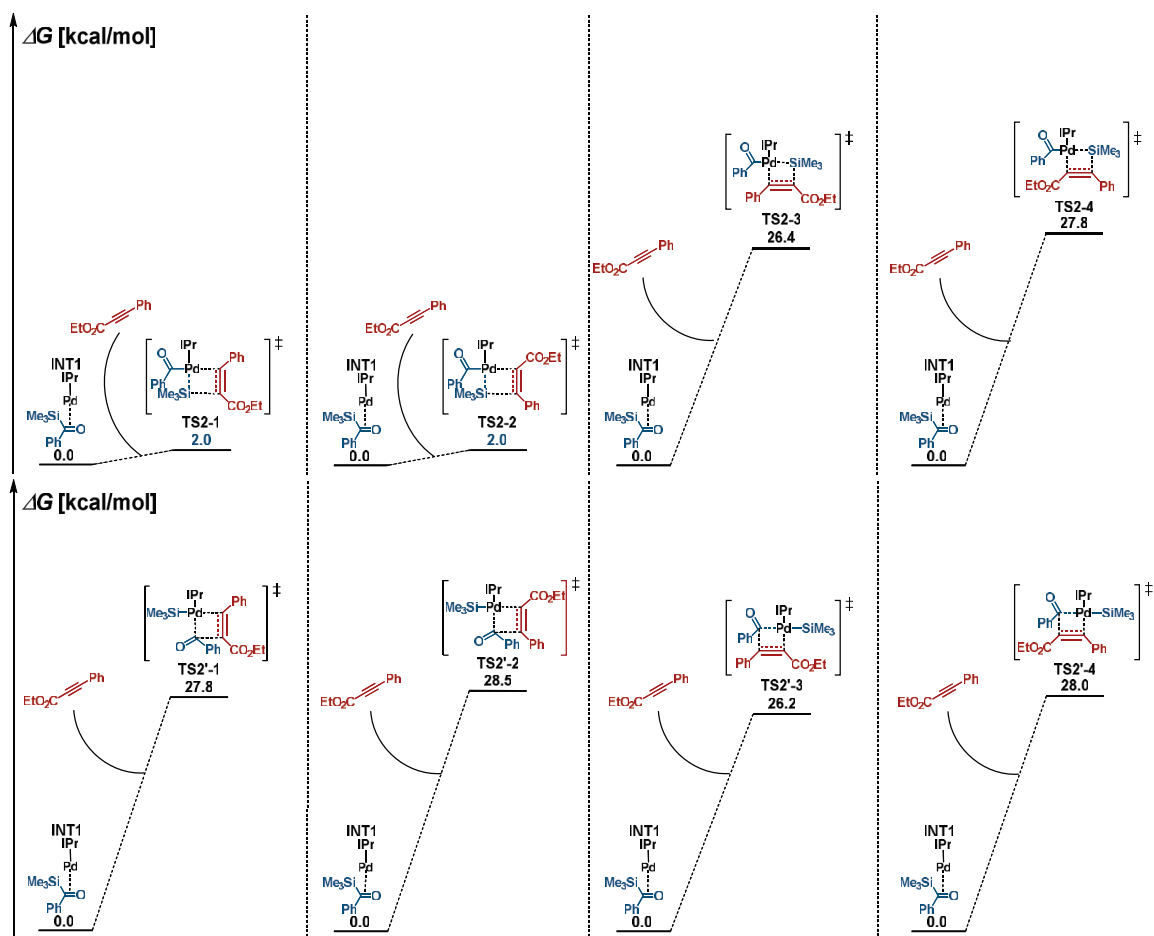


Figure S3. Energy comparison of possible eight transition states for silylpalladation and benzoylpalladation at the ω B97XD/SDD-6-311+G**// ω B97XD/LANL2DZ-6-31G* level of theory.

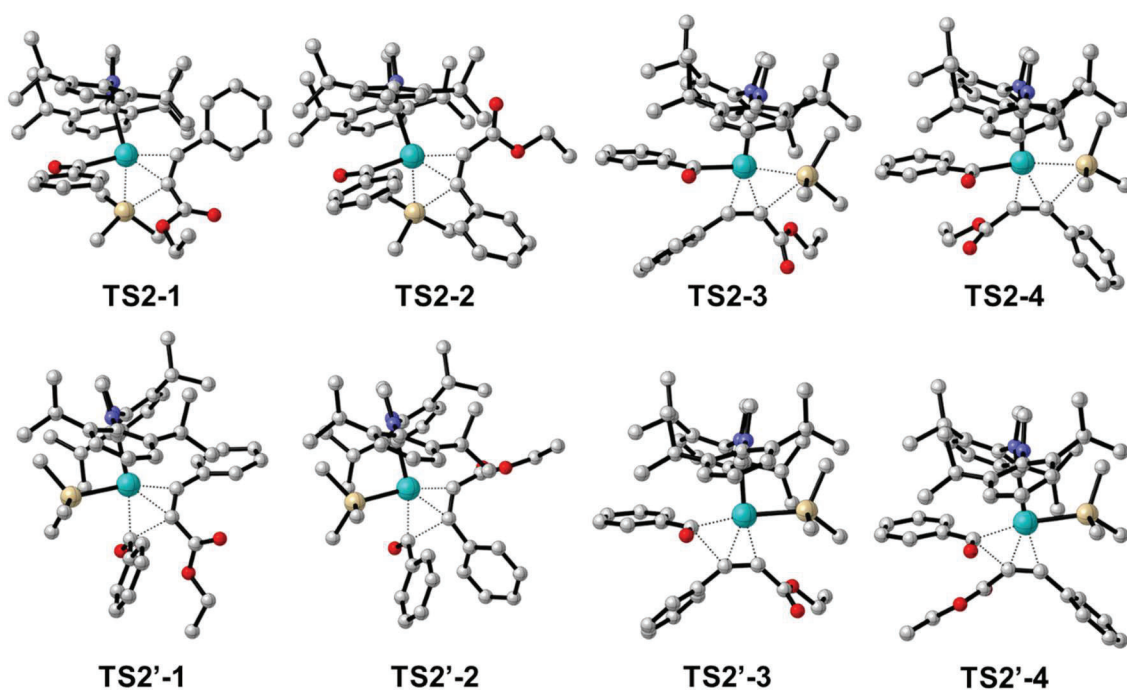


Figure S4. Structures of the transition states shown in **Figure S3**.

If the numbers of atoms for the two species to be compared are different, the free energy (G) must be used for the comparison because of the large influence of the entropy term. In contrast, in insertion reactions from π -complexes, the number of atoms are unchanged and can be regarded as intramolecular reactions in terms of the computational model. Therefore, the total electron energy (E) may be used for more accurate comparison. Therefore, E_s of **TS2-1** and **TS2-2** were compared, which revealed that **TS2-1** is more favored than **TS2-2**.

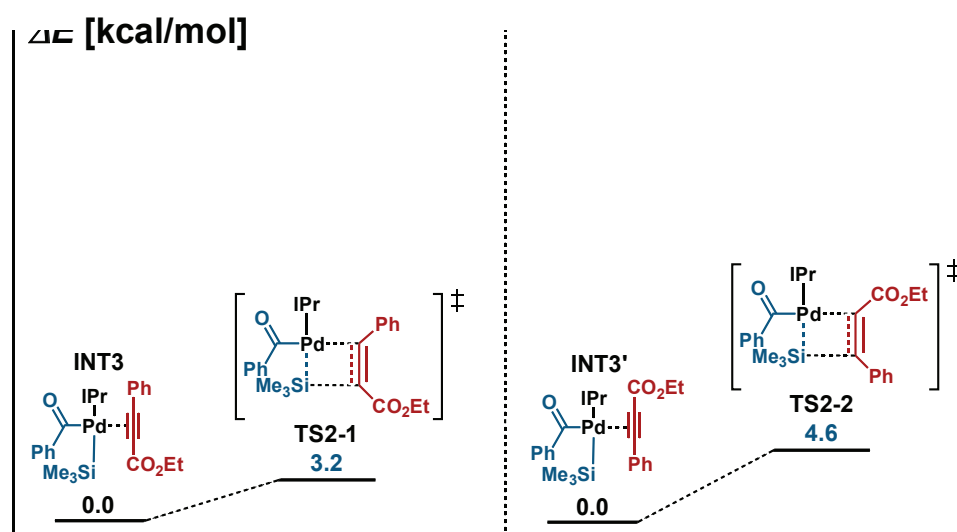


Figure S5. Comparison of **TS2-1** and **TS2-2** with the total electron energy at the ω B97XD/SDD-6-

311+G*// ω B97XD/LANL2DZ-6-31G* level of theory.

VIII. Cartesian Coordinates and Energies of Optimized Structures

INT1				C	2.49033100	-0.08138500	4.56814200
SCF Done: E(R ω B97XD) = -2040.60093966	A.U.			H	3.33965700	0.60513000	4.47813300
Sum of electronic and thermal Free Energies = -2039.896292	A.U.			H	1.82496100	0.32887700	5.33499200
SCF Done (single point): E(R ω B97XD) = -2042.15554812	A.U.			H	2.86833300	-1.04616400	4.92265600
no imaginary frequency				C	1.27705700	1.15469200	2.73054500
N	-1.63525200	-1.59252600	0.89482900	H	0.60250800	1.63016800	3.45171100
N	0.43565900	-1.88271700	1.30498700	H	2.14204400	1.81377200	2.59261200
C	-0.40277900	-1.14589500	0.52658000	H	0.75462200	1.07354100	1.77192000
C	-2.85216500	-1.07117100	0.34679000	C	-3.56385200	-3.96435500	-1.79006500
C	-3.46723700	0.00133300	1.00369600	H	-4.38689500	-3.71234300	-2.46811400
C	-4.63321900	0.51628000	0.43771000	H	-3.00537300	-4.79034000	-2.24369400
C	-5.15524300	-0.01920000	-0.73273300	H	-3.99948000	-4.32041100	-0.85051500
C	-4.51955700	-1.08176600	-1.36231500	C	-2.02185400	-2.26820700	-2.87102300
C	-3.35086200	-1.63155000	-0.83573700	H	-1.47055800	-3.07714500	-3.36363900
C	-2.87623700	0.62645900	2.25621000	H	-2.79540000	-1.91271700	-3.56133400
C	-2.63777900	-2.76447300	-1.55607400	H	-1.32557800	-1.43868000	-2.69051100
C	1.86156600	-1.78036200	1.23863600	C	2.35546100	-4.85117300	-0.60759600
C	2.53079600	-2.48527000	0.23269700	H	1.76967600	-5.53067300	-1.23615700
C	3.91480000	-2.31970400	0.14918100	H	3.39807800	-4.90847000	-0.93999100
C	4.59020400	-1.50776200	1.04943800	H	2.31132000	-5.21534400	0.42443000
C	3.89971000	-0.85168600	2.06314000	C	1.84154400	-2.91884200	-2.16572700
C	2.51539300	-0.96970200	2.17815100	H	1.29766200	-3.61030500	-2.81928000
C	1.80418200	-3.42308300	-0.71929900	H	1.37306000	-1.93155100	-2.24061500
C	1.72998800	-0.22024200	3.24571300	H	2.86933000	-2.83852600	-2.53863200
H	-5.13085000	1.35777600	0.91135400	C	-2.35867200	2.03769900	1.95680100
H	-4.93246000	-1.48346800	-2.28333500	H	-3.17145600	2.70562200	1.65080700
H	-2.01355500	0.02799400	2.56549700	H	-1.88528500	2.46926300	2.84570500
H	-1.81427400	-3.10719300	-0.92161100	H	-1.62028100	2.01752900	1.15034400
H	4.46842100	-2.83487200	-0.63087600	C	-3.87479500	0.62206500	3.42003300
H	4.44793100	-0.22667500	2.76063900	H	-4.22934700	-0.39127400	3.63782400
H	0.75168100	-3.45882600	-0.42243100	H	-3.40294900	1.02270800	4.32377000
H	0.82337600	-0.79793300	3.45653000	H	-4.75044600	1.24387300	3.20193400

H	5.66597600	-1.38608100	0.96501500	Sum of electronic and thermal Free Energies = -2039.881515 A.U.			
H	-6.06076100	0.39946100	-1.16201200	SCF Done (single point): E(RoB97XD) = -2042.13858055 A.U.			
Pd	-0.08149700	0.13883800	-1.02937900	$v_i = -123.18 \text{ cm}^{-1}$			
C	0.03326700	3.14698700	-0.80139300	N	0.41968500	2.15387100	0.87459700
C	0.55168900	3.70813500	0.36897300	N	-1.53709600	1.37944700	1.20947500
H	1.49354100	3.34780600	0.76691300	C	-0.38327500	1.10868800	0.54297400
C	-1.19783500	3.60842600	-1.28288100	C	1.75290800	2.28518500	0.36766900
H	-1.59387100	3.16451200	-2.19029400	C	2.80980800	1.77030600	1.12820200
C	-1.88984300	4.60510400	-0.60830100	C	4.09395700	1.87518400	0.59401600
H	-2.84172100	4.95746200	-0.99614300	C	4.30492500	2.46341500	-0.64653100
C	-0.14593900	4.70050200	1.04980700	C	3.23327800	2.95288900	-1.38217200
H	0.26687600	5.11888600	1.96347700	C	1.93029700	2.86898400	-0.89283700
C	-1.36731500	5.15584400	0.56169700	C	2.57920300	1.07187700	2.45857800
H	-1.90988400	5.93530700	1.08902900	C	0.75898100	3.35276500	-1.73165000
C	0.77697700	2.09497300	-1.57166800	C	-2.69073900	0.52936000	1.19015400
C	-1.56643900	-2.57664500	1.86542400	C	-3.60297100	0.65139700	0.12992900
C	-0.25322300	-2.76242600	2.12487500	C	-4.73689800	-0.15943200	0.16865300
H	-2.45093400	-3.03904500	2.27345900	C	-4.93057400	-1.07190900	1.19894400
H	0.25723900	-3.42646800	2.80418200	C	-3.98734900	-1.20132400	2.20825700
O	0.17410100	1.54631800	-2.56328500	C	-2.84512000	-0.39921100	2.22700300
Si	2.69678300	2.03081800	-1.69061300	C	-3.33794400	1.60056100	-1.03075800
C	3.16812100	0.45463400	-2.59221500	C	-1.77191100	-0.58943300	3.28822600
H	3.18845700	-0.38333200	-1.88826800	H	4.93860600	1.47709900	1.14920700
H	2.43987100	0.22606900	-3.37612500	H	3.40921400	3.39243100	-2.35982800
H	4.16068400	0.54609700	-3.04891000	H	1.52368300	1.18621500	2.72453700
C	3.63943600	2.07701500	-0.05914100	H	-0.15735000	3.21932300	-1.14892100
H	3.61141300	3.05373400	0.43472300	H	-5.47081100	-0.09841300	-0.62754100
H	3.25457500	1.31891000	0.62842800	H	-4.13816600	-1.94049900	2.98878800
H	4.69200400	1.83593800	-0.25297600	H	-2.25812900	1.57310000	-1.21890700
C	3.15222200	3.55172000	-2.71348100	H	-1.17363400	0.32654000	3.33461200
H	4.23553900	3.62048400	-2.86692800	C	-2.34703900	-0.82374100	4.68901500
H	2.67126200	3.51206400	-3.69690600	H	-2.85021300	-1.79386400	4.76798700
H	2.82208800	4.47118400	-2.21675900	H	-1.53917700	-0.81912300	5.42822700
				H	-3.06689100	-0.04565300	4.96367400
TS1				C	-0.82766400	-1.72797000	2.87399600
SCF Done: E(RoB97XD) = -2040.59617319 A.U.				H	-0.02709500	-1.85353700	3.61216200

H	-1.37537200	-2.67538000	2.79638500	C	1.93490800	-3.96646300	1.31693100
H	-0.36841200	-1.51753100	1.90234200	H	1.39693500	-4.48023700	2.10816600
C	0.87680900	4.84648300	-2.05911700	C	3.32405500	-3.89842500	1.34317400
H	1.75978100	5.05555500	-2.67365900	H	3.87456400	-4.36173400	2.15699700
H	-0.00357100	5.18251800	-2.61797200	C	1.17273700	-1.94322600	-1.80912000
H	0.95298000	5.44728500	-1.14636400	C	-0.20852200	3.04806500	1.72482100
C	0.61356400	2.50337300	-3.00161200	C	-1.44864200	2.55622700	1.94066400
H	-0.28592900	2.79941500	-3.55440300	H	0.28409900	3.93487800	2.09020700
H	1.47543800	2.63055200	-3.66681400	H	-2.26853800	2.91842400	2.54048300
H	0.53559400	1.43968000	-2.75196600	O	1.79932900	-1.38033600	-2.71859200
C	-3.72602100	3.04601800	-0.68553700	Si	-0.76114500	-2.30122300	-2.32183400
H	-3.50093200	3.70962100	-1.52802100	C	-1.22397400	-1.04289800	-3.64344900
H	-4.79949900	3.11732800	-0.47425300	H	-1.60485500	-0.11627800	-3.20420200
H	-3.18062200	3.41798400	0.18621400	H	-0.32738500	-0.79594700	-4.22062000
C	-4.02924400	1.16575200	-2.32654100	H	-1.98176100	-1.44608800	-4.32622700
H	-3.64642400	1.75736700	-3.16450100	C	-2.19288500	-2.63734100	-1.12532400
H	-3.84432800	0.10960200	-2.54563800	H	-1.95555300	-3.43081200	-0.40819400
H	-5.11327900	1.32478500	-2.28365100	H	-2.49016200	-1.75090700	-0.56007800
C	2.85309500	-0.43223500	2.33228100	H	-3.05842500	-2.97773200	-1.71026300
H	3.90011700	-0.62457800	2.07281600	C	-0.42141100	-3.96171200	-3.17094000
H	2.64100400	-0.94106800	3.27959700	H	-1.33826300	-4.34209400	-3.63821300
H	2.22759900	-0.87937500	1.55330200	H	0.34308900	-3.85525600	-3.94743600
C	3.40586800	1.70265000	3.58557900	H	-0.07214300	-4.71347300	-2.45405200
H	3.19967400	2.77408800	3.68108300				
H	3.17162400	1.22162800	4.54153200	INT2			
H	4.48103800	1.58212000	3.41160900	SCF Done: $E(R\omega B97XD) = -2040.61071434$	A.U.		
H	-5.81637000	-1.70035800	1.20290200	Sum of electronic and thermal Free Energies = -2039.893007	A.U.		
H	5.31123600	2.53143000	-1.04936300	SCF Done (single point): $E(R\omega B97XD) = -2042.15610189$	A.U.		
Pd	0.19383500	-0.46628600	-0.65976700	no imaginary frequency			
C	1.91221800	-2.69235500	-0.74309500	N	-0.07866200	1.76098100	1.37018500
C	1.23191600	-3.36643300	0.27589000	N	-1.94968600	0.74284500	1.39533700
H	0.14751600	-3.41234500	0.26275300	C	-0.74301800	0.73253900	0.78379500
C	3.31105600	-2.63416200	-0.71109200	C	1.26204300	2.09766700	0.97968000
H	3.81969400	-2.09808900	-1.50586600	C	2.32523500	1.58032100	1.73414200
C	4.01107200	-3.23458100	0.32438500	C	3.61673200	1.83578200	1.27642100
H	5.09582100	-3.18081900	0.34914000	C	3.83039700	2.57934700	0.12224500

C	2.75727100	3.08260600	-0.59944800	C	-5.37174100	2.25063900	-0.63584000
C	1.44425600	2.84646900	-0.19159500	H	-5.26453500	3.28737700	-0.97128800
C	2.08485100	0.70572900	2.95489700	H	-5.93339800	1.71851300	-1.41158700
C	0.27726600	3.38952900	-1.00015100	H	-5.96948300	2.24706300	0.28178800
C	-3.00605400	-0.17558100	1.08828700	C	-3.19709400	1.56480000	-1.72746100
C	-4.03607300	0.26018600	0.24096700	H	-3.11510000	2.56035700	-2.17895100
C	-5.05566600	-0.64683300	-0.04221000	H	-2.18571700	1.17571100	-1.56839800
C	-5.03369100	-1.93273900	0.48653400	H	-3.70088900	0.90516400	-2.44368900
C	-3.99221100	-2.33629100	1.30880100	C	2.15680500	-0.77647100	2.56283300
C	-2.95267200	-1.46250300	1.63301000	H	3.14463500	-1.02584200	2.16001300
C	-3.98747700	1.63512500	-0.41068500	H	1.96649000	-1.41465900	3.43404000
C	-1.80380400	-1.92533000	2.51481700	H	1.41811900	-1.01674600	1.79108900
H	4.46749500	1.42931800	1.81365800	C	3.04511700	1.01987000	4.10749700
H	2.93948300	3.64792500	-1.50804400	H	3.04118800	2.08705900	4.35318100
H	1.07115300	0.90028100	3.32111100	H	2.74961200	0.46040300	5.00139800
H	-0.64159400	2.93496800	-0.61943400	H	4.07478900	0.73063000	3.87074100
H	-5.86947400	-0.35418000	-0.69744000	H	-5.83114900	-2.62869200	0.24412300
H	-3.98124700	-3.34820200	1.70356200	H	4.84421100	2.75849000	-0.22354900
H	-3.44171400	2.30906200	0.25849700	Pd	0.30987500	-0.33457600	-0.74412900
H	-1.17160500	-1.06001500	2.73749000	C	2.93442200	-1.49975900	-1.03865700
C	-2.29995300	-2.48388300	3.85409800	C	2.57545200	-2.66336600	-0.35805700
H	-2.88589800	-3.39978500	3.71878700	H	1.55113300	-3.01918700	-0.42260400
H	-1.44772500	-2.73157400	4.49622100	C	4.24314200	-1.02073000	-0.93912700
H	-2.92694900	-1.75741300	4.38149500	H	4.50630400	-0.11302000	-1.47304600
C	-0.93076000	-2.94368200	1.76959400	C	5.17624000	-1.69175900	-0.15700200
H	-0.07656000	-3.24063900	2.38880700	H	6.18809400	-1.30586600	-0.06812400
H	-1.50180700	-3.84588100	1.51948500	C	3.51722600	-3.35514100	0.39636300
H	-0.54587900	-2.50895100	0.84024500	H	3.23487600	-4.26976600	0.90973800
C	0.15298200	4.90734400	-0.80912100	C	4.81642200	-2.86418400	0.50654500
H	1.04900800	5.42366900	-1.17240400	H	5.54808100	-3.39449800	1.10968500
H	-0.70795900	5.29294100	-1.36628200	C	1.92899100	-0.70034400	-1.83874400
H	0.02065900	5.16514500	0.24757100	C	-0.85139500	2.40273900	2.32153500
C	0.38059900	3.01308700	-2.48298000	C	-2.03682700	1.75190600	2.34425100
H	-0.54674300	3.28336700	-3.00025700	H	-0.48459200	3.24507100	2.88611600
H	1.20263000	3.54241500	-2.97846200	H	-2.92879000	1.90593100	2.93041100
H	0.55040700	1.93956000	-2.60817100	O	2.30380200	-0.05890700	-2.80358300

Si	-0.50106000	-1.59852500	-2.54072300	C	-2.27634700	-3.41995800	1.41995700
C	-0.74150300	-0.43188100	-4.00764200	C	1.44792100	-0.28110900	2.96640400
H	-1.44594800	0.37122400	-3.76666300	H	-3.61820500	4.17317400	-1.88269100
H	0.21806900	0.02337900	-4.27246000	H	-5.14497800	0.34041600	-2.99584000
H	-1.12481900	-0.97434200	-4.88124000	H	-1.49923500	2.74424500	0.84481500
C	-2.19283200	-2.23819200	-1.96729600	H	-2.98265100	-1.49861300	-0.66130500
H	-2.09343500	-2.94650600	-1.13763200	H	-0.34608000	-5.25168500	1.85888800
H	-2.84331000	-1.42600000	-1.63045600	H	2.79448400	-2.65093000	3.13291600
H	-2.69525200	-2.75712100	-2.79516700	H	-2.75469400	-2.46036300	1.21580800
C	0.42309800	-3.12948400	-3.17693700	H	0.91950300	0.40935200	2.31388000
H	-0.14754100	-3.57967100	-3.99977300	C	1.07334900	0.06983100	4.41263200
H	1.42065400	-2.88413500	-3.55516500	H	1.57024600	-0.60538000	5.11909100
H	0.53597500	-3.89320000	-2.39905200	H	1.37322200	1.09795700	4.64242200
				H	-0.00792700	-0.01027300	4.57292100
INT3				C	2.94029800	-0.05942300	2.71586800
SCF Done: E(RoB97XD) = -2616.03434930	A.U.			H	3.16861800	1.00767400	2.80706900
Sum of electronic and thermal Free Energies = -2615.137539	A.U.			H	3.56629300	-0.59544900	3.43877700
SCF Done (single point): E(RwB97XD) = -2617.71873195	A.U.			H	3.22223700	-0.38020000	1.70846000
no imaginary frequency				C	-5.07277900	-1.55082100	-0.13007700
N	-2.44899200	0.55339700	0.70484500	H	-6.03863500	-1.23087900	-0.53860300
N	-1.21886000	-0.76080400	1.87779300	H	-5.10798900	-2.63744900	0.00981400
C	-1.26500000	-0.11023700	0.68155400	H	-4.95148700	-1.09155300	0.85498600
C	-3.08839700	1.16107500	-0.44027500	C	-4.08971500	-1.94798900	-2.40395700
C	-2.97245200	2.53995500	-0.64674700	H	-3.94628900	-3.01560200	-2.21183500
C	-3.68652900	3.10404100	-1.70555700	H	-5.08847400	-1.82368300	-2.83924300
C	-4.47549600	2.31851900	-2.53066800	H	-3.34387700	-1.64214800	-3.14052900
C	-4.54730000	0.94711600	-2.32436500	C	-3.07338700	-4.08911800	2.54884800
C	-3.85206300	0.33251600	-1.28429300	H	-4.12129200	-4.21436000	2.25437100
C	-2.11156200	3.41065100	0.24208600	H	-2.66720800	-5.07949100	2.78415800
C	-3.93378000	-1.17480600	-1.09072900	H	-3.04507900	-3.49154200	3.46673300
C	-0.34228000	-1.88124600	2.13771400	C	-2.35200500	-4.23806000	0.12679000
C	-0.84537800	-3.16378600	1.86837700	H	-3.40121400	-4.40077900	-0.14611000
C	0.01062900	-4.24742200	2.06723000	H	-1.86099400	-3.71141100	-0.69604900
C	1.31095000	-4.06295700	2.50865700	H	-1.88632100	-5.22354200	0.23984300
C	1.77503800	-2.78535700	2.78722500	C	-1.14590400	4.28456800	-0.56277700
C	0.95968700	-1.66951500	2.61314800	H	-1.67264600	5.02286500	-1.17771600

H	-0.48143300	4.82763900	0.11716000	H	1.06285100	2.43548700	-4.50649900
H	-0.52579100	3.66575700	-1.21873700	H	0.98138000	3.04140900	-2.84560100
C	-2.96318700	4.25070100	1.20060900	H	2.46382600	2.27357900	-3.44206200
H	-3.61228600	3.61648700	1.81511900	C	2.04616700	1.52426100	-0.52242400
H	-2.31566400	4.82736200	1.87029100	C	1.27731800	1.94428000	0.41293100
H	-3.60194200	4.95276900	0.65179100	C	1.19543400	2.90792300	1.49620600
H	1.96949000	-4.91734400	2.63050500	C	0.22372500	2.81861900	2.50193000
H	-5.02468200	2.77219100	-3.35042800	C	2.11649800	3.96696200	1.54046800
Pd	0.39671200	0.28349300	-0.59777200	C	0.15998300	3.76627100	3.51538400
C	1.28962500	-2.57884300	-1.10803900	H	-0.48547200	1.99654500	2.49053600
C	2.51927200	-2.15161900	-0.60765100	C	2.04533600	4.91790300	2.55192400
H	2.69341900	-1.09117500	-0.46826600	H	2.88354900	4.02209900	0.77407500
C	1.08685500	-3.94466000	-1.33040600	C	1.06651500	4.82366600	3.53887000
H	0.13568800	-4.26836300	-1.73939000	H	-0.60048300	3.67971100	4.28578600
C	2.08753600	-4.86398100	-1.04458800	H	2.76133000	5.73414500	2.57109900
H	1.91878900	-5.92245100	-1.22197900	H	1.01351000	5.56951500	4.32647300
C	3.52327200	-3.06998600	-0.31853100	C	3.40066800	1.68872600	-1.03674100
H	4.47231500	-2.72227200	0.08078500	O	4.13696800	2.60714000	-0.73658700
C	3.30902100	-4.42778700	-0.53358900	O	3.75978700	0.68563800	-1.85490200
H	4.09262400	-5.14621400	-0.30877200	C	5.09018900	0.72024800	-2.38552900
C	0.16783300	-1.61260500	-1.43649500	H	5.02010900	0.17841200	-3.33100700
C	-3.10172900	0.36896100	1.91658500	C	6.06324000	0.05257000	-1.43137600
C	-2.32944200	-0.45873300	2.65327800	H	7.06490100	0.02888400	-1.87246900
H	-4.05298900	0.83280900	2.12285400	H	6.11266900	0.60451200	-0.48882100
H	-2.47090100	-0.88484100	3.63361800	H	5.74953900	-0.97614200	-1.22904700
O	-0.84283600	-2.06193300	-1.94949500	H	5.37009400	1.75827300	-2.58007500
Si	0.66098900	0.54043400	-2.99095700				
C	-1.14179400	0.62169700	-3.52932500	TS2			
H	-1.68282500	-0.26012200	-3.18270600	SCF Done: E(RωB97XD) = -2616.02966757	A.U.		
H	-1.62926800	1.51367100	-3.12113500	Sum of electronic and thermal Free Energies = -2615.132624	A.U.		
H	-1.20387600	0.67092900	-4.62447000	SCF Done (single point): E(RωB97XD) = -2617.71367806	A.U.		
C	1.62022900	-0.74850600	-3.98418300	$\nu_i = -115.95 \text{ cm}^{-1}$			
H	1.07502000	-1.69356500	-4.06353200	N	1.63606000	1.91382500	0.78204700
H	1.79871300	-0.36683500	-4.99741700	N	-0.13854800	1.43537700	1.89758100
H	2.58886900	-0.95114700	-3.51761200	C	0.49005200	1.18990400	0.71686500
C	1.37171000	2.23351000	-3.47214700	C	2.52242400	2.17032900	-0.32862500

C	3.71958000	1.45278000	-0.43352000	H	-0.71252200	4.79483300	-2.34571600
C	4.59200800	1.79147000	-1.46948800	H	0.90658200	5.24898400	-2.88871100
C	4.26910900	2.78961200	-2.37500500	H	0.27038500	3.61286100	-3.20951900
C	3.06028300	3.46428800	-2.26613100	C	-2.20807900	4.63583100	2.46523700
C	2.15727000	3.17409600	-1.24471700	H	-1.80413800	5.60589800	2.15492000
C	4.07740900	0.35008100	0.54066000	H	-3.27583400	4.76543500	2.67578300
C	0.84660300	3.93859900	-1.13266000	H	-1.71643300	4.34437100	3.39984700
C	-1.54048500	1.17757700	2.12832700	C	-2.64954600	4.01430100	0.05124300
C	-2.43685900	2.21685100	1.83907700	H	-2.31976200	5.02407800	-0.21993200
C	-3.79566500	1.97156200	2.04255200	H	-2.37569600	3.33821300	-0.76237700
C	-4.23777500	0.74909500	2.52210500	H	-3.74172700	4.03519300	0.13414600
C	-3.32599600	-0.25907500	2.80613900	C	4.57347900	-0.91610800	-0.16370500
C	-1.96119200	-0.07262000	2.60398400	H	5.53272100	-0.75648400	-0.66903300
C	-1.98347400	3.58967500	1.36412500	H	4.71267100	-1.71699000	0.56966600
C	-0.96252500	-1.17356800	2.89833100	H	3.84421000	-1.25924600	-0.90469500
H	5.53335300	1.25985000	-1.56846000	C	5.09062700	0.83400900	1.58513800
H	2.81075600	4.22672900	-2.99551600	H	4.72235800	1.71529300	2.12175500
H	3.16335400	0.07900100	1.06682900	H	5.28164600	0.04255300	2.31849200
H	0.09773700	3.24545900	-0.74240400	H	6.04377900	1.10224900	1.11447200
H	-4.51713600	2.75045200	1.81457200	H	-5.29987900	0.57434500	2.66297700
H	-3.68625500	-1.21677100	3.16742700	H	4.95767700	3.03875700	-3.17704100
H	-0.90910200	3.55374700	1.17331900	Pd	0.05406100	-0.34787400	-0.58771600
H	-0.13561500	-1.03440800	2.20391300	C	-2.89149800	0.31101800	-1.21940800
C	-0.41090600	-1.04064500	4.32378900	C	-3.17823200	-0.88582100	-0.56573600
H	-1.21397500	-1.14242500	5.06312200	H	-2.35836200	-1.52805900	-0.26095500
H	0.33720300	-1.81723800	4.51651900	C	-3.94870700	1.12164100	-1.64553900
H	0.06629500	-0.06573000	4.47592500	H	-3.71454100	2.03899300	-2.17628600
C	-1.49627800	-2.58524100	2.64493500	C	-5.26459300	0.75397700	-1.39969600
H	-0.66672500	-3.29912000	2.68224300	H	-6.07866700	1.39319300	-1.73041000
H	-2.23225700	-2.89318900	3.39679800	C	-4.49591200	-1.26211400	-0.32465100
H	-1.96045100	-2.66385400	1.65659300	H	-4.70586100	-2.19178800	0.19757500
C	0.98378800	5.12611900	-0.16661600	C	-5.54092400	-0.44074900	-0.73485600
H	1.73520100	5.83527000	-0.53364400	H	-6.57051100	-0.73018500	-0.54241300
H	0.02884400	5.65780500	-0.08419800	C	-1.46328800	0.74207500	-1.48811300
H	1.27677900	4.81156200	0.83927900	C	1.74442800	2.56155500	2.00546400
C	0.30858100	4.42514800	-2.48063000	C	0.62975600	2.26180800	2.70594900

H	2.59449700	3.18008300	2.24472200	H	-2.35198300	-5.36967300	0.11327700
H	0.29253900	2.57332300	3.68157200	H	-3.66607300	-4.28209800	-0.40377700
O	-1.29190000	1.74613600	-2.16614300	H	-1.54174700	-5.52137200	-2.24617600
Si	0.36321400	-1.23142700	-2.89954400				
C	1.43603700	0.26821900	-3.30503600	INT3'			
H	0.91234300	1.19899700	-3.07315000	SCF Done: E(RωB97XD) = -2616.03351668	A.U.		
H	2.38613700	0.25631500	-2.76056900	Sum of electronic and thermal Free Energies = -2615.141504	A.U.		
H	1.66300000	0.24841000	-4.37997000	SCF Done (single point): E(RωB97XD) = -2617.71843703	A.U.		
C	-1.23835300	-1.22775200	-3.89424500	no imaginary frequency			
H	-1.57162800	-0.20194300	-4.07513200	N	-1.69308000	1.92402900	0.86192000
H	-1.07356900	-1.71935300	-4.86082600	N	-1.54639800	0.07905200	1.93677500
H	-2.03702600	-1.75746900	-3.36944400	C	-1.16920600	0.67690800	0.77604100
C	1.39646000	-2.70889100	-3.48497500	C	-1.76468700	2.88116200	-0.21190900
H	1.64289600	-2.53496700	-4.54085200	C	-0.81559900	3.90622300	-0.27012500
H	2.33567600	-2.78975200	-2.92800400	C	-0.97634700	4.88353100	-1.25491300
H	0.88033300	-3.67159500	-3.42055200	C	-2.03437200	4.82534600	-2.14856500
C	0.38594200	-2.40448600	-0.81124100	C	-2.94272700	3.77537100	-2.08907100
C	1.14698600	-1.97639000	0.16400900	C	-2.82884900	2.77365200	-1.12691700
C	1.99996200	-2.53495400	1.19767600	C	0.34745800	3.97158600	0.69931100
C	2.32212500	-1.80086200	2.34949100	C	-3.81393000	1.61295000	-1.08931600
C	2.57110300	-3.80799500	1.03620800	C	-1.50627900	-1.34189400	2.16777800
C	3.18368700	-2.31622700	3.30872100	C	-2.63111500	-2.08886300	1.78201500
H	1.89479700	-0.81232200	2.48648300	C	-2.59790200	-3.46436800	2.01050300
C	3.44717800	-4.31503200	1.98868100	C	-1.50093200	-4.06191200	2.61391800
H	2.30964500	-4.38878000	0.15896500	C	-0.41253000	-3.29375400	3.00493200
C	3.75801300	-3.57281800	3.12572800	C	-0.38845100	-1.91681300	2.78484700
H	3.41561400	-1.73212000	4.19470200	C	-3.88859400	-1.44033900	1.22226900
H	3.88757300	-5.29706500	1.84351900	C	0.77574100	-1.06415800	3.24492400
H	4.44430400	-3.97107800	3.86742900	H	-0.26034200	5.69751900	-1.31997600
C	-0.26047100	-3.69356500	-1.08075700	H	-3.74446300	3.72836600	-2.81793300
O	0.19193100	-4.77790700	-0.77569000	H	0.38880400	3.02746000	1.24494100
O	-1.45050800	-3.53358300	-1.68716100	H	-3.25573200	0.72940100	-0.76936600
C	-2.21571300	-4.71796800	-1.93910400	H	-3.44573500	-4.07497500	1.71505800
H	-2.86634200	-4.44790600	-2.77332400	H	0.43657600	-3.77254400	3.48284800
C	-3.01951100	-5.10913500	-0.71231700	H	-3.66497500	-0.39628000	0.99416000
H	-3.64911600	-5.97632100	-0.93661800	H	0.74893100	-0.13047600	2.68334700

C	0.61435400	-0.69470900	4.72606600	C	0.07565400	-3.21955600	-0.43811300
H	0.65157700	-1.58699100	5.36303500	H	0.68553100	-2.54236300	0.15144700
H	1.41425500	-0.01232800	5.03142300	C	-1.64516400	-3.58438300	-2.08027300
H	-0.34191200	-0.19154600	4.90481600	H	-2.36521300	-3.17024700	-2.77920000
C	2.13941600	-1.71324600	2.99193900	C	-1.50915700	-4.95722100	-1.92128100
H	2.93409700	-0.99705200	3.22750900	H	-2.12480700	-5.63436500	-2.50663800
H	2.30107100	-2.59620900	3.62122800	C	0.20906600	-4.59361700	-0.26975600
H	2.25731800	-2.00865000	1.94471500	H	0.92552700	-4.97885700	0.44969400
C	-4.95643700	1.86879700	-0.09409600	C	-0.57991100	-5.46492400	-1.01388900
H	-5.52685500	2.75946500	-0.38381800	H	-0.47163500	-6.53863400	-0.88826300
H	-5.64397400	1.01477800	-0.08560000	C	-1.02551300	-1.21167900	-1.56393800
H	-4.59376400	2.01301700	0.92696700	C	-2.33779300	2.11861700	2.07521800
C	-4.39875900	1.26485700	-2.46121800	C	-2.24801600	0.95454700	2.75112300
H	-4.92331100	0.30686200	-2.39186700	H	-2.80153200	3.05935200	2.32475100
H	-5.12217100	2.01547100	-2.80210600	H	-2.62373500	0.65546000	3.71627100
H	-3.61729000	1.15736100	-3.21680500	O	-2.02325500	-0.84653800	-2.16439900
C	-4.99179200	-1.44076500	2.29133200	Si	0.85854500	0.25189100	-2.91747200
H	-5.87644300	-0.90812600	1.92524900	C	-0.39895800	1.57499700	-3.37434800
H	-5.29169400	-2.46415500	2.54495700	H	-1.41030100	1.23124700	-3.15085200
H	-4.65604900	-0.95269000	3.21257700	H	-0.21669600	2.50433300	-2.82429700
C	-4.38369800	-2.08087700	-0.07808700	H	-0.32775000	1.79428600	-4.44791400
H	-5.30078600	-1.57715200	-0.40571600	C	0.74796900	-1.19517900	-4.12925200
H	-3.64275900	-1.98101700	-0.87409700	H	-0.25769600	-1.62130100	-4.17796200
H	-4.61917600	-3.14311800	0.05102100	H	1.01018000	-0.82457600	-5.12878100
C	1.68308400	4.12807900	-0.03566800	H	1.45100200	-1.99681300	-3.88267300
H	1.75130600	5.08398100	-0.56730600	C	2.56175300	1.03753900	-3.19252600
H	2.51084200	4.09453400	0.68050000	H	2.55200000	1.52078300	-4.17830700
H	1.82506700	3.32051600	-0.76110400	H	2.78637700	1.80366500	-2.44352500
C	0.14834100	5.08739400	1.73245200	H	3.37385600	0.30546100	-3.18389400
H	-0.79645100	4.96151600	2.27212400	C	2.42054500	-0.23799900	-0.38209600
H	0.96121000	5.06973300	2.46612600	C	2.06824100	0.65036700	0.46749700
H	0.13396800	6.07477600	1.25537600	C	3.48019300	-1.08751600	-0.89166300
H	-1.49333500	-5.13526400	2.77905000	C	4.81669400	-0.74143400	-0.64381300
H	-2.14543500	5.59331900	-2.90852500	C	3.19518200	-2.25883700	-1.60088100
Pd	0.35263200	-0.01448800	-0.57429500	C	5.84307600	-1.55625200	-1.10435400
C	-0.84984900	-2.70118700	-1.34270400	H	5.02879700	0.17051200	-0.09547600

C	4.22558400	-3.07150100	-2.05698100	C	-2.75044700	3.99482600	-1.44910600
H	2.15980200	-2.52412200	-1.78522500	C	-1.60462400	3.59735100	-2.12174100
C	5.55095000	-2.72135300	-1.81163200	C	-1.28216700	2.24744400	-2.25906500
H	6.87640900	-1.28151400	-0.91386600	C	-4.34813400	0.65437600	-0.53397000
H	3.99188400	-3.97965000	-2.60446000	C	-0.05444600	1.82803500	-3.04643000
H	6.35620100	-3.35522200	-2.17133800	H	1.23101700	-5.70423800	-0.11563100
C	2.57418100	1.44090600	1.57457100	H	-2.16793300	-4.93557200	2.35568400
O	1.93964600	1.82791400	2.53674500	H	0.87822500	-2.47579700	-1.95238600
O	3.88456000	1.72509400	1.41817900	H	-2.76637700	-1.59524000	0.94513400
C	4.48216200	2.50340900	2.46194200	H	-4.51260400	3.37171400	-0.40495700
H	3.95809900	3.46196000	2.53834200	H	-0.94116900	4.34976800	-2.53742100
H	4.35488300	1.98164000	3.41550400	H	-3.84408600	-0.31306000	-0.47041000
C	5.94196100	2.68582500	2.10487900	H	0.08167700	0.75415300	-2.89634000
H	6.04457900	3.20216300	1.14603800	C	-0.28936200	2.05762200	-4.54650800
H	6.44331300	3.28009900	2.87493700	H	-0.42530300	3.12340300	-4.76350400
H	6.44636300	1.71751900	2.03294800	H	0.56842400	1.70057300	-5.12732600
				H	-1.18387700	1.52922400	-4.89402900
INT4'				C	1.22680500	2.52289400	-2.57410900
SCF Done: E(RωB97XD) = -2616.04645032	A.U.			H	2.07428700	2.20560100	-3.19053400
Sum of electronic and thermal Free Energies = -2615.153374	A.U.			H	1.14773300	3.61321500	-2.65365700
SCF Done (single point): E(RωB97XD) = -2617.72811859	A.U.			H	1.46387100	2.26420500	-1.53891400
no imaginary frequency				C	-4.29854700	-2.99197300	0.36001300
N	-1.39466800	-2.08351100	-1.14187000	H	-4.59654700	-4.02881400	0.55553600
N	-1.86240400	-0.08928000	-1.78379700	H	-5.13046800	-2.33894000	0.64846400
C	-1.17257900	-0.77992900	-0.83738700	H	-4.14478000	-2.87862200	-0.71727300
C	-1.03101600	-3.20300000	-0.31318100	C	-3.35189200	-2.65811200	2.66488300
C	0.10550400	-3.95012600	-0.64285400	H	-4.06859900	-1.86456800	2.89653300
C	0.36421800	-5.09346000	0.11526600	H	-3.79739000	-3.61014400	2.97787300
C	-0.46333900	-5.45287000	1.16868600	H	-2.45382300	-2.47621400	3.26085700
C	-1.55414800	-4.66136900	1.50443500	C	-5.49822700	0.51188700	-1.54324600
C	-1.86128000	-3.51167500	0.77827600	H	-6.18912300	-0.27703100	-1.22614600
C	1.03269000	-3.54348700	-1.77462900	H	-6.06211300	1.44877700	-1.62075900
C	-3.04125600	-2.63044400	1.16606300	H	-5.13157200	0.26173800	-2.54397500
C	-2.16162900	1.31551700	-1.69892200	C	-4.89604800	0.95345600	0.86431000
C	-3.34631800	1.68368600	-1.03873500	H	-5.59015300	0.15811600	1.15940000
C	-3.61580800	3.04619800	-0.92223800	H	-4.09091100	0.98793600	1.60072400

H	-5.45232100	1.89689800	0.89726700	H	1.21374700	-0.02902700	5.27567400
C	2.50881100	-3.72831500	-1.40689100	H	1.89910900	1.32371700	4.35609800
H	2.78312800	-4.78734900	-1.34126100	C	3.57108400	-1.48632100	3.55162500
H	3.14457200	-3.26795900	-2.16964300	H	3.47816300	-1.99443800	4.51913600
H	2.73230700	-3.25005600	-0.44894900	H	3.93072200	-2.21921800	2.81944500
C	0.69908800	-4.29981400	-3.06805300	H	4.31955800	-0.69453000	3.64620100
H	-0.33218800	-4.12070300	-3.38901900	C	2.26320200	0.14638400	1.36300900
H	1.36581300	-3.98124600	-3.87701200	C	2.14144900	-0.43884300	0.11260100
H	0.82576900	-5.37976500	-2.92863600	C	3.12336100	-0.38669800	-0.95807600
H	-2.96801900	5.05138200	-1.32824500	C	2.72315700	-0.43101600	-2.30057100
H	-0.24531900	-6.34596600	1.74698000	C	4.49957400	-0.39964700	-0.67386900
Pd	0.18358500	-0.09703600	0.49486000	C	3.65713400	-0.43208700	-3.32705300
C	-1.18023000	2.46982000	1.57048900	H	1.66112800	-0.46347500	-2.51931300
C	-0.17933000	3.18168700	0.91325900	C	5.43672200	-0.43182700	-1.69813200
H	0.58551000	2.63959400	0.36861100	H	4.82528800	-0.39656200	0.36309000
C	-2.15507800	3.16405400	2.29486300	C	5.01930200	-0.43647700	-3.02804500
H	-2.91719500	2.59805600	2.82097500	H	3.32563200	-0.44789400	-4.36160300
C	-2.13667000	4.55121800	2.34128300	H	6.49653000	-0.44764400	-1.46116300
H	-2.89856000	5.08694700	2.90061200	H	5.75319500	-0.45641500	-3.82830600
C	-0.14908300	4.57151400	0.97267300	C	3.08762100	1.37929400	1.53123000
H	0.63926900	5.11696800	0.46127600	O	3.78879900	1.64997000	2.48535400
C	-1.13142700	5.25749300	1.67933900	O	2.93857100	2.21832000	0.48137100
H	-1.11220500	6.34308700	1.72404500	C	3.72416400	3.41250900	0.47308800
C	-1.21008800	0.96522600	1.52435000	H	3.15105400	4.10817200	-0.14555000
C	-2.17978400	-2.20386900	-2.27860300	C	5.09707800	3.15225900	-0.12026700
C	-2.46946200	-0.95003600	-2.68516300	H	5.64867300	4.09330500	-0.21727500
H	-2.46281800	-3.16674300	-2.67211900	H	5.66954100	2.48114700	0.52593400
H	-3.05301500	-0.58342300	-3.51384000	H	5.00513600	2.69245800	-1.10887400
O	-1.98544900	0.35649300	2.24555000	H	3.79430900	3.80615500	1.48987200
Si	1.91229500	-0.77023400	3.00824900				
C	0.69581200	-2.19059100	2.80673500	INT4			
H	-0.32621000	-1.82482600	2.66416800	SCF Done: E(R ω B97XD) = -2616.06893906	A.U.		
H	0.94512100	-2.84563100	1.96573400	Sum of electronic and thermal Free Energies = -2615.173144	A.U.		
H	0.70874700	-2.79841500	3.72100300	SCF Done (single point): E(R ω B97XD) = -2617.74884640	A.U.		
C	1.25594200	0.44151100	4.28614000	no imaginary frequency			
H	0.24273000	0.76575400	4.02552000	N	-1.13531500	1.38907300	-2.10048000

