Supporting Information

Gold-catalyzed dual C-C bond cleavage of biphenylenes bearing a pendant alkyne at ambient temperature

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1) General information

^{1}H NMR spectra were recorded with JEOL ECX-500 (500 MHz) spectrometer. Chemical shift values for protons are reported in parts per million (δ) relative to internal standard tetramethylsilane (0.00 ppm). ^{13}C NMR spectra were obtained by JEOL ECX-500 (125 MHz) spectrometers and referenced to the internal solvent signals (central peak is 77.16 ppm in $CDCl_3$). ^{19}F NMR spectra were obtained by JEOL ECX-500 (470.5 MHz) spectrometers and referenced to the external standard trifluoroacetic acid (76.55 ppm). 2D NMR spectra were recorded with Bruker AVANCE 600. Data are presented as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublets), coupling constant in Hz, and area integration. HRMS were measured with a direct analysis in real time DART-orbitrap mass spectrometer.[S1] X-ray structure was obtained by a Rigaku R-AXIS RAPID diffractometer. PTLC was performed with silica gel-precoated glass plates (Merck 60 GF254) prepared in author's laboratory. All reagents except for metal reagents were weighed and handled in air and backfilled under argon at room temperature. All reactions were performed under an argon atmosphere. Unless otherwise noted, organic compounds and solvents were purchased from Tokyo Kasei Co., Aldrich Inc., and other commercial suppliers and were used without further purification. Compounds **1** were synthesized by reported procedures.[S2]

2) Experimental procedures

A) General procedure for gold-catalyzed skeletal rearrangement

$AuCl_3$ (0.005 mmol), $AgSbF_6$ (0.015 mmol), and **1** (0.05 mmol) were placed in a Schlenk tube, which was then evacuated and backfilled with argon (x3). To the reaction vessel was added dehydrated DCE (0.5 mL, pretreated by argon bubbling for 30 sec). The solution was then stirred at room temperature and, after **1** was completely consumed as judged by TLC, the solvent was evaporated to dryness. The obtained crude products were purified by PTLC to give products **3**.

B) Preparation of compound 1aa-^{13}C and ^{13}C-labbeled experiment

Compound **1aa-^{13}C** was synthesized from 2-(biphenylen-1-yl)benzaldehyde and ^{13}C-labbeled benzyl phenyl sulfone by a reported procedure.[S2] ^{13}C-labbeled Benzyl phenyl sulfone was synthesized from benzoic acid-α-^{13}C.[S3]

Experimental procedure for gold-catalyzed skeletal rearrangement of 1aa-^{13}C

$AuCl_3$ (0.005 mmol), $AgSbF_6$ (0.015 mmol), and **1aa-^{13}C** (0.05 mmol) were placed in a Schlenk tube, which was then evacuated and backfilled with argon (x3). To the reaction vessel was added dehydrated DCE (0.5 mL, pretreated by argon bubbling for 30 sec). The solution was then stirred at room temperature for 2.5 h and the solvent was evaporated to dryness. The obtained crude products were purified by PTLC to give products **3aa-^{13}C**.