N	-2.78320000	0.24185700	-1.37237000	H	0.32140700	-0.65520100	-5.52603000
C	-1.47225800	0.49116500	-1.13828900	H	-0.54413900	0.80835000	-5.03083600
C	0.13449100	2.06133700	-2.16573700	C	2.34133300	-0.60809700	-3.66939200
C	0.27733200	3.25961600	-1.45014000	H	2.16560400	-1.62289900	-4.04082400
C	1.45935900	3.97778900	-1.62904800	H	3.06837000	-0.14574200	-4.34632400
C	2.46092100	3.50583900	-2.46511600	H	2.79694500	-0.68056400	-2.67562400
C	2.32241600	2.27821300	-3.10062400	C	-3.48857900	-2.48519300	-3.14568300
C	1.16004800	1.51981300	-2.95748000	H	-2.87239200	-2.96523800	-3.91367800
C	-0.76652000	3.74479200	-0.45814500	H	-4.47195200	-2.96970000	-3.14706400
C	1.01867200	0.16729600	-3.63779900	H	-3.62471300	-1.43880000	-3.43353800
C	-3.63510300	-0.55348000	-0.52877300	C	-2.54097200	-4.10350200	-1.47652100
C	-3.65408300	-1.94570300	-0.69381400	H	-1.82596500	-4.48749500	-2.21044900
C	-4.49871400	-2.67145700	0.14595800	H	-2.10762300	-4.23489800	-0.48194200
C	-5.28516500	-2.03409100	1.09724500	H	-3.44999900	-4.71174000	-1.55659000
C	-5.25073200	-0.65326800	1.22821300	C	-0.18932400	3.71048300	0.96424400
C	-4.42770000	0.12152500	0.41083700	H	0.64233100	4.41451300	1.07716800
C	-2.82057600	-2.62775700	-1.76809500	H	-0.96193300	3.97342000	1.69458800
C	-4.37362600	1.63415600	0.57254500	H	0.19187900	2.71293000	1.20443400
H	1.60216900	4.91113400	-1.09244200	C	-1.30943500	5.13164600	-0.81940300
H	3.13716500	1.89950300	-3.70775500	H	-1.75048800	5.13649500	-1.82193100
H	-1.61109600	3.05007100	-0.47758100	H	-2.08336500	5.43052700	-0.10409900
H	0.30916100	-0.42594900	-3.04911900	H	-0.52222400	5.89328800	-0.79353300
H	-4.53813300	-3.75150500	0.06195300	H	-5.92989900	-2.62254300	1.74370600
H	-5.86619100	-0.17276800	1.98161100	H	3.37438100	4.07855300	-2.59525900
H	-1.85238600	-2.11736300	-1.80611000	Pd	0.10660500	-0.22323900	0.04696000
H	-4.02228800	2.06811800	-0.36929600	C	-1.32138900	-0.81073800	2.57973500
C	-5.74631100	2.25429800	0.85640700	C	-0.76997600	0.34266300	3.13491200
H	-6.11015000	2.00197900	1.85837500	H	0.07024400	0.82107800	2.64499200
H	-5.67460600	3.34583900	0.80511400	C	-2.41759900	-1.42176400	3.19423600
H	-6.49591600	1.92505200	0.12932800	H	-2.84058900	-2.31341000	2.74405700
C	-3.36018900	2.01941300	1.65584400	C	-2.95864100	-0.87534600	4.35155600
H	-3.32163300	3.10896900	1.77437200	H	-3.82042500	-1.34326400	4.81867400
H	-3.63119000	1.57588700	2.62000800	C	-1.29269100	0.87145700	4.30965100
H	-2.35767600	1.66535400	1.40176800	H	-0.84725200	1.76153300	4.74383500
C	0.43793700	0.32453600	-5.05054200	C	-2.39092200	0.26626400	4.91623500
H	1.10283800	0.93096200	-5.67659600	H	-2.80815200	0.68582200	5.82738500

C	-0.78479300	-1.43013000	1.32129100	H	6.50166200	-1.55203500	2.64131000
C	-2.21245800	1.70091600	-2.91301800	C	6.27903100	0.47737200	1.90285500
C	-3.25291200	0.97240000	-2.45482000	H	7.32095500	0.75595900	2.09465600
H	-2.13243200	2.41008600	-3.72122400	H	5.94281600	0.98254300	0.99419100
H	-4.27956500	0.90680900	-2.77822200	H	5.66038400	0.82314300	2.73580800
O	-1.00759500	-2.58748200	1.05820900	H	6.74223400	-1.38056100	0.88287800
Si	2.36374100	-3.28714200	-0.38290800				
C	0.88329700	-3.26227300	-1.53897000	TS3			
H	0.99638300	-2.53480700	-2.34674400	SCF Done: E(RoB97XD) = -2616.05519466	A.U.		
H	0.74313400	-4.25423700	-1.98661100	Sum of electronic and thermal Free Energies = -2615.160201	A.U.		
H	-0.01103000	-3.01687700	-0.96124900	SCF Done (single point): E(RoB97XD) = -2617.73295508	A.U.		
C	1.98382500	-4.42340000	1.07029500	$v_i = -240.28 \text{ cm}^{-1}$			
H	1.07671600	-4.08117000	1.57882000	N	1.95600100	2.39073300	-0.20310300
H	1.82010000	-5.45511700	0.73668700	N	3.02314100	0.68677800	0.52370300
H	2.80480300	-4.42519900	1.79569700	C	1.78806100	1.08617800	0.13215500
C	3.87487800	-3.93210200	-1.31185400	C	0.90039900	3.14790600	-0.81402000
H	3.66138500	-4.91126900	-1.75631800	C	0.70732700	3.00696300	-2.19594300
H	4.16933600	-3.24478000	-2.11155300	C	-0.33568800	3.73097600	-2.77521500
H	4.73928100	-4.04792800	-0.64823900	C	-1.15661600	4.54122800	-2.00370300
C	2.80735000	-1.58414900	0.30964600	C	-0.95689600	4.63957700	-0.63255900
C	1.97569200	-0.61846400	0.75418400	C	0.07190300	3.93838200	-0.00453500
C	2.51663100	0.62955400	1.36144300	C	1.58676000	2.11441900	-3.05780400
C	2.57123000	0.80078800	2.75210400	C	0.28920400	4.03428500	1.49619200
C	2.95065200	1.68206800	0.54574700	C	3.33350900	-0.69596100	0.76835200
C	3.02304700	1.99349900	3.30418500	C	3.03429000	-1.25824000	2.01949900
H	2.25777500	-0.01613900	3.39584000	C	3.25073400	-2.62680300	2.16457000
C	3.40913900	2.87355400	1.10020200	C	3.73387500	-3.39580300	1.11199200
H	2.93379100	1.55398400	-0.53243300	C	4.03866200	-2.80647600	-0.10381800
C	3.44136500	3.03926000	2.48079500	C	3.85129900	-1.43743800	-0.30015600
H	3.05946900	2.10586700	4.38457000	C	2.51249700	-0.40242900	3.16474000
H	3.74007000	3.67375000	0.44359500	C	4.19574600	-0.80878100	-1.64278300
H	3.79757100	3.96880800	2.91524700	H	-0.51180800	3.65277700	-3.84395500
C	4.27472400	-1.29131600	0.35375500	H	-1.62258700	5.25917200	-0.04135200
O	4.92953600	-0.97041600	-0.61704600	H	2.22480900	1.51974400	-2.39842900
O	4.79707700	-1.42620400	1.58587500	H	0.78246400	3.11074600	1.81841800
C	6.16668200	-1.02879200	1.74292900	H	3.01534800	-3.11108800	3.10508500

H	4.40839100	-3.41984700	-0.92029700	H	-1.96888700	5.08980100	-2.47093900
H	1.74381600	0.26071400	2.75210100	Pd	-0.05029200	0.13664200	0.10156500
H	4.08612700	0.27584200	-1.55741200	C	0.10802300	-2.85624900	0.14546600
C	5.65571100	-1.07969500	-2.02849200	C	0.43292000	-2.78167600	-1.20744700
H	5.83733200	-2.14713400	-2.19477200	H	0.29092100	-1.84395500	-1.73528600
H	5.90559900	-0.55321800	-2.95618500	C	0.27545300	-4.06639300	0.82464600
H	6.34289000	-0.74159400	-1.24573900	H	0.02417100	-4.10679100	1.87951600
C	3.23369900	-1.26758700	-2.74205700	C	0.76176400	-5.18355800	0.15860800
H	3.48819900	-0.78774700	-3.69439900	H	0.88982100	-6.12107600	0.69219200
H	3.27813800	-2.35306300	-2.88288100	C	0.92088400	-3.89875300	-1.87609300
H	2.20485600	-1.00148600	-2.48565600	H	1.16151700	-3.82938600	-2.93274500
C	1.22025300	5.20852100	1.83367100	C	1.08637400	-5.10074200	-1.19478800
H	0.78016400	6.15603400	1.50174800	H	1.46375000	-5.97533000	-1.71746300
H	1.38494300	5.26910300	2.91485700	C	-0.39761400	-1.67376100	0.92641900
H	2.19591200	5.10163900	1.34867900	C	3.26991400	2.79707700	-0.03728700
C	-1.02383000	4.14386400	2.27738800	C	3.94342500	1.71982400	0.42705300
H	-0.82801400	4.02778600	3.34778000	H	3.59577100	3.79865500	-0.26788800
H	-1.50316500	5.11932300	2.13714800	H	4.98270100	1.58171300	0.67985400
H	-1.73162500	3.36584300	1.97688500	O	-0.56015700	-1.76289200	2.12909000
C	3.63649800	0.46770300	3.75084000	Si	-2.75741000	0.15258200	2.79012000
H	3.24894600	1.08270300	4.57041700	C	-1.12179300	0.86120900	3.40234300
H	4.44061900	-0.16202200	4.14928200	H	-0.52414700	1.24865800	2.56977200
H	4.06973700	1.14200600	3.00654700	H	-1.29763000	1.67509400	4.11471200
C	1.85073900	-1.21340500	4.27985800	H	-0.53672100	0.07773000	3.88650500
H	1.41068900	-0.52924800	5.01277000	C	-3.26588200	-1.39021900	3.74359900
H	1.05359600	-1.84809400	3.88372800	H	-2.51006400	-2.17288900	3.64095400
H	2.57701900	-1.83578700	4.81670800	H	-3.39358500	-1.16293000	4.80871600
C	0.75623500	1.12231000	-3.87906600	H	-4.21797100	-1.77654600	3.36304700
H	0.09188200	1.63130300	-4.58616800	C	-4.08934800	1.46463900	3.08328500
H	1.41571900	0.46858000	-4.45938200	H	-4.05220200	1.79845900	4.12746200
H	0.13793500	0.49667500	-3.22750300	H	-3.95189100	2.33928000	2.43903500
C	2.50528100	2.95932400	-3.95040900	H	-5.09671700	1.07886100	2.89280500
H	3.13576300	3.62422400	-3.35011900	C	-2.88134000	-0.25514900	0.92717400
H	3.15933400	2.31309900	-4.54633800	C	-1.96733600	-0.68664200	0.03468900
H	1.92328100	3.58061600	-4.64086700	C	-2.34991100	-1.04522700	-1.35957200
H	3.86415600	-4.46551700	1.24255800	C	-2.64808200	-2.36684700	-1.70813000

C	-2.41685200	-0.05769200	-2.35114900	C	1.60674700	2.86175300	-0.29794500
C	-2.97979100	-2.69679800	-3.01803600	C	2.12858300	2.87835200	1.00278100
H	-2.61519200	-3.13657200	-0.94382400	C	3.51583000	2.95290400	1.12963200
C	-2.75844800	-0.38792600	-3.65862200	C	4.33357300	3.01518800	0.01010900
H	-2.20238600	0.97456000	-2.08672500	C	3.78870900	2.94827600	-1.26516700
C	-3.03424100	-1.71018000	-3.99900600	C	2.41056900	2.84799400	-1.44754500
H	-3.19969000	-3.73033700	-3.27048000	C	1.21576500	2.84683400	2.21924300
H	-2.80726100	0.39164100	-4.41367800	C	1.80949600	2.62748700	-2.82872800
H	-3.29388800	-1.96813600	-5.02164900	H	-4.49392200	-0.88142100	-2.75768900
C	-4.26266800	-0.04430100	0.38241400	H	-5.88336700	0.86054400	0.88798600
O	-4.68786900	1.02067100	-0.00690300	H	-1.15165100	0.64731400	-2.51584700
O	-4.98275900	-1.17975200	0.38624600	H	-2.68527100	2.71999200	1.46845500
C	-6.27815400	-1.10643800	-0.23122500	H	3.96690500	2.95616200	2.11548500
H	-6.83730500	-1.93458400	0.20942000	H	4.44893700	2.95263700	-2.12678600
C	-6.16603000	-1.24720400	-1.73887500	H	0.34891900	2.23112900	1.95958300
H	-7.16287800	-1.21858600	-2.19185600	H	0.77764400	2.99340200	-2.82138200
H	-5.57034900	-0.43075900	-2.15568900	C	2.54333800	3.37589400	-3.94527200
H	-5.68529000	-2.19225500	-2.00435100	H	3.54365100	2.96515100	-4.12174300
H	-6.75111600	-0.16093600	0.04501500	H	1.98726800	3.28120200	-4.88381700
				H	2.64936800	4.44122600	-3.71549500
				C	1.75184400	1.11981000	-3.12551000
INT5				H	1.25479800	0.93436900	-4.08509900
SCF Done: E(RωB97XD) = -2616.11697116			A.U.	H	2.76200100	0.69552600	-3.17700800
Sum of electronic and thermal Free Energies = -2615.223571			A.U.	H	1.20132200	0.58595500	-2.34330900
SCF Done (single point): E(RωB97XD) = -2617.79248781			A.U.	C	-4.51105300	3.81955600	1.22130700
no imaginary frequency				H	-5.58974500	3.63875100	1.14861000
N	-1.84613800	2.27623500	-0.75461800	H	-4.33384800	4.48522800	2.07315400
N	0.18281600	2.88403200	-0.48290000	H	-4.20033400	4.34370400	0.31271100
C	-0.62782400	1.80150900	-0.39059200	C	-4.15729100	1.84167600	2.73422000
C	-3.02891300	1.46363900	-0.81770100	H	-3.83085900	2.47004100	3.56985500
C	-3.17996600	0.58595300	-1.90327700	H	-5.24359800	1.72506200	2.81846100
C	-4.34589800	-0.17511400	-1.94829300	H	-3.69992400	0.85647900	2.84884600
C	-5.31439200	-0.06152700	-0.95899600	C	0.71157900	4.25877800	2.55295300
C	-5.12772500	0.80176600	0.11096000	H	0.01785600	4.22420100	3.40039100
C	-3.96950200	1.57338500	0.21452000	H	1.54697700	4.91589400	2.82245800
C	-2.12215400	0.48620100	-2.99272900	H	0.18505300	4.70987100	1.70527100
C	-3.75589400	2.49496600	1.40592800				

C	1.86063800	2.19354300	3.44326600	H	-0.03396100	0.05770900	3.73540700
H	1.11364600	2.10034400	4.23812500	C	-0.96916200	-3.15840900	3.86647600
H	2.23072200	1.18983400	3.21168400	H	0.07156600	-3.09492200	4.19356800
H	2.68773100	2.79137900	3.84372100	H	-1.62035000	-3.11484500	4.74795600
C	-2.05435400	-0.89393300	-3.65139700	H	-1.12101100	-4.12734400	3.37889600
H	-2.91678900	-1.08372300	-4.30176600	C	-3.21418700	-1.86478500	2.25324000
H	-1.15831700	-0.95129500	-4.28068700	H	-3.81594400	-1.61195300	3.13505800
H	-2.00544700	-1.68275800	-2.89542000	H	-3.48215600	-1.17454900	1.44544800
C	-2.31606200	1.58894300	-4.04409700	H	-3.50598900	-2.87228700	1.93519400
H	-2.27649700	2.58663600	-3.59439300	C	-0.51367000	-2.08618400	0.99061600
H	-1.52957700	1.53129500	-4.80547700	C	0.84591100	-1.99263400	0.64119400
H	-3.28468900	1.48003200	-4.54603800	C	1.38622100	-2.77144800	-0.52333900
H	5.41010800	3.08077800	0.13469700	C	2.31433900	-3.79153300	-0.29450200
H	-6.21531400	-0.66532900	-1.01439000	C	0.96575000	-2.53229200	-1.83555100
Pd	-0.17606200	-0.15389100	0.17436900	C	2.81530500	-4.54678400	-1.34908700
C	3.16491000	-0.95317300	1.19841500	H	2.64706900	-3.99290300	0.72027700
C	3.46044800	-0.58416800	-0.11685900	C	1.46644000	-3.28597600	-2.89162400
H	2.68484400	-0.59413100	-0.87291200	H	0.24262800	-1.74276400	-2.01939800
C	4.16994400	-0.88335200	2.16721900	C	2.39450500	-4.29530500	-2.65301400
H	3.92369900	-1.15475500	3.18853200	H	3.53909300	-5.33216700	-1.15166200
C	5.45648800	-0.48624100	1.82424800	H	1.12663200	-3.08252800	-3.90325600
H	6.23123700	-0.44570600	2.58422100	H	2.78849200	-4.88289900	-3.47705500
C	4.74961700	-0.19969600	-0.46109400	C	-1.35482200	-2.97914000	0.12689200
H	4.96767200	0.07870600	-1.48752100	O	-2.13516200	-2.63431000	-0.73285300
C	5.75176600	-0.15681900	0.50396700	O	-1.16148700	-4.26335400	0.47713500
H	6.76045300	0.13945700	0.22922200	C	-1.84520200	-5.25597000	-0.30107100
C	1.81626600	-1.44430500	1.64501700	H	-1.86763200	-6.13563500	0.34562600
C	-1.79534800	3.62432800	-1.07307000	C	-1.10493400	-5.53748700	-1.59612400
C	-0.51323200	4.01028800	-0.89798600	H	-1.56772800	-6.38488000	-2.11314500
H	-2.66751100	4.16878300	-1.39637900	H	-1.13683900	-4.66598800	-2.25402300
H	-0.02450800	4.96115900	-1.03840400	H	-0.05616000	-5.77577500	-1.39447100
O	1.54636000	-1.43202800	2.84093600	H	-2.86806900	-4.91993200	-0.49019800
Si	-1.37251800	-1.75812100	2.67486200				
C	-1.08323800	-0.07549400	3.46861500	TS4			
H	-1.37752600	0.73637900	2.79593900	SCF Done:	E(RωB97XD) = -2040.58037750	A.U.	
H	-1.69060500	-0.00102600	4.38028100	Sum of electronic and thermal Free Energies =	-2039.864235	A.U.	

SCF Done (single point): E(R ω B97XD) = -2042.12266109 A.U.				H	0.41511000	-2.07326000	-2.01778900
$\nu_i = -111.31 \text{ cm}^{-1}$				C	-0.56403500	3.91677400	3.40744700
N	0.17641000	2.26678500	-0.19362500	H	-1.52511300	4.08613800	3.90586000
N	2.00855300	1.27043800	-0.62856100	H	0.20769600	3.87214600	4.18333400
C	0.76772800	1.04311800	-0.12313000	H	-0.35861000	4.78308700	2.76950200
C	-1.20592500	2.48960300	0.12056400	C	-0.83413900	1.39444100	3.48770900
C	-2.12968300	2.48585500	-0.93566700	H	-0.06249900	1.31696900	4.26185400
C	-3.47054000	2.70002900	-0.61674800	H	-1.80749400	1.46965400	3.98663400
C	-3.86940700	2.89315200	0.70038600	H	-0.82497100	0.47374700	2.89192700
C	-2.93323600	2.87045500	1.72531500	C	5.31299800	2.24372700	0.75106800
C	-1.57811500	2.67025700	1.45843400	H	5.42033700	2.99283800	1.54316900
C	-1.71648500	2.18213300	-2.36817400	H	6.29552800	1.78985000	0.57732500
C	-0.57232500	2.61546100	2.59558000	H	5.02111900	2.76080800	-0.16835500
C	2.98920800	0.24640900	-0.84382400	C	4.71526600	0.50745400	2.47210600
C	4.09151000	0.17683300	0.02155300	H	4.75078400	1.25904600	3.26803800
C	5.03094200	-0.82593900	-0.21390100	H	4.01246800	-0.27484600	2.76906800
C	4.86991600	-1.72394500	-1.26078200	H	5.71443400	0.06390600	2.39942100
C	3.77089500	-1.62653200	-2.10301000	C	-2.07639400	0.73384200	-2.73042900
C	2.80477100	-0.63602000	-1.91733000	H	-3.15892400	0.57093300	-2.67546100
C	4.29004400	1.17102400	1.15659500	H	-1.74524900	0.50490800	-3.75021000
C	1.64501000	-0.51461300	-2.89491200	H	-1.59905500	0.02665000	-2.04182000
H	-4.21592900	2.69405900	-1.40629800	C	-2.31211500	3.17423500	-3.37380400
H	-3.25985500	3.00481200	2.75246600	H	-2.09024200	4.21009900	-3.09587200
H	-0.62789000	2.27179500	-2.43835700	H	-1.89563500	2.99029100	-4.36982800
H	0.42379500	2.49135700	2.16098400	H	-3.39992000	3.07085400	-3.45267000
H	5.89636500	-0.91221500	0.43582000	H	5.60779800	-2.50414300	-1.42214900
H	3.65980600	-2.33243100	-2.92101200	H	-4.91921900	3.05112300	0.92957900
H	3.33125500	1.66676300	1.34094700	Pd	-0.40363600	-0.66973200	0.38876600
H	0.95987000	0.25324600	-2.52644000	C	-3.12974700	-2.07554900	0.09954300
C	2.15482100	-0.05475800	-4.26790900	C	-3.74869100	-0.82401600	0.04970900
H	2.83848400	-0.79089200	-4.70638900	H	-3.16220200	0.06039400	0.28453600
H	1.31563500	0.07832900	-4.95971700	C	-3.87109700	-3.22469100	-0.19663100
H	2.69058200	0.89782400	-4.19175800	H	-3.38125300	-4.19214600	-0.14563600
C	0.83331500	-1.81018400	-2.99468900	C	-5.21005300	-3.11666000	-0.55046000
H	0.00190200	-1.67462700	-3.69531000	H	-5.78279000	-4.00835800	-0.78896100
H	1.44034900	-2.64901900	-3.35401700	C	-5.09213400	-0.71646900	-0.28968000

H	-5.56633100	0.26047500	-0.31854900	C	-1.93965900	3.35217100	-1.23228500
C	-5.82133700	-1.86315800	-0.59630800	C	1.13707900	3.77886500	1.05965100
H	-6.87005600	-1.78240900	-0.86906400	C	-3.16958000	2.46338000	-1.35515900
C	-1.68930300	-2.14660600	0.45929600	C	-2.03145400	-1.00593000	2.01979300
C	1.02018100	3.22611300	-0.72592400	C	-3.27346800	-1.45534500	1.54360100
C	2.17894800	2.59245900	-1.00972900	C	-3.59104000	-2.79689200	1.75192800
H	0.71215200	4.25093300	-0.85900900	C	-2.71584300	-3.64144200	2.42084200
H	3.09770200	2.94827600	-1.44662200	C	-1.49775600	-3.16384300	2.88507200
O	-1.24768600	-3.32162700	0.72775900	C	-1.12089200	-1.83598300	2.68257200
Si	0.48463600	-2.87448300	1.41419000	C	-4.28533400	-0.51890100	0.89740800
C	0.03806700	-3.86942000	2.96864600	C	0.20556000	-1.31023300	3.19516300
H	-0.63421700	-3.28415900	3.60906000	H	1.22640600	5.60633400	-0.96945300
H	-0.47452300	-4.80537900	2.72636400	H	-2.36821900	4.49868100	-2.99536400
H	0.93373300	-4.09598000	3.55896500	H	0.95875700	2.79502400	1.50236500
C	1.78681600	-1.68910100	2.19013300	H	-2.88664800	1.46807700	-1.00293500
H	2.29472100	-1.08483100	1.43687700	H	-4.53800400	-3.18486300	1.38845000
H	1.35686800	-1.01979800	2.94353900	H	-0.82196400	-3.83536300	3.40609600
H	2.53809800	-2.32411700	2.68650800	H	-3.79952300	0.44261000	0.71612300
C	1.48558400	-3.84408000	0.14322800	H	0.41159400	-0.35393000	2.71186200
H	2.20824200	-4.47958100	0.67168400	C	0.12931400	-1.04718200	4.70490100
H	0.86151500	-4.48368800	-0.48741400	H	-0.04024200	-1.97723700	5.26128800
H	2.05716700	-3.16634100	-0.49902900	H	1.06503100	-0.59823700	5.05284800
				H	-0.68734500	-0.35724900	4.94517300
TS2-2				C	1.38137800	-2.23274800	2.85767400
SCF Done: E(RωB97XD) = -2616.02688968	A.U.			H	2.31227200	-1.76503100	3.19202600
Sum of electronic and thermal Free Energies = -2615.132531	A.U.			H	1.30116400	-3.20760200	3.35280900
SCF Done (single point): E(RωB97XD) = -2617.71108549	A.U.			H	1.46417800	-2.39956800	1.77871200
$\nu_i = -119.00 \text{ cm}^{-1}$				C	-4.32827900	2.98406700	-0.49033300
N	-1.30746700	2.23851500	0.84246200	H	-4.63813900	3.98206700	-0.82258900
N	-1.72081900	0.38546200	1.83331400	H	-5.19154300	2.31411500	-0.57880100
C	-1.10760100	0.90184600	0.73957700	H	-4.06287400	3.04495900	0.56877100
C	-1.01586200	3.20499700	-0.18193000	C	-3.64475700	2.27980600	-2.79864200
C	0.14145600	3.98205800	-0.06841400	H	-4.39582700	1.48465700	-2.82901400
C	0.34513900	4.97537300	-1.02960100	H	-4.10933900	3.19003000	-3.19706200
C	-0.56050500	5.16439100	-2.06249400	H	-2.82424800	1.98071500	-3.45456200
C	-1.68411800	4.35411600	-2.16634500	C	-5.44877300	-0.26126600	1.86662300

H	-6.14705700	0.46785300	1.44078600	C	0.53566500	1.61534600	-3.08919200
H	-6.00268300	-1.18514400	2.06901900	H	-0.53698300	1.42633700	-3.00856100
H	-5.08966700	0.13002700	2.82463400	H	0.79506800	2.46322700	-2.44693500
C	-4.79721200	-1.01584500	-0.45848500	H	0.77077000	1.89327800	-4.12603000
H	-5.54498100	-0.31336900	-0.84533200	C	1.21434200	-1.32538400	-3.86276300
H	-3.98800000	-1.07876000	-1.18885500	H	0.21834100	-1.75990400	-3.74629400
H	-5.27487300	-1.99875100	-0.38248800	H	1.29057500	-0.92054500	-4.88022200
C	2.58305800	3.78859800	0.55374700	H	1.95806300	-2.12150900	-3.76502900
H	2.87554600	4.76687400	0.15622000	C	3.34383000	0.62823300	-2.90956300
H	3.26337100	3.55769400	1.37917400	H	3.42327600	1.07764500	-3.90796400
H	2.72913600	3.03879100	-0.22998900	H	3.63149500	1.38495300	-2.17239700
C	0.94011600	4.83245600	2.15858900	H	4.05821200	-0.19703400	-2.84857400
H	-0.07199400	4.79408700	2.57488000	C	2.26773900	-0.63652900	-0.56102700
H	1.64730900	4.66162000	2.97731700	C	2.11895700	0.26910800	0.37288500
H	1.10474400	5.84325300	1.76663200	C	3.13262100	-1.79976400	-0.80924400
H	-2.98176000	-4.68313000	2.57418500	C	4.50440100	-1.73873400	-0.52811000
H	-0.38418300	5.94019300	-2.80187900	C	2.59142700	-2.99598800	-1.29045900
Pd	0.23538900	-0.04739800	-0.50595400	C	5.30838200	-2.85574600	-0.71941700
C	-1.47451100	-2.42918400	-1.44575400	H	4.92417400	-0.80855100	-0.16145700
C	-0.79021900	-3.15847000	-0.47642800	C	3.39843800	-4.11373500	-1.47385900
H	-0.10846800	-2.64040100	0.19044000	H	1.53071100	-3.04702300	-1.51317400
C	-2.36604500	-3.09451400	-2.29431100	C	4.75958000	-4.04665400	-1.19148200
H	-2.89224400	-2.51444300	-3.04638500	H	6.37110400	-2.79510400	-0.50261900
C	-2.56485500	-4.46316700	-2.17181200	H	2.95939100	-5.03636500	-1.84187700
H	-3.25585100	-4.97407500	-2.83654200	H	5.39166000	-4.91717900	-1.34049500
C	-0.98442800	-4.52997900	-0.35061100	C	2.86051400	0.70918600	1.54092900
H	-0.44881900	-5.08114600	0.41672800	O	2.39429500	0.92671000	2.64418200
C	-1.87186400	-5.18431000	-1.19878800	O	4.16894100	0.91538700	1.26605600
H	-2.02632000	-6.25553800	-1.10333600	C	4.97431200	1.36853100	2.35907500
C	-1.25773700	-0.93890700	-1.61358000	H	4.52746000	2.27096600	2.78826200
C	-1.99817300	2.55385300	2.00348100	H	4.97940800	0.60171300	3.14029700
C	-2.25706800	1.38665200	2.62814200	C	6.36177000	1.63034900	1.81273500
H	-2.24196500	3.57303700	2.25575900	H	6.32979000	2.39507500	1.03129000
H	-2.77695000	1.16365200	3.54565400	H	7.02058700	1.97921700	2.61398800
O	-1.97097100	-0.35065300	-2.41331800	H	6.79064200	0.71823900	1.38677100
Si	1.54930000	0.08376900	-2.66000200				

TS2-3				C	-1.07665100	4.26401200	1.57306200
SCF Done: E(RoB97XD) = -2615.99152104 A.U.				H	-1.97760300	4.82737400	1.30493100
Sum of electronic and thermal Free Energies = -2615.091271 A.U.				H	-0.42474400	4.93994300	2.13607700
SCF Done (single point): E(RoB97XD) = -2617.67796495 A.U.				H	-0.56113500	3.98767700	0.65210300
$\nu_i = -85.65 \text{ cm}^{-1}$				C	-5.80114300	-2.50010100	0.15114600
N	-2.74016200	-0.27462400	0.41882500	H	-6.51682500	-2.60871100	-0.67168900
N	-1.33537500	0.15757800	1.98901500	H	-6.01225400	-3.28016800	0.89090300
C	-1.39973900	-0.11841200	0.64883900	H	-5.99098900	-1.52723900	0.61615300
C	-3.37694300	-0.30602200	-0.87705800	C	-4.16645300	-4.00649300	-1.00481400
C	-3.38099700	0.88190500	-1.63677400	H	-4.28976900	-4.78393100	-0.24268500
C	-3.92195600	0.81818000	-2.91950100	H	-4.90940100	-4.19967500	-1.78648300
C	-4.49372600	-0.35029100	-3.40455300	H	-3.17480100	-4.11328600	-1.44612900
C	-4.59468600	-1.46283100	-2.58539900	C	-0.05711500	-2.04847500	4.23903300
C	-4.05591100	-1.46118700	-1.29721100	H	-0.12984000	-3.13971800	4.17517800
C	-2.97444500	2.22690000	-1.04256700	H	0.40189900	-1.79258400	5.20120700
C	-4.35757900	-2.62639500	-0.36793300	H	-1.07508800	-1.64555700	4.22878500
C	-0.22529600	0.79117900	2.65958200	C	2.15006300	-2.17072900	3.02532900
C	0.83377000	0.01389300	3.14958600	H	2.01764300	-3.24055600	2.83148200
C	1.88735500	0.67641500	3.77680500	H	2.76750300	-1.76743000	2.21924600
C	1.86380300	2.05520200	3.94827500	H	2.69105900	-2.07769600	3.97486800
C	0.78172700	2.79428900	3.49643900	C	-2.68901700	3.31354900	-2.08153700
C	-0.28312100	2.18425200	2.83130200	H	-3.60845000	3.65215800	-2.57390100
C	0.78009400	-1.49816700	3.07506600	H	-2.24911100	4.18185500	-1.57920200
C	-1.47094900	3.02853700	2.38928500	H	-1.98366600	2.96253900	-2.83687200
H	-3.90644200	1.70035600	-3.54872600	C	-4.08695200	2.72440900	-0.10114000
H	-5.10799900	-2.34844900	-2.94659100	H	-4.27213500	2.03816600	0.72923700
H	-2.06072800	2.08975600	-0.45755400	H	-3.81521300	3.69727100	0.32327600
H	-3.68669800	-2.56598000	0.48953400	H	-5.02487900	2.84750300	-0.65478100
H	2.73138400	0.10644800	4.15017800	H	2.69080600	2.55274300	4.44678600
H	0.76902100	3.86963400	3.64526900	H	-4.90011400	-0.37791400	-4.41114200
H	0.27102900	-1.74762700	2.14469100	Pd	0.32172200	-0.46731300	-0.47867100
H	-2.10867500	2.41738600	1.74780200	C	-3.46808600	-0.16819600	1.59736100
C	-2.30679800	3.44151900	3.61079300	C	-2.58817000	0.09709000	2.57941500
H	-1.73333600	4.10629100	4.26693600	H	-4.53926600	-0.27876200	1.61462300
H	-3.20871200	3.97500600	3.29125200	H	-2.72701000	0.27488000	3.63323500
H	-2.61590000	2.57558000	4.20513300	C	2.08723200	-1.61430600	-0.94878200

C	2.18994100	-0.41594200	-1.39480400	H	6.22510700	1.79129300	-1.31631700
Si	-0.08928700	-2.94825200	-0.35578900	H	5.78365300	2.93235900	-3.47664000
C	-0.85427200	-3.05390400	-2.08169200	C	3.08500300	-2.69849500	-1.00059400
H	-0.07207700	-2.81910700	-2.81231800	O	3.43408900	-3.26343800	-2.01036900
H	-1.21023100	-4.06979500	-2.29437900	O	3.62174000	-2.93741200	0.20628600
H	-1.67222200	-2.34540200	-2.24034900	C	4.60785700	-3.97708800	0.25020900
C	-1.28779200	-3.36628900	1.07469000	H	4.17609300	-4.88960000	-0.17258700
H	-1.97700300	-4.14976700	0.73569500	H	5.45804100	-3.68872300	-0.37552700
H	-0.70507500	-3.79751200	1.89682000	C	5.00495300	-4.15978700	1.69960400
H	-1.87384100	-2.54261200	1.48491900	H	4.14444800	-4.46487300	2.30236900
C	0.99000800	-4.50687600	-0.20578900	H	5.77528200	-4.93305000	1.77915700
H	0.28760600	-5.34579700	-0.11457900	H	5.40341900	-3.22919500	2.11458300
H	1.62278100	-4.70423700	-1.07380800				
H	1.61453200	-4.50290600	0.69388600	TS2-4			
C	0.24358600	1.36675800	-1.46676500	SCF Done: E(RoB97XD) = -2615.98682276	A.U.		
O	-0.33876900	1.39250000	-2.53207100	Sum of electronic and thermal Free Energies = -2615.089402	A.U.		
C	0.93892500	2.59917500	-0.95504800	SCF Done (single point): E(RoB97XD) = -2617.67300933	A.U.		
C	1.72397000	2.55378800	0.19459900	$v_i = -104.63 \text{ cm}^{-1}$			
C	0.83299000	3.79619300	-1.66994800	N	-2.66965100	-0.64161300	0.46794700
C	2.39041500	3.69266300	0.63374100	N	-1.50127800	0.52381800	1.84581300
H	1.81416500	1.61676000	0.73895300	C	-1.40911500	-0.14062900	0.65108900
C	1.48350400	4.93870800	-1.22380300	C	-3.18323200	-1.19318000	-0.76317100
H	0.24171200	3.80677400	-2.57976500	C	-3.34828800	-0.31685600	-1.85533700
C	2.26531200	4.88680800	-0.06950800	C	-3.74925700	-0.87549500	-3.06727400
H	3.00052500	3.64607500	1.53052000	C	-4.04264000	-2.22836800	-3.17531800
H	1.39303300	5.86894800	-1.77738900	C	-4.00733900	-3.03676700	-2.05063300
H	2.78106400	5.77823300	0.27662300	C	-3.59327400	-2.53514500	-0.81481300
C	3.15538600	0.49120000	-1.99438100	C	-3.27330500	1.19866800	-1.69629000
C	2.91173900	1.13469800	-3.21146300	C	-3.75401100	-3.39846000	0.42751500
C	4.35764100	0.73331300	-1.31856900	C	-0.61208100	1.56355900	2.30461000
C	3.85934500	2.00174000	-3.74159700	C	0.56717400	1.23373900	2.98441300
H	1.97135800	0.96421300	-3.72458200	C	1.37652300	2.27909400	3.42760300
C	5.29736500	1.60754800	-1.85055200	C	1.00969700	3.60299600	3.22636000
H	4.53873600	0.23633300	-0.36966800	C	-0.17270300	3.90272300	2.56697800
C	5.05093700	2.24545200	-3.06343200	C	-1.00419100	2.89464800	2.07800200
H	3.66169300	2.49602900	-4.68815200	C	0.92106100	-0.20678100	3.28668800

C	-2.29582100	3.27562800	1.36670500	H	-2.28233800	1.57084100	-3.59982400
H	-3.84412300	-0.24177200	-3.94119900	C	-4.54765600	1.69361700	-0.98683600
H	-4.31218600	-4.07564400	-2.12908200	H	-4.67227500	1.25648800	0.00777200
H	-2.41122300	1.44541800	-1.07039000	H	-4.51689800	2.78286500	-0.87163300
H	-3.19470100	-2.93920400	1.24349900	H	-5.43346400	1.44099300	-1.58104000
H	2.30173000	2.05396400	3.94793300	H	1.64907300	4.40350500	3.58728700
H	-0.44778400	4.94114900	2.40907700	H	-4.34222600	-2.64307300	-4.13308400
H	0.43235300	-0.82011300	2.53089200	Pd	0.43495400	-0.44624300	-0.28544600
H	-2.72579800	2.37446100	0.92584900	C	-3.48790700	-0.35764100	1.55418800
C	-3.31649900	3.82957800	2.37219700	C	-2.75329300	0.36385100	2.41984800
H	-2.95995000	4.76721500	2.81384600	H	-4.51197800	-0.68891100	1.59562600
H	-4.27073800	4.03070800	1.87316000	H	-2.99784700	0.80335600	3.37298300
H	-3.50257800	3.12707700	3.19081000	C	2.45765700	-1.39399900	-0.46739800
C	-2.08275500	4.27114400	0.22025700	C	2.33272600	-0.25197100	-1.03309700
H	-3.04754400	4.50997000	-0.24103100	Si	0.52285900	-2.86395800	0.55304200
H	-1.64425000	5.21240200	0.56818300	C	-0.11960600	-3.63821800	-1.04980900
H	-1.42840000	3.86069000	-0.55109700	H	0.63015700	-3.48608300	-1.83385600
C	-5.23961700	-3.42800800	0.83005600	H	-0.26905300	-4.71959700	-0.94139200
H	-5.83395200	-3.94150700	0.06576700	H	-1.04791300	-3.17914900	-1.40139000
H	-5.36995200	-3.96179700	1.77787500	C	-0.69005600	-2.99794700	2.03014600
H	-5.65986600	-2.42292800	0.94228600	H	-1.18909800	-3.97404700	1.98263400
C	-3.24111900	-4.83329000	0.27246700	H	-0.10194000	-2.99617400	2.95544100
H	-3.30981400	-5.35318500	1.23436900	H	-1.45146700	-2.22380500	2.12468300
H	-3.83798600	-5.40412400	-0.44735600	C	1.79854500	-4.09956600	1.23792200
H	-2.20152900	-4.85514300	-0.05543100	H	1.20838300	-4.91822100	1.67182600
C	0.36320600	-0.61417000	4.65656800	H	2.46818500	-4.53181500	0.49301700
H	0.59608700	-1.66346800	4.86903400	H	2.41646700	-3.68381800	2.04100900
H	0.79717200	-0.00000400	5.45444000	C	0.08739400	0.97887700	-1.74822000
H	-0.72547700	-0.49688700	4.69148600	O	-0.41336100	0.56065400	-2.76721300
C	2.41951600	-0.49091400	3.18254600	C	0.48450000	2.42531400	-1.62622600
H	2.59236900	-1.57113400	3.23908600	C	1.11984200	2.90426700	-0.48311500
H	2.81205500	-0.13050600	2.22647000	C	0.23604700	3.29429300	-2.69434200
H	2.98947800	-0.02647800	3.99568500	C	1.48958800	4.24350600	-0.39712900
C	-3.11289500	1.96457300	-3.01140100	H	1.32983400	2.22076800	0.33468400
H	-4.03027700	1.93059600	-3.61129400	C	0.59841400	4.63166300	-2.60697800
H	-2.90794800	3.01754400	-2.78941600	H	-0.23344600	2.89615800	-3.58771200

C	1.22557200	5.10818200	-1.45458500	C	-5.02376900	-1.34457000	0.69485800
H	1.97334200	4.60972700	0.50316400	C	-4.91911300	-1.80710400	1.99864700
H	0.40114200	5.30472900	-3.43632300	C	-3.92781000	-1.30963600	2.83295900
H	1.50960700	6.15461900	-1.38472700	C	-3.04617200	-0.31788100	2.39780200
C	3.09582000	0.70044000	-1.83589300	C	-4.30324400	0.07723000	-1.24970600
O	3.05242000	0.79212400	-3.04037500	C	-2.01947200	0.25893200	3.35232100
O	3.82321500	1.50951100	-1.04582600	C	0.13803300	2.65803500	-1.43800600
C	4.44979200	2.61348300	-1.71252900	C	0.80568400	3.88068700	-1.26384400
H	5.16128800	2.23304000	-2.45165900	C	1.93791300	4.11514400	-2.04965400
H	3.67920500	3.18233700	-2.24313600	C	2.39077300	3.17417800	-2.95744000
C	5.12874300	3.44839100	-0.64845000	C	1.66283600	2.00913900	-3.16928700
H	5.88697000	2.86435600	-0.11837800	C	0.49900600	1.74335600	-2.45036000
H	5.61474500	4.31472800	-1.10814700	C	0.31612700	4.99452500	-0.34802600
H	4.39433700	3.80719900	0.07842500	C	-0.43236800	0.61427900	-2.88280900
C	3.54852000	-2.37404900	-0.41328700	H	-5.78299600	-1.75945600	0.03831200
C	3.72960900	-3.26399900	-1.47738400	H	-3.84547100	-1.68360400	3.84895300
C	4.45828700	-2.38333600	0.64671300	H	-3.50094200	0.77910200	-1.48683500
C	4.78574600	-4.16819400	-1.46271300	H	-1.33993500	0.88235600	2.77135000
H	3.03469100	-3.24033200	-2.31114200	H	2.48139200	5.04682400	-1.92954100
C	5.51623600	-3.28472800	0.65494100	H	1.99405900	1.30934500	-3.92808300
H	4.32992200	-1.68221400	1.46413600	H	-0.41600300	4.58182500	0.34854200
C	5.67764500	-4.18689400	-0.39315600	H	-0.87623500	0.15185000	-1.99949000
H	4.91343500	-4.85888200	-2.29105500	C	-1.57316500	1.22008100	-3.71934100
H	6.21776000	-3.28323200	1.48415400	H	-1.17771100	1.69535400	-4.62459900
H	6.49943900	-4.89659700	-0.38140600	H	-2.27630800	0.43681700	-4.02202200
				H	-2.13201100	1.97681000	-3.15759500
				C	0.25343100	-0.50707400	-3.66175800
				H	-0.48808400	-1.27700000	-3.89316500
				H	0.66025700	-0.15912700	-4.61822600
				H	1.05419300	-0.98214300	-3.08582800
				C	-2.70186600	1.16073500	4.38914400
				H	-3.39899900	0.59080100	5.01477300
				H	-1.95365800	1.61652400	5.04695400
				H	-3.26295100	1.96644200	3.90301800
				C	-1.16987900	-0.82870800	4.01676300
				H	-0.45663300	-0.36771400	4.70709200
TS2'-1							
SCF Done: E(RωB97XD) = -2615.98681255 A.U.							
Sum of electronic and thermal Free Energies = -2615.091454 A.U.							
SCF Done (single point): E(RωB97XD) = -2617.67089012 A.U.							
$\nu_i = -277.69 \text{ cm}^{-1}$							
N	-2.39984500	1.25393600	0.60858700	H	-3.39899900	0.59080100	5.01477300
N	-0.99560000	2.33277600	-0.61339600	H	-1.95365800	1.61652400	5.04695400
C	-1.11743500	1.20286200	0.14931300	H	-3.26295100	1.96644200	3.90301800
C	-3.19150900	0.14733500	1.08581100	C	-1.16987900	-0.82870800	4.01676300
C	-4.15365800	-0.37376100	0.19978400	H	-0.45663300	-0.36771400	4.70709200

H	-1.77890000	-1.52915700	4.59928500	H	2.83911600	2.77662800	0.08810200
H	-0.59769000	-1.39457000	3.27437200	H	2.42171700	1.74027400	4.19414200
C	-0.37532500	6.08467400	-1.18558300	H	1.52752800	0.21329800	4.03129500
H	-0.81117700	6.84961200	-0.53373300	H	3.14260000	0.36282800	3.34475200
H	0.34876300	6.57559600	-1.84575600	C	2.14741900	-1.28750200	1.17153700
H	-1.16879200	5.68414700	-1.82576400	O	2.02698400	-1.83823700	2.24075200
C	1.42294800	5.63008200	0.50061200	C	3.47323100	-0.91043000	0.58553400
H	0.97932600	6.33003700	1.21674300	C	3.56190300	-0.29772800	-0.66366700
H	1.97996500	4.87691500	1.05780600	C	4.63167100	-1.17252900	1.31799800
H	2.13207300	6.19746500	-0.11214000	C	4.80288000	0.04895500	-1.18254300
C	-4.16839900	-1.08006900	-2.24613700	H	2.65160200	-0.06501200	-1.20997200
H	-4.91294700	-1.86367400	-2.07267100	C	5.87242800	-0.81809300	0.80246700
H	-4.31502400	-0.70208800	-3.26430600	H	4.53637000	-1.65099200	2.28797000
H	-3.17996600	-1.54075400	-2.18833800	C	5.95885000	-0.20979600	-0.44982400
C	-5.63769600	0.80908700	-1.45693000	H	4.86520000	0.53402500	-2.15179200
H	-5.76237000	1.63977500	-0.75466400	H	6.77486300	-1.01493800	1.37380500
H	-5.69903600	1.21034400	-2.47429800	H	6.92925200	0.06600800	-0.85240800
H	-6.48391100	0.12749200	-1.31405000	C	2.03250100	-3.04764800	-0.79196300
H	3.29364600	3.36213100	-3.53087700	O	2.12599800	-3.18358600	-1.99332100
H	-5.60616100	-2.56528900	2.36305100	O	2.75984200	-3.72564900	0.09064400
Pd	0.35560800	-0.14247000	0.55138300	C	3.82301700	-4.52605100	-0.44702300
C	-3.02887700	2.42452100	0.20627600	H	3.39077100	-5.35456100	-1.01595300
C	-2.16050900	3.08754200	-0.57666800	H	4.40727700	-3.90719700	-1.13498500
H	-4.04542200	2.64295100	0.48836900	C	4.65222000	-5.00404700	0.72500800
H	-2.25970000	4.01389600	-1.11581600	H	4.04233500	-5.58804600	1.41976400
C	1.05968000	-2.10601800	-0.17450200	H	5.47303400	-5.63317900	0.36673000
C	-0.22027000	-2.00103700	-0.31785900	H	5.07460000	-4.15077500	1.26285200
Si	1.47407700	1.58510200	1.89824400	C	-1.26458200	-2.84694600	-0.87555100
C	0.28536800	2.93526100	2.56806600	C	-1.14669300	-3.41776700	-2.15135100
C	2.98626300	2.44167900	1.11754000	C	-2.36913600	-3.17592800	-0.08259400
C	2.20588800	0.90081400	3.51942400	C	-2.13146200	-4.27658500	-2.62695700
H	-0.17312800	2.57324600	3.49610900	H	-0.26686300	-3.20239200	-2.74700400
H	0.84220800	3.84422600	2.82730800	C	-3.33406100	-4.05881500	-0.55192100
H	-0.53176700	3.21988200	1.89864900	H	-2.45427700	-2.73855900	0.90689300
H	3.28159400	3.30477100	1.72911400	C	-3.22570700	-4.60322200	-1.82887800
H	3.83294700	1.74809400	1.11967600	H	-2.03147300	-4.70956200	-3.61815500

H	-4.18044000	-4.30961200	0.08100400	H	-1.73580800	-0.60500500	-4.64607400
H	-3.98658600	-5.28447100	-2.19875900	H	-1.02727300	-1.99357400	-3.79250000
				H	-2.48403600	-1.20961700	-3.15613000
TS2'-2				C	0.73998200	0.06820500	-3.49523000
SCF Done: E(RωB97XD) = -2615.98728466	A.U.			H	1.26688600	-0.88598900	-3.43053900
Sum of electronic and thermal Free Energies = -2615.089243	A.U.			H	0.66798700	0.34525200	-4.55365700
SCF Done (single point): E(RωB97XD) = -2617.67252833	A.U.			H	1.34804000	0.82069200	-2.98151500
$\nu_i = -248.89 \text{ cm}^{-1}$				C	-2.87363900	-1.13342700	4.21238200
N	-2.36472600	-1.27174500	0.69904500	H	-2.85623800	-1.95533500	4.93782600
N	-2.59908800	0.34194300	-0.70834100	H	-3.08886100	-0.20490000	4.75294900
C	-1.69124500	-0.22734000	0.13972700	H	-3.69704700	-1.31595300	3.51255000
C	-1.74519100	-2.40197800	1.34990000	C	-0.39041600	-0.67174800	4.42694700
C	-1.63418400	-3.59094200	0.60978000	H	-0.60395900	0.28936400	4.90742100
C	-1.02781100	-4.67978400	1.23507500	H	-0.27226600	-1.41106400	5.22768400
C	-0.54100600	-4.58496700	2.52905400	H	0.55796000	-0.57615000	3.88925600
C	-0.67740800	-3.40077100	3.23901600	C	-5.68365100	2.61726600	-1.36743000
C	-1.28890300	-2.28633100	2.66876700	H	-6.51061100	2.70914900	-0.65505000
C	-2.19634400	-3.76236400	-0.79720300	H	-5.80055300	3.40171000	-2.12371200
C	-1.53221000	-1.02581500	3.47383400	H	-5.78329700	1.65646600	-1.88344800
C	-2.36056400	1.41151300	-1.64411400	C	-4.27447000	4.12105000	0.06578000
C	-3.17961900	2.55423100	-1.61155300	H	-5.02513400	4.15743500	0.86232400
C	-2.93515400	3.55633500	-2.55405400	H	-3.29288900	4.29330700	0.50938000
C	-1.91062600	3.44408300	-3.47684900	H	-4.48684500	4.94590900	-0.62326200
C	-1.13828500	2.29120900	-3.51060200	C	-1.16189700	-4.26602700	-1.80665200
C	-1.36131100	1.23845400	-2.62445800	H	-0.69432500	-5.20312400	-1.48772900
C	-4.33591100	2.76057500	-0.64166100	H	-1.64405300	-4.44188600	-2.77532400
C	-0.63335000	-0.08292600	-2.83697200	H	-0.37780500	-3.52131200	-1.95243600
H	-0.91702700	-5.61306400	0.69145900	C	-3.41878300	-4.69266400	-0.76601900
H	-0.30097200	-3.34058900	4.25466700	H	-4.17270200	-4.34786400	-0.05036900
H	-2.53106200	-2.79067800	-1.16762000	H	-3.88527300	-4.74976000	-1.75568800
H	-1.61196100	-0.20305200	2.76552800	H	-3.12897800	-5.70755800	-0.47096600
H	-3.55178500	4.44968900	-2.54867200	H	-1.72379000	4.24501600	-4.18584500
H	-0.36362200	2.19814700	-4.26328400	H	-0.05212400	-5.43912200	2.98703300
H	-4.28591700	1.99615900	0.13538500	Pd	0.22908800	0.26944800	0.59948600
H	-0.45590400	-0.55403900	-1.87085900	C	-3.67785500	-1.31163700	0.25886400
C	-1.52591200	-1.02787000	-3.65647500	C	-3.81986700	-0.31886700	-0.63772900

H	-4.36646300	-2.06709900	0.59973000	H	0.40885400	2.13973100	3.88783000
H	-4.66115600	-0.02406600	-1.24099500	H	1.21277100	3.38472000	2.92558000
C	2.31571900	-0.49638200	0.28412600	C	2.10388900	1.07229400	1.45364700
C	1.42348800	-1.36915700	-0.04297400	O	2.32384000	0.77207000	2.60672400
C	3.77054100	-0.38871000	0.03540400	C	2.72336300	2.27279500	0.80394100
C	4.71853300	-0.37777000	1.05967200	C	2.43681200	2.60342100	-0.51886100
C	4.19573200	-0.36563000	-1.29754500	C	3.60010600	3.06544500	1.54465000
C	6.07396500	-0.35271400	0.75276200	C	3.02468500	3.71770000	-1.10360000
H	4.38662000	-0.38031200	2.09291000	H	1.72886700	1.99248000	-1.07383100
C	5.55218000	-0.33535700	-1.59878800	C	4.18237200	4.18548000	0.96444700
H	3.45261600	-0.37701300	-2.08808800	H	3.80953800	2.78994200	2.57357800
C	6.49478600	-0.32714400	-0.57450300	C	3.89755600	4.51001300	-0.36084700
H	6.80550700	-0.35028800	1.55518800	H	2.79627800	3.97261500	-2.13401100
H	5.87260000	-0.31421100	-2.63644600	H	4.85932000	4.80645700	1.54348500
H	7.55492000	-0.29866400	-0.80868500	H	4.35510400	5.38434600	-0.81475400
C	1.66919500	-2.69667200	-0.59512200				
O	1.79565900	-3.71505900	0.04264500	TS2[‡]-3			
O	1.79053300	-2.65508600	-1.94628800	SCF Done: E(RoB97XD) = -2615.99087147	A.U.		
C	2.22209400	-3.86948400	-2.57268700	Sum of electronic and thermal Free Energies = -2615.091920	A.U.		
H	3.27371100	-4.03622300	-2.31700400	SCF Done (single point): E(RoB97XD) = -2617.67699709	A.U.		
H	1.64497300	-4.70859300	-2.17737600	$\nu_i = -134.86 \text{ cm}^{-1}$			
C	2.02581900	-3.70190700	-4.06456600	N	2.76097100	-0.14147700	0.33122200
H	2.60070500	-2.85099200	-4.44241100	N	1.36620500	-0.49981300	1.92949600
H	2.35776400	-4.60339800	-4.58881000	C	1.42069800	-0.11952900	0.61449000
H	0.96912700	-3.53593600	-4.29771200	C	3.33415200	-0.04618200	-0.98962900
Si	-0.66405700	2.31300600	1.60301500	C	3.06440800	-1.09120100	-1.89690100
C	-2.43915800	2.12460700	2.30019800	C	3.51889100	-0.93744500	-3.20499600
C	-0.59854300	3.81645100	0.44033300	C	4.27341200	0.16634000	-3.58030600
C	0.24275200	2.93569800	3.15652100	C	4.64874300	1.10176400	-2.63072200
H	-2.37404300	1.73079000	3.32100800	C	4.20287900	1.01016300	-1.31009700
H	-2.92239400	3.10570300	2.37588500	C	2.47131100	-2.42039700	-1.43897800
H	-3.10350200	1.45995300	1.74041700	C	4.79794000	1.94292700	-0.26603800
H	-1.11026900	4.67075100	0.90376800	C	0.21006700	-1.04100200	2.60080600
H	0.44665400	4.10835800	0.29583600	C	-0.73377500	-0.18630400	3.18791300
H	-1.03321500	3.64627700	-0.54712100	C	-1.82018700	-0.77314900	3.83711000
H	-0.37997700	3.70989800	3.62507700	C	-1.94005900	-2.15290100	3.93455200

C	-0.97435200	-2.97466000	3.37444500	C	1.97198100	-3.31053600	-2.57812700
C	0.11324700	-2.44169400	2.68206200	H	2.80332200	-3.70164300	-3.17650200
C	-0.52948800	1.31544700	3.22122400	H	1.44237300	-4.17035300	-2.15434000
C	1.15676000	-3.38820800	2.10140000	H	1.28387600	-2.76972000	-3.23060000
H	3.29303900	-1.69847500	-3.94246900	C	3.53696600	-3.19549800	-0.64103700
H	5.30480700	1.91868400	-2.91426000	H	3.86880600	-2.65739400	0.25094000
H	1.62098500	-2.22330400	-0.77925500	H	3.13653800	-4.16277400	-0.31833900
H	4.18344700	1.89506300	0.63314400	H	4.41531500	-3.38464800	-1.26879600
H	-2.57239600	-0.14049000	4.29611000	H	-2.78739100	-2.58799700	4.45676300
H	-1.07502700	-4.05244100	3.45996500	H	4.60680400	0.27117000	-4.60839700
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H	1.85128000	-2.80740000	1.49186000	C	3.50850300	-0.46022100	1.45805300
C	1.96827800	-4.04240000	3.22952500	C	2.63621300	-0.67456600	2.45906800
H	1.33300300	-4.69247600	3.84218200	H	4.58392600	-0.51121400	1.43173500
H	2.77478600	-4.65465300	2.81151200	H	2.78578700	-0.95840400	3.48791900
H	2.41575000	-3.29647900	3.89433400	C	-1.84392000	1.79976800	-1.01315800
C	0.55846500	-4.45878300	1.18273200	C	-2.17654600	0.61632500	-1.36628600
H	1.35154800	-5.13107600	0.83686400	Si	0.71211600	2.90605300	0.04298800
H	-0.19006400	-5.07250700	1.69422700	C	1.43223400	3.34615500	-1.65389600
H	0.08454600	-4.01171300	0.30722800	H	0.59428200	3.38896500	-2.35956400
C	6.21117800	1.45045500	0.09639200	H	1.91048200	4.33425000	-1.64972500
H	6.88484700	1.55323200	-0.76199400	H	2.14210800	2.60577600	-2.03346200
H	6.62258800	2.03955100	0.92340300	C	1.99804100	3.01886300	1.45946200
H	6.22301600	0.39432800	0.38626600	H	2.77050400	3.75367000	1.20065100
C	4.86923000	3.41312900	-0.69019300	H	1.49304100	3.39858500	2.35557900
H	5.21306700	4.02049000	0.15429700	H	2.49185000	2.08654700	1.74164600
H	5.58081600	3.56679200	-1.50902300	C	-0.34713300	4.42628100	0.48861200
H	3.89683200	3.78965400	-1.00828400	H	0.33123700	5.20221100	0.86628300
C	0.24743700	1.69656500	4.48960100	H	-0.85824800	4.83908600	-0.38494300
H	0.43673300	2.77537100	4.51231900	H	-1.09302300	4.22708000	1.26343700
H	-0.31720600	1.42980700	5.39100700	C	-0.69469700	-1.06206700	-1.56517000
H	1.21484200	1.18424600	4.53094700	O	-0.16606800	-1.03842000	-2.65235000
C	-1.82560300	2.11793900	3.09876300	C	-1.38530400	-2.28788000	-1.04822400
H	-1.58999500	3.18704000	3.11068400	C	-2.05861700	-2.27157800	0.17035900
H	-2.34098700	1.90247500	2.15770800	C	-1.43849800	-3.42872400	-1.85463000
H	-2.51394900	1.93523800	3.93185500	C	-2.77981700	-3.38650900	0.58276400

H	-2.02854800	-1.37391500	0.78290900	C	-1.40466000	0.31384100	0.53966600
C	-2.14238600	-4.54908600	-1.43472300	C	-3.16547500	-0.17204900	-1.16273400
H	-0.93965900	-3.41173700	-2.81751700	C	-2.76098900	0.58493800	-2.28201000
C	-2.81854700	-4.52580300	-0.21528900	C	-3.08924600	0.09150100	-3.54286500
H	-3.30784100	-3.36286400	1.53032200	C	-3.85761700	-1.05639800	-3.68827600
H	-2.18057300	-5.43464300	-2.06236400	C	-4.37191000	-1.68934400	-2.56928400
H	-3.38248700	-5.39615700	0.10826300	C	-4.05131700	-1.25633000	-1.28008500
C	-3.35294000	-0.11228800	-1.83758500	C	-2.16665200	1.98239400	-2.13170000
C	-3.39444000	-0.77279600	-3.06811300	C	-4.78929000	-1.86541300	-0.09577800
C	-4.48905500	-0.11048800	-1.01912800	C	-0.38866700	1.71189000	2.36534100
C	-4.55577100	-1.42121300	-3.47055500	C	0.52219500	1.05301300	3.20085200
H	-2.51074300	-0.78274000	-3.69804800	C	1.48716600	1.82825200	3.84752000
C	-5.64641500	-0.76268300	-1.42604500	C	1.53487700	3.20445500	3.68425900
H	-4.44959100	0.40868000	-0.06618300	C	0.62542200	3.83180400	2.84598500
C	-5.68203800	-1.42307800	-2.65138900	C	-0.34378700	3.10436700	2.15689300
H	-4.57983300	-1.93035700	-4.42938800	C	0.46381800	-0.43957900	3.45909000
H	-6.52197100	-0.75658700	-0.78322900	C	-1.30728600	3.85086600	1.24180300
H	-6.58514500	-1.93652900	-2.96779900	H	-2.75636700	0.61979600	-4.42843300
C	-2.54005700	3.08548300	-1.07417200	H	-5.03813700	-2.53707600	-2.69371900
O	-2.50175600	3.86422100	-1.99784800	H	-1.38967900	1.96159000	-1.36238300
O	-3.26158100	3.28118800	0.04364800	H	-4.26295600	-1.59722100	0.82071400
C	-3.94233600	4.53887000	0.13549200	H	2.20309100	1.34374700	4.50348500
H	-3.22129400	5.34303700	-0.03906400	H	0.67868800	4.90786400	2.70922100
H	-4.70344900	4.59229600	-0.64900000	H	-0.16315900	-0.88498300	2.68632300
C	-4.54623000	4.61759500	1.52139700	H	-1.90820000	3.12079700	0.69694500
H	-3.76479600	4.55123800	2.28449400	C	-2.26928700	4.72529400	2.05882000
H	-5.07250800	5.56906600	1.64554100	H	-1.72855100	5.52493900	2.57809500
H	-5.25847400	3.80313800	1.68384200	H	-3.00880400	5.19200700	1.39890800
				H	-2.80691200	4.14395300	2.81445500
TS2'-4				C	-0.58437900	4.69392700	0.18524900
SCF Done: E(RøB97XD) = -2615.98769114	A.U.			H	-1.31891900	5.23512600	-0.42142700
Sum of electronic and thermal Free Energies = -2615.089091	A.U.			H	0.08131800	5.43837800	0.63408400
SCF Done (single point): E(RøB97XD) = -2617.67377260	A.U.			H	0.01269200	4.06758700	-0.47993300
$\nu_i = -171.77 \text{ cm}^{-1}$				C	-6.20522100	-1.26356500	-0.02857100
N	-2.71319700	0.26167700	0.13574500	H	-6.79592400	-1.57929200	-0.89612700
N	-1.46622800	0.99397200	1.72791300	H	-6.72293900	-1.60097800	0.87600300

H	-6.19430500	-0.16834300	-0.03218200	H	-2.89119100	-3.30134900	1.96561200
C	-4.89258100	-3.39359000	-0.12122300	H	-1.67136400	-2.62324200	3.03591600
H	-5.36186800	-3.74206500	0.80524200	H	-2.63008800	-1.54832600	2.02752500
H	-5.51336700	-3.74813600	-0.95148400	C	0.21650300	-4.16139200	1.62471900
H	-3.91205400	-3.86211700	-0.20362000	H	-0.51813800	-4.80471100	2.12782800
C	-0.19500400	-0.72240100	4.81477100	H	0.80039100	-4.79124500	0.95040300
H	-0.27033300	-1.80235200	4.98306800	H	0.89759500	-3.78063600	2.39192400
H	0.38703600	-0.28963600	5.63717200	C	1.02022700	0.73691100	-1.50771200
H	-1.20552900	-0.30126400	4.85633200	O	0.63599400	0.44158300	-2.61067100
C	1.84466100	-1.09390400	3.35001100	C	1.62439800	2.07164700	-1.19730600
H	1.74925800	-2.17888100	3.45098300	C	2.13834700	2.35470700	0.06521400
H	2.30193900	-0.88105100	2.37850400	C	1.77363700	2.99962100	-2.23409400
H	2.52769000	-0.75405800	4.13660200	C	2.80724800	3.55477200	0.28999000
C	-1.53320400	2.53738200	-3.40836900	H	2.03235500	1.62609100	0.86386100
H	-2.28915400	2.74800700	-4.17406900	C	2.42205600	4.20484500	-2.00367500
H	-1.03370600	3.48411400	-3.17638200	H	1.39190100	2.74705900	-3.21764800
H	-0.79048300	1.84882600	-3.81650600	C	2.94645600	4.47980000	-0.73929200
C	-3.27892500	2.94530300	-1.67463300	H	3.21721600	3.76069000	1.27282100
H	-3.71536800	2.65726600	-0.71422300	H	2.53389700	4.92562600	-2.80838100
H	-2.88046000	3.96037900	-1.57154100	H	3.46679600	5.41653400	-0.56111300
H	-4.08395200	2.97037700	-2.41798200	C	2.55823300	-3.28867500	-0.28773100
H	2.28519700	3.78861600	4.20925100	C	3.43051400	-3.56184700	0.77098500
H	-4.09315100	-1.42911600	-4.68060300	C	2.29877200	-4.28164700	-1.23705300
Pd	0.27972800	-0.73669000	-0.09557400	C	4.00556600	-4.82088600	0.89393500
C	-3.55684000	0.83260100	1.07954200	H	3.64609100	-2.78254100	1.49469700
C	-2.77778100	1.27739100	2.08079500	C	2.88410800	-5.53666800	-1.11439500
H	-4.62370800	0.87400400	0.94043600	H	1.63602200	-4.05977600	-2.06773200
H	-3.01649700	1.79183600	2.99706400	C	3.72983300	-5.81399200	-0.04290100
C	1.95526900	-1.96875200	-0.40971200	H	4.67572600	-5.02672700	1.72355000
C	2.35162600	-0.78231300	-0.68478500	H	2.67521500	-6.30167200	-1.85644000
Si	-0.76023600	-2.79248900	0.72807600	H	4.17902900	-6.79755200	0.05759700
C	-1.42253700	-3.66573700	-0.82204200	C	3.64717500	-0.10457900	-0.86455400
H	-0.56184200	-3.92257900	-1.44912400	O	4.44581200	0.03415000	0.03477300
H	-1.93303400	-4.60495300	-0.57213900	O	3.83153200	0.34170800	-2.10928300
H	-2.08842100	-3.04393900	-1.42626600	C	4.96576900	1.20009700	-2.29948200
C	-2.12741200	-2.51713100	2.04398200	H	4.87537000	2.04256200	-1.60505500

H	5.87883800	0.65081900	-2.05243500	H	-2.40623100	-2.13042600	0.13426100
C	4.94425900	1.65587200	-3.74209500	H	-1.69850100	2.09518700	-0.12626100
H	4.01683200	2.19409700	-3.95653300	H	-4.14683200	2.50688900	-0.12364000
H	5.78823300	2.32643600	-3.93214300	H	-5.72298000	0.59769900	0.01185600
H	5.01680100	0.80242800	-4.42222300	C	-0.49145800	-0.28206200	-0.00488200
				C	0.70043700	-0.48301000	-0.01404800
Alkyne 5j				C	2.11328900	-0.79561100	-0.03779300
SCF Done: E(RωB97XD) = -575.391144876	A.U.			O	2.56082100	-1.91725700	-0.09519400
Sum of electronic and thermal Free Energies = -575.248203	A.U.			O	2.85462700	0.31882300	0.00999600
SCF Done (single point): E(RωB97XD) = -575.524304443	A.U.			C	4.27688600	0.11387300	-0.01975700
no imaginary frequency				H	4.55715800	-0.55165100	0.80202400
C	-4.16516100	-0.88498200	0.08284700	H	4.54094400	-0.38554600	-0.95703800
C	-2.79629200	-1.11936200	0.07864200	C	4.93056200	1.47357700	0.10273200
C	-1.90145500	-0.04302700	0.00305200	H	4.65594300	1.95314400	1.04642100
C	-2.39660500	1.26641400	-0.06842700	H	6.01885300	1.36248000	0.07365800
C	-3.76702800	1.49153500	-0.06572800	H	4.62666200	2.12698400	-0.71995200
C	-4.65207700	0.41826900	0.00983400				
H	-4.85517800	-1.72098000	0.14141500				

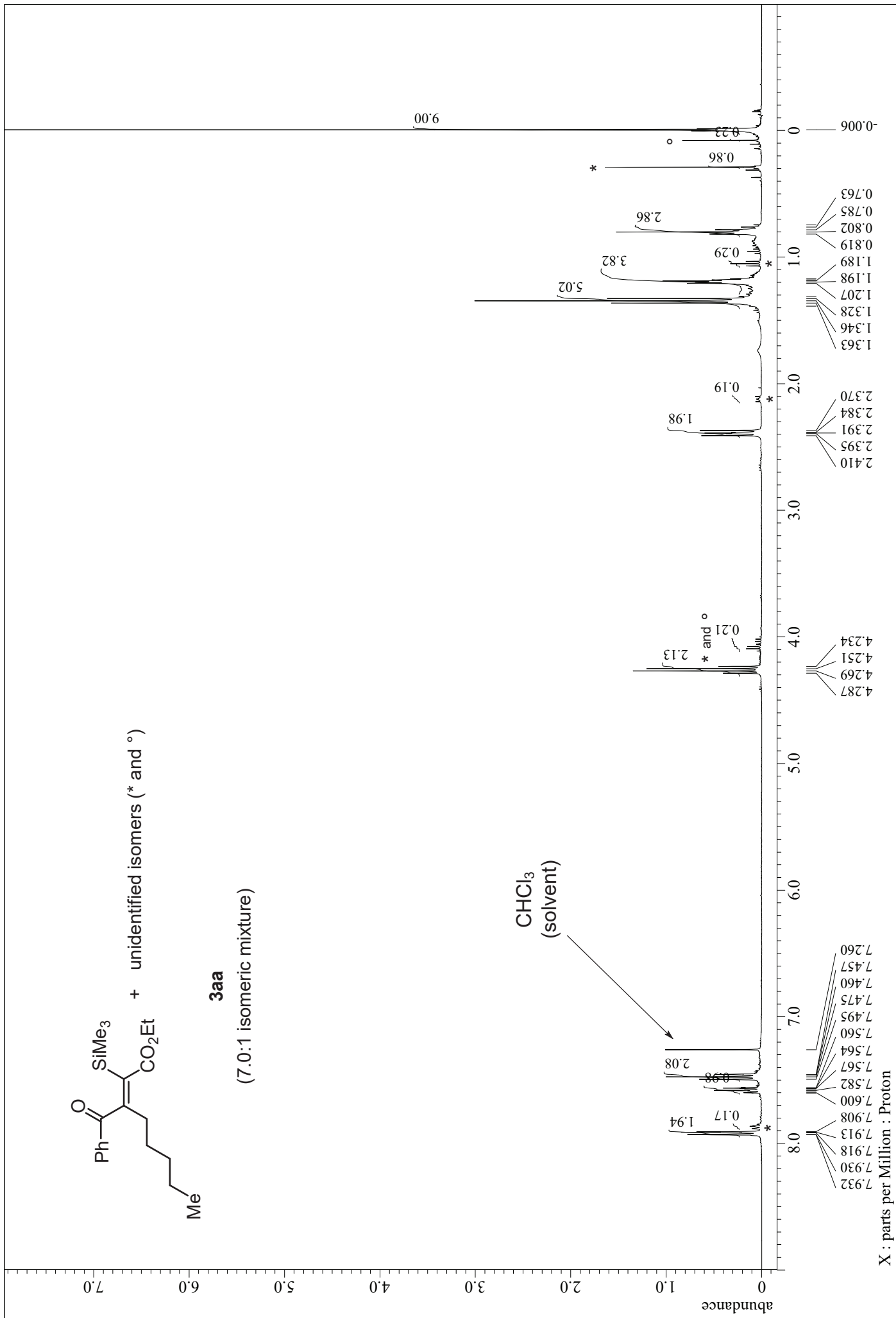
IX. References

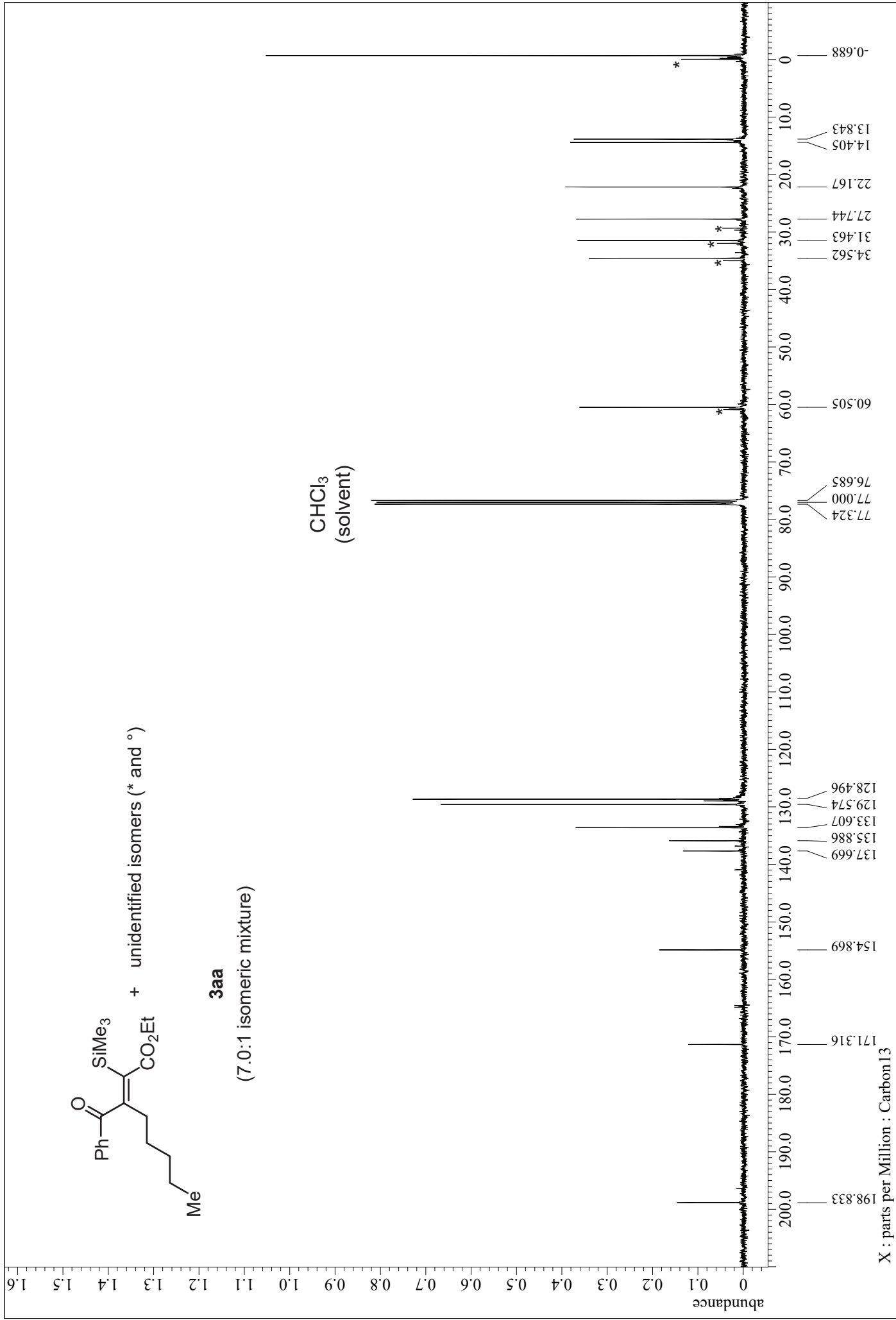
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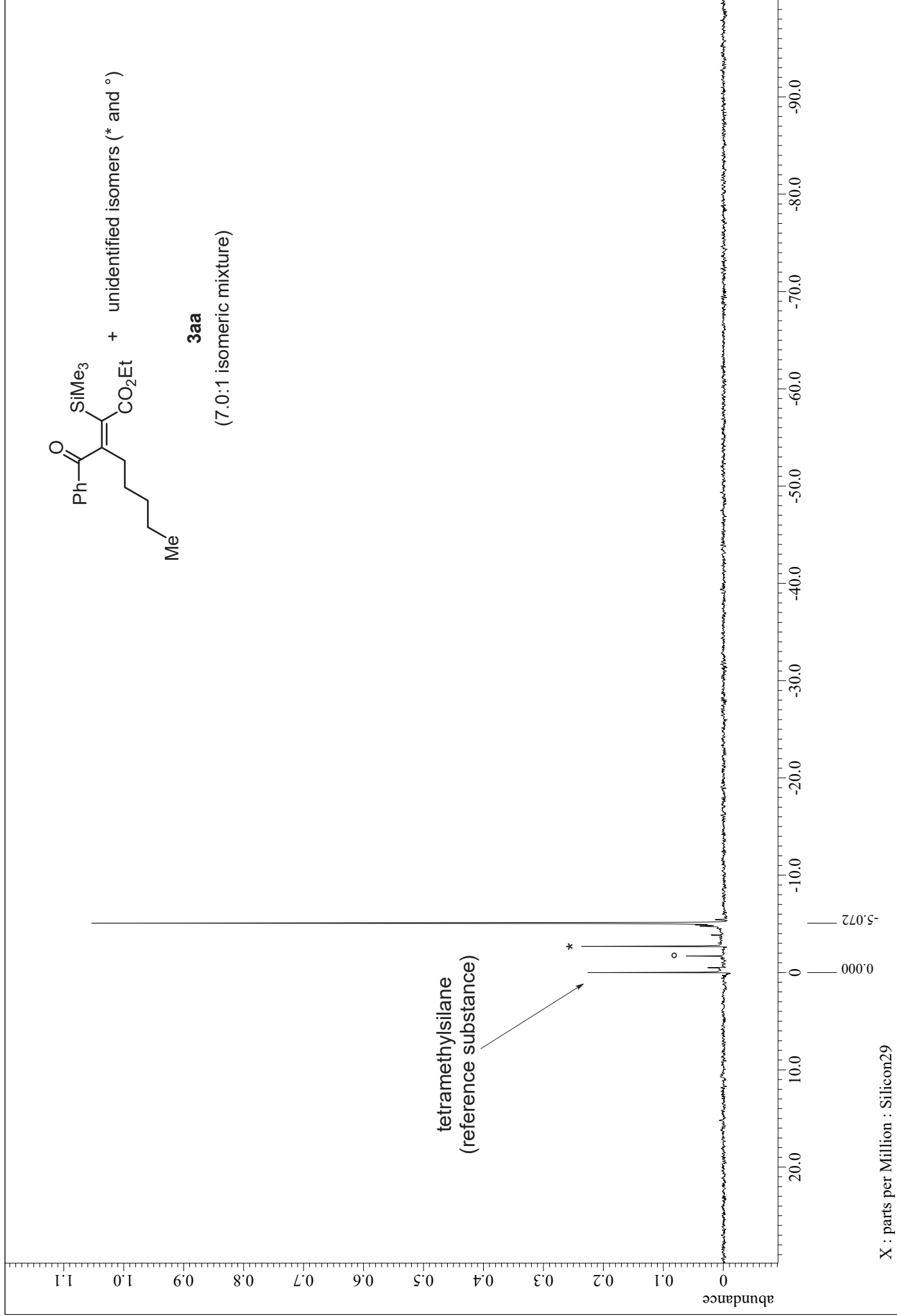
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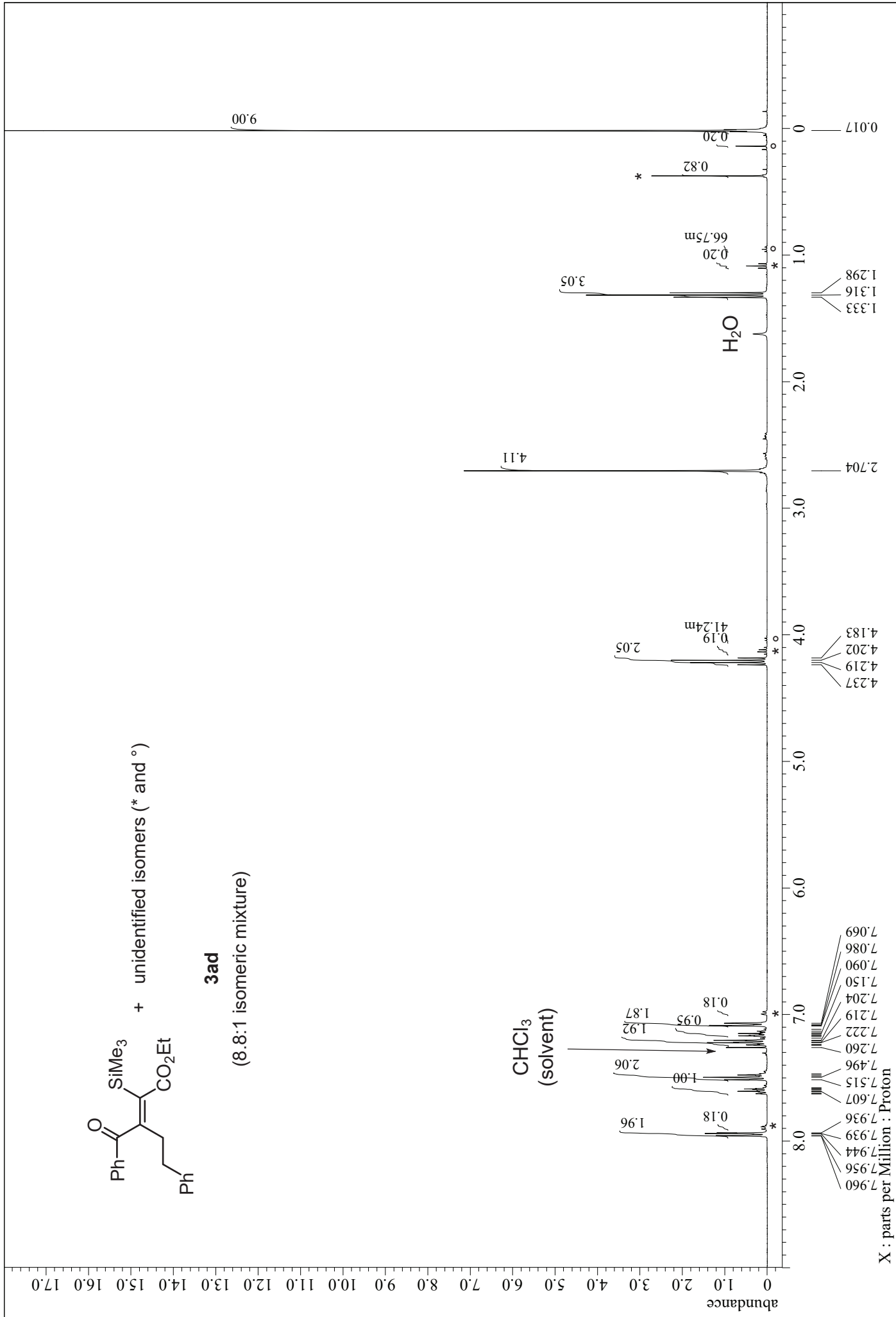
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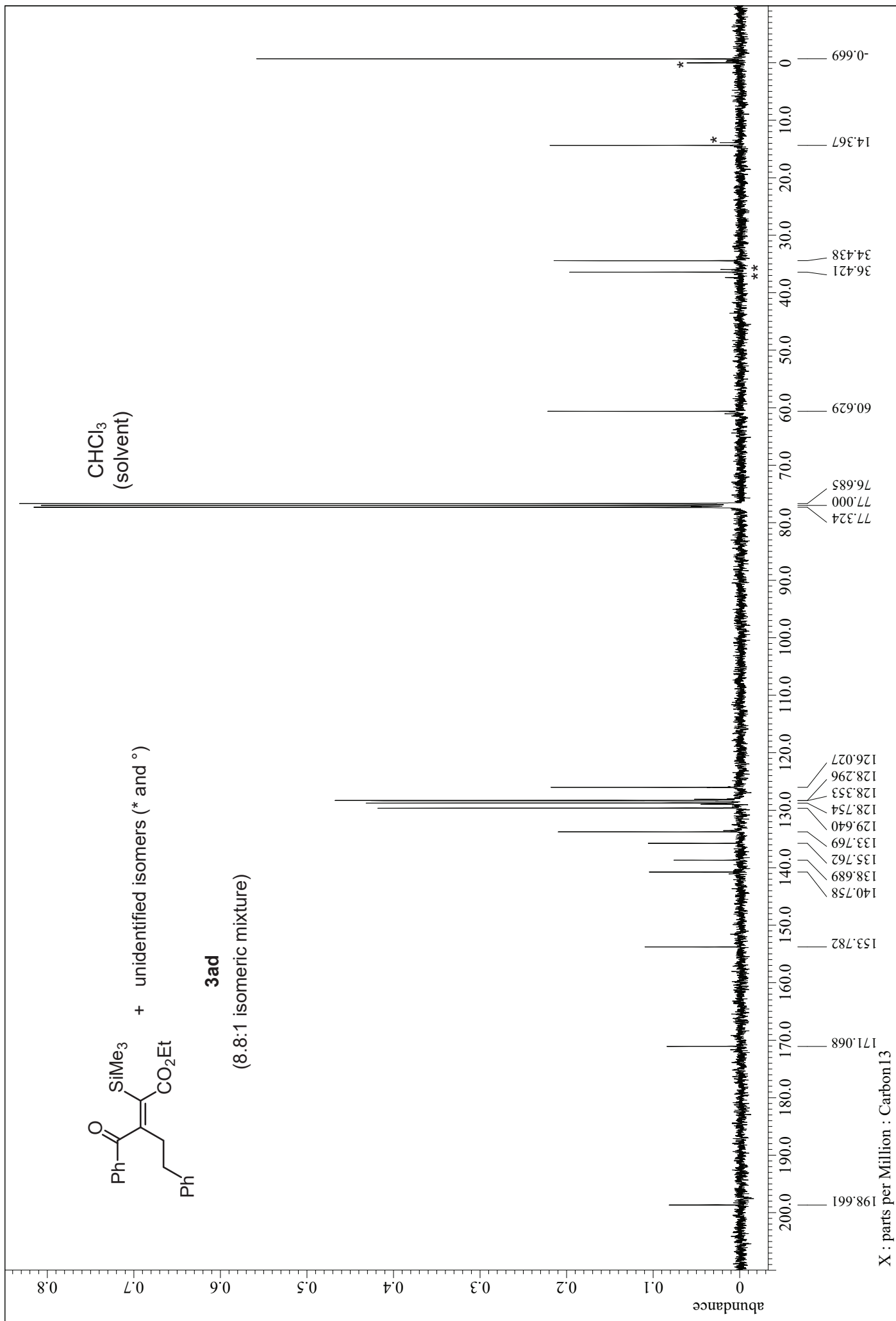
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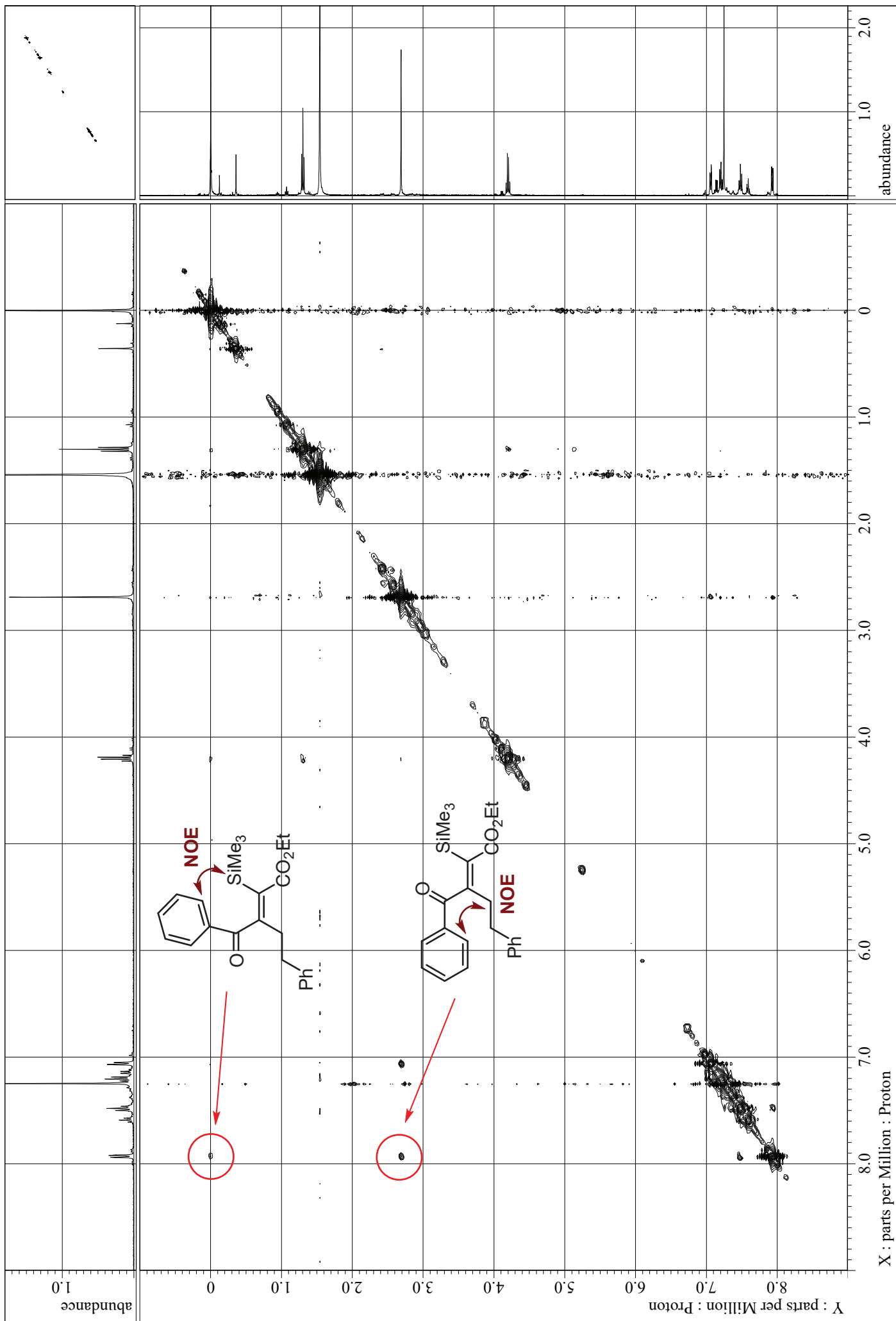


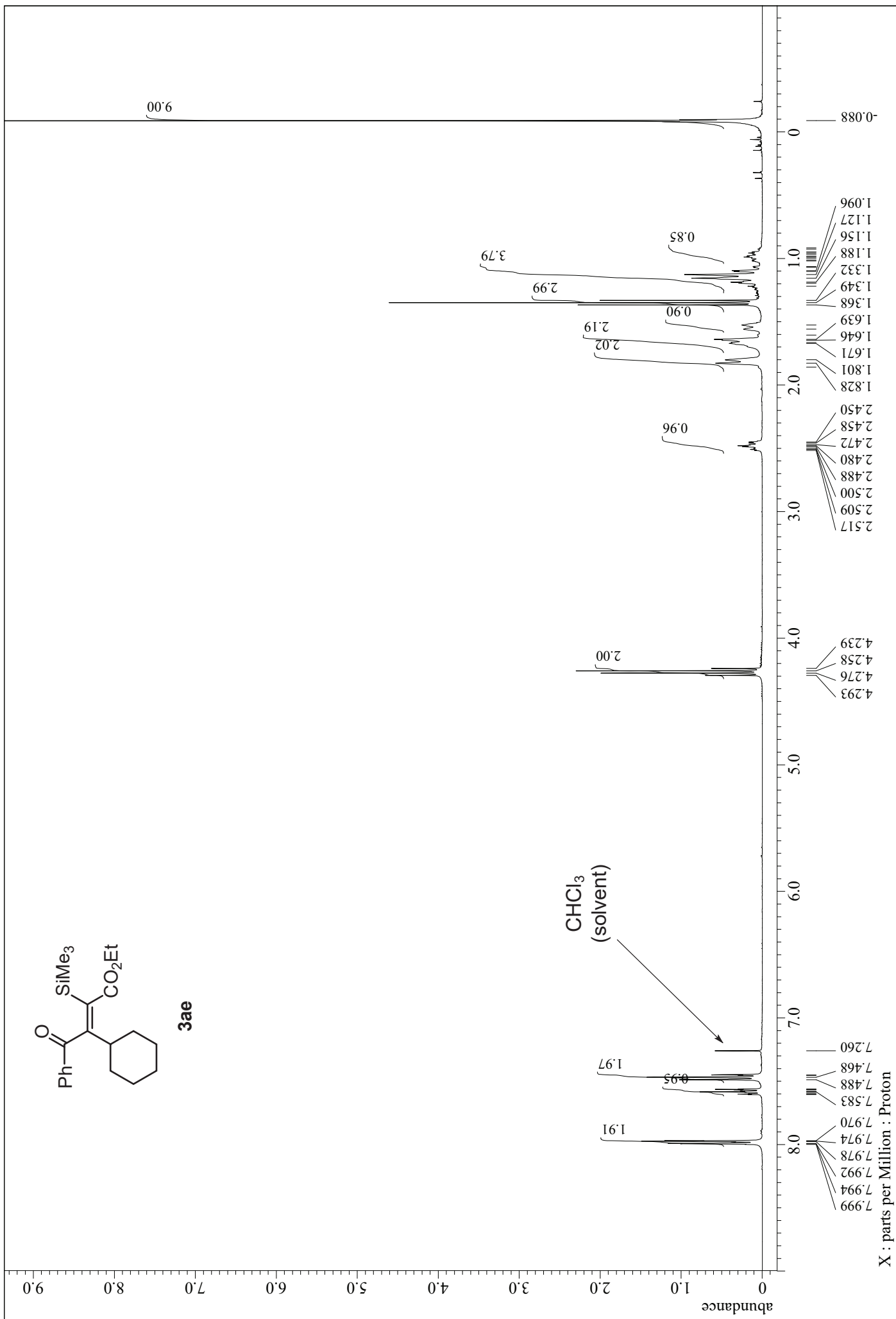


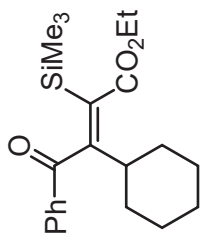






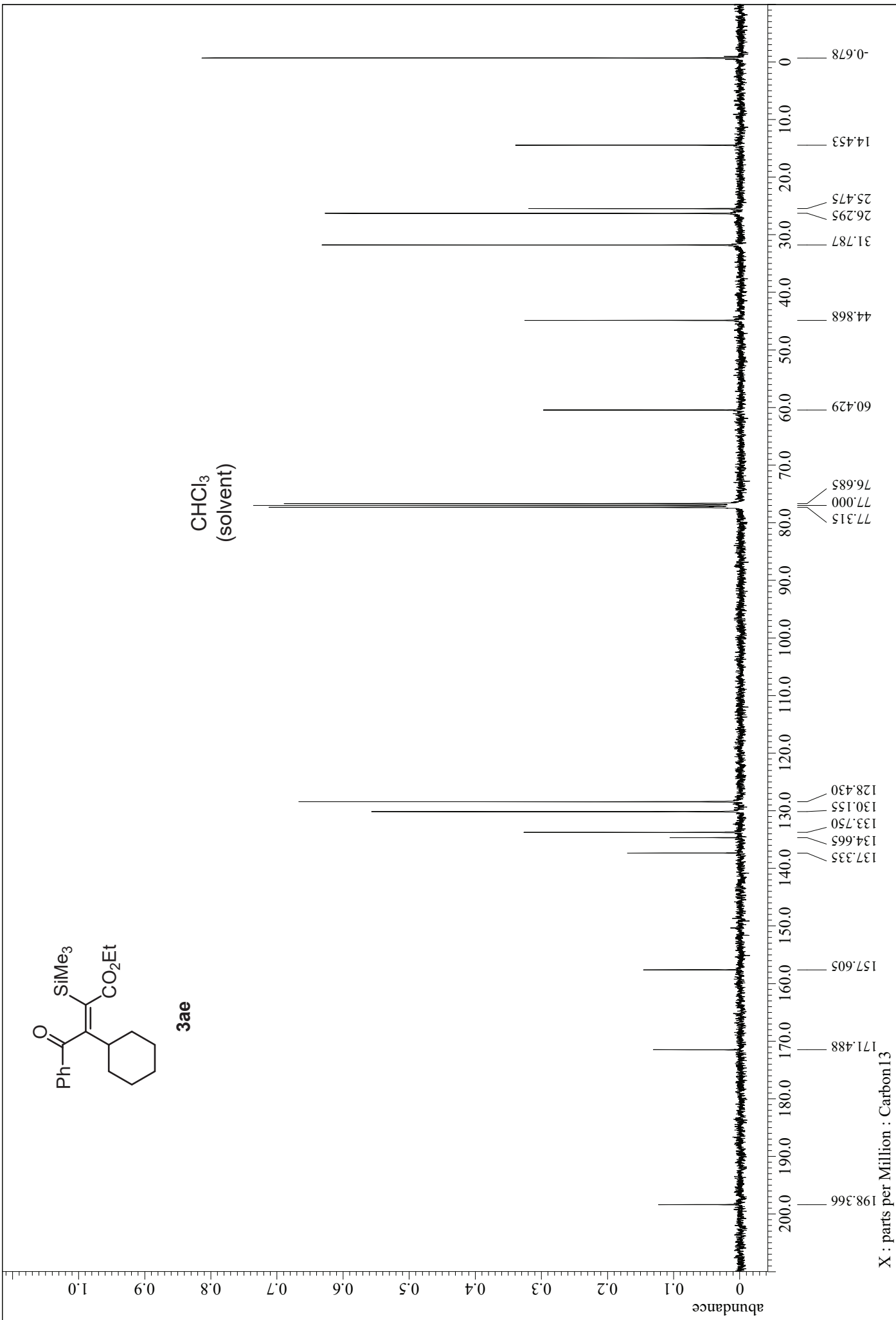






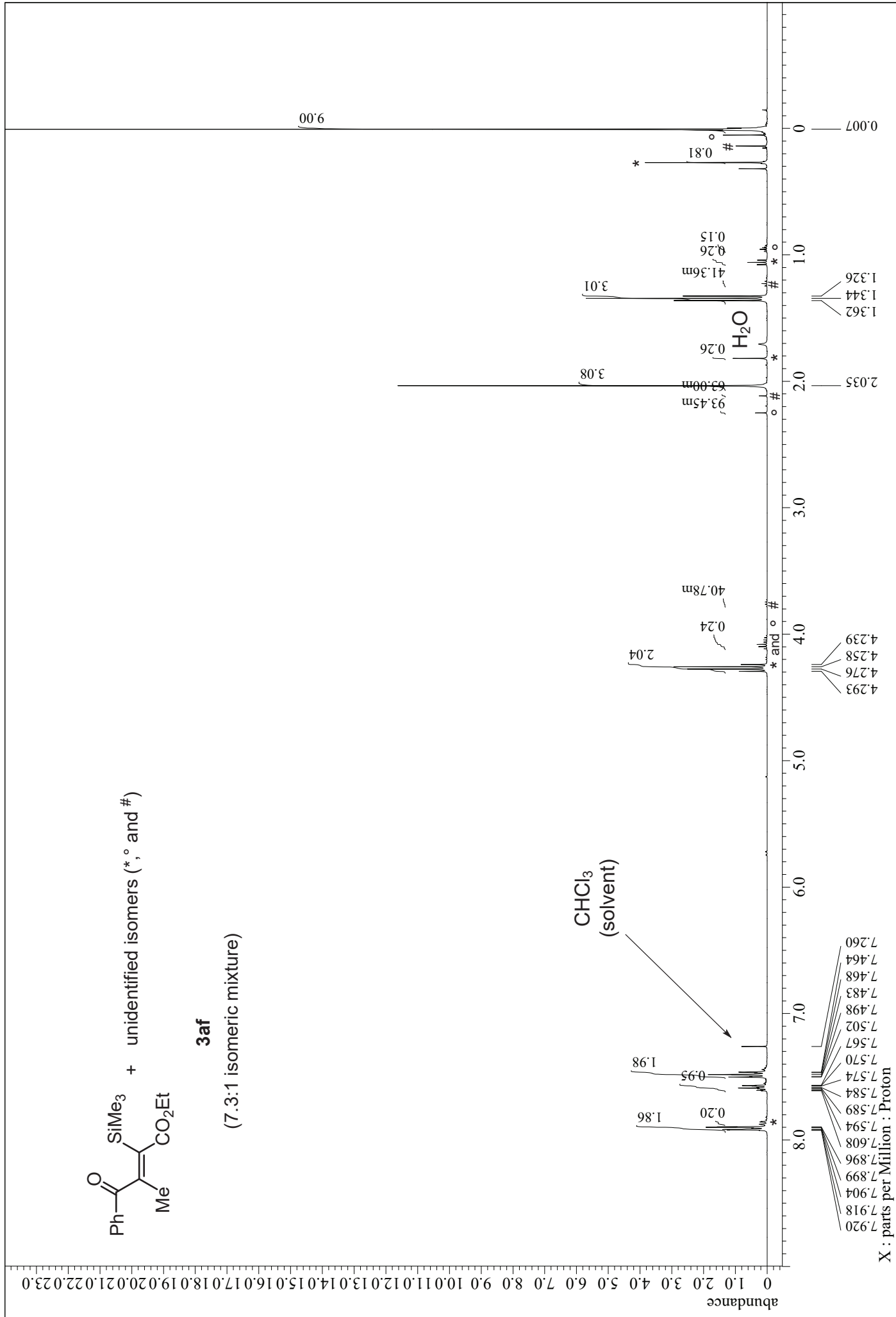
3ae

CHCl₃
(solvent)