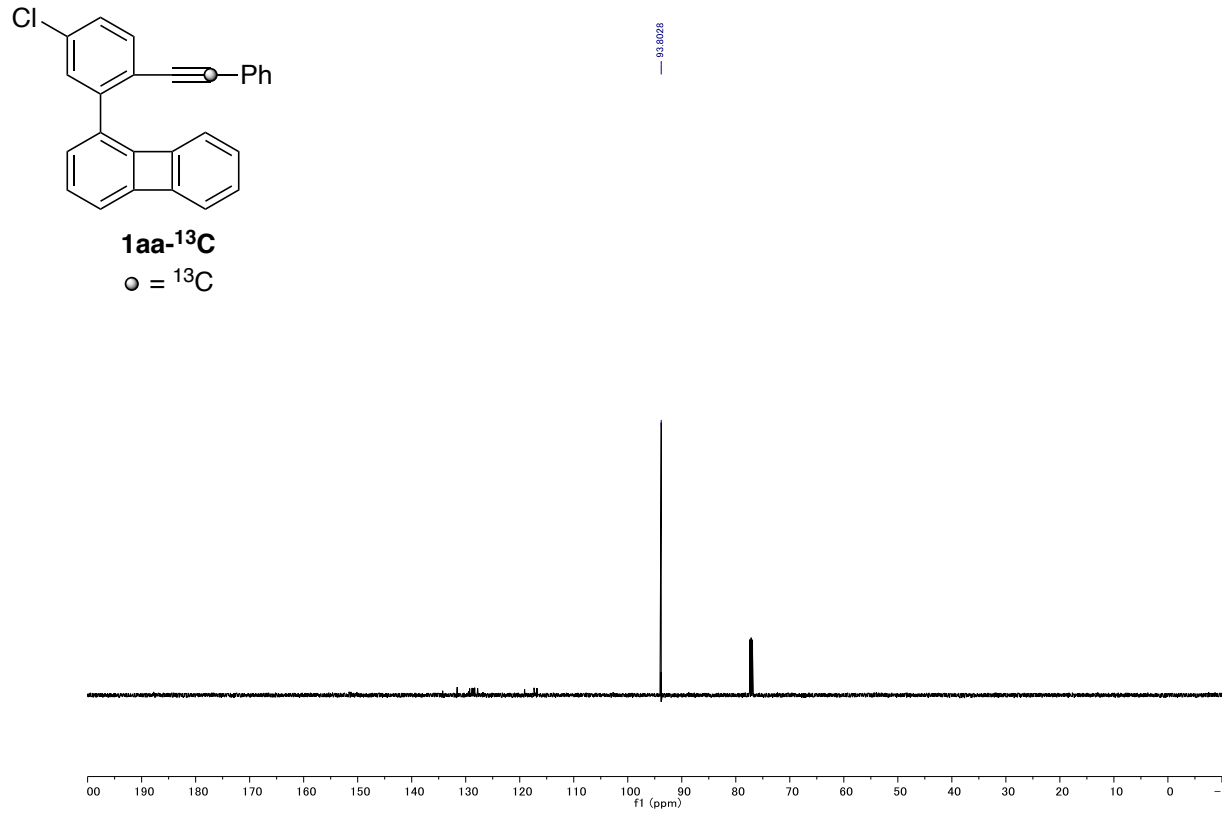


Figure S1. ^{13}C NMR spectrum of **^{13}C-1aa**

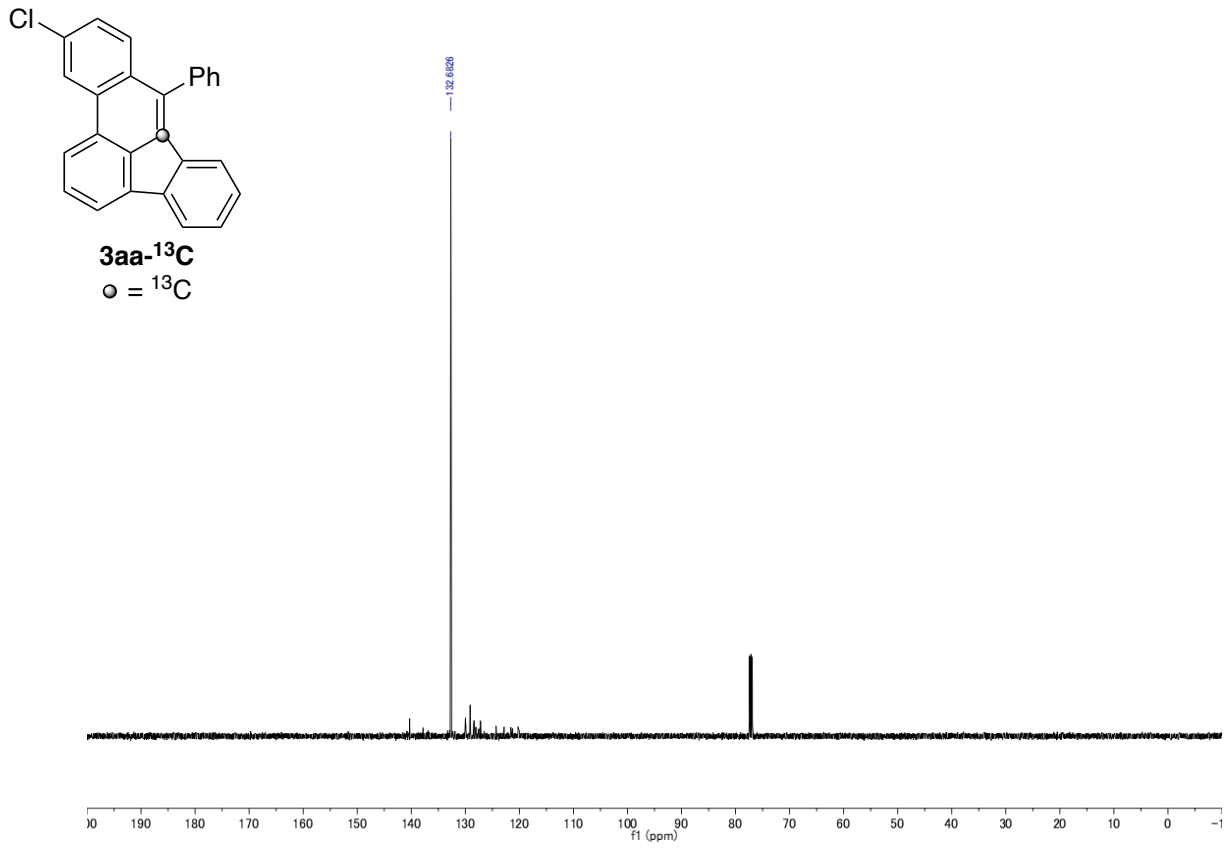