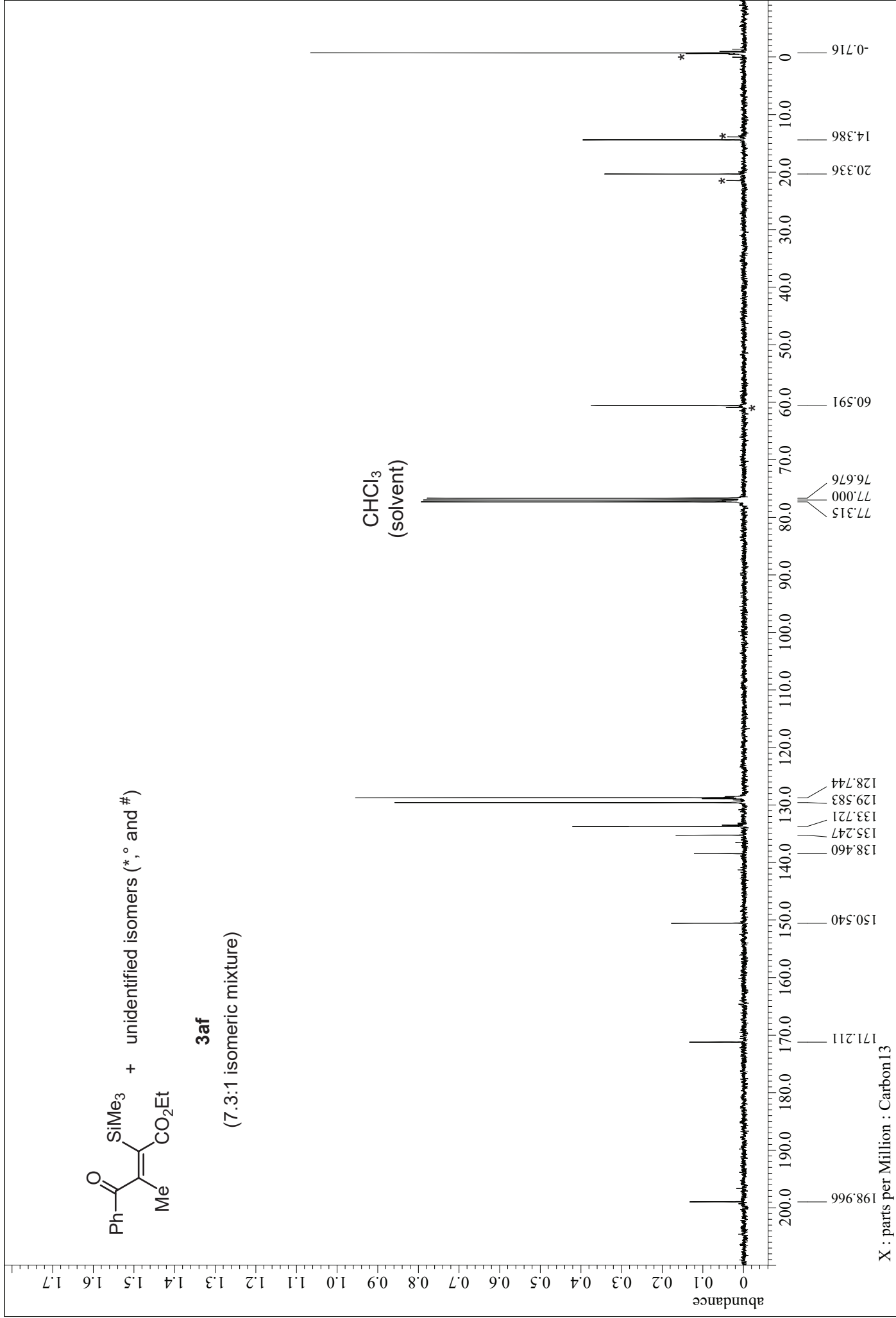


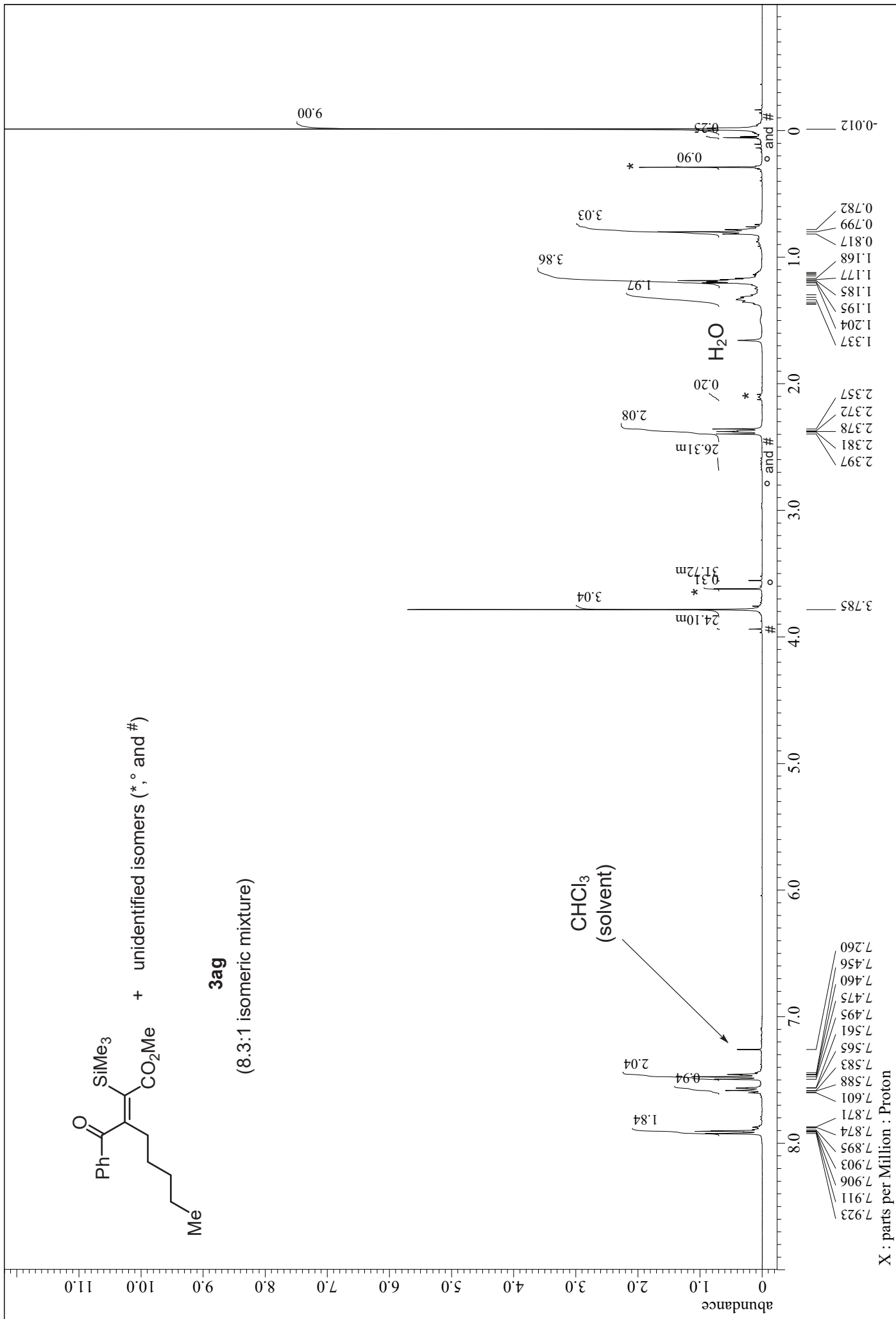
3af
(7.3:1 isomeric mixture)

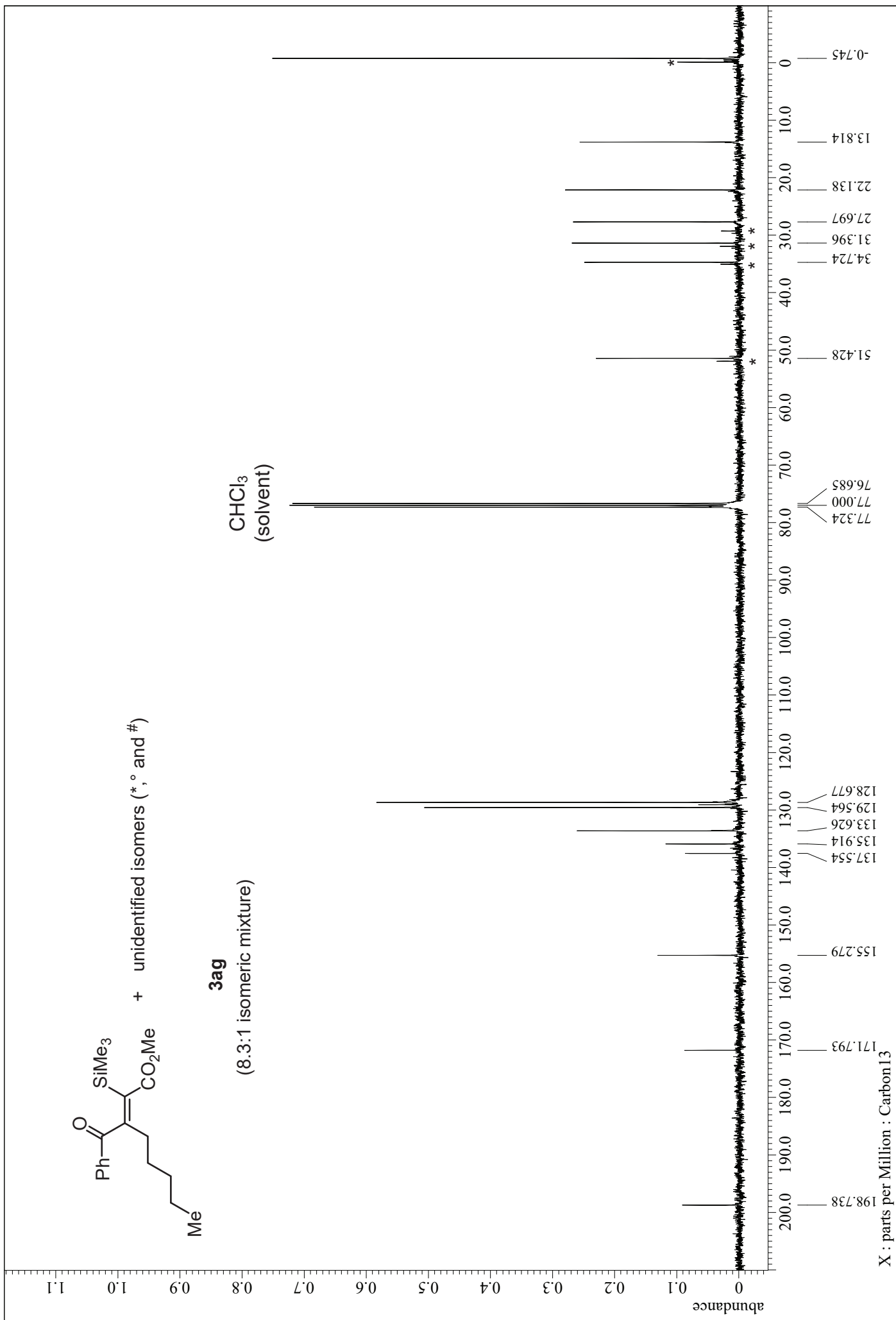


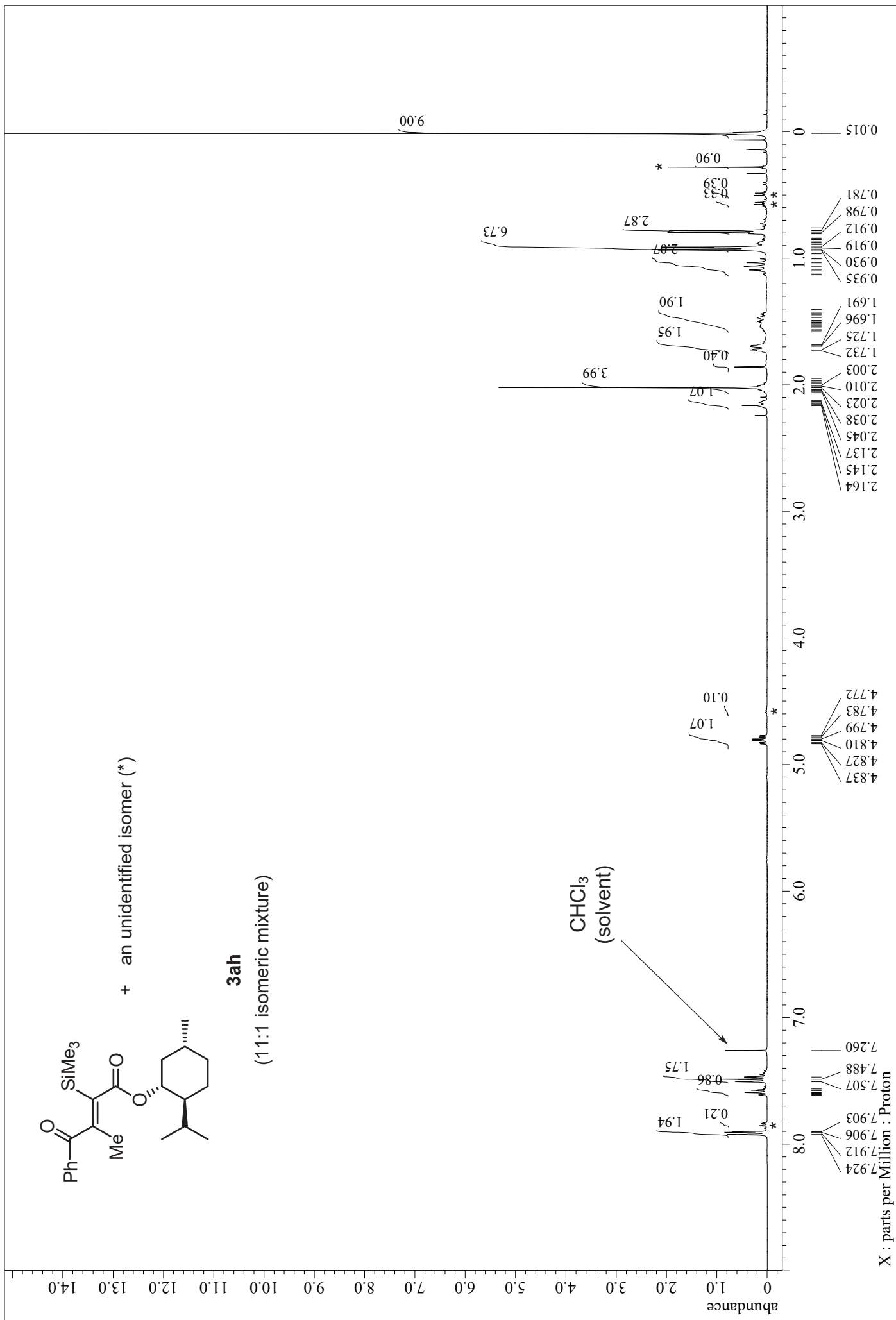


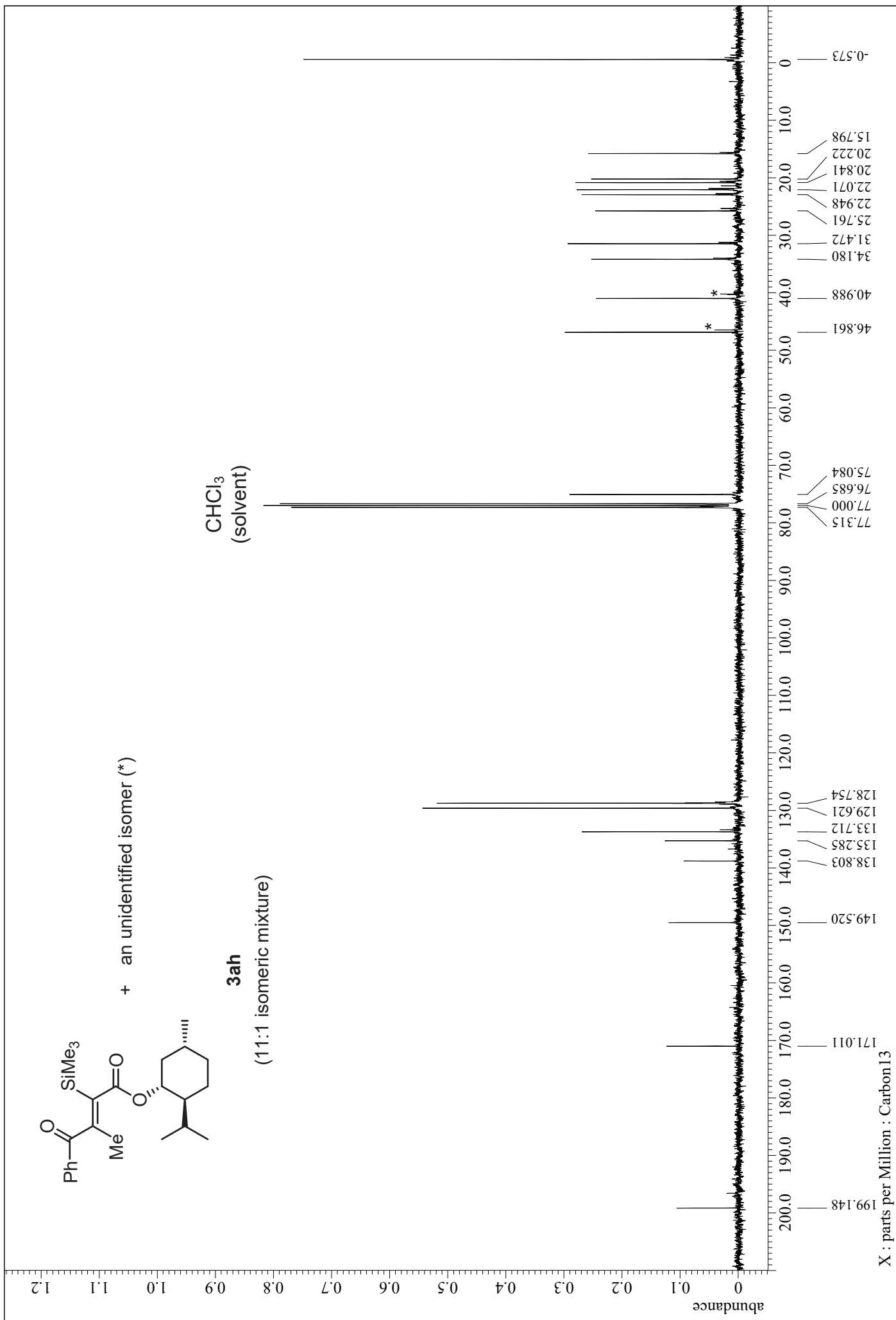
3af
 (7.3:1 isomeric mixture)

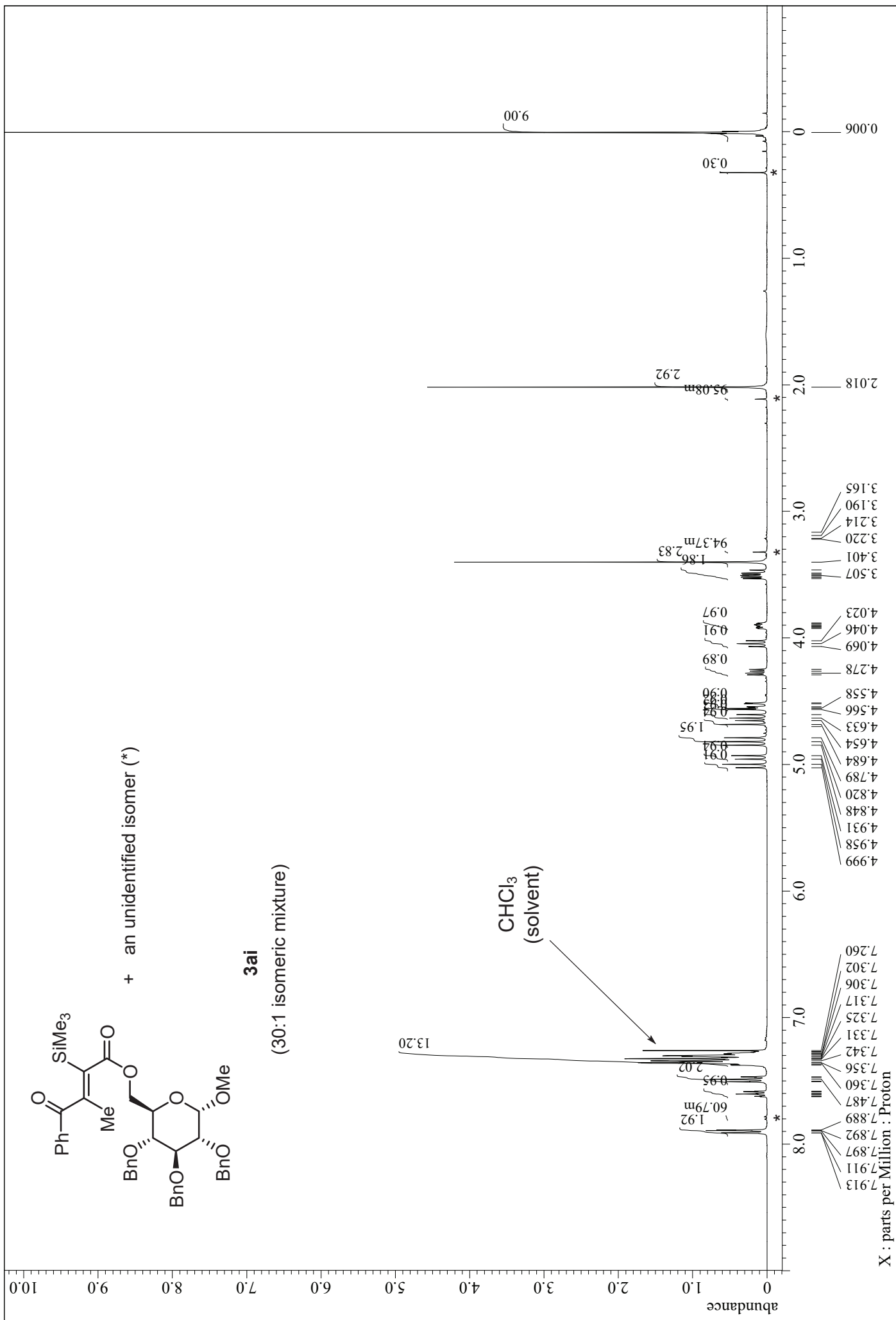


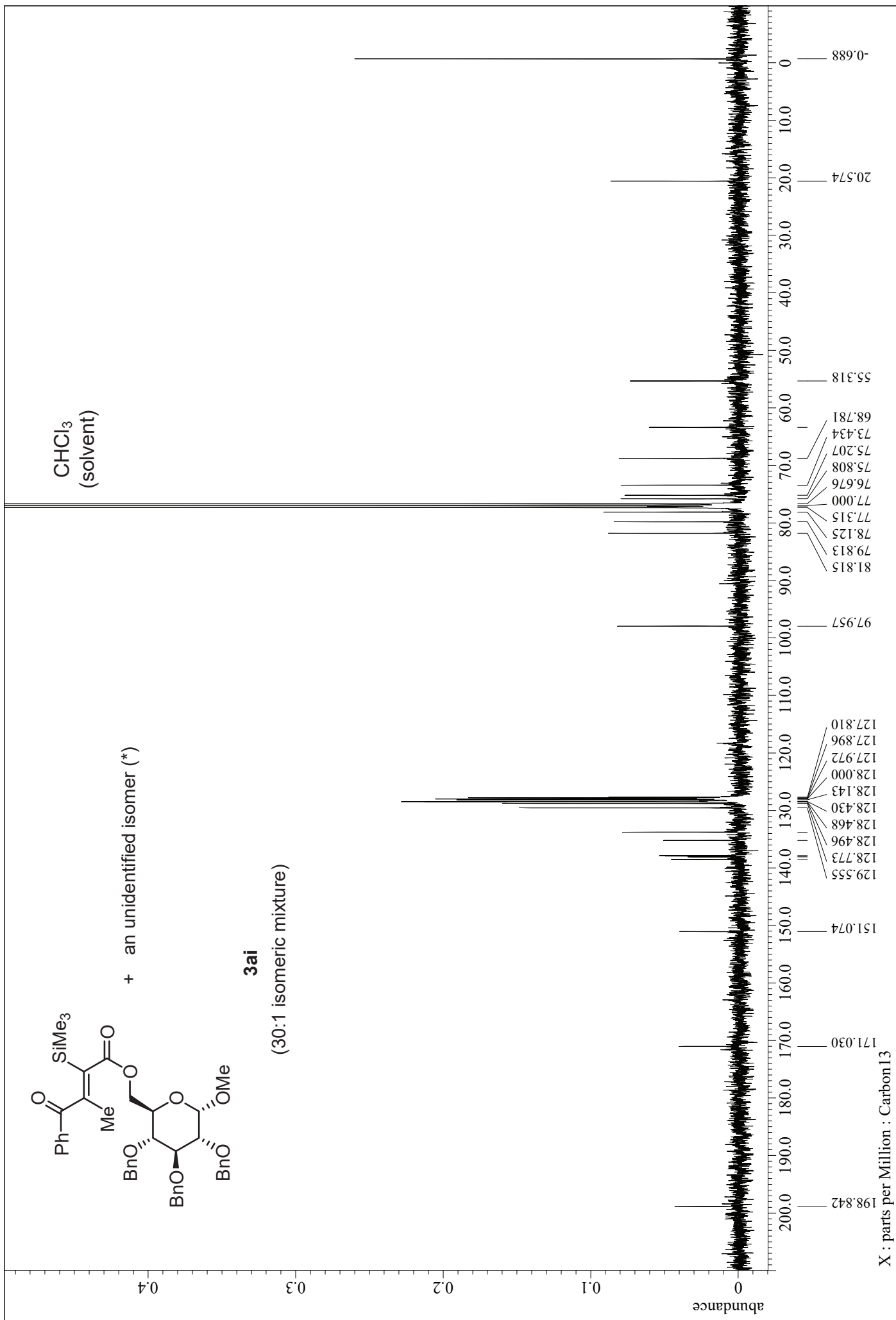


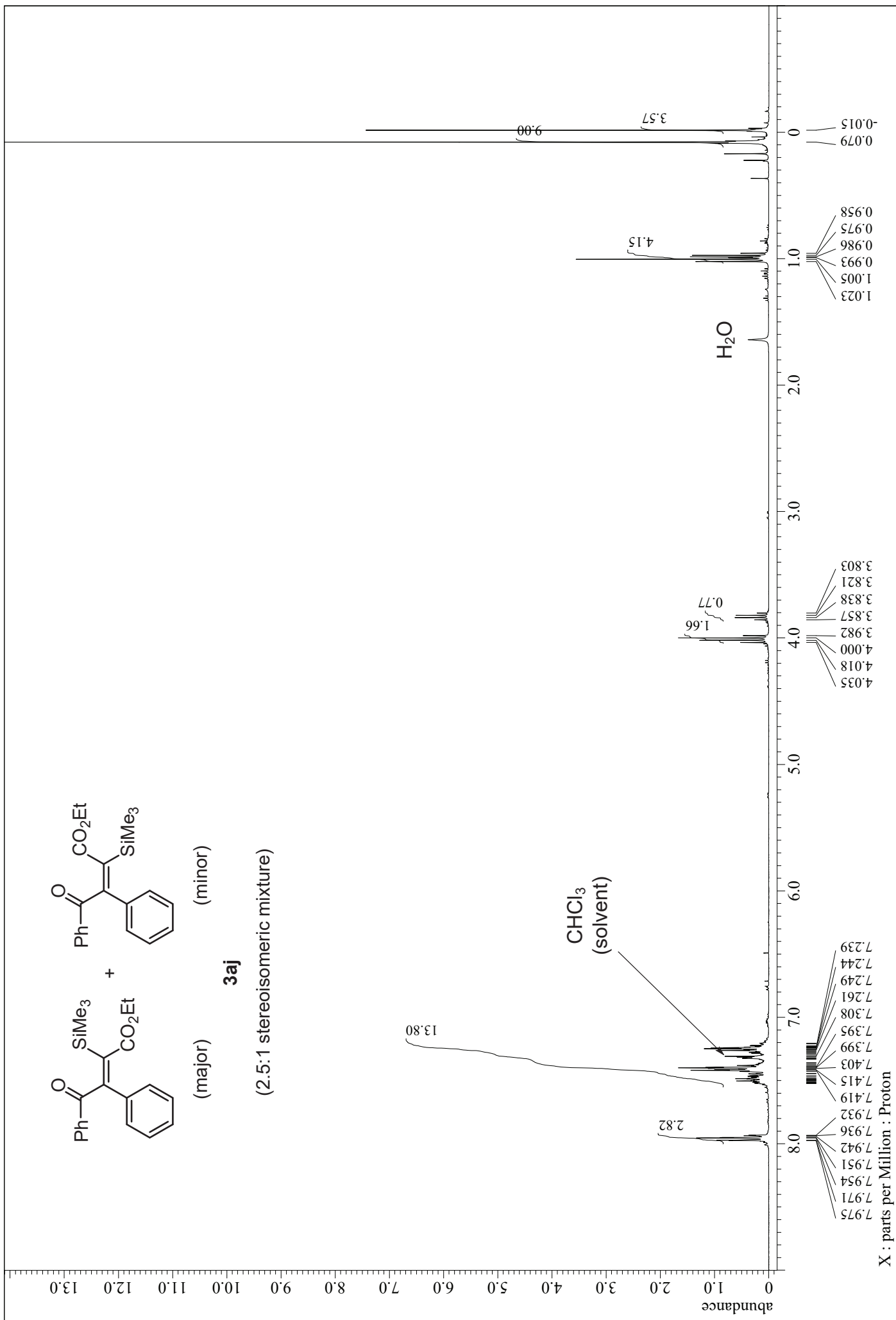


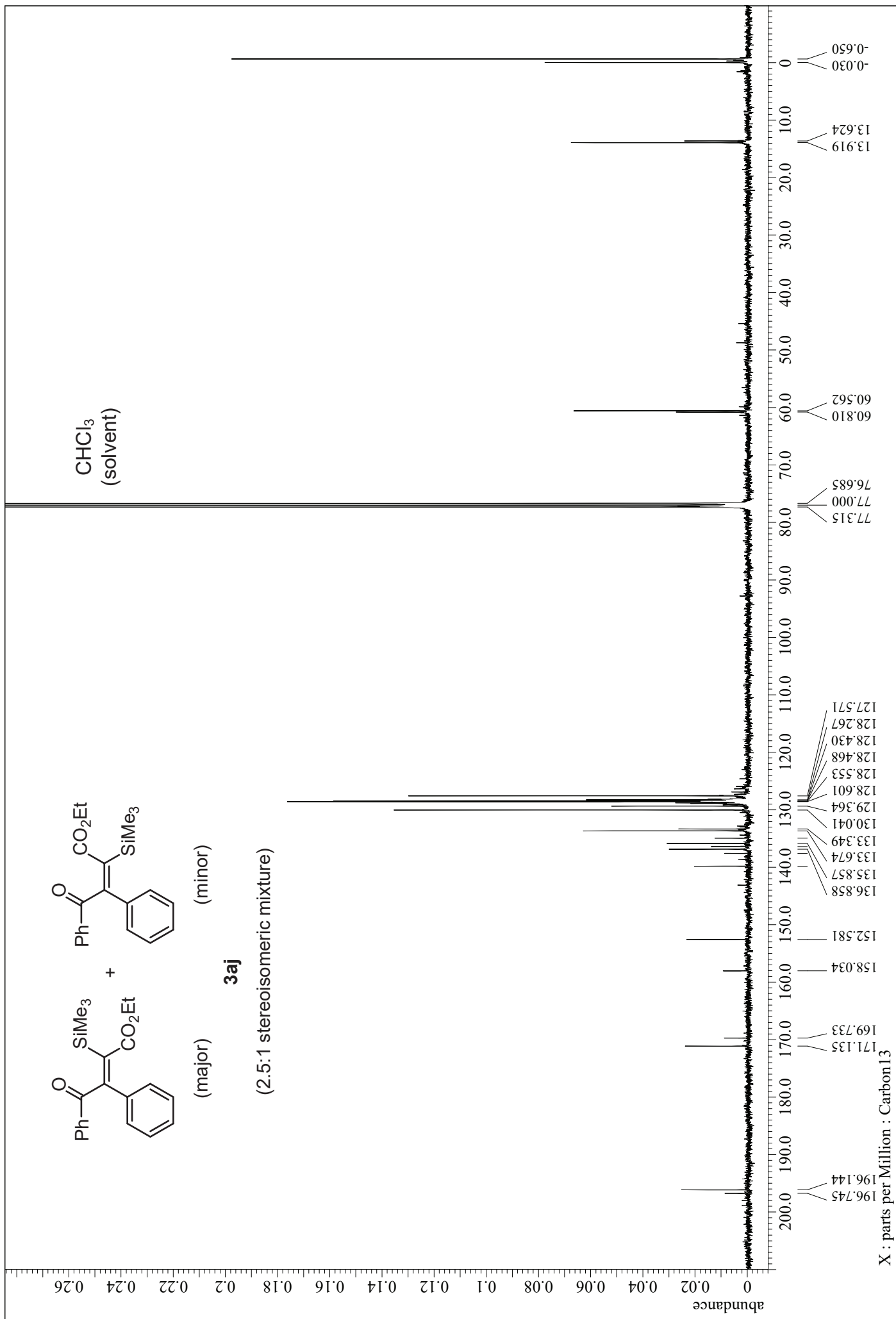


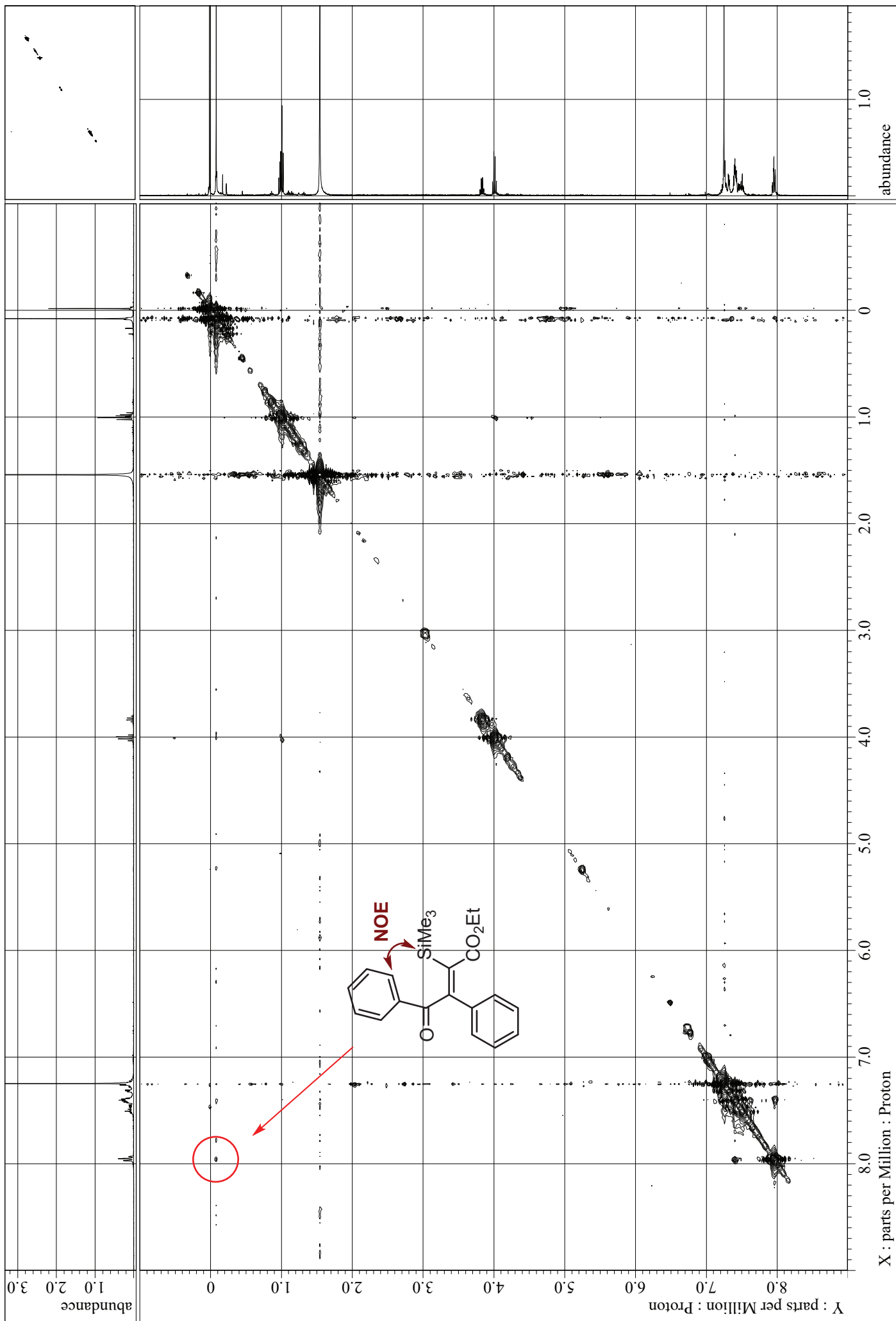


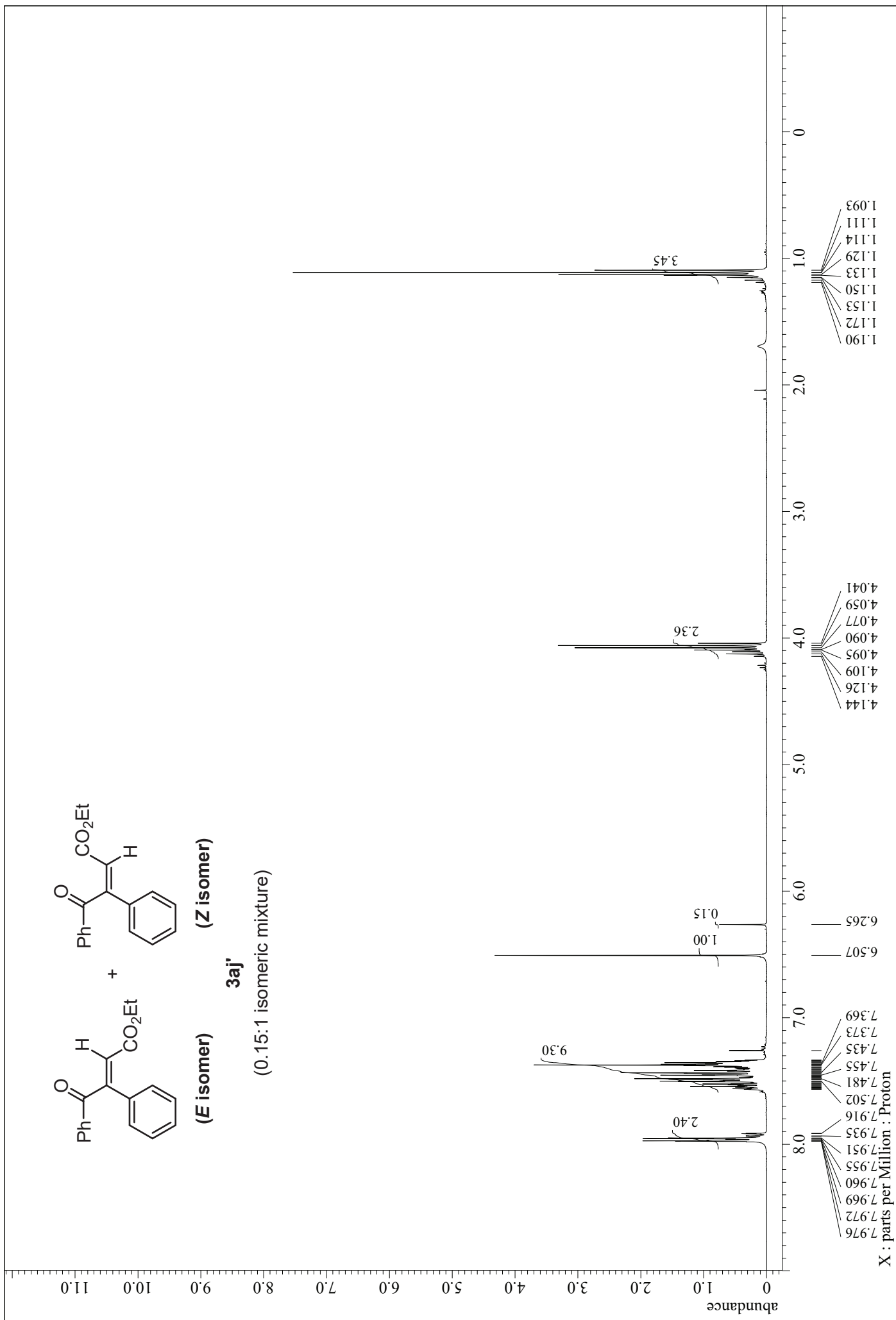


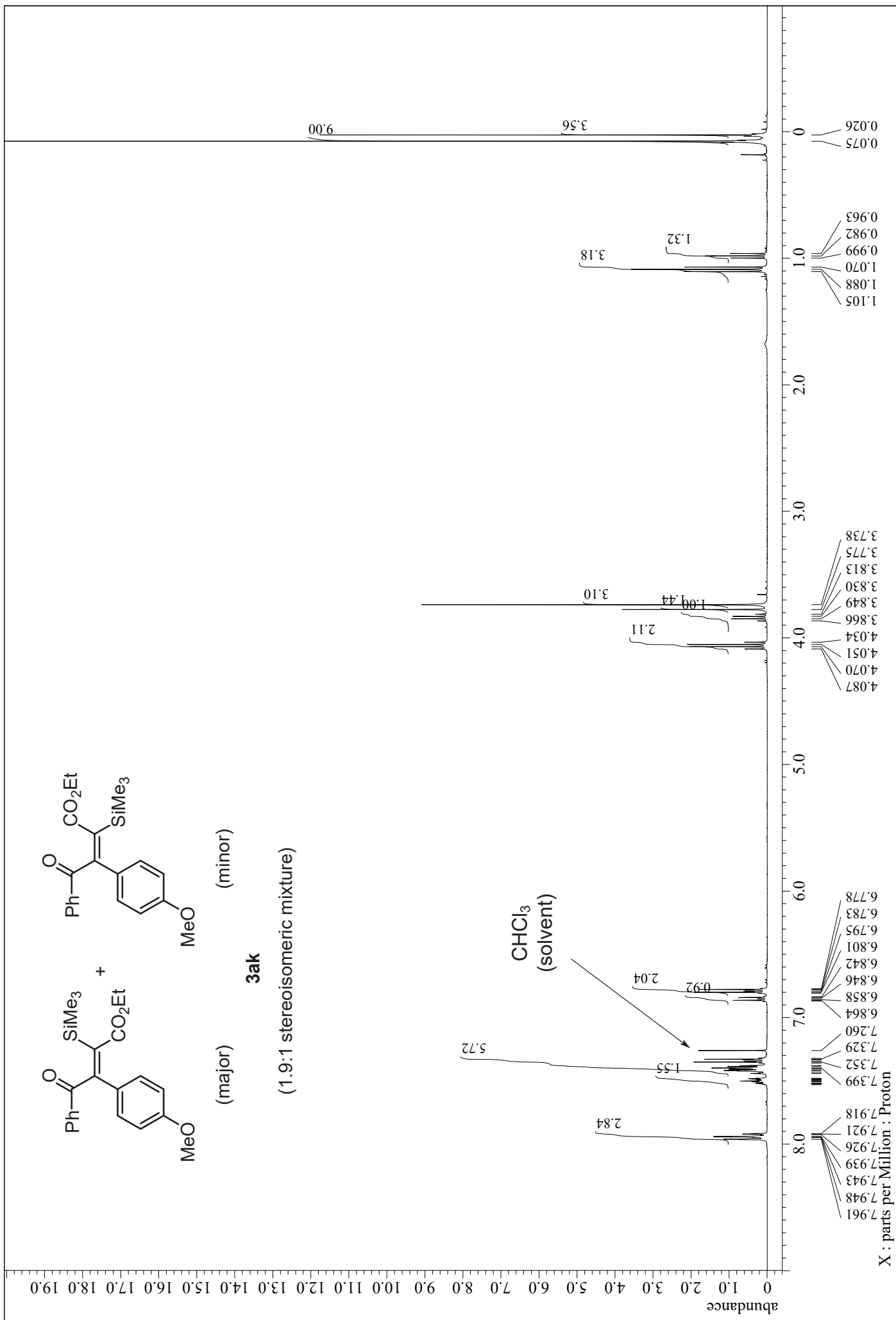


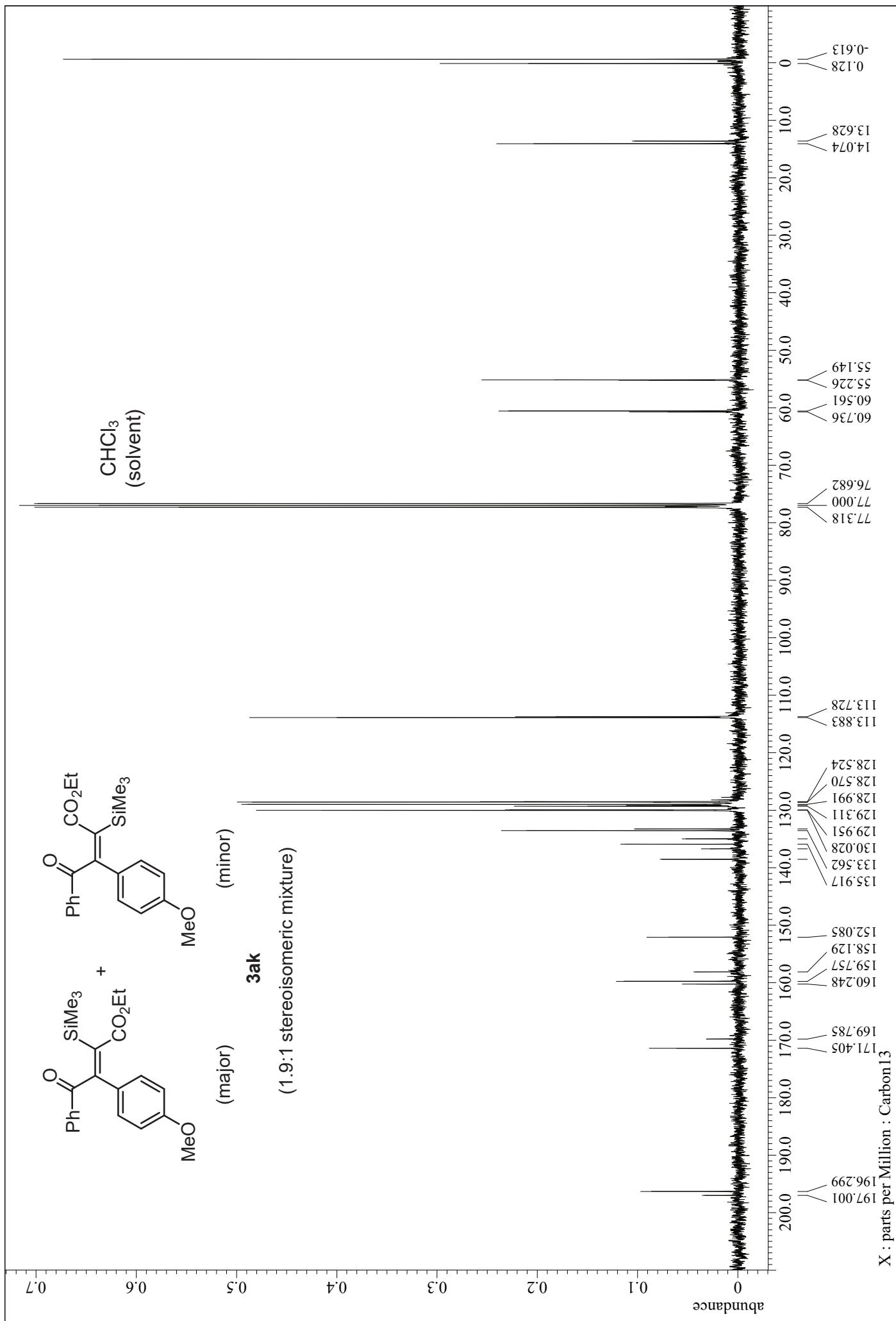






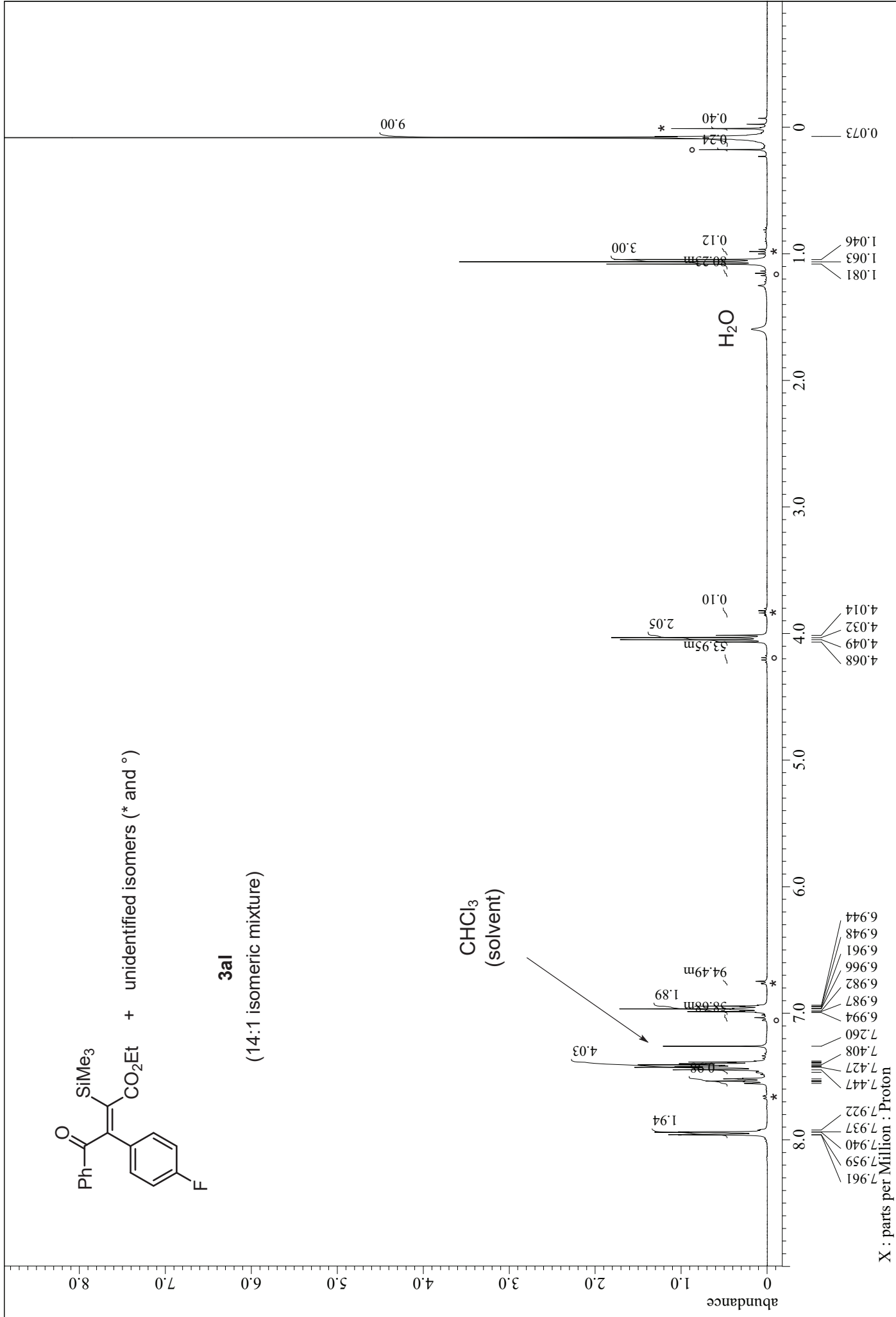


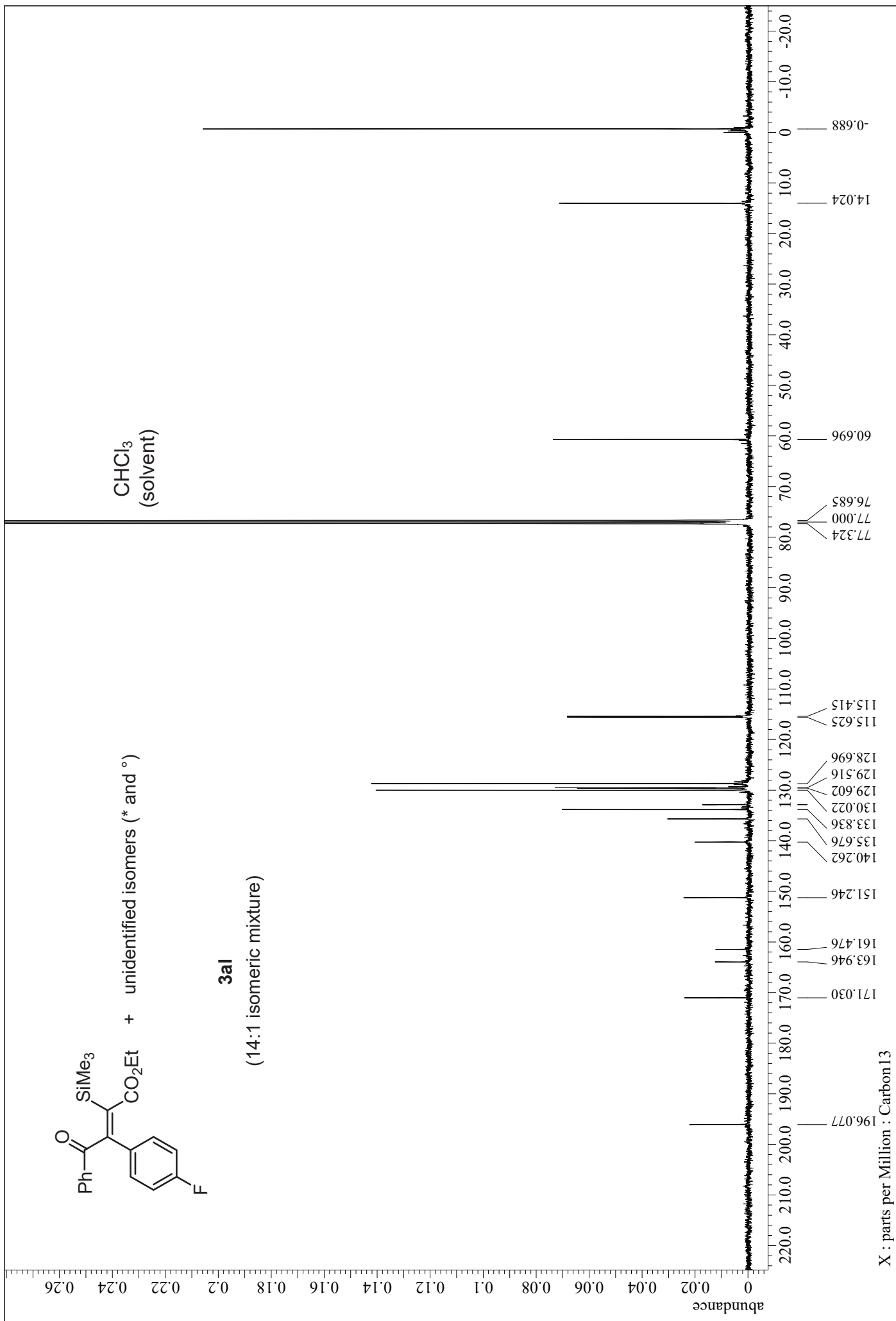


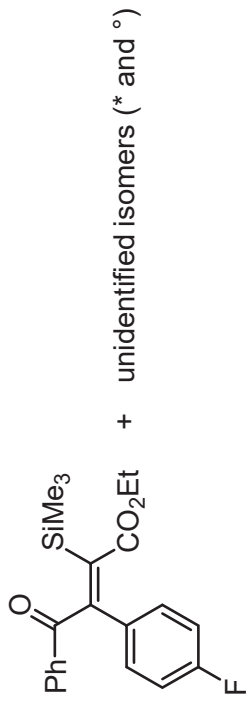




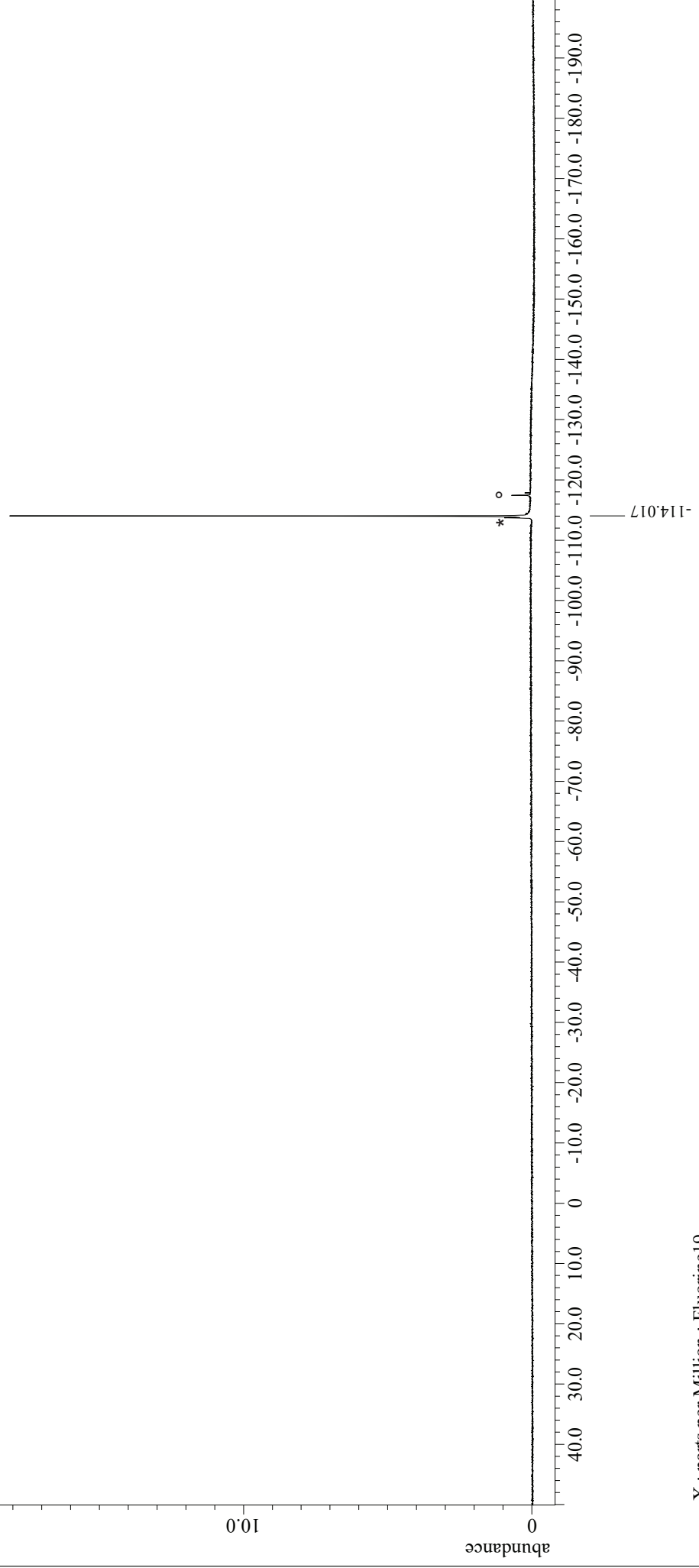
3al
(14:1 isomeric mixture)

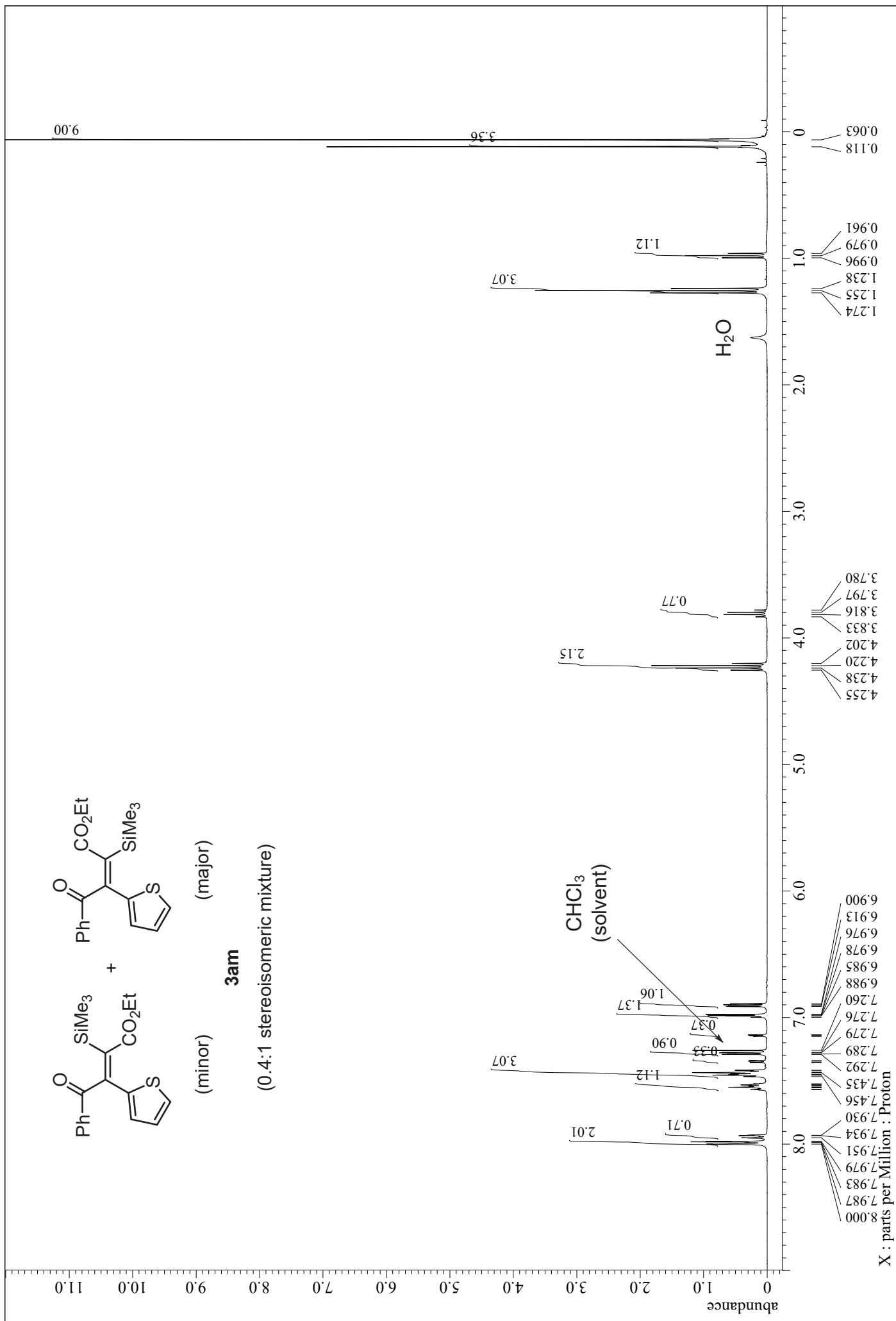


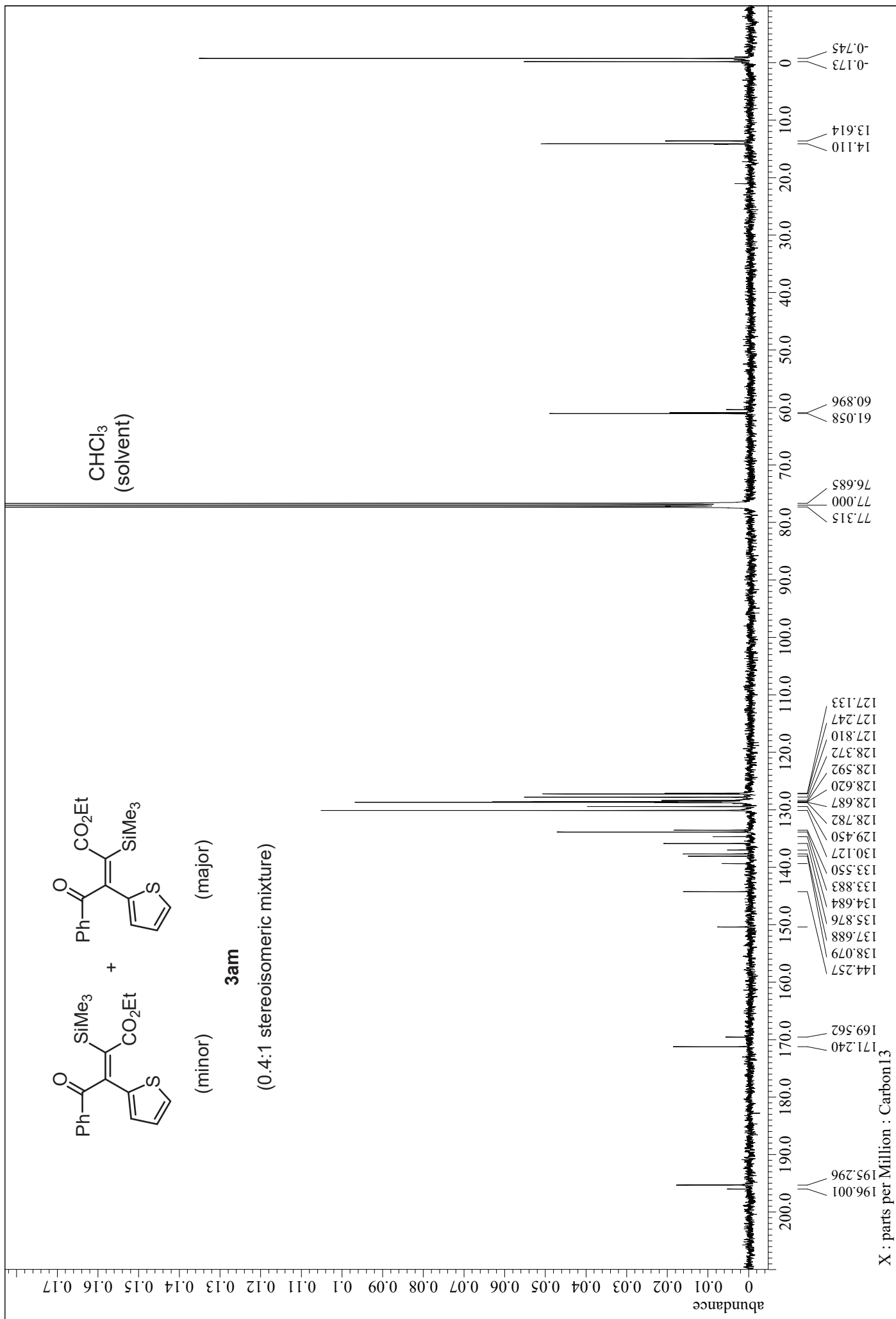


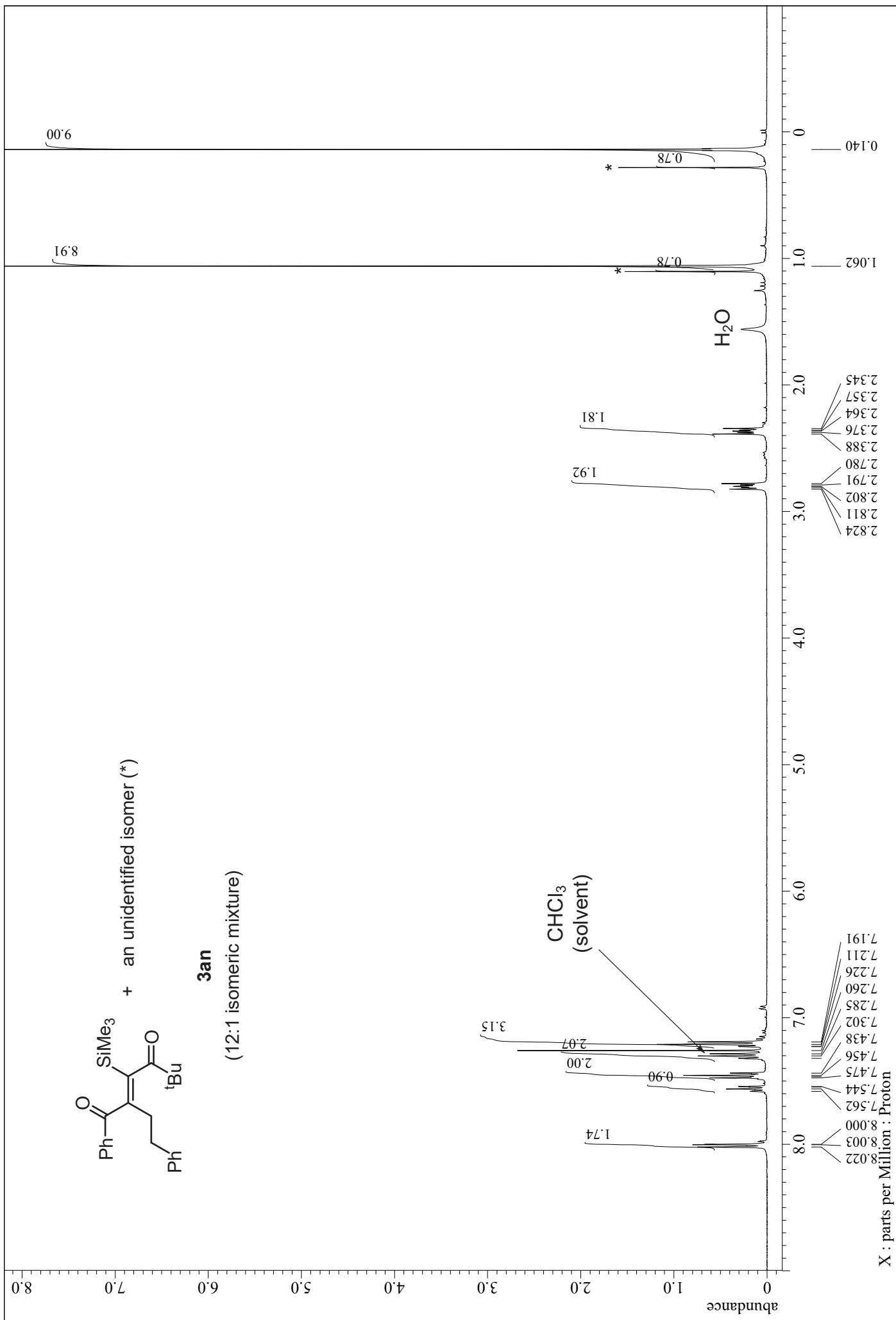


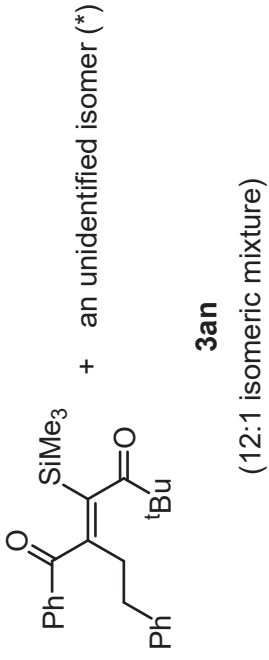
3al
(14:1 isomeric mixture)



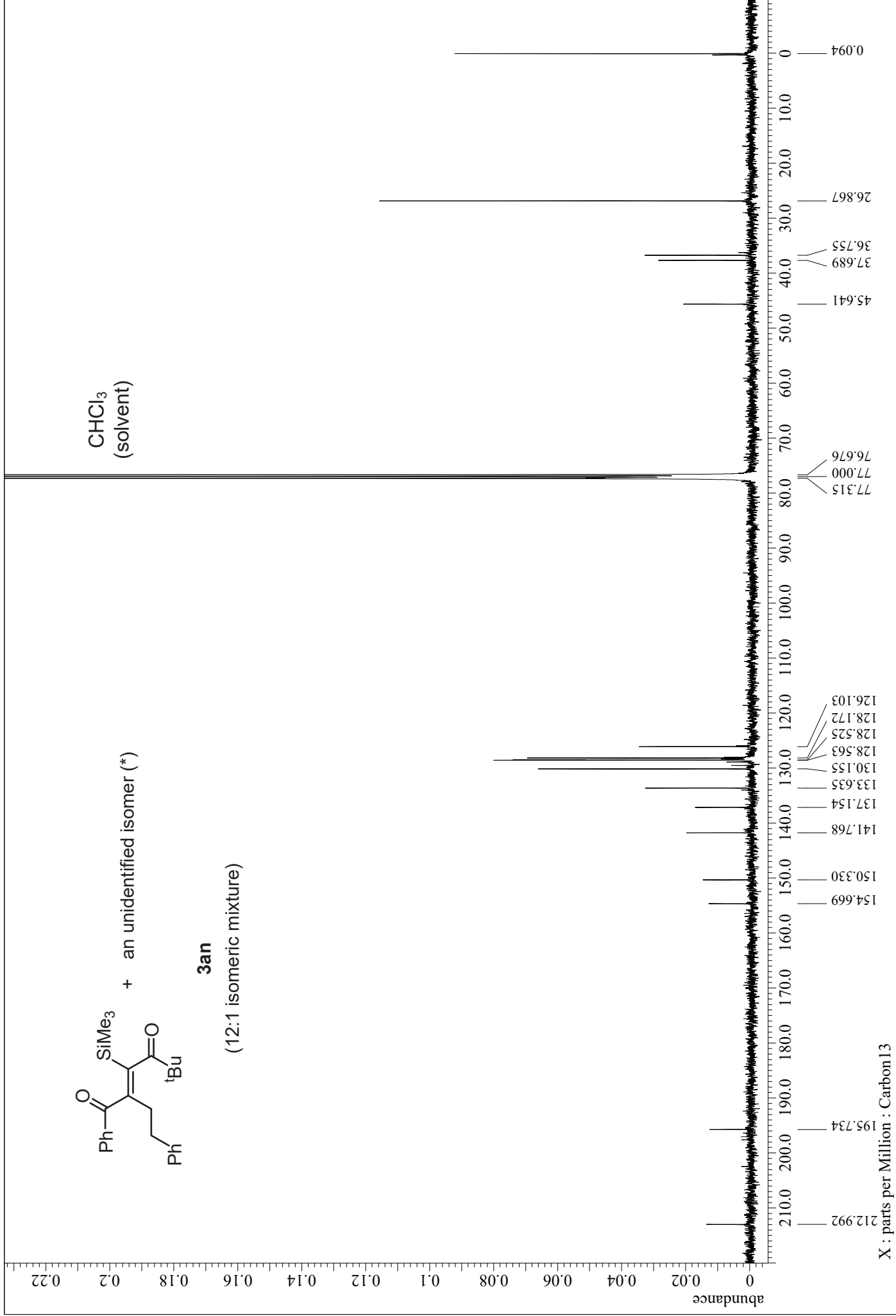


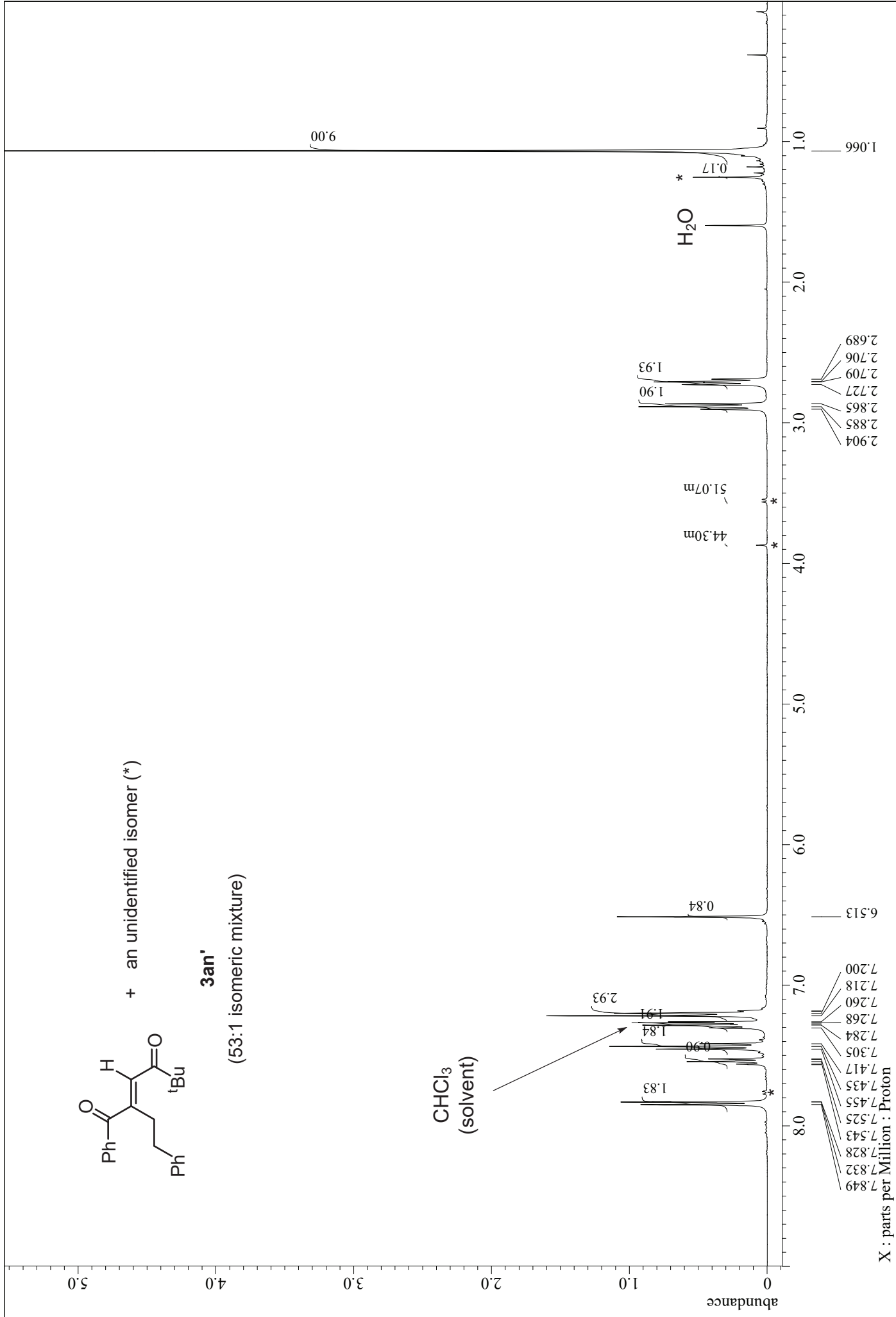
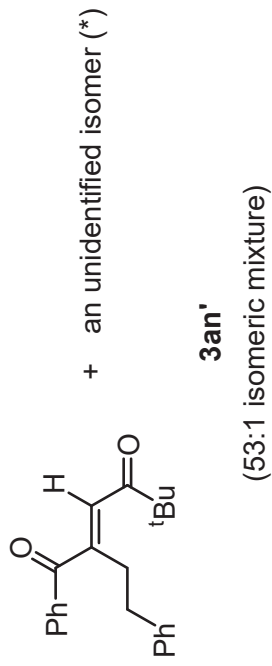


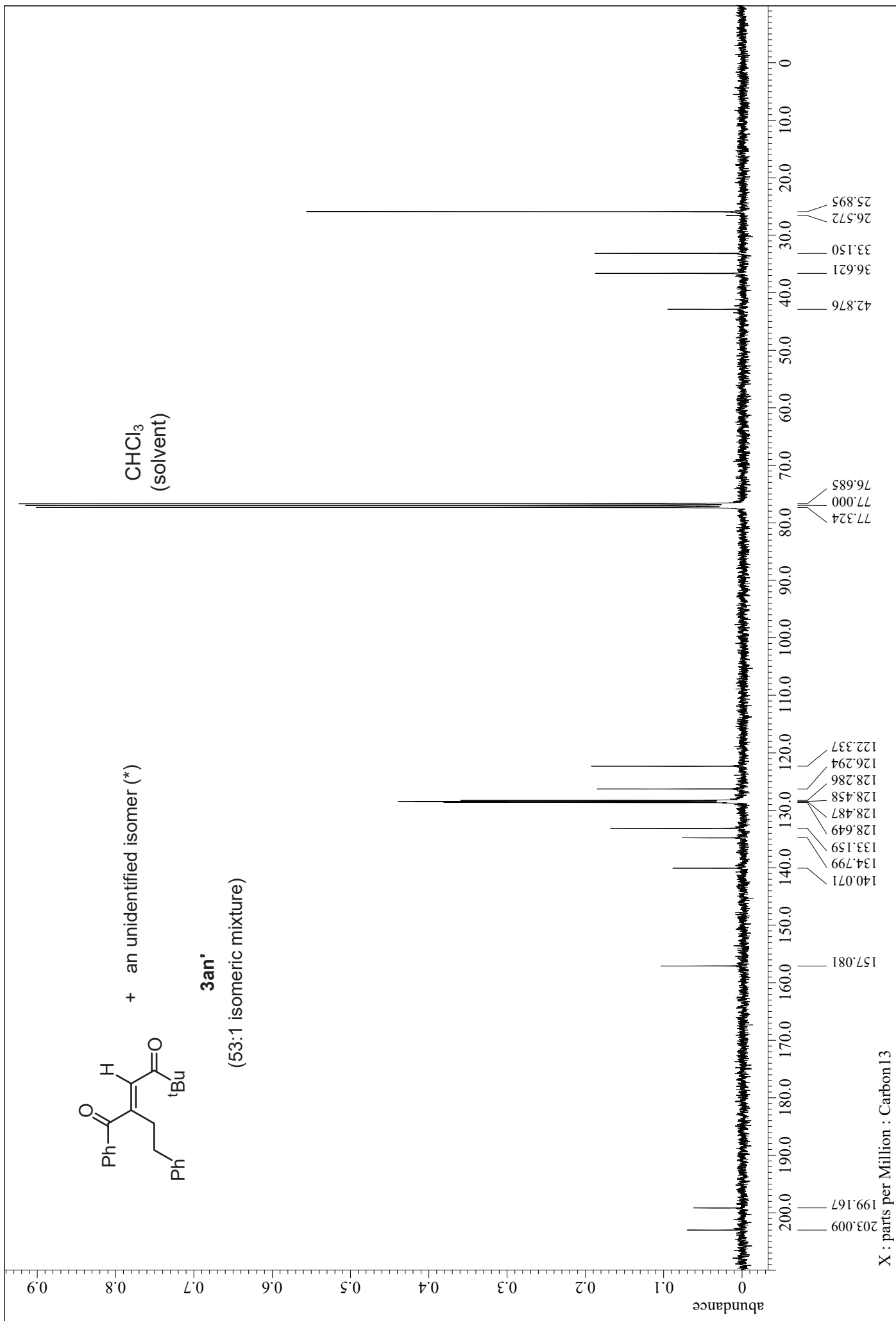


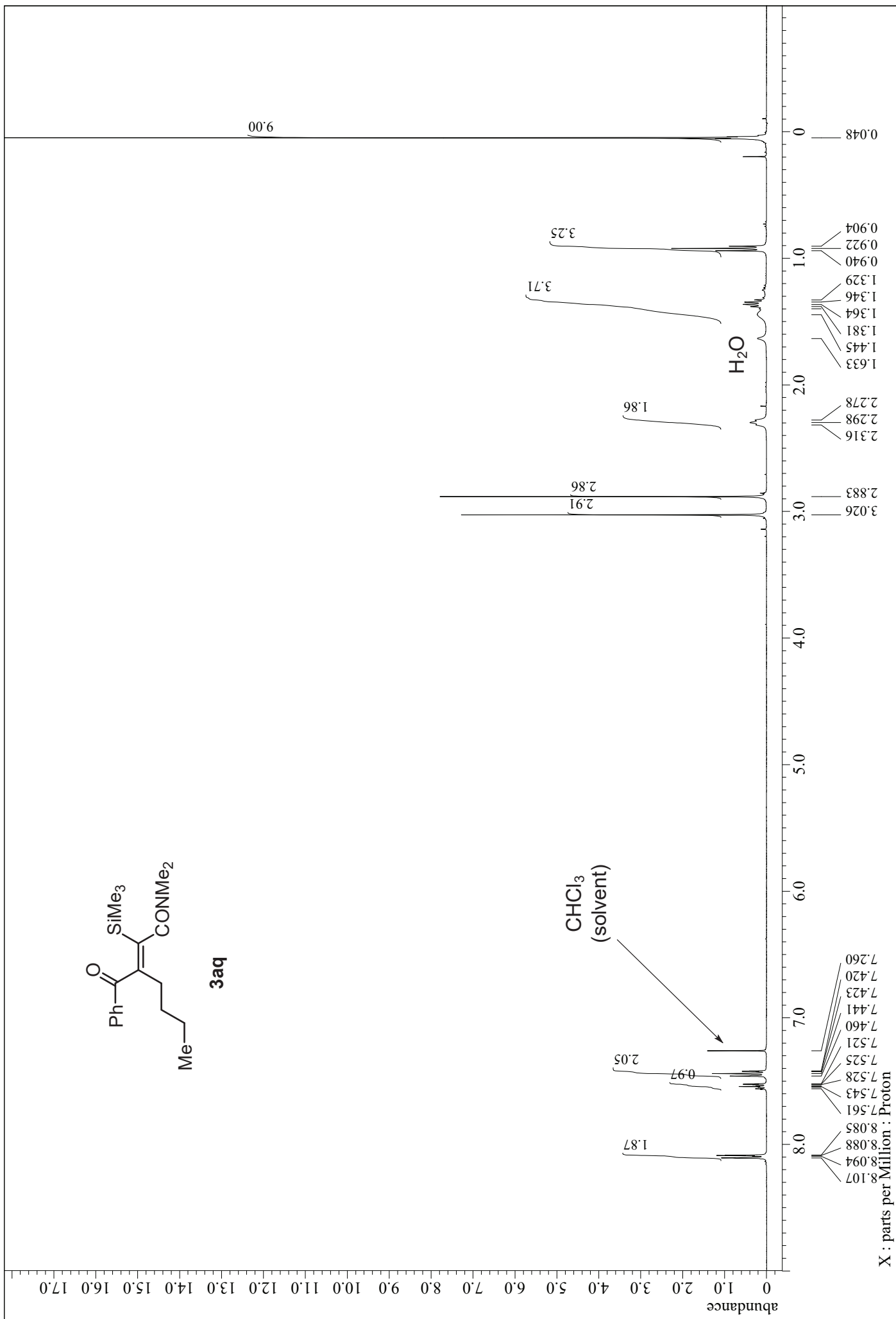


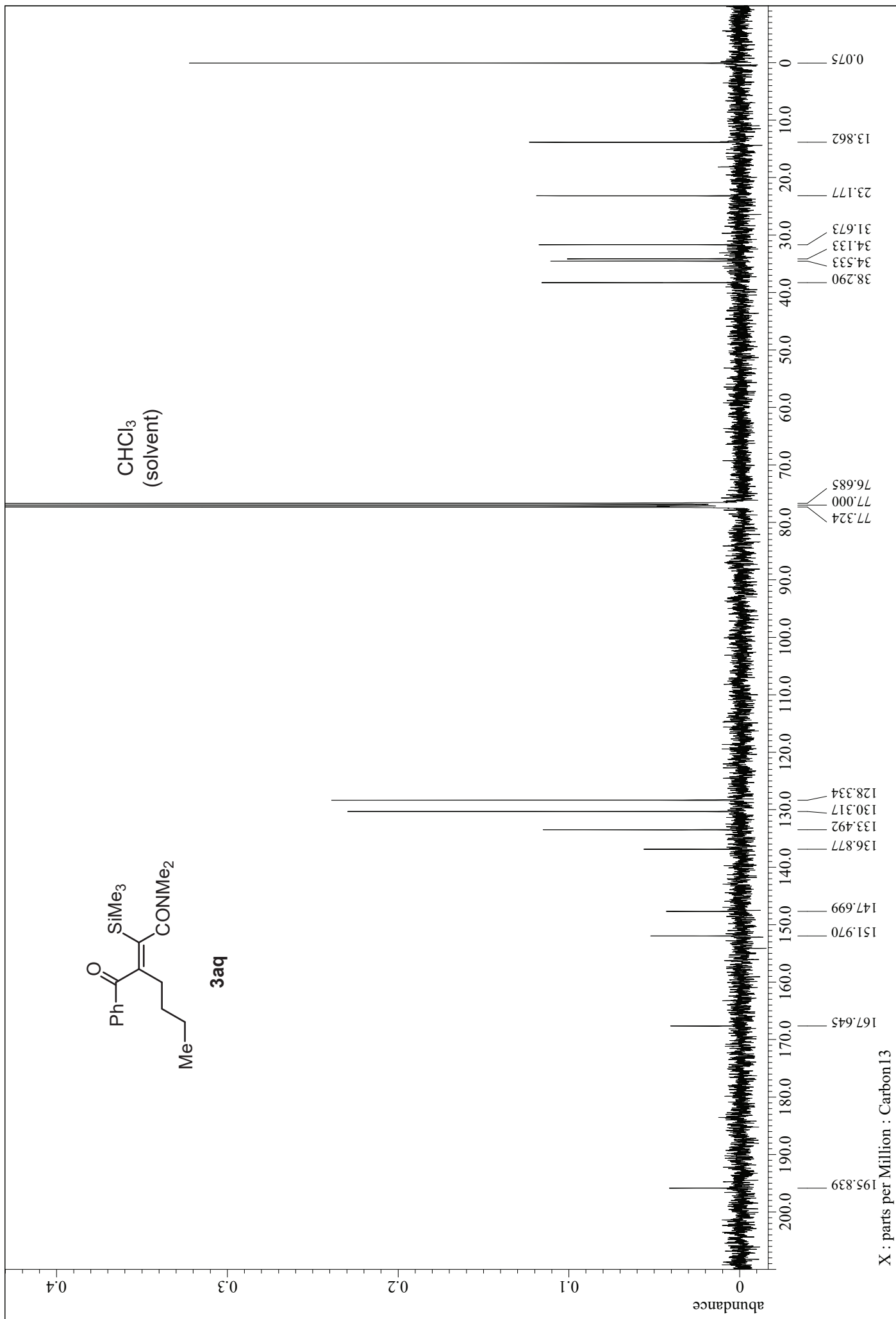
CHCl₃
(solvent)