Figure S2. ^{13}C NMR spectrum of **^{13}C-3aa**

3) Structural analysis for 3aa and 3aa-^{13}C by 2D NMR spectra

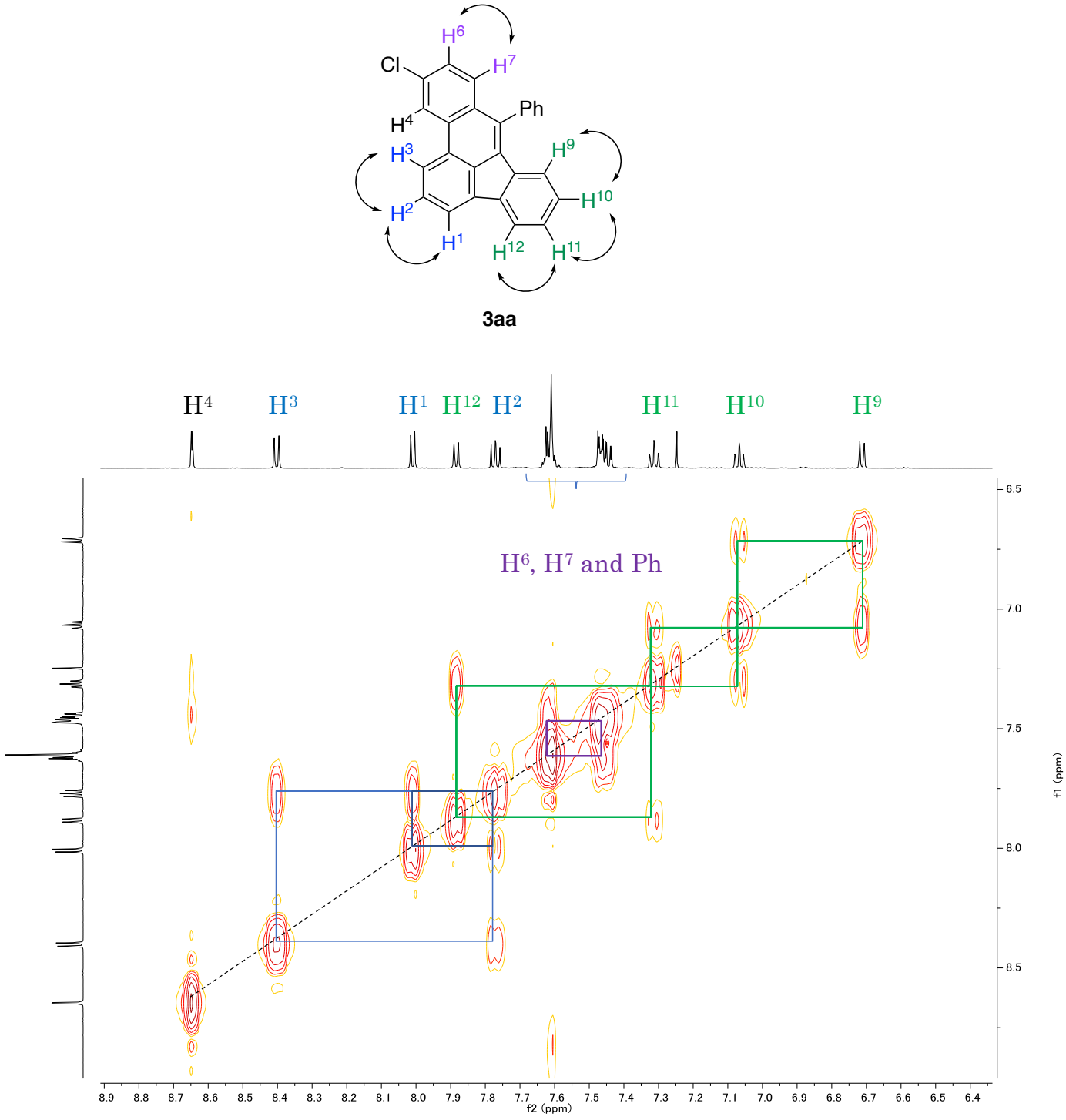