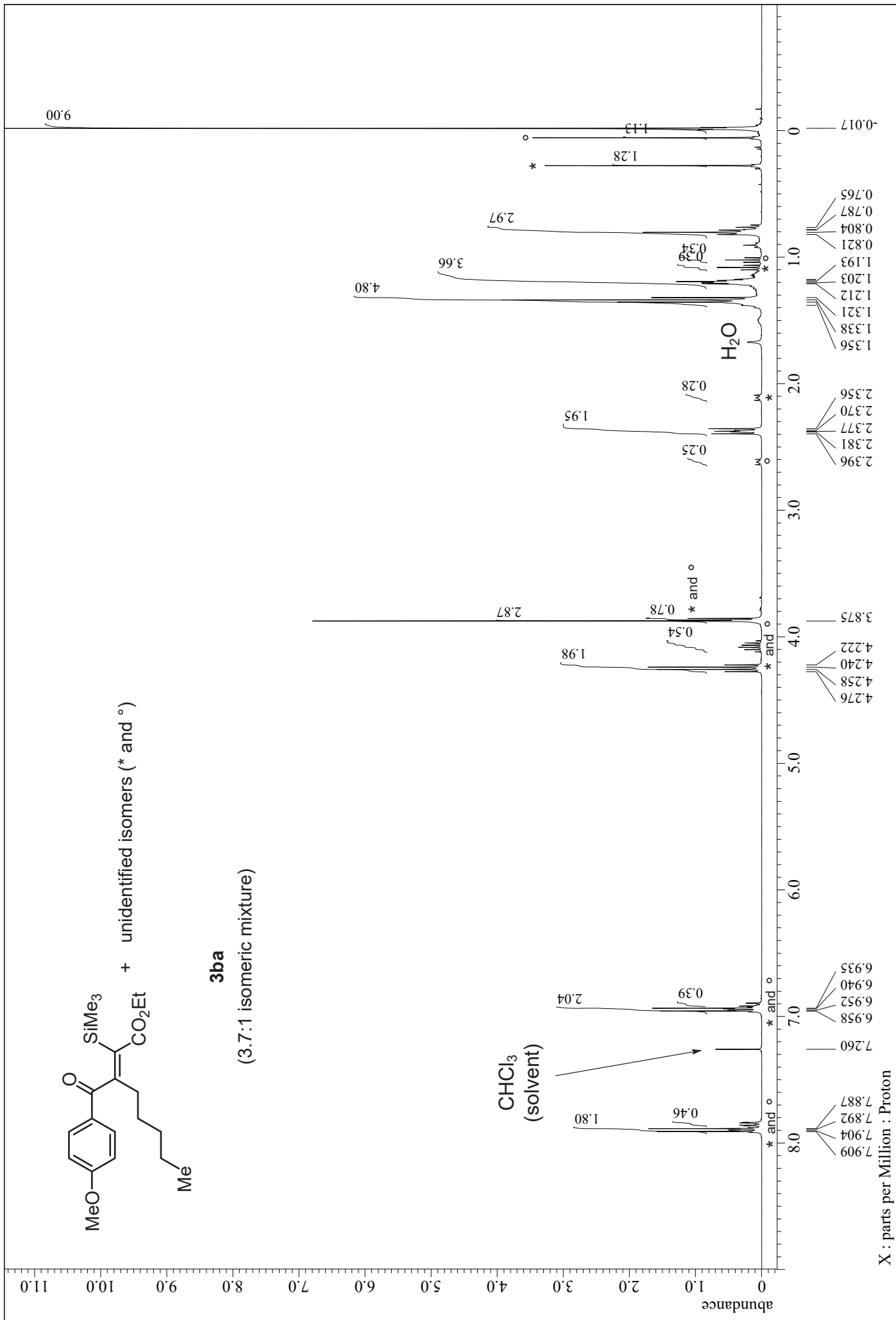


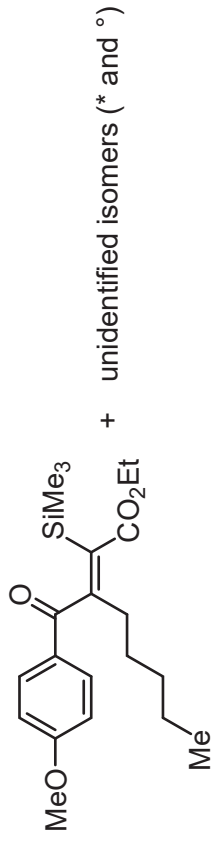






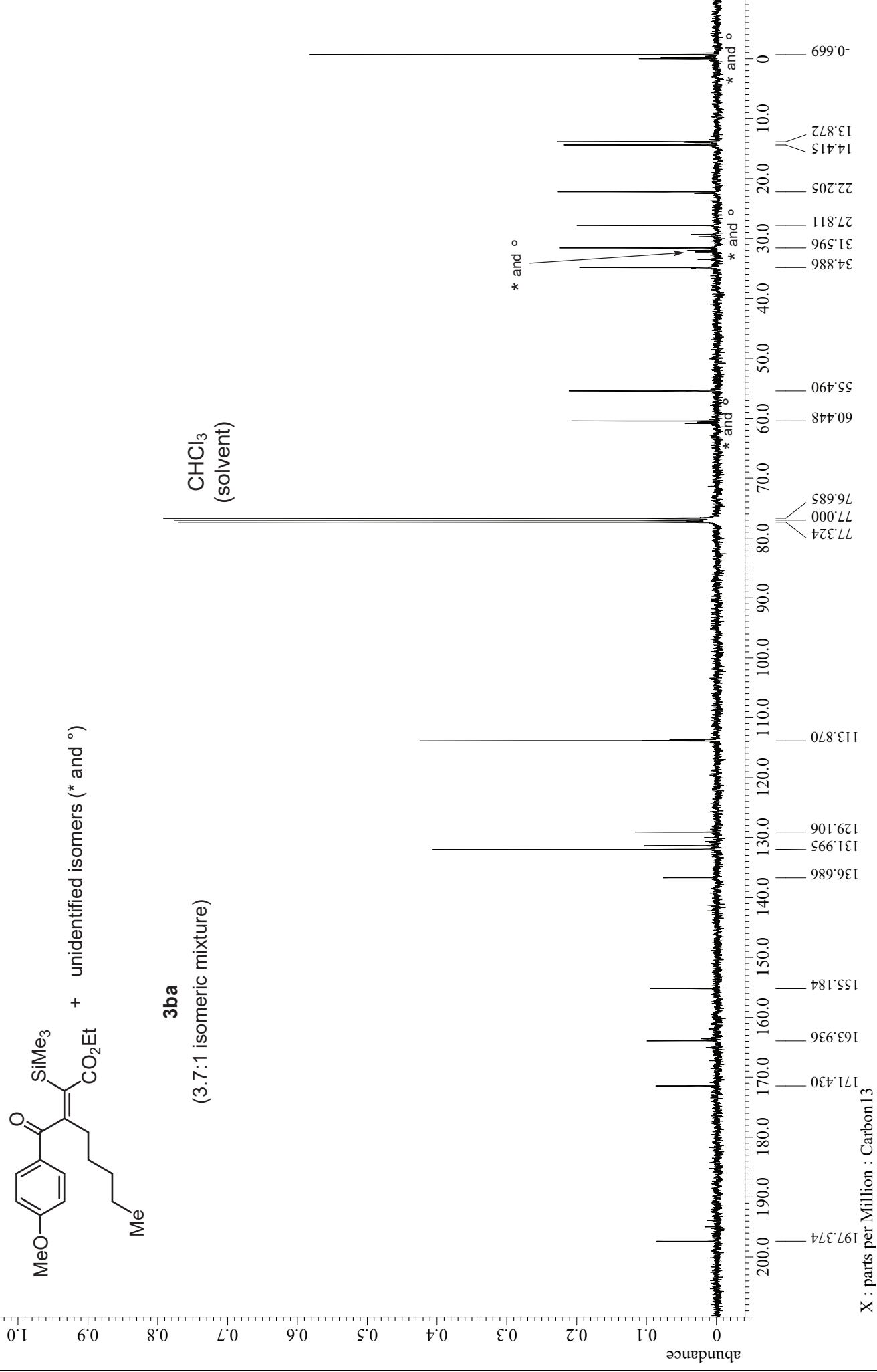


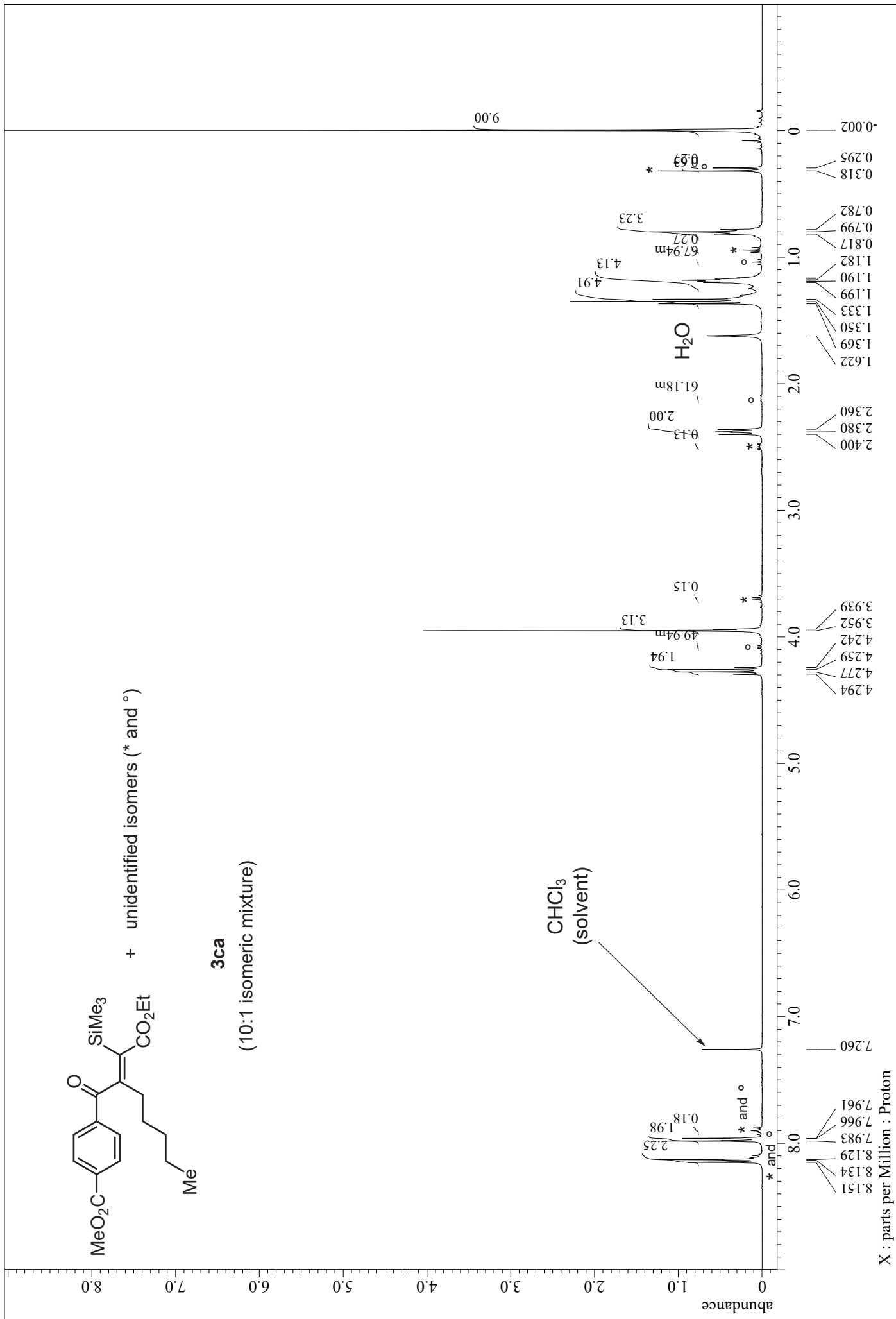


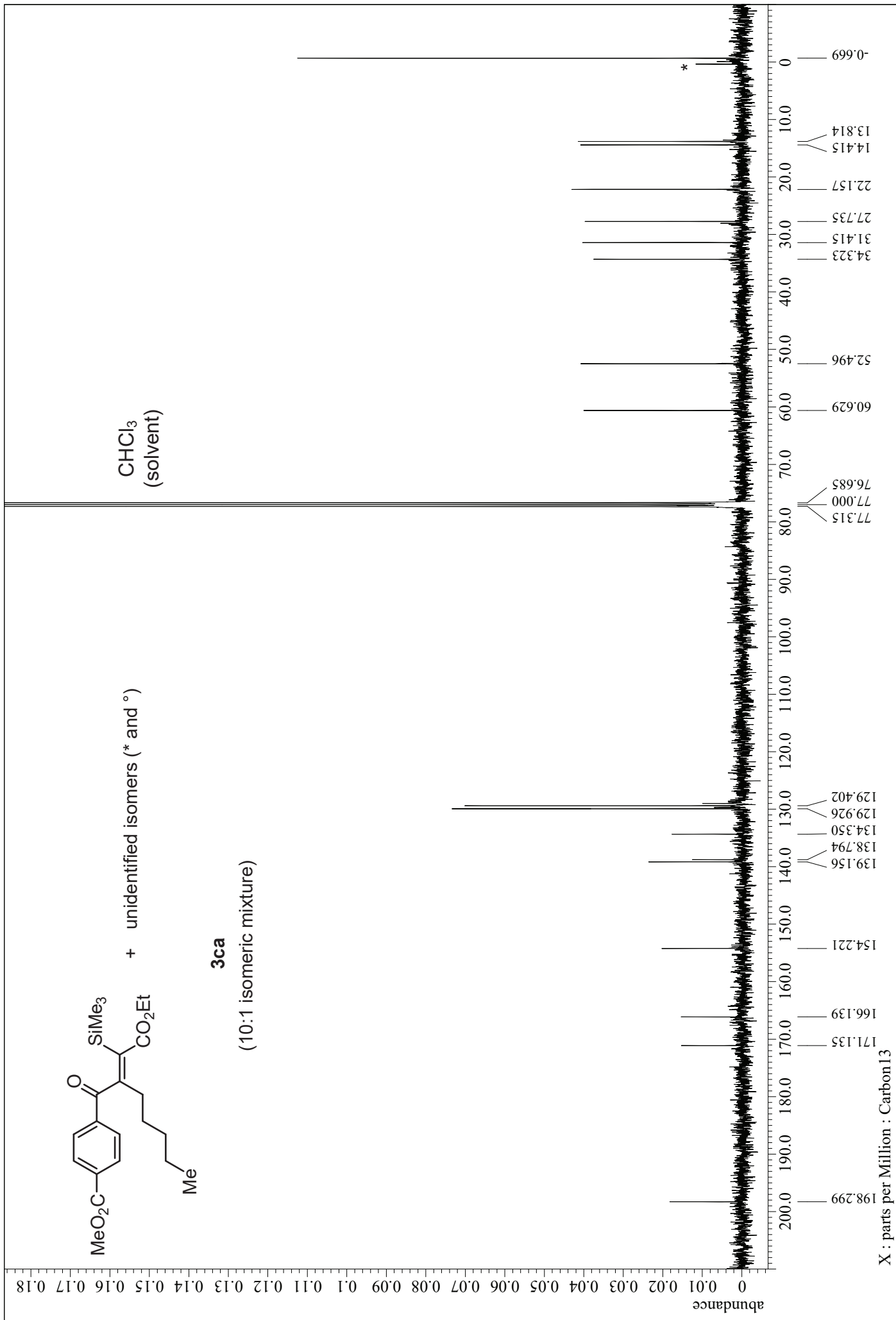


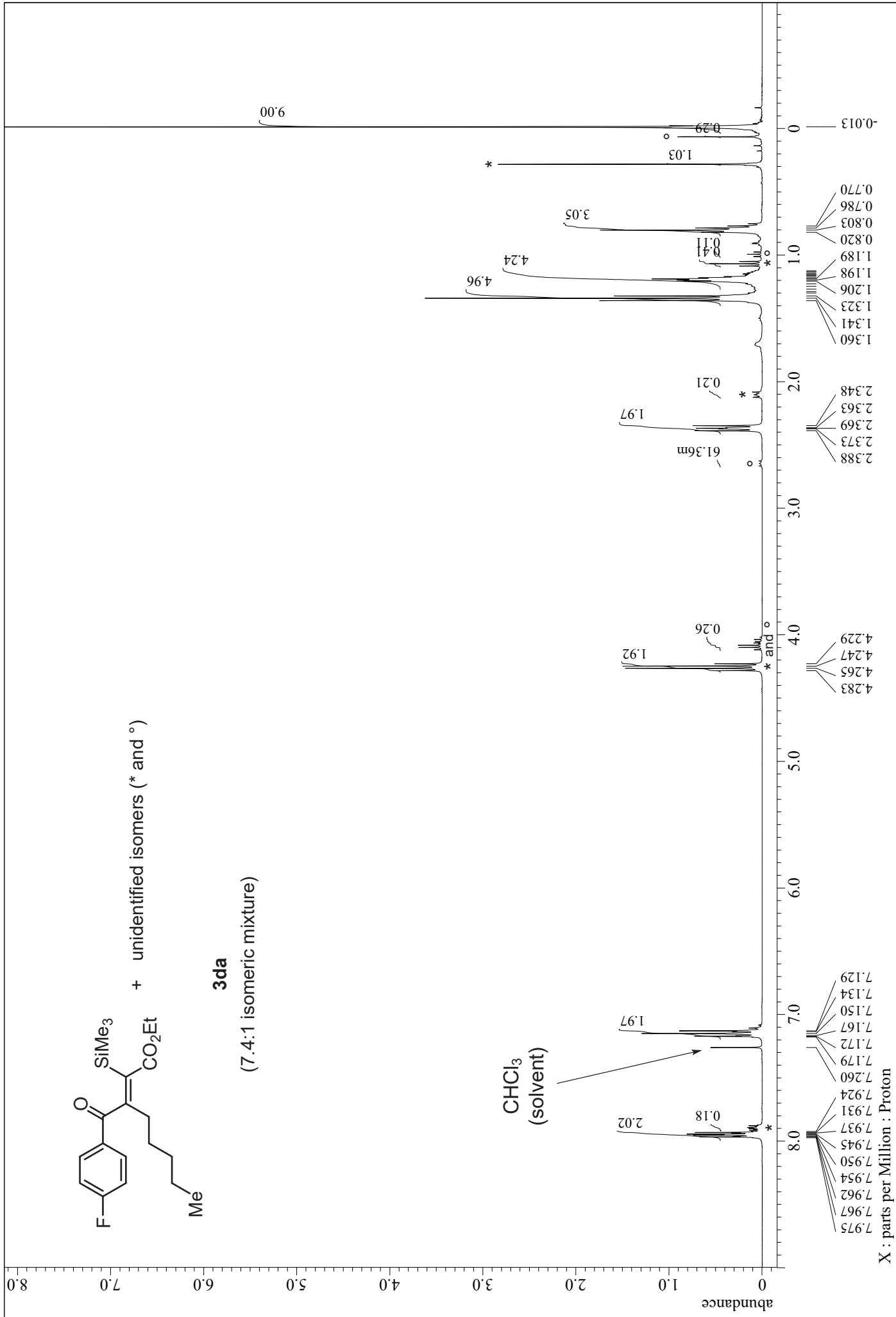
3ba
(3.7:1 isomeric mixture)

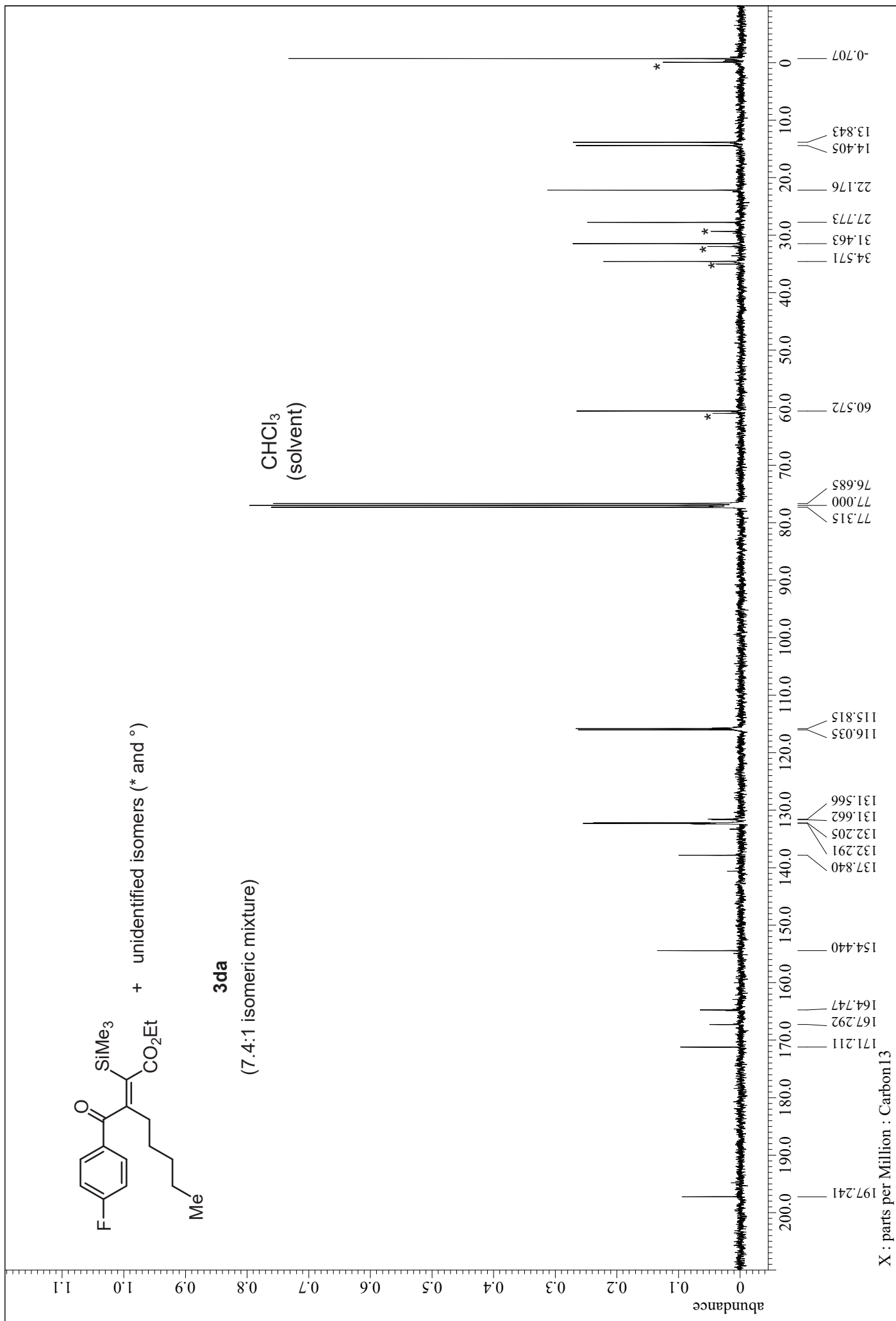
CHCl₃
(solvent)

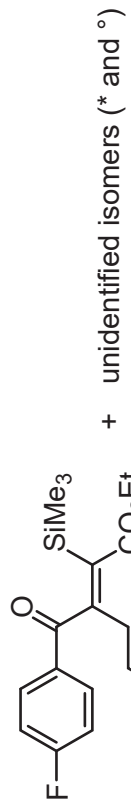




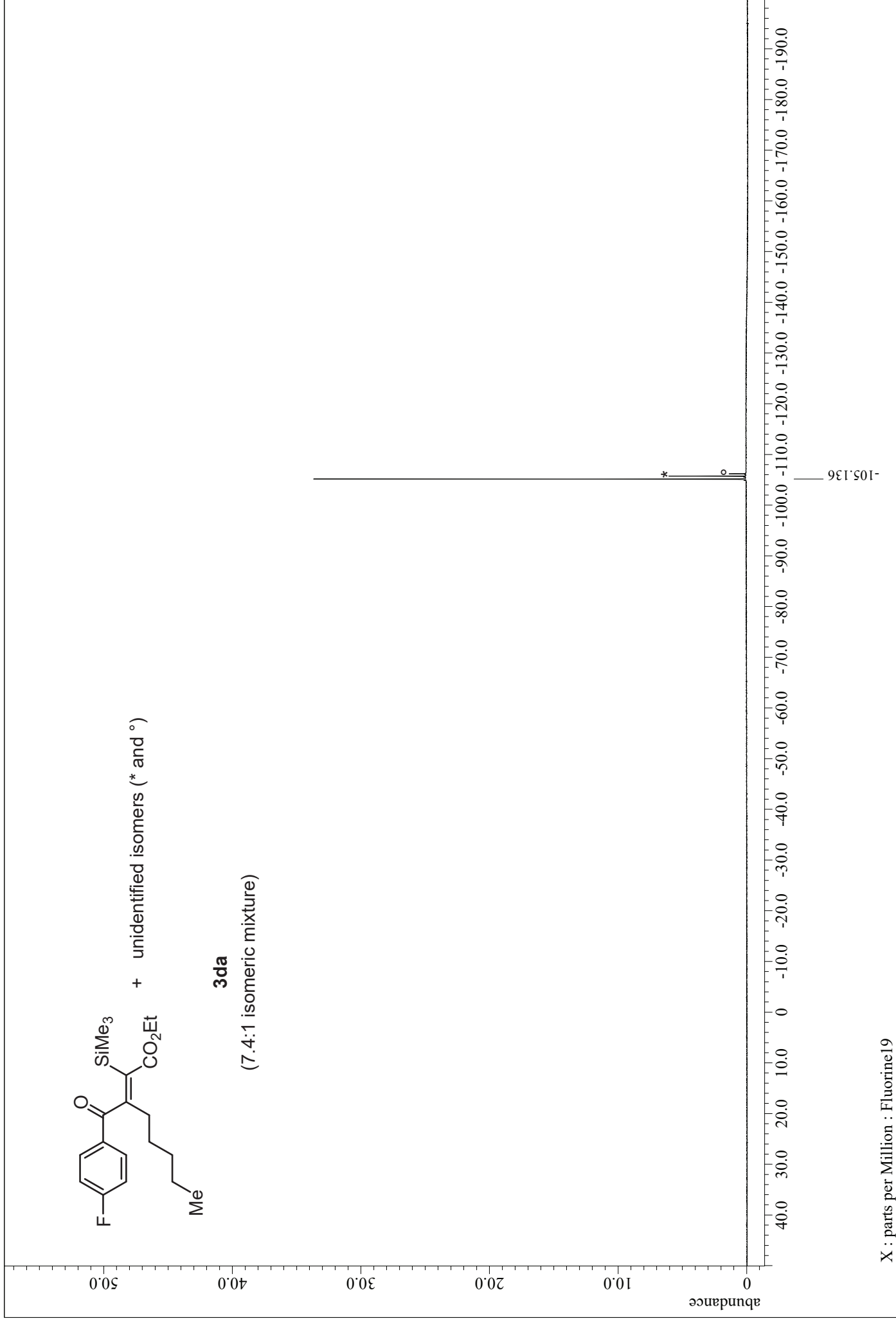




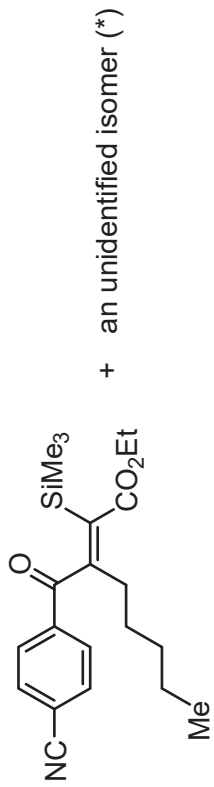




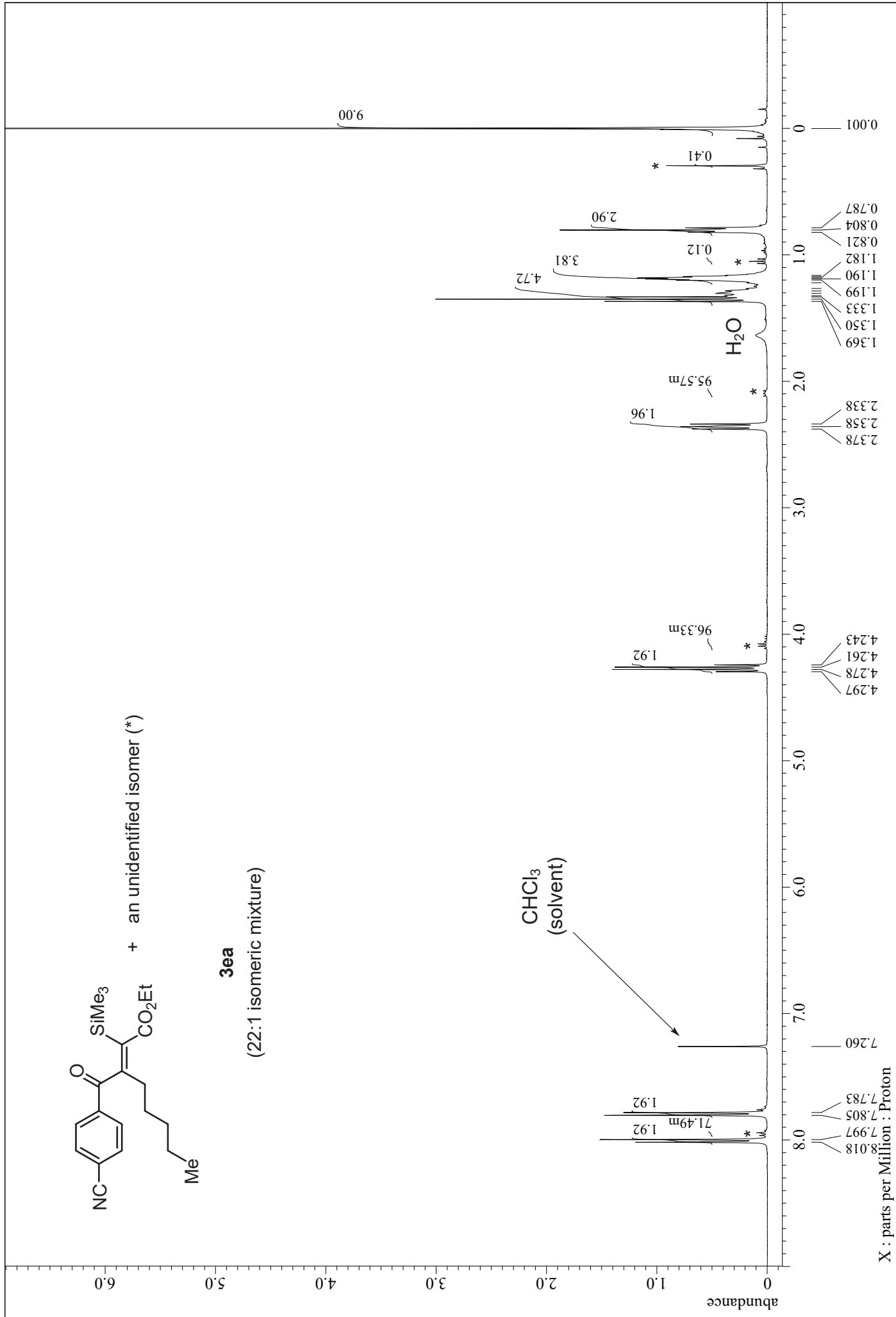
3da
(7.4:1 isomeric mixture)

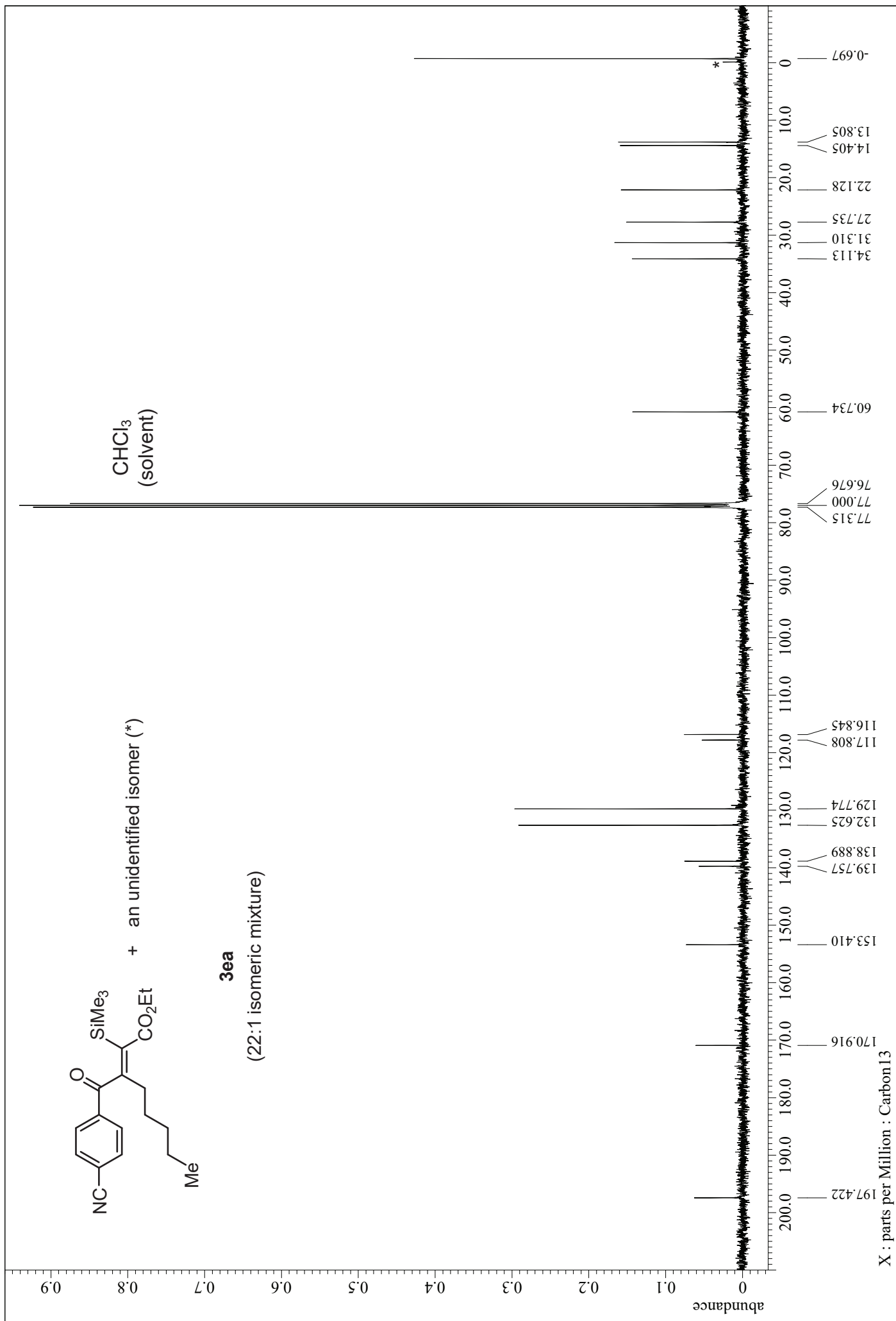


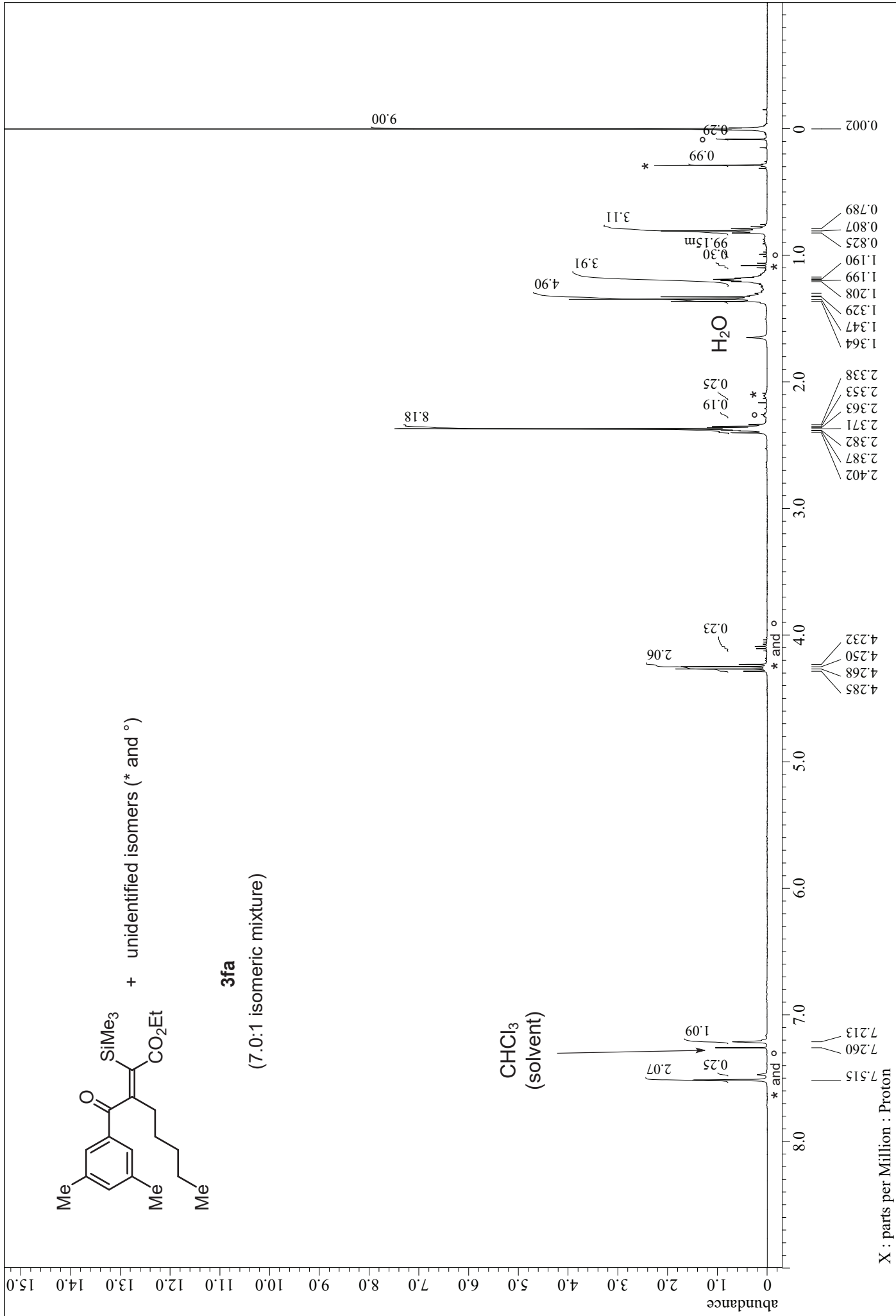
X : parts per Million : Fluorine19

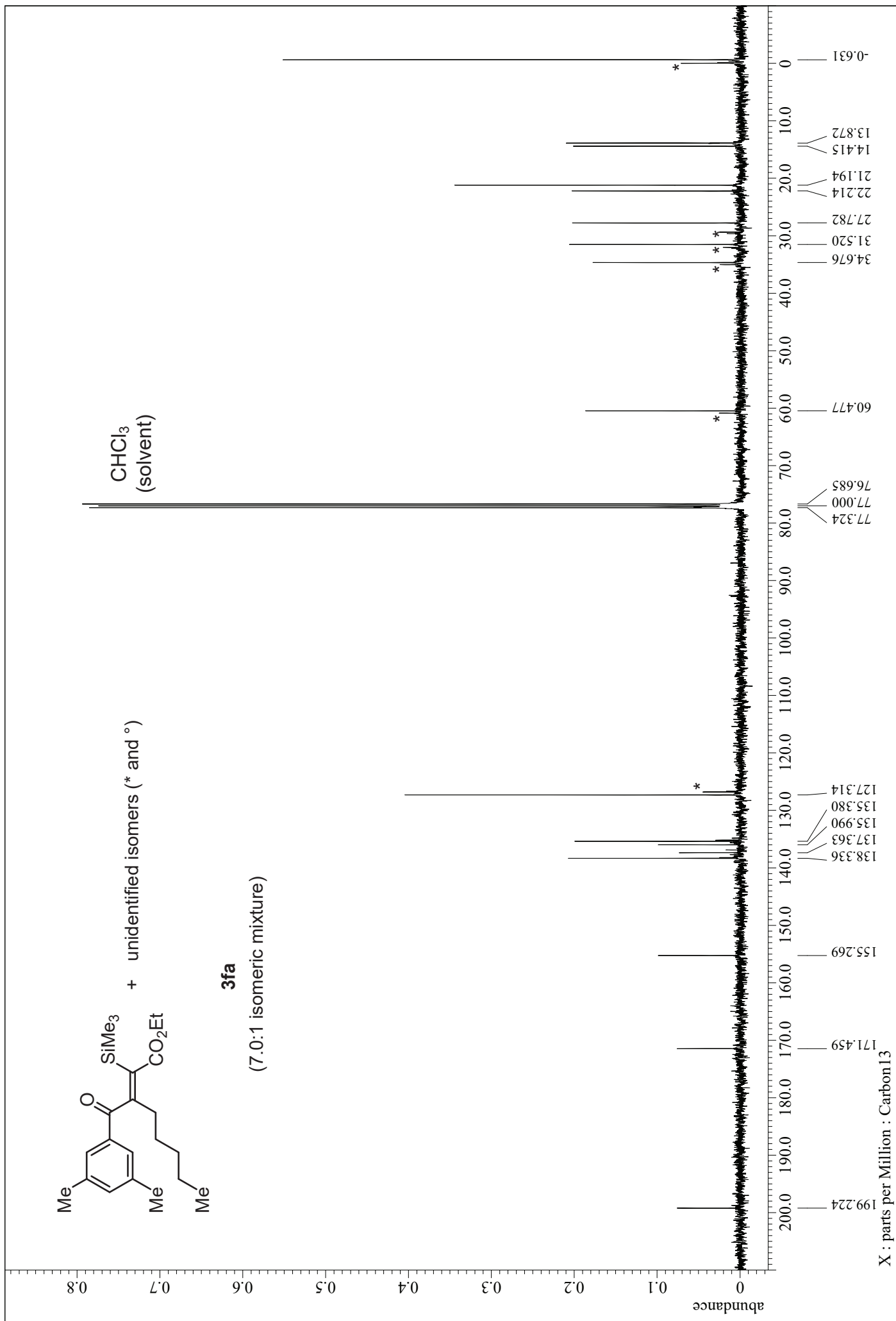


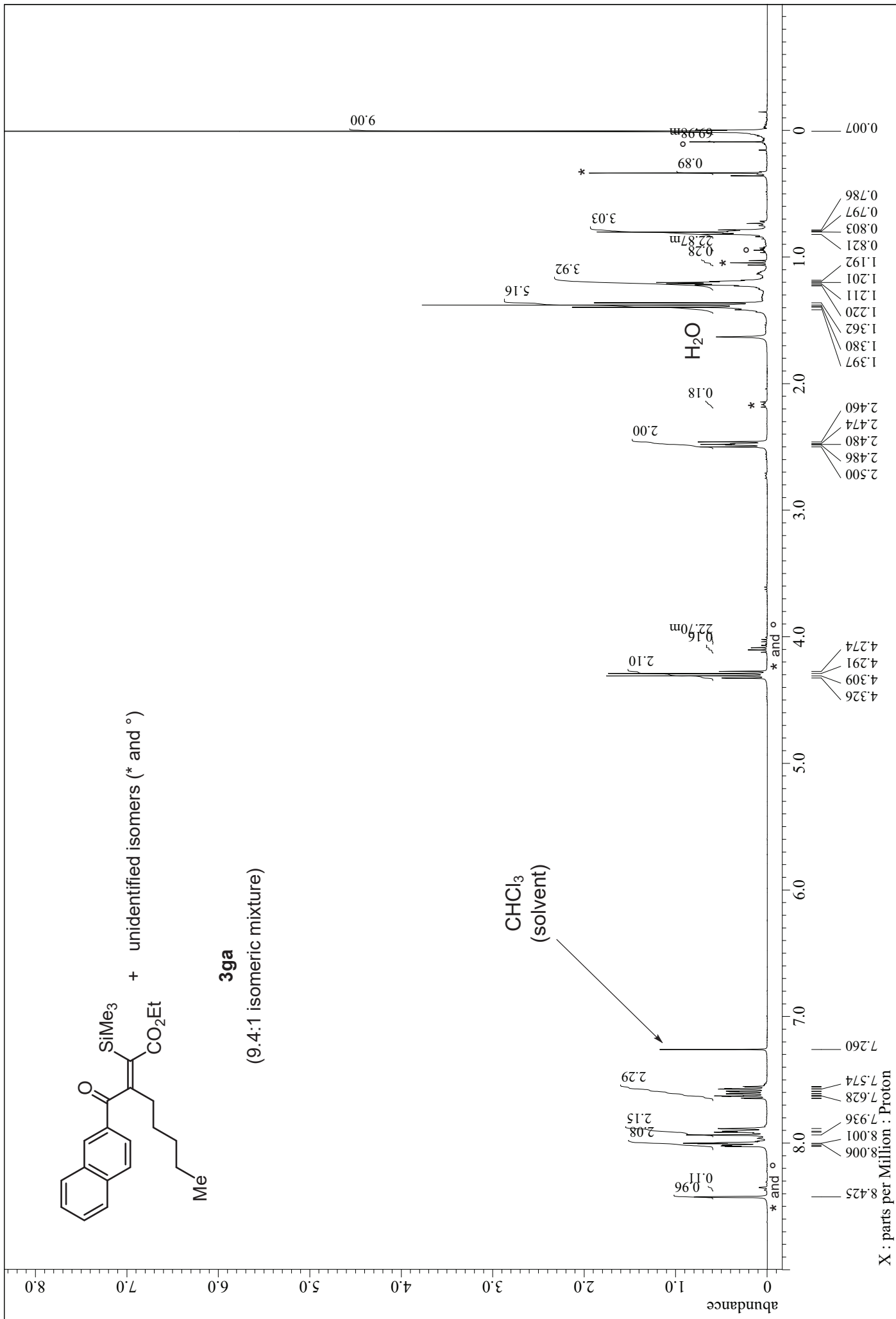
3ea
(22:1 isomeric mixture)

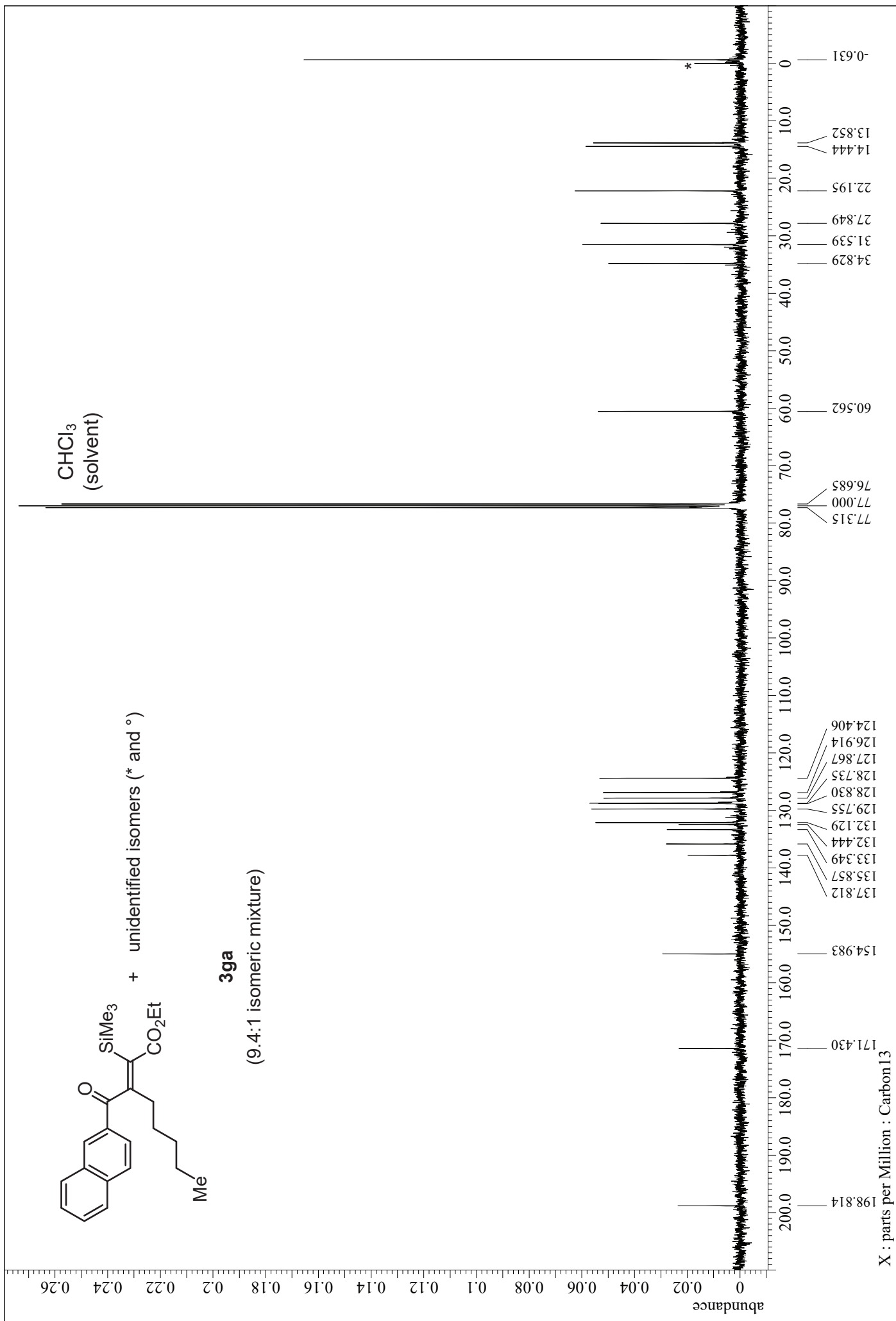


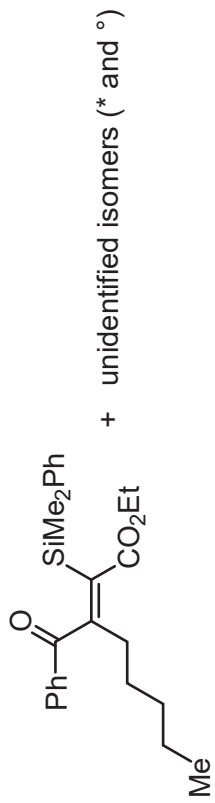






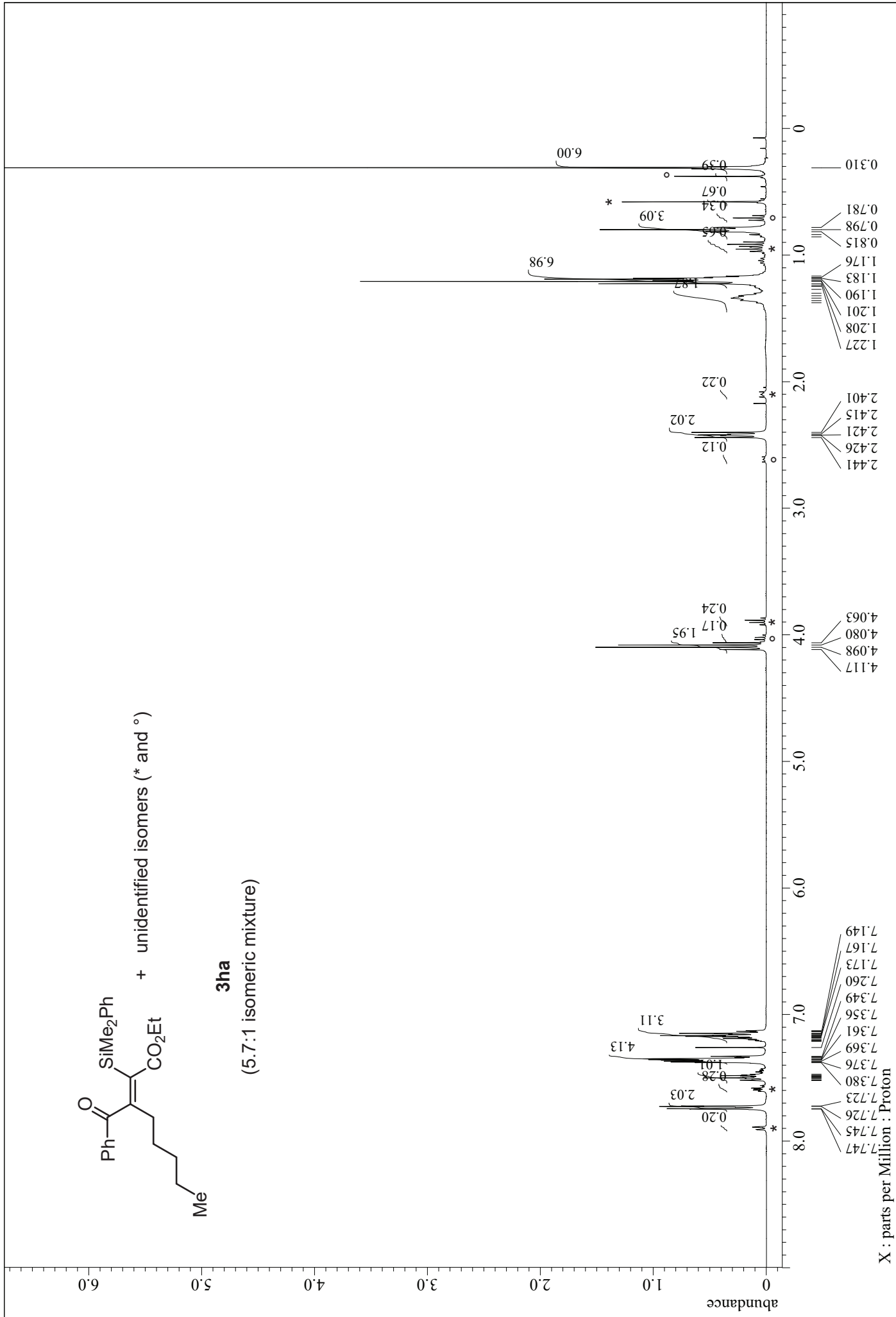


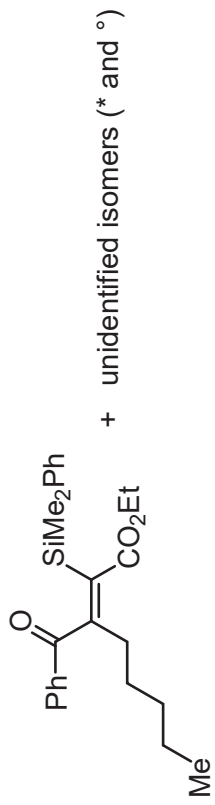




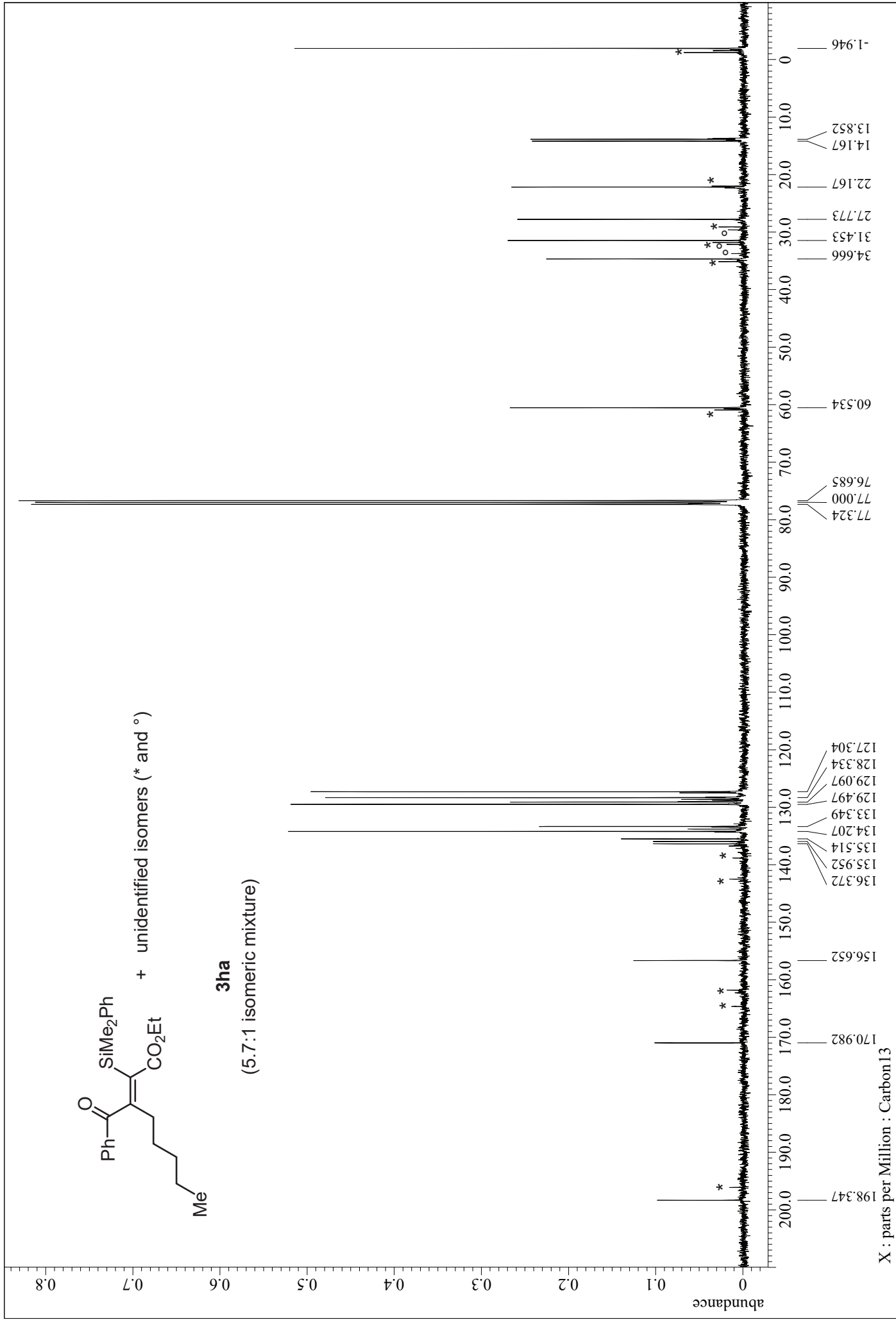
3ha

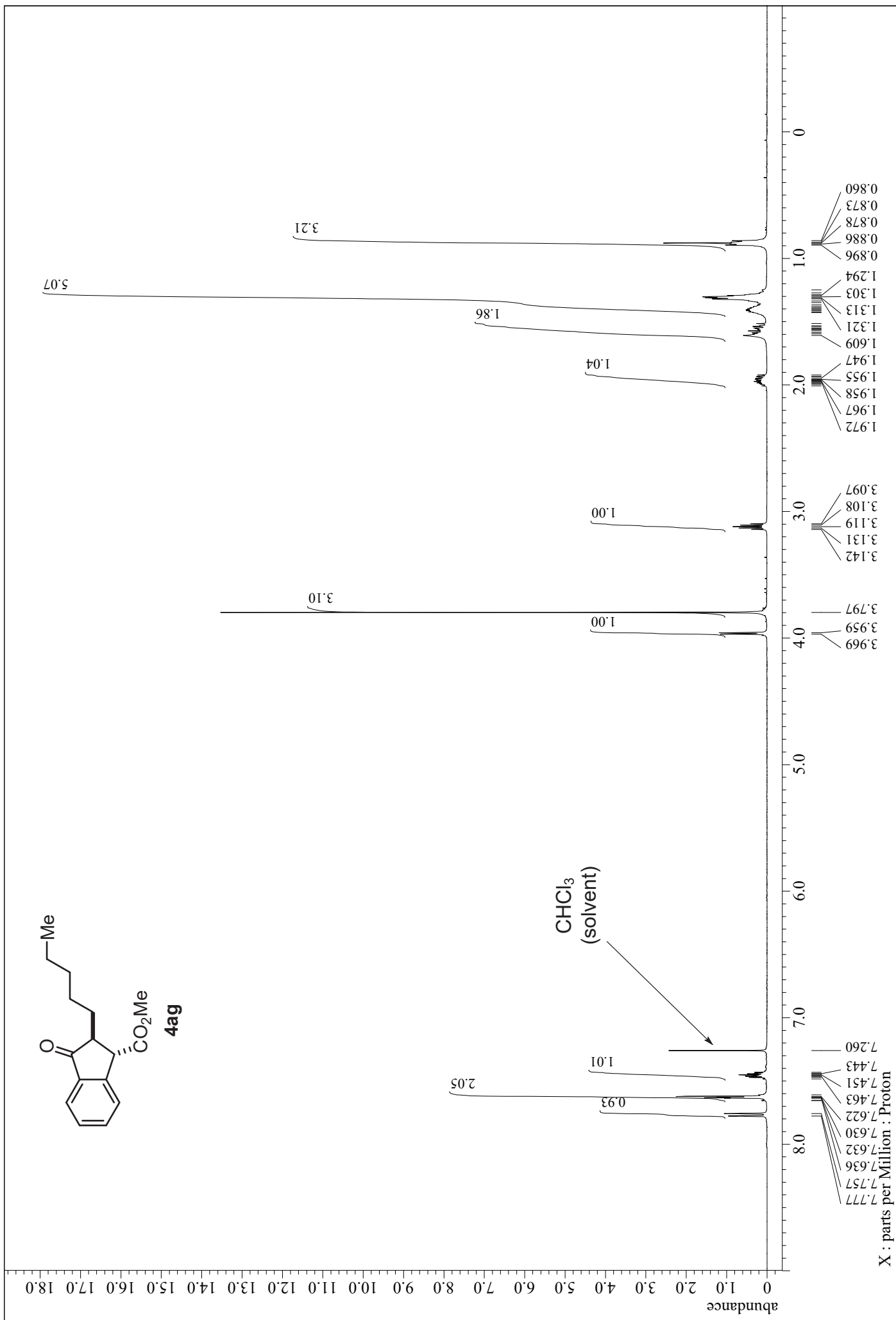
(5.7:1 isomeric mixture)

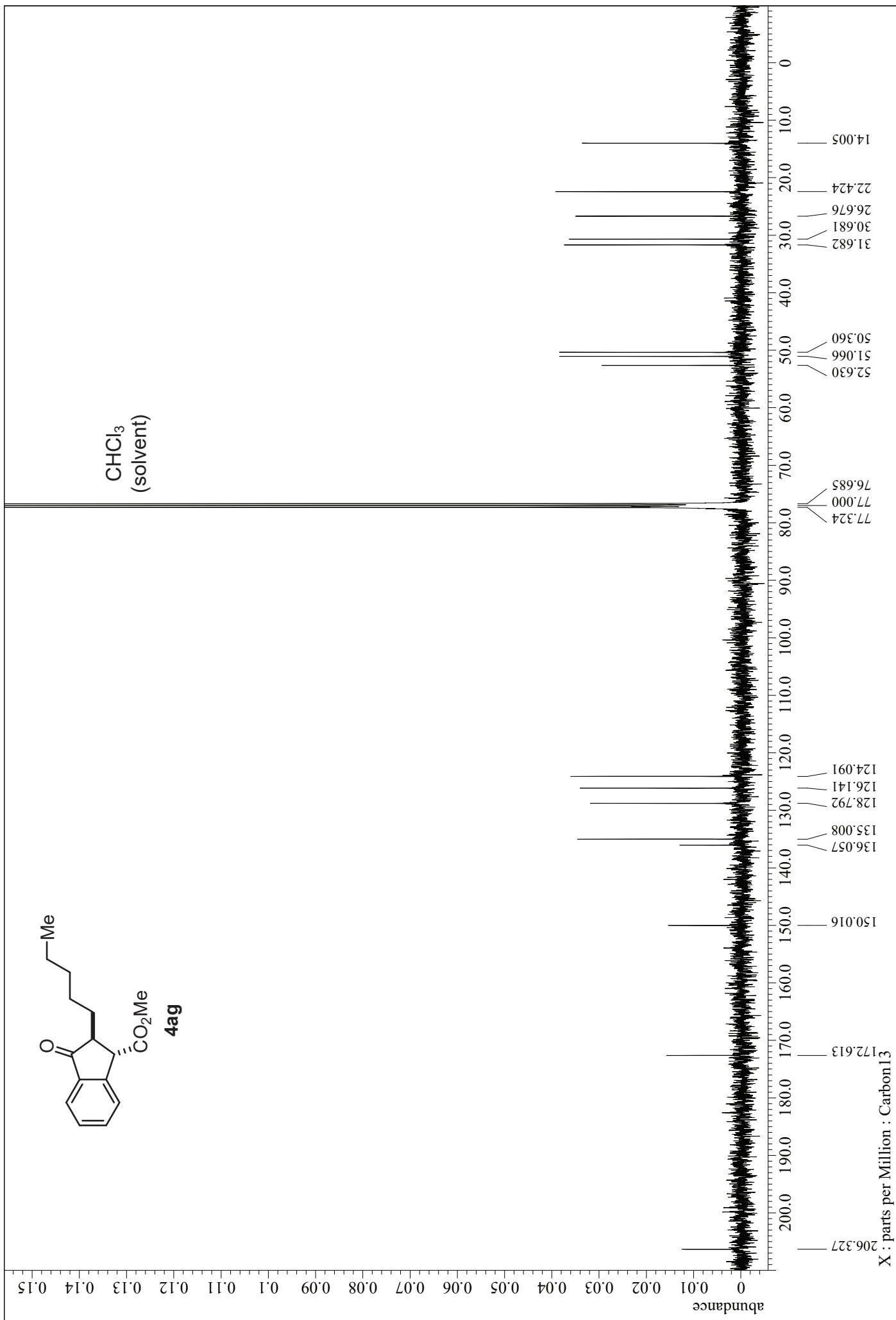


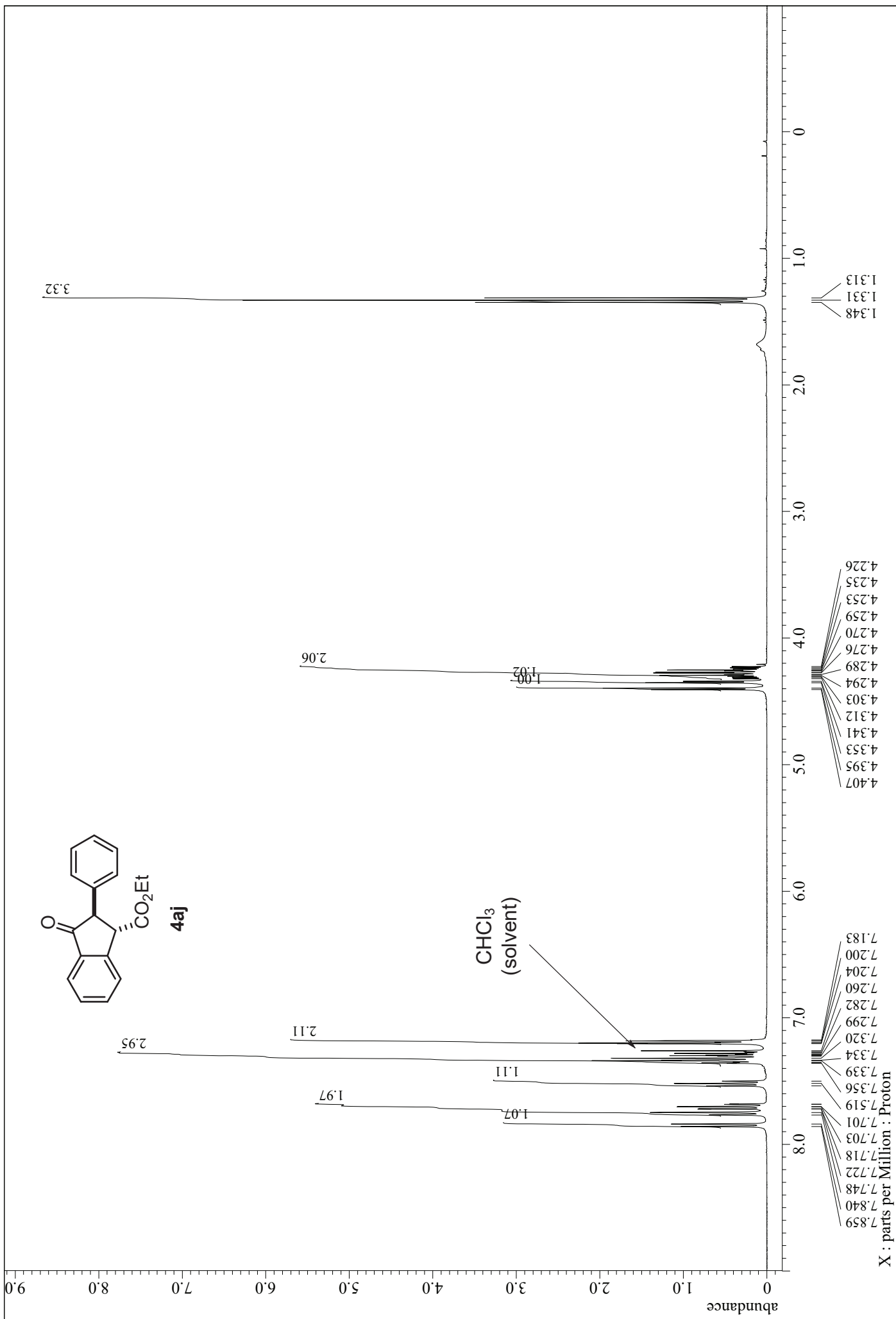


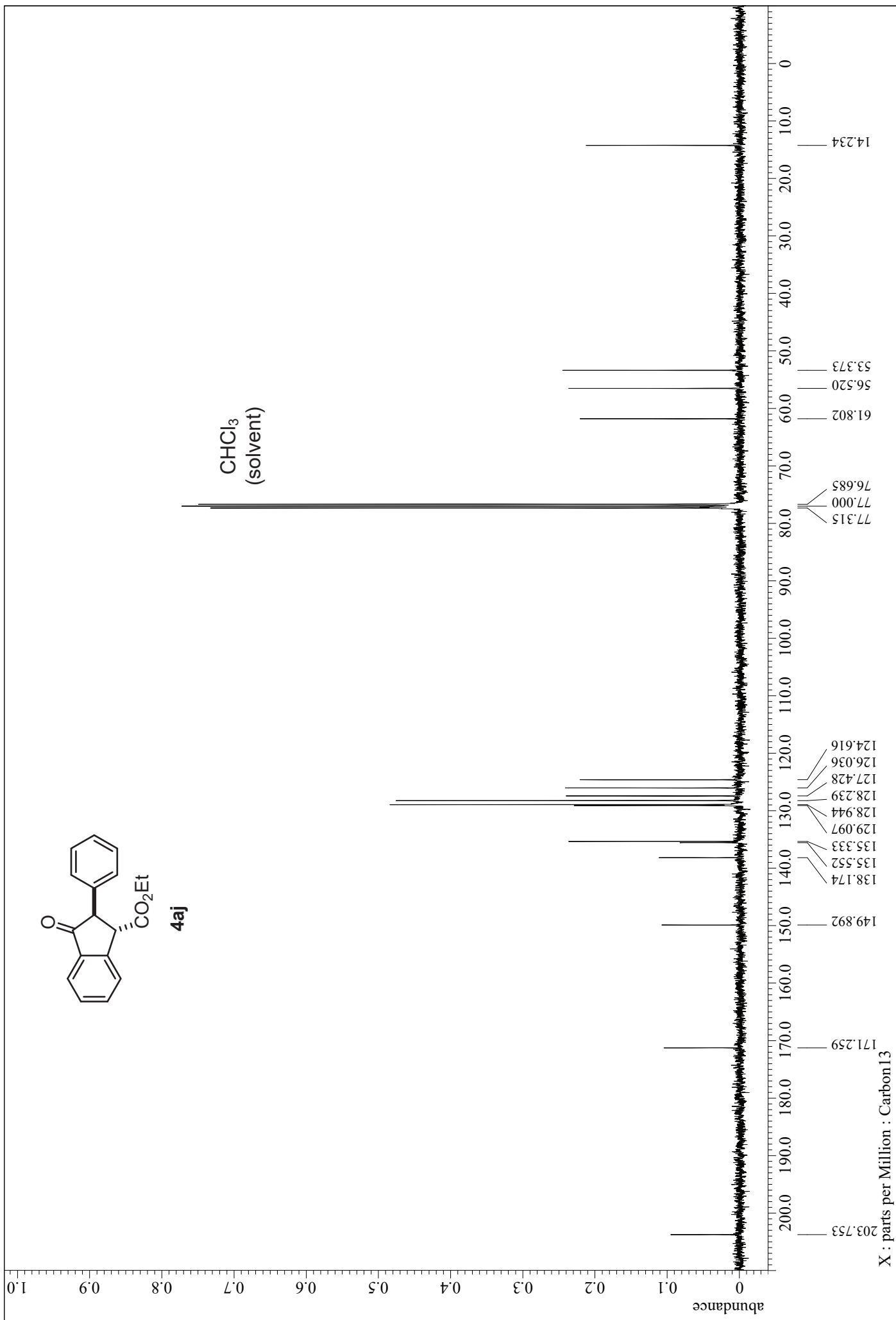
3ha
(5.7:1 isomeric mixture)

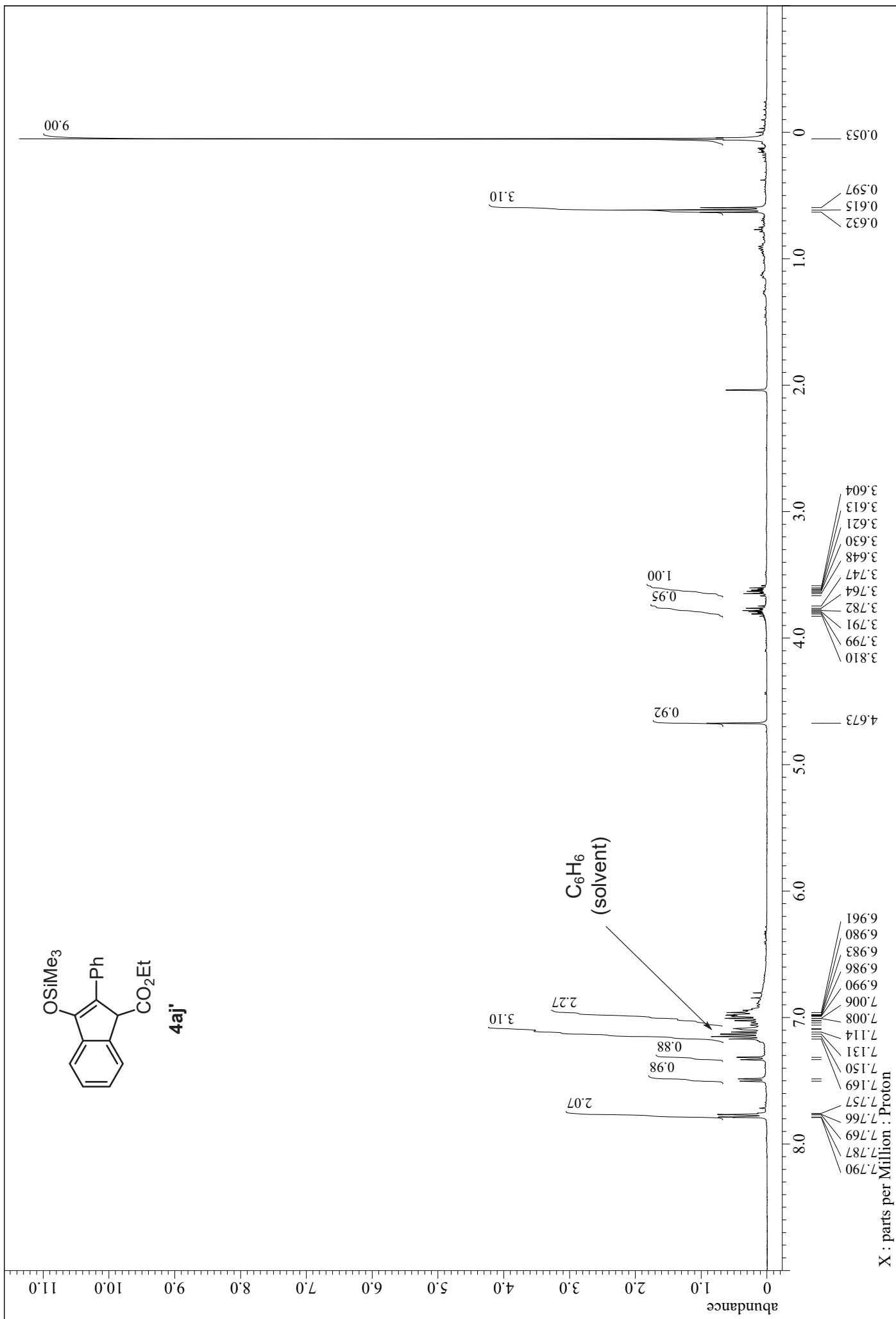


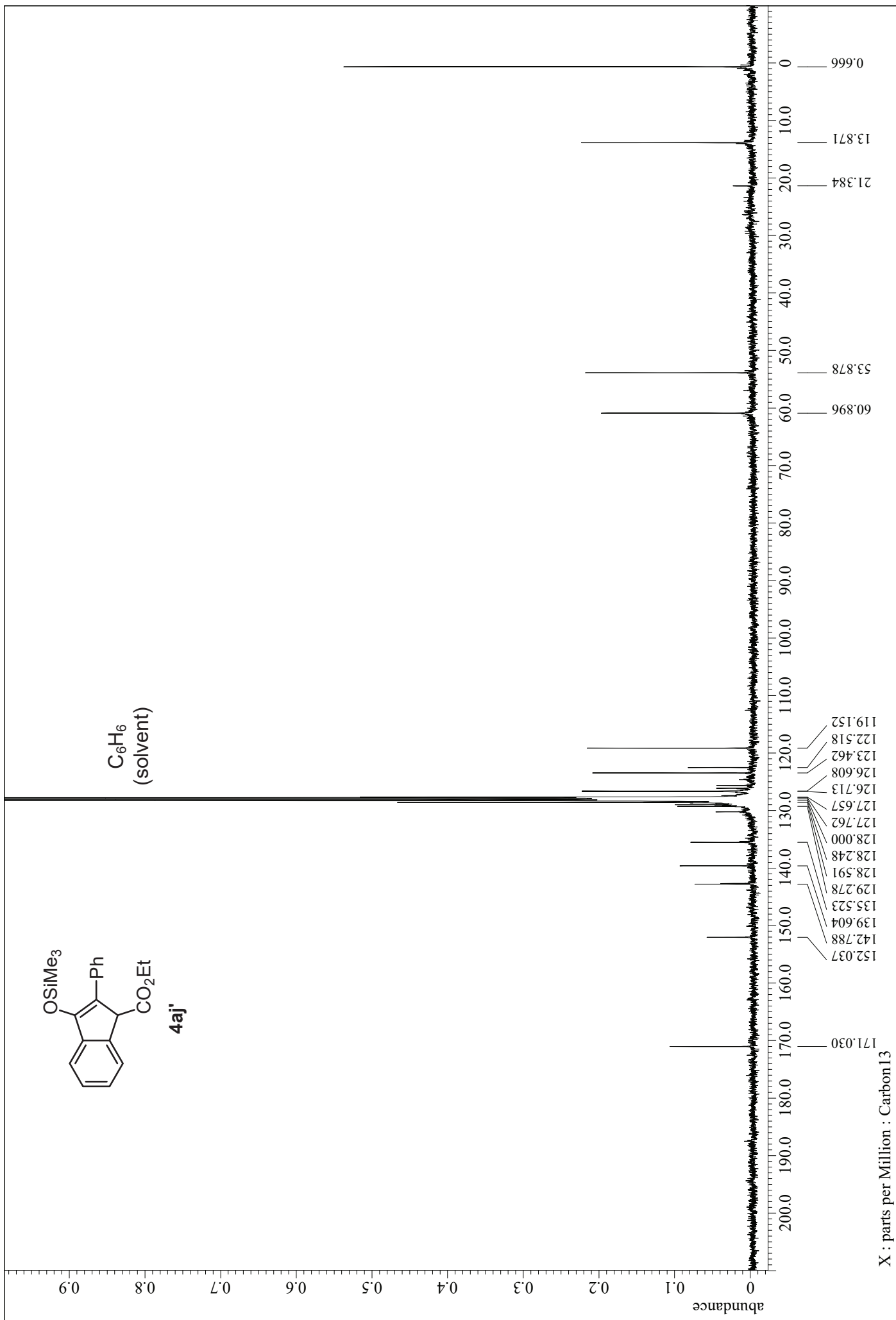


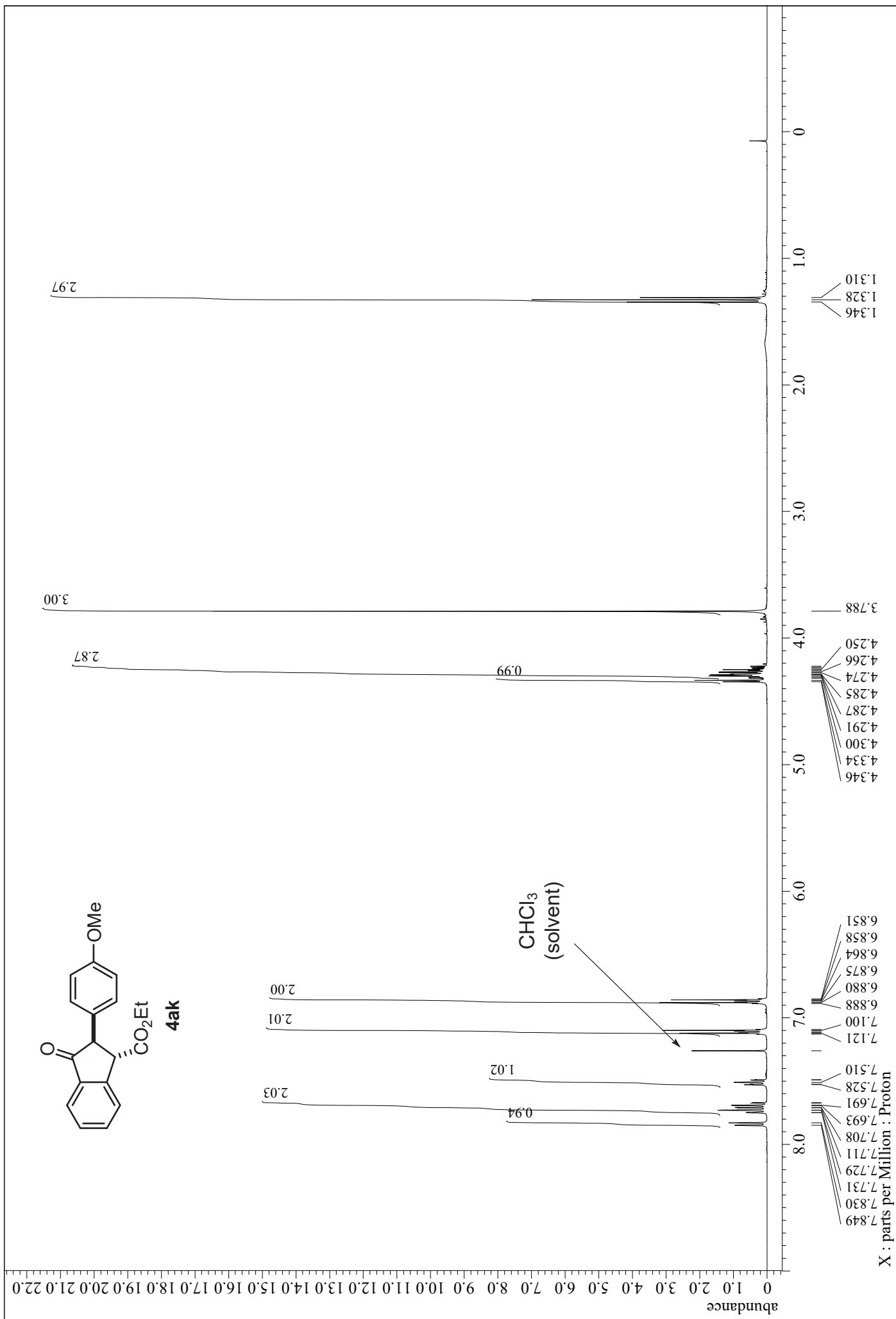


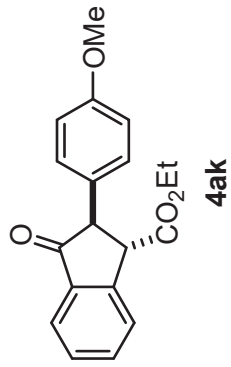




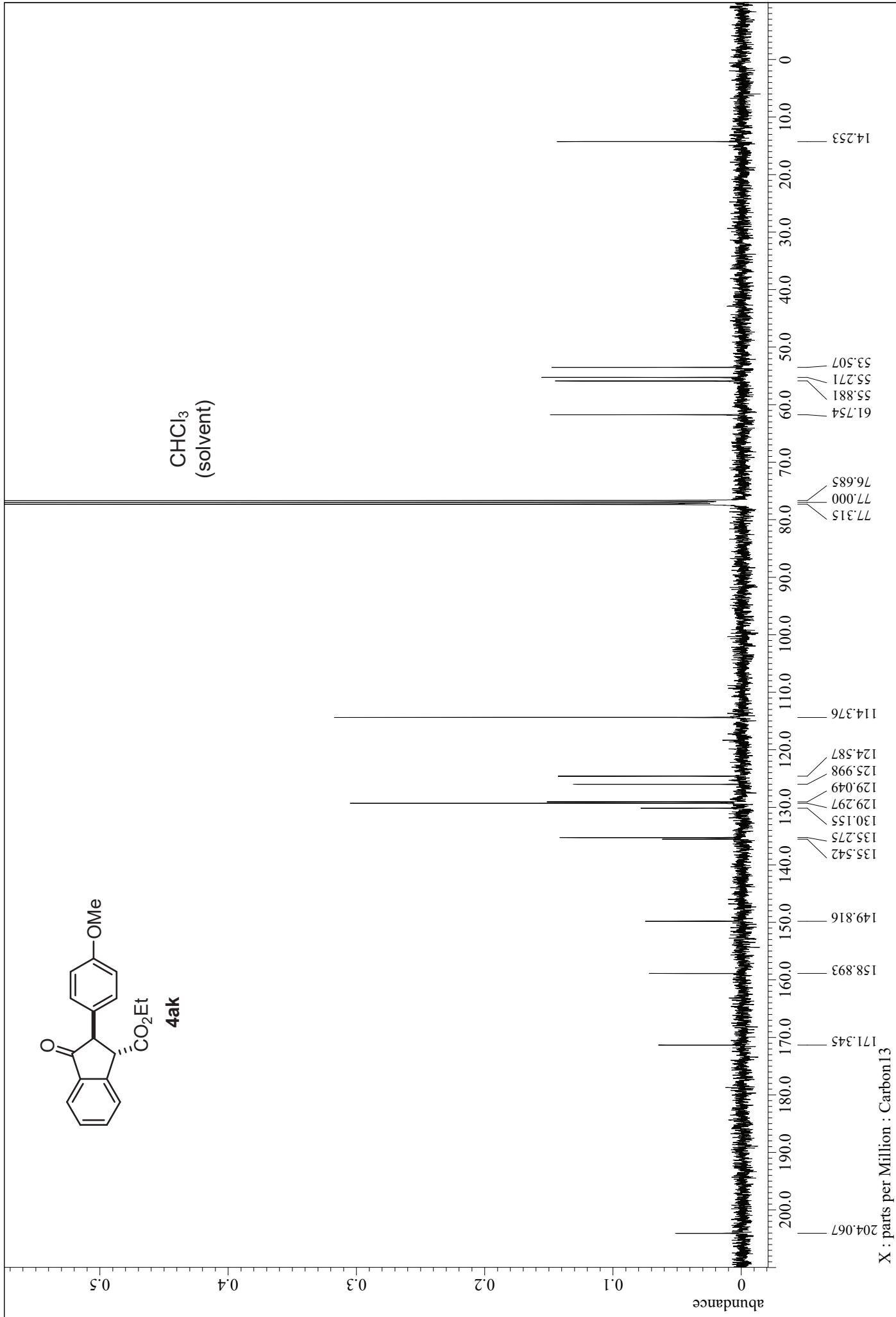


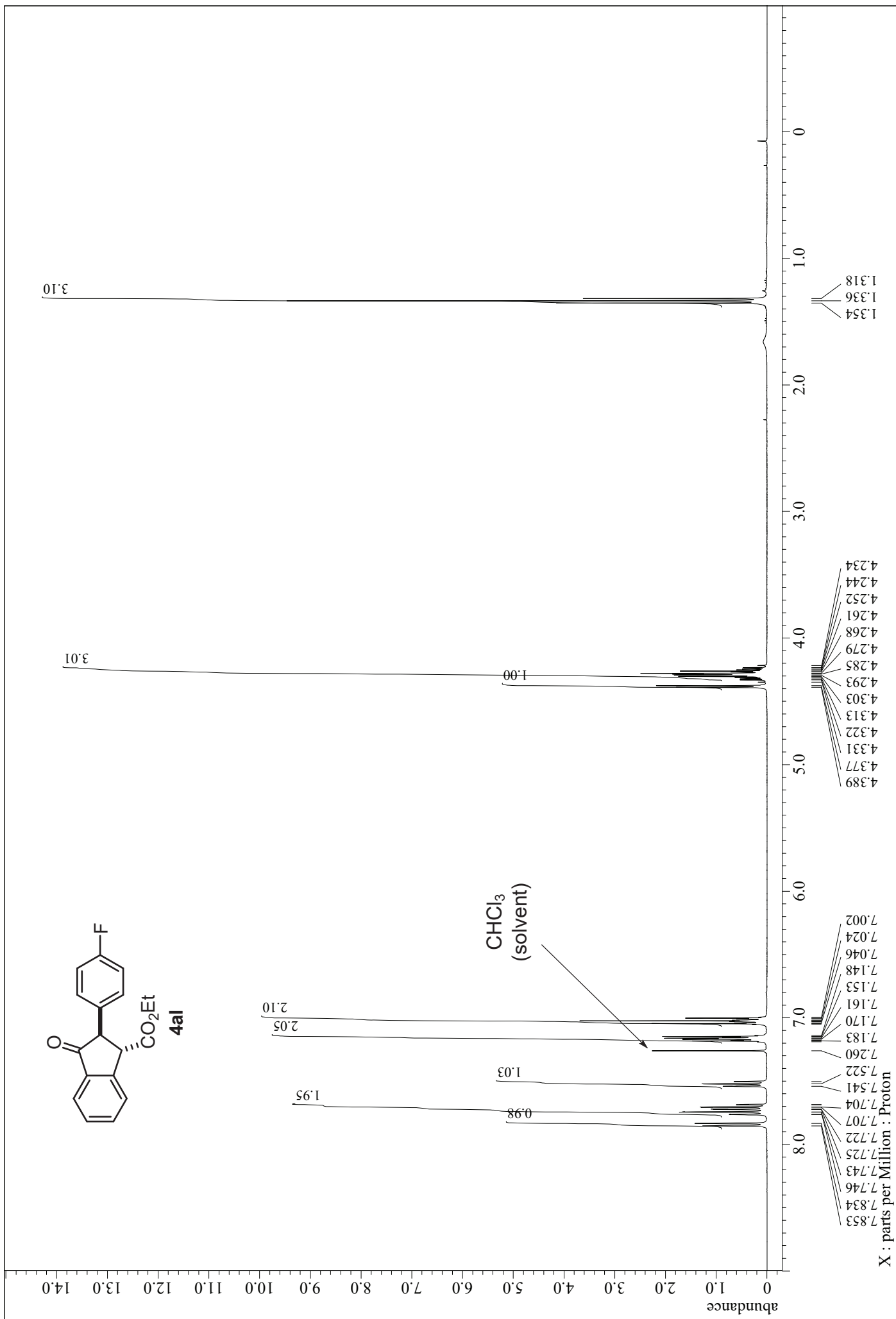


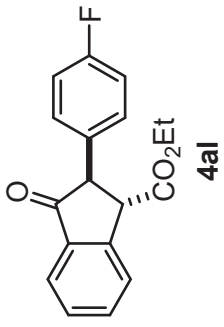




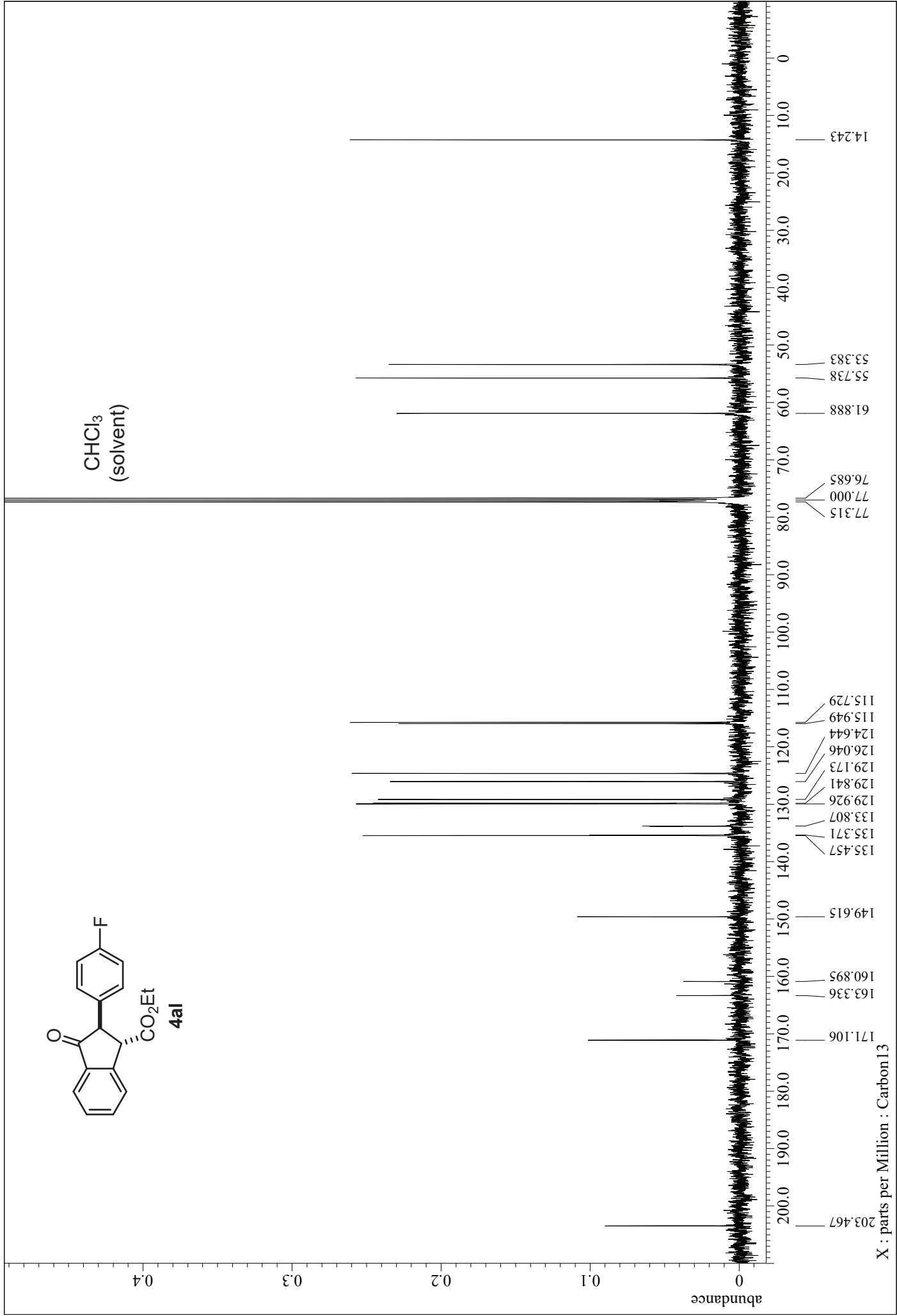
CHCl_3
(solvent)

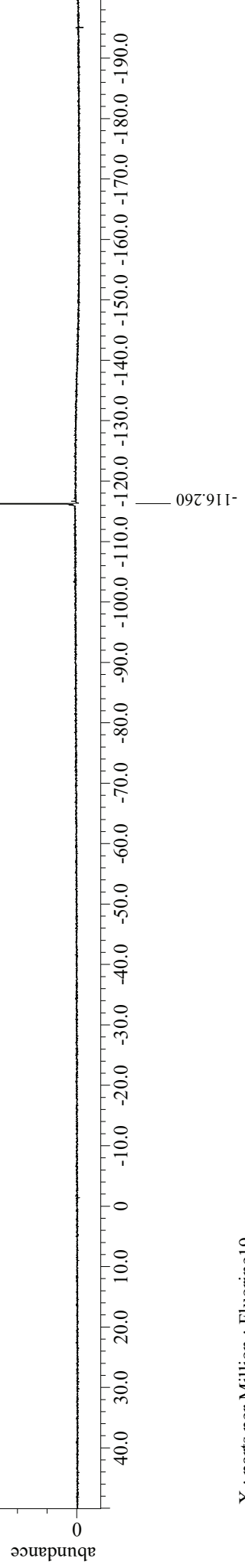
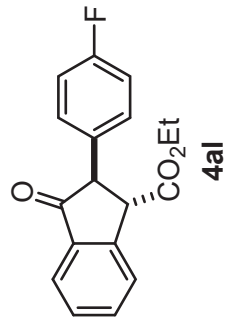


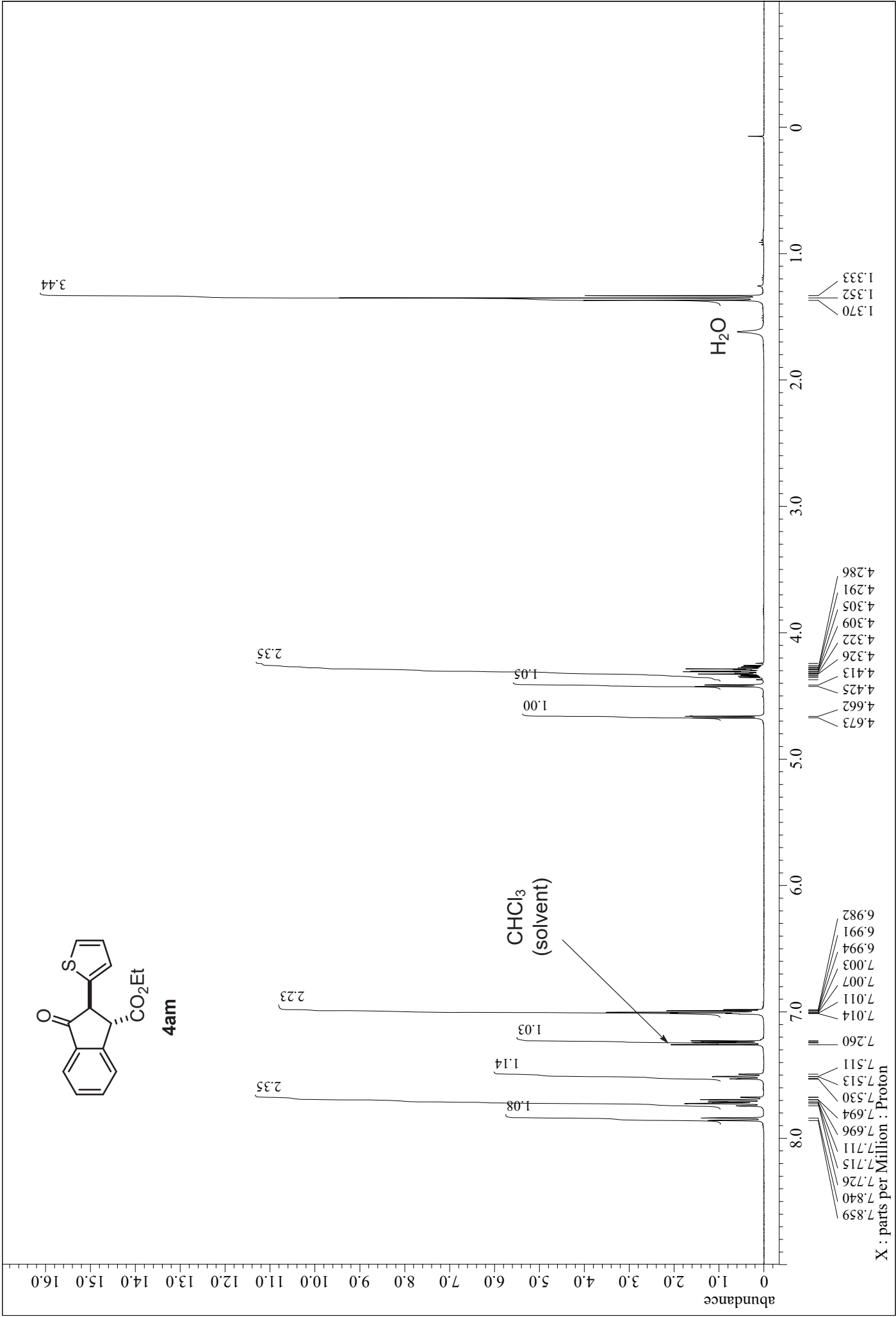


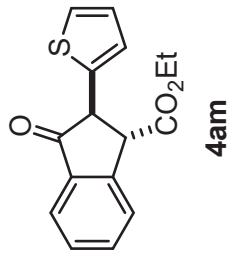


CHCl₃
(solvent)

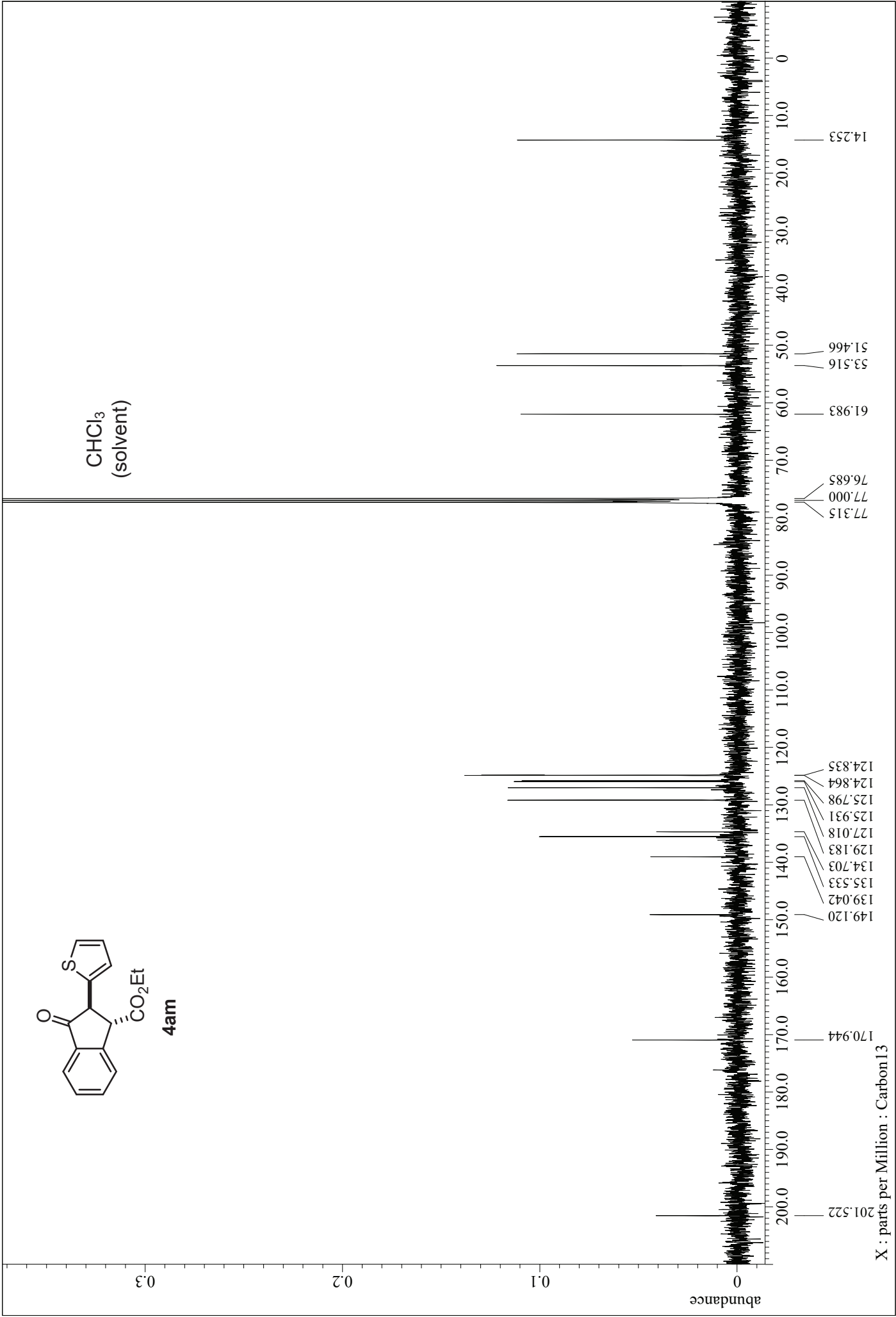


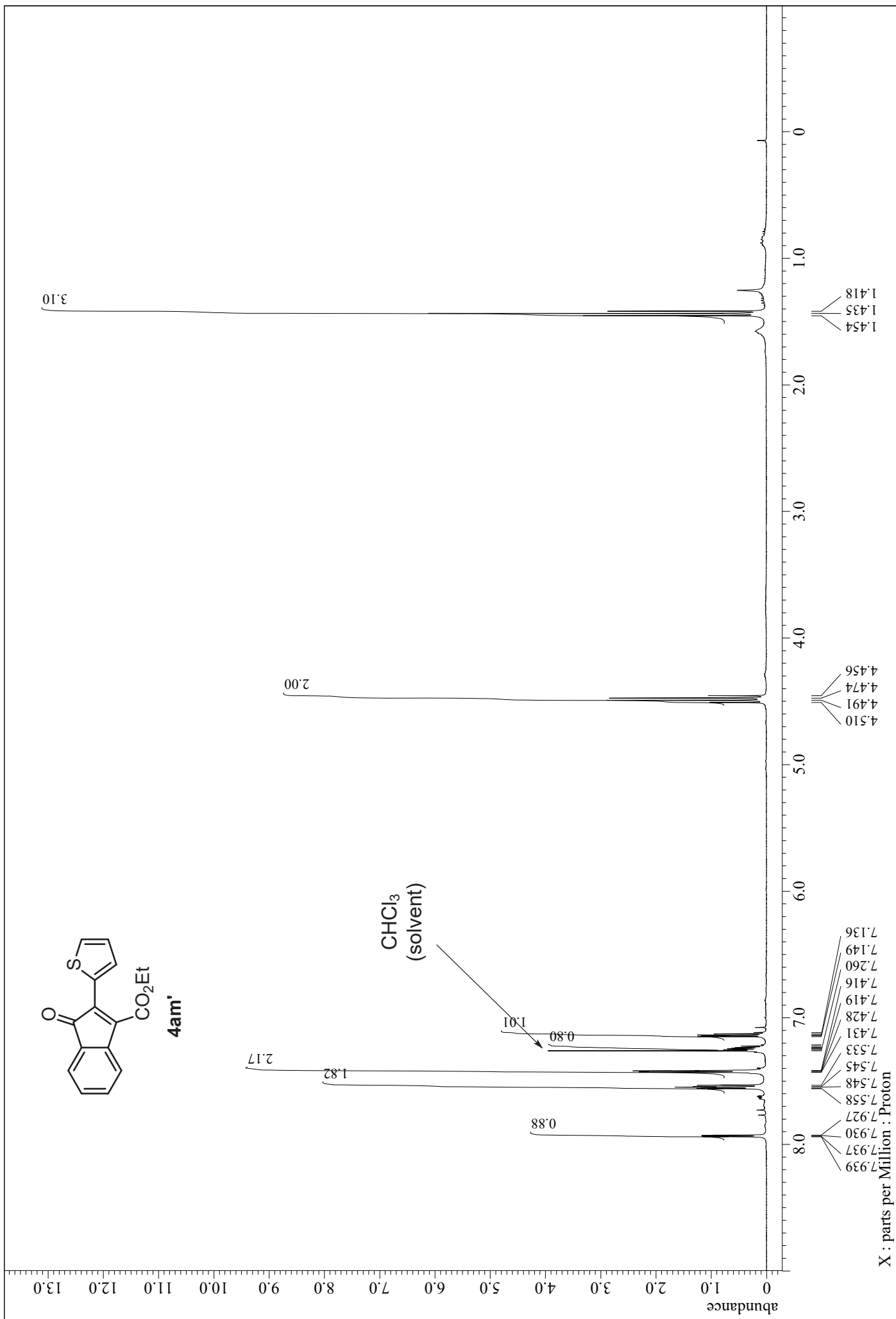


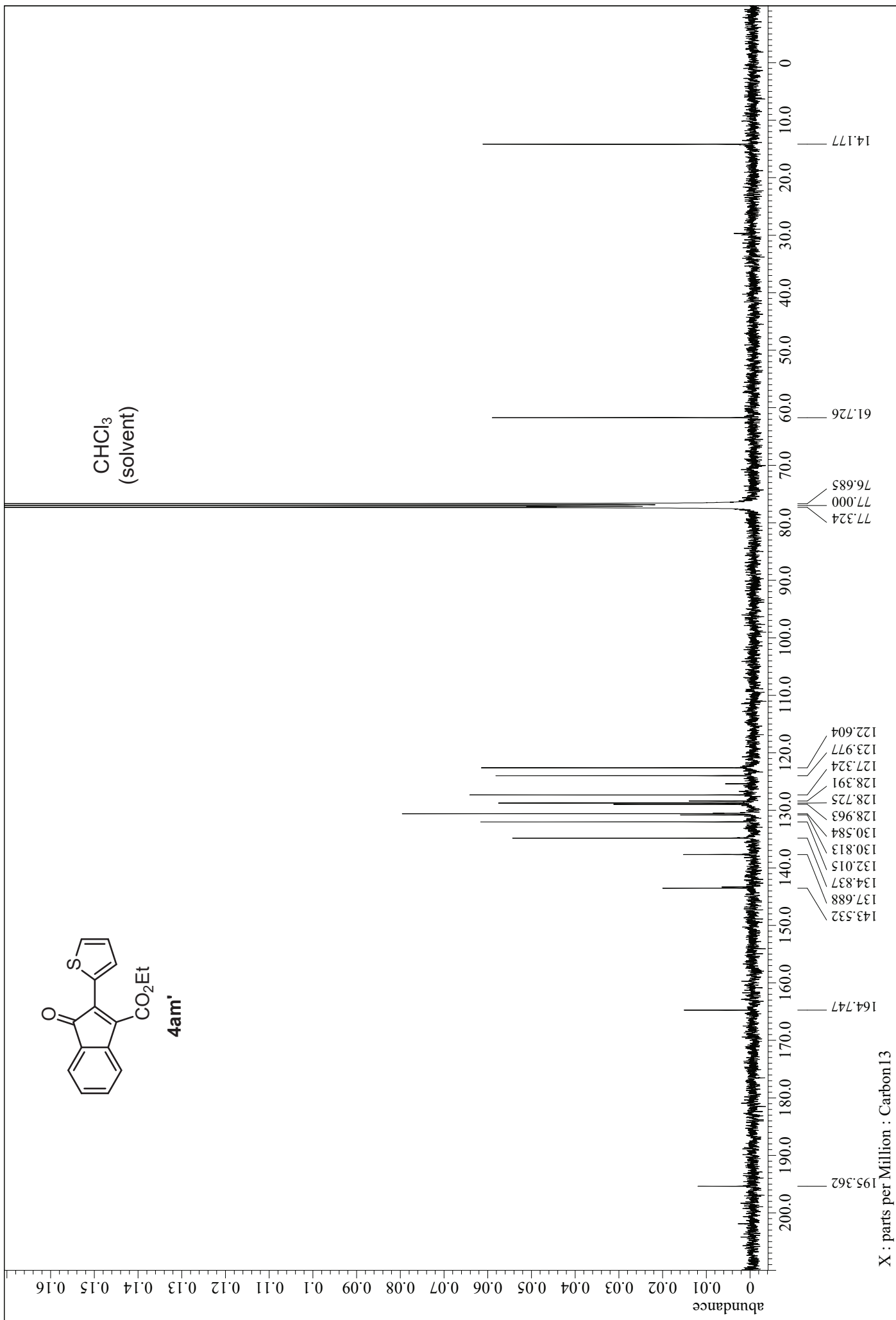


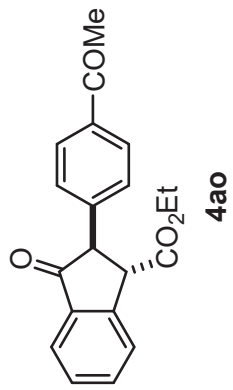


CHCl₃
(solvent)









CHCl₃
(solvent)

abundance

0.9

0.8

0.7

0.6

0.5

0.4

0.3

0.2

0.1

0

0

10.0

20.0

30.0

40.0

50.0

60.0

70.0

80.0

90.0

100.0

110.0

120.0

130.0

140.0

150.0

160.0

170.0

180.0

190.0

200.0

14.205

26.572

52.887

56.348

61.954

76.676

77.000

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128.544

128.944

129.259

135.266

135.552

136.210

143.370

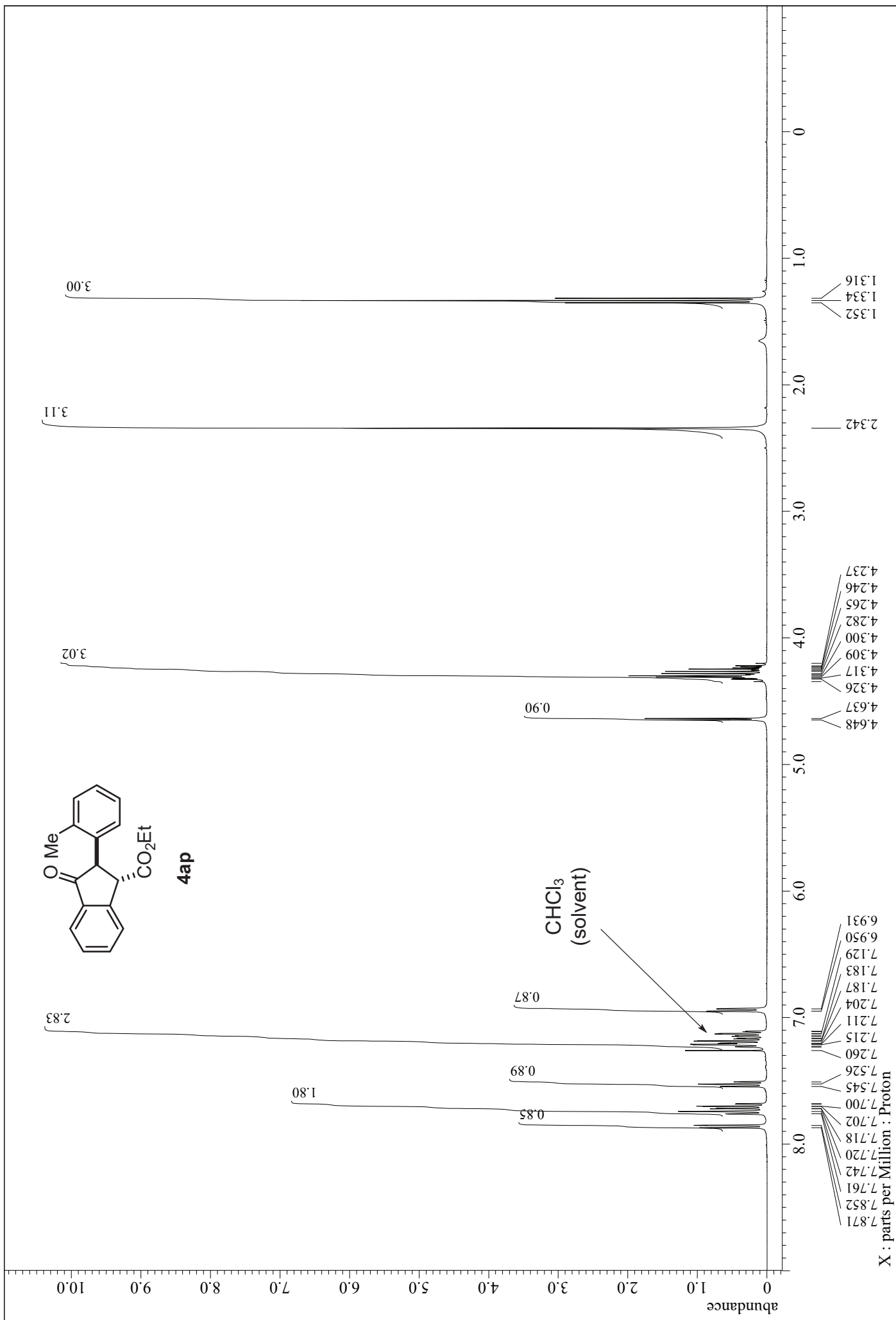
149.587

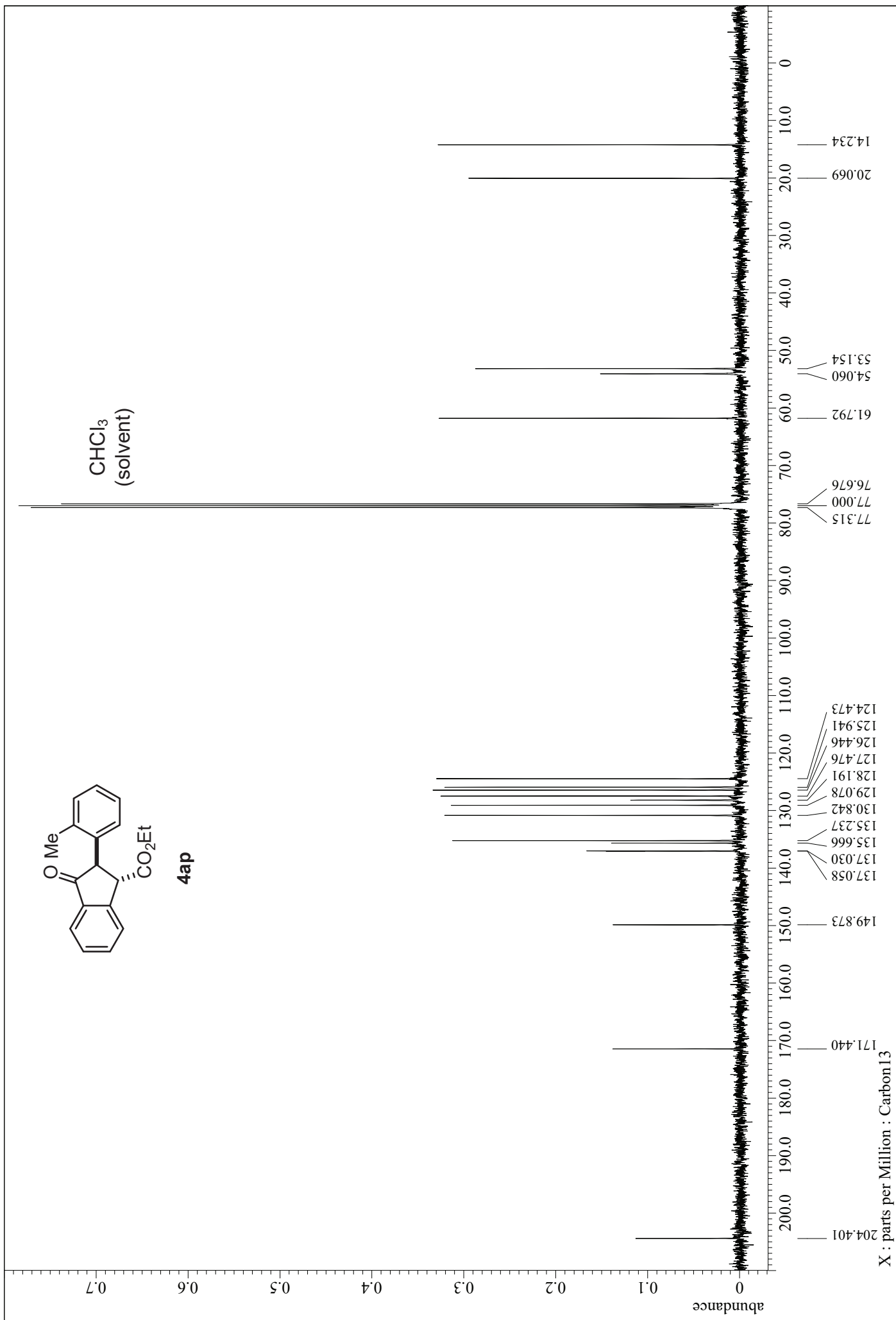
170.897

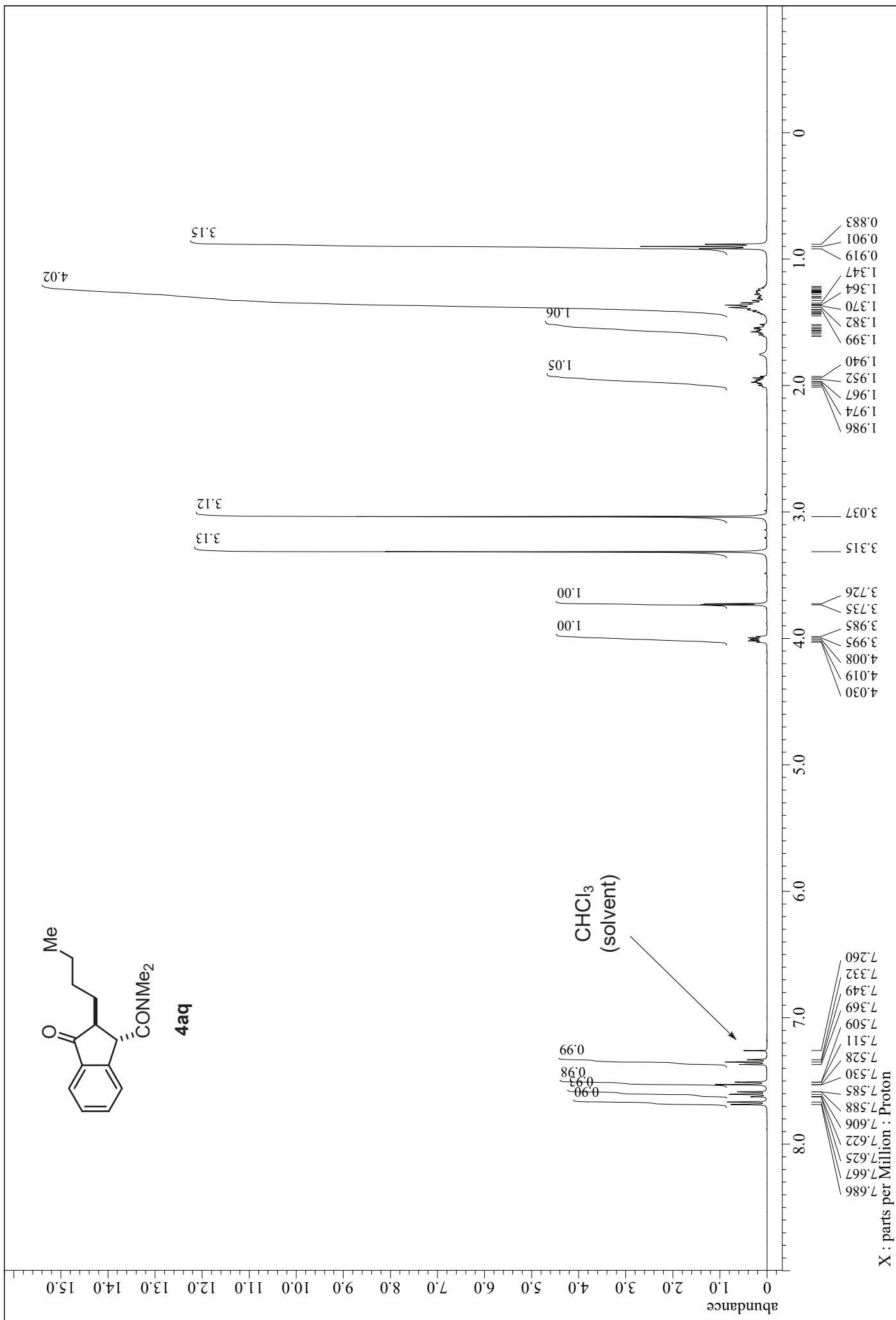
197.565

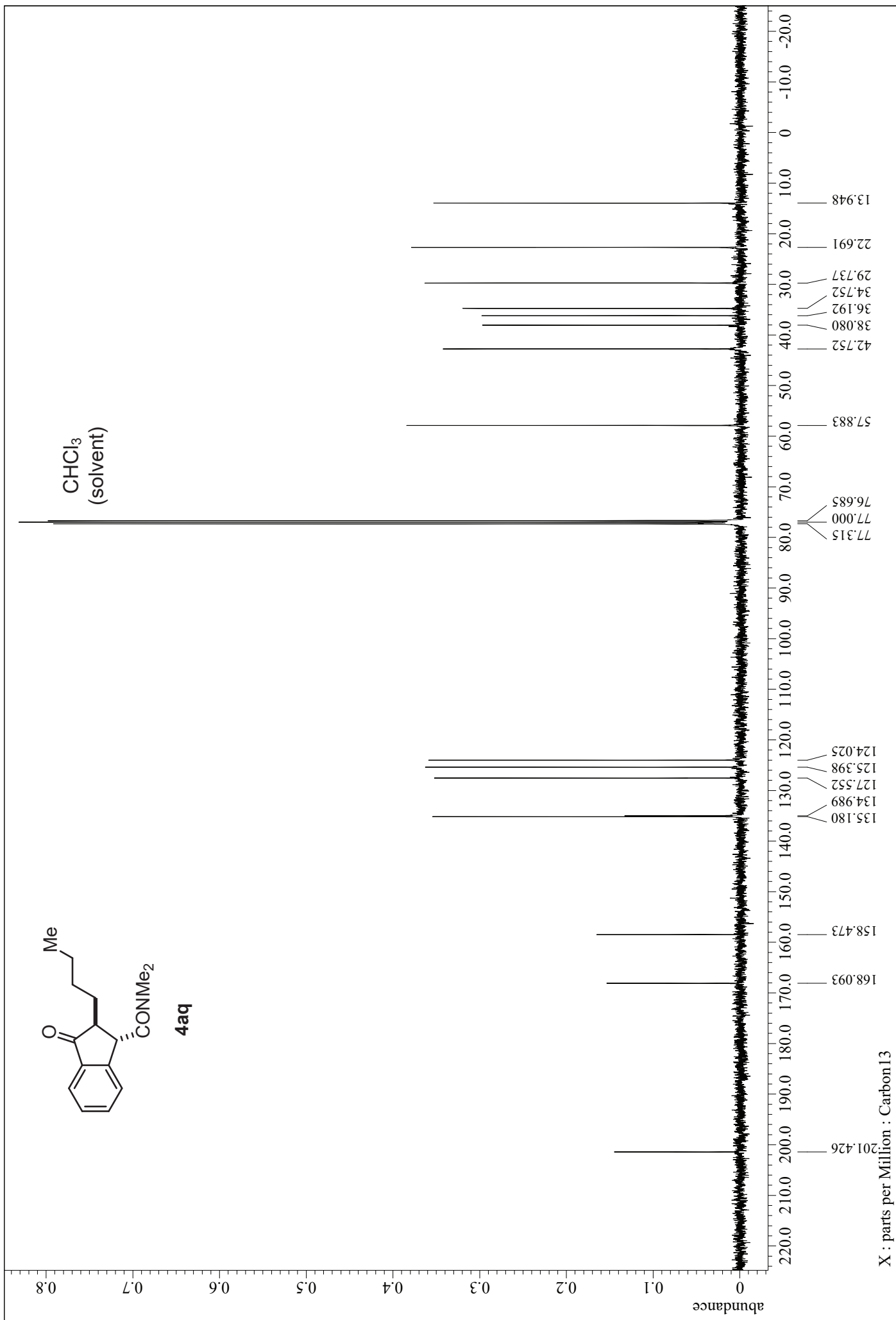
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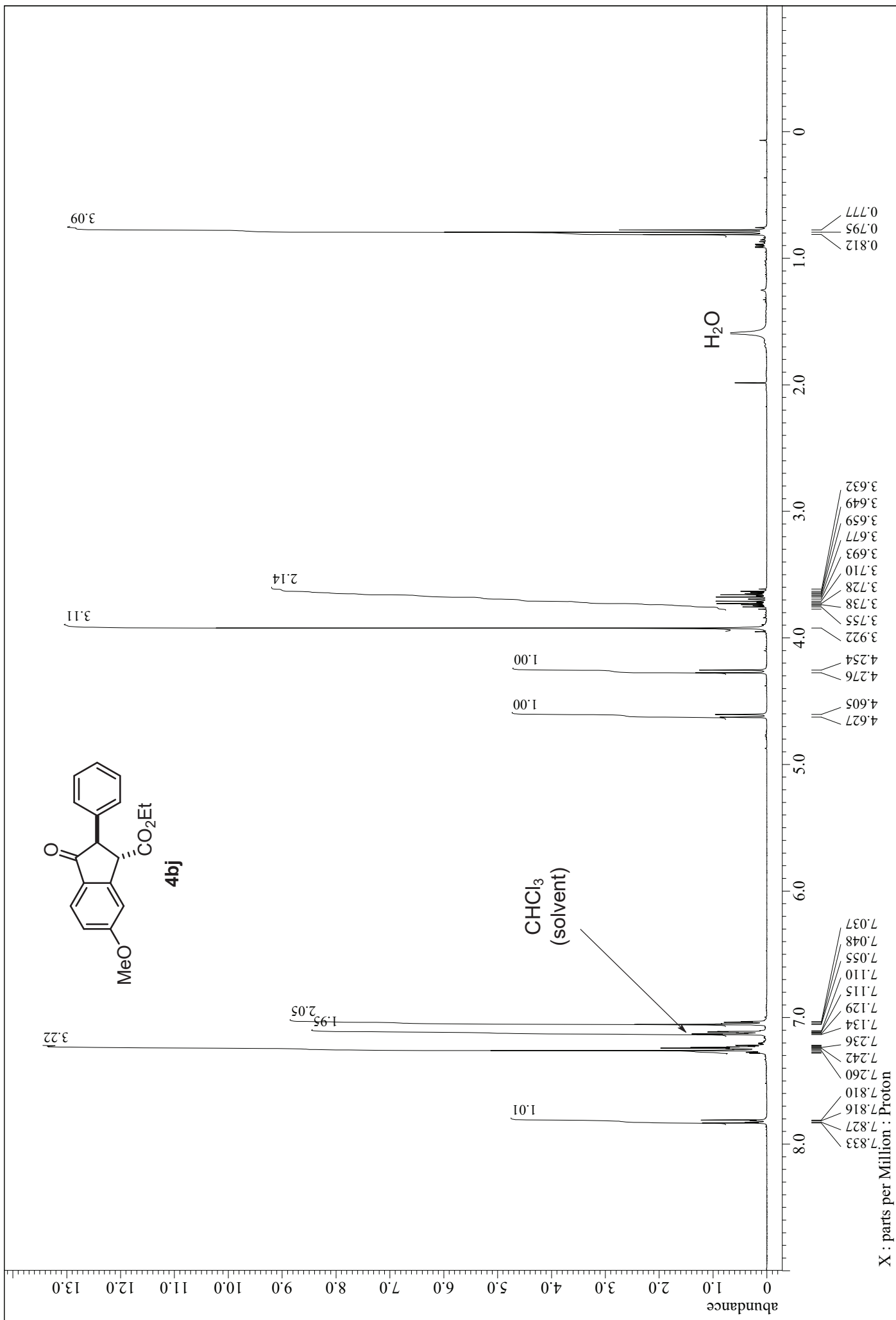
X : parts per Million : Carbon13

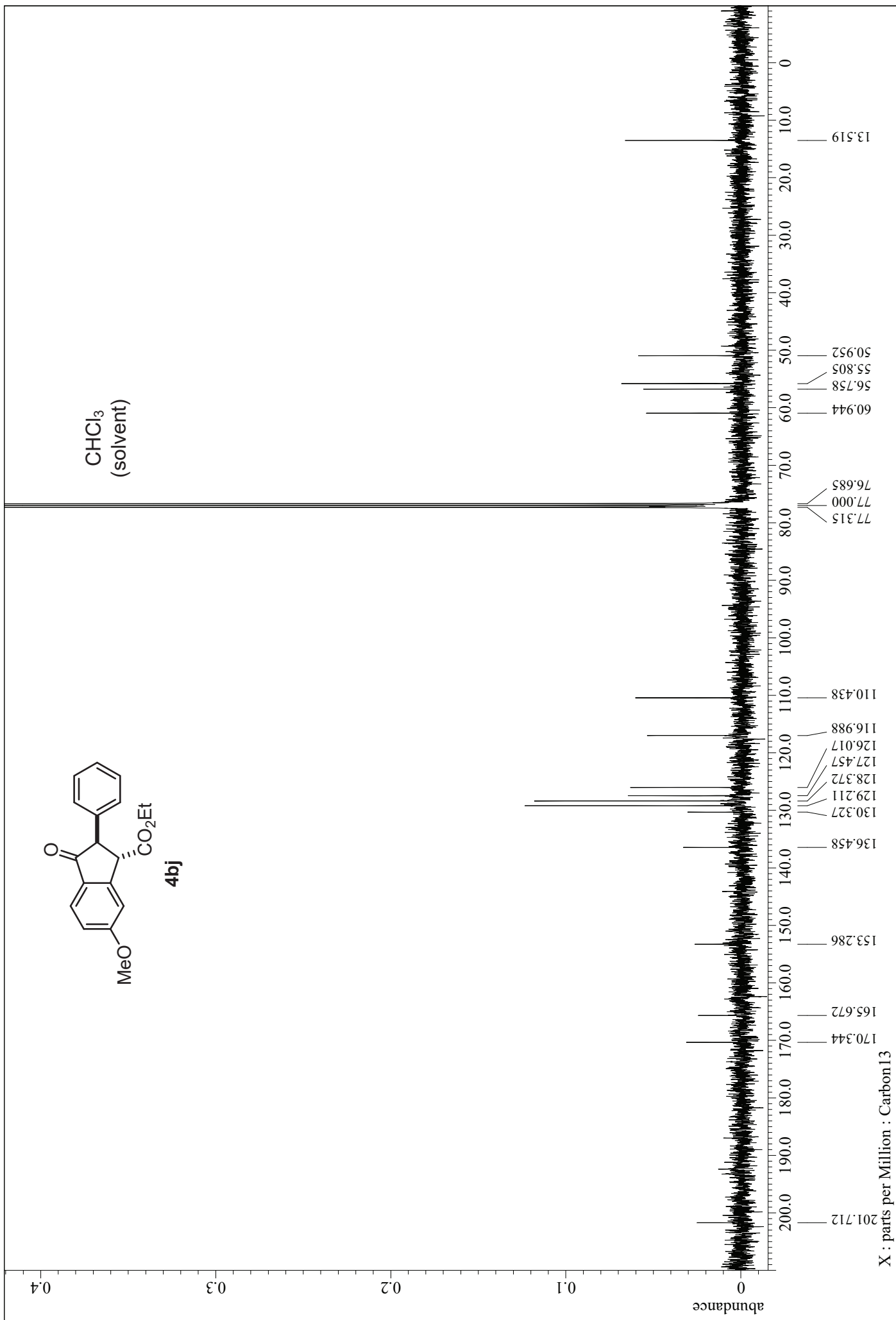


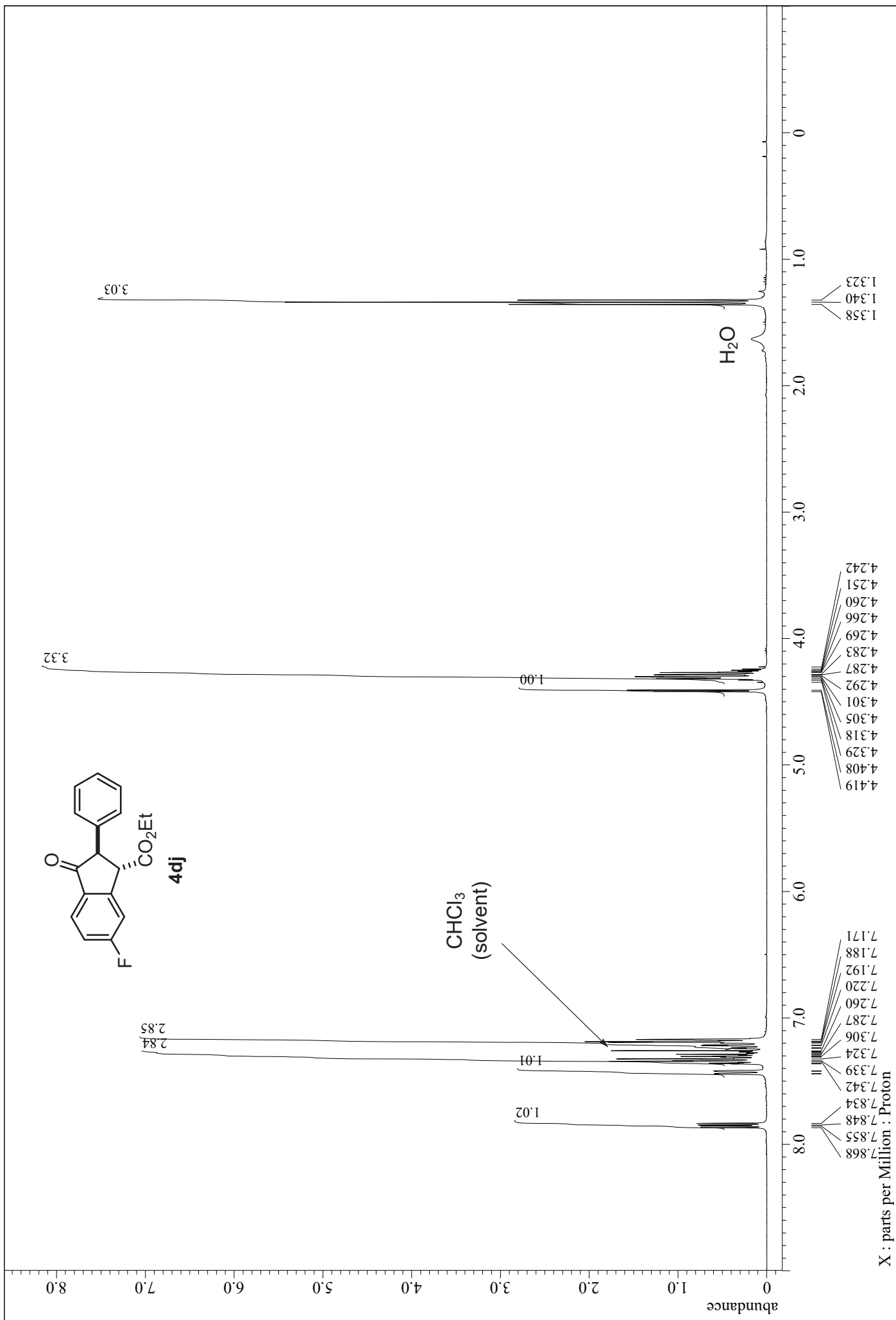


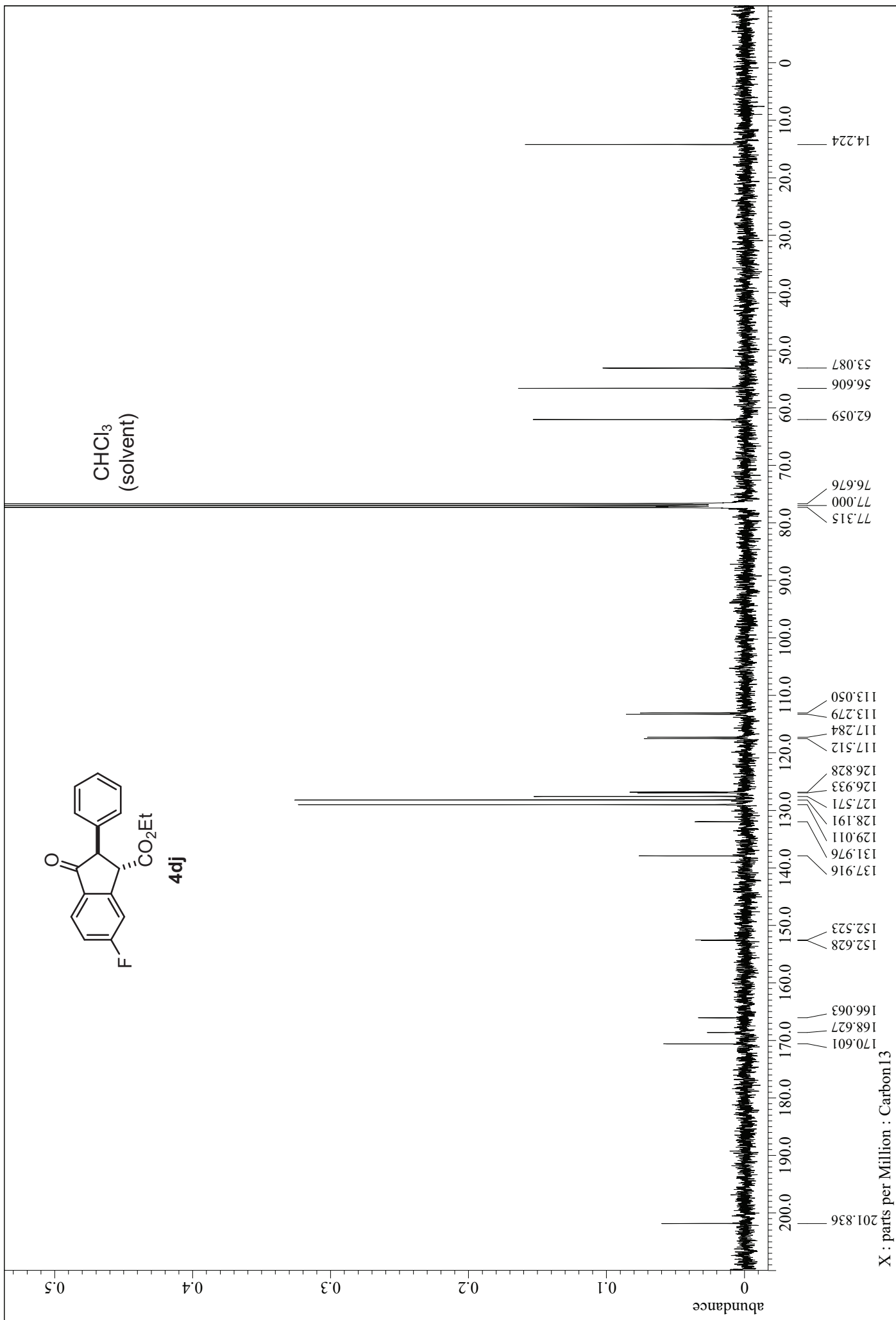


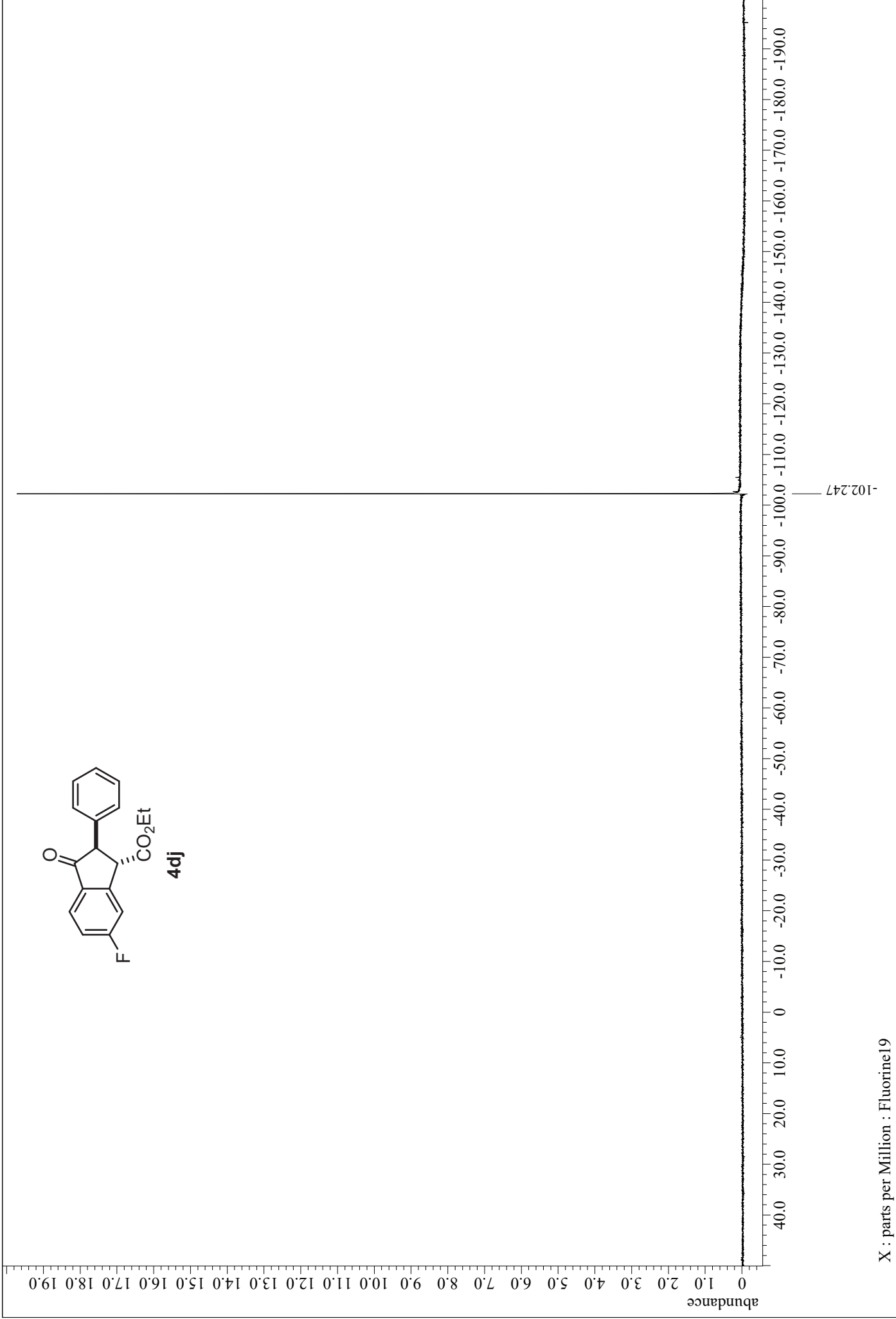
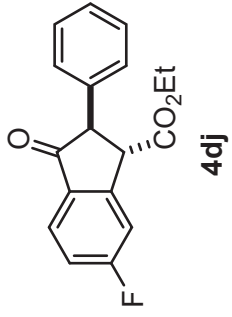












X : parts per Million : Fluorine19