Figure S3. ^{1}H-^{1}H Cosy spectrum of **3aa**

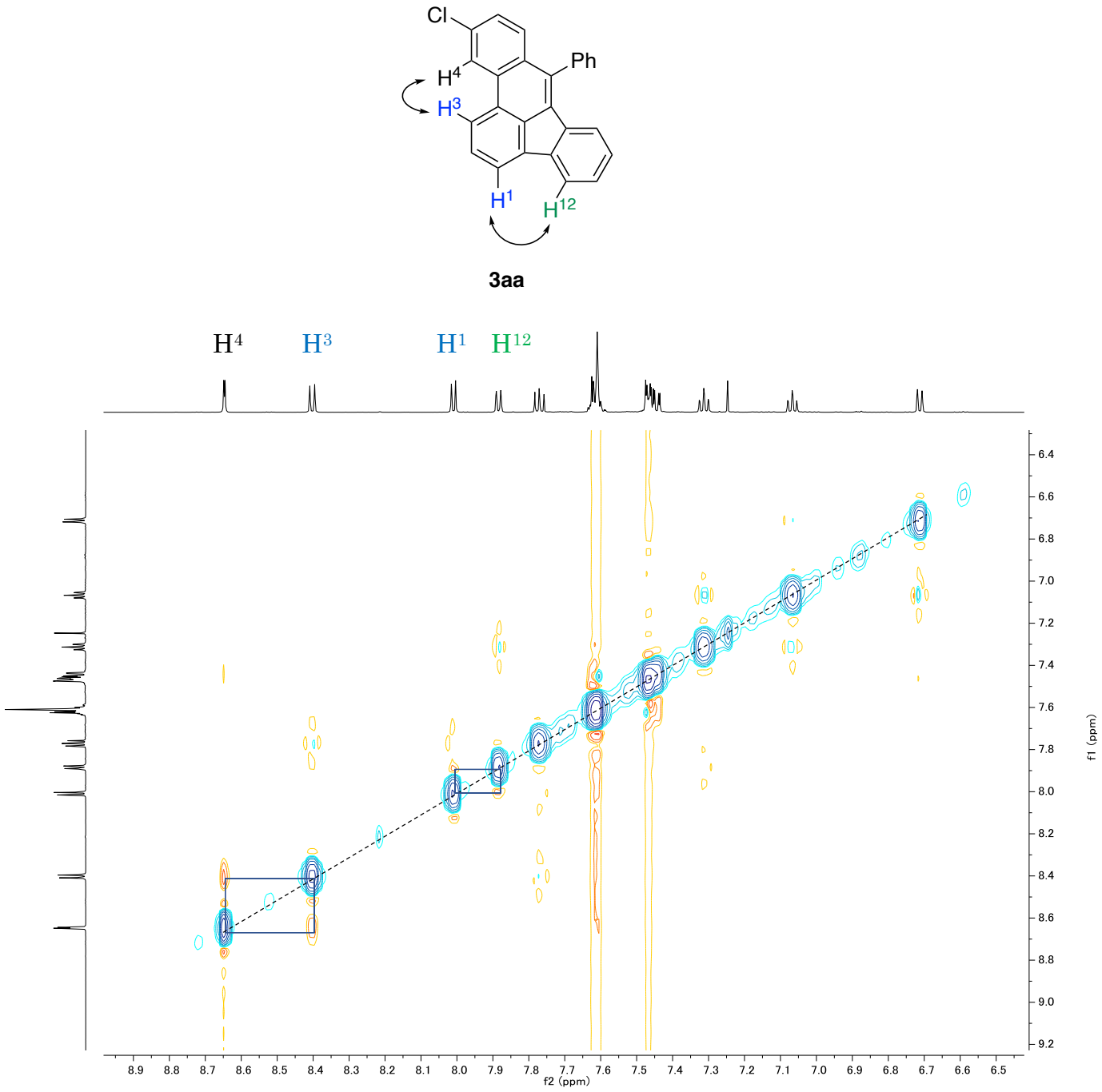


Figure S4. ^{1}H-^{1}H NOESY spectrum of **3aa**

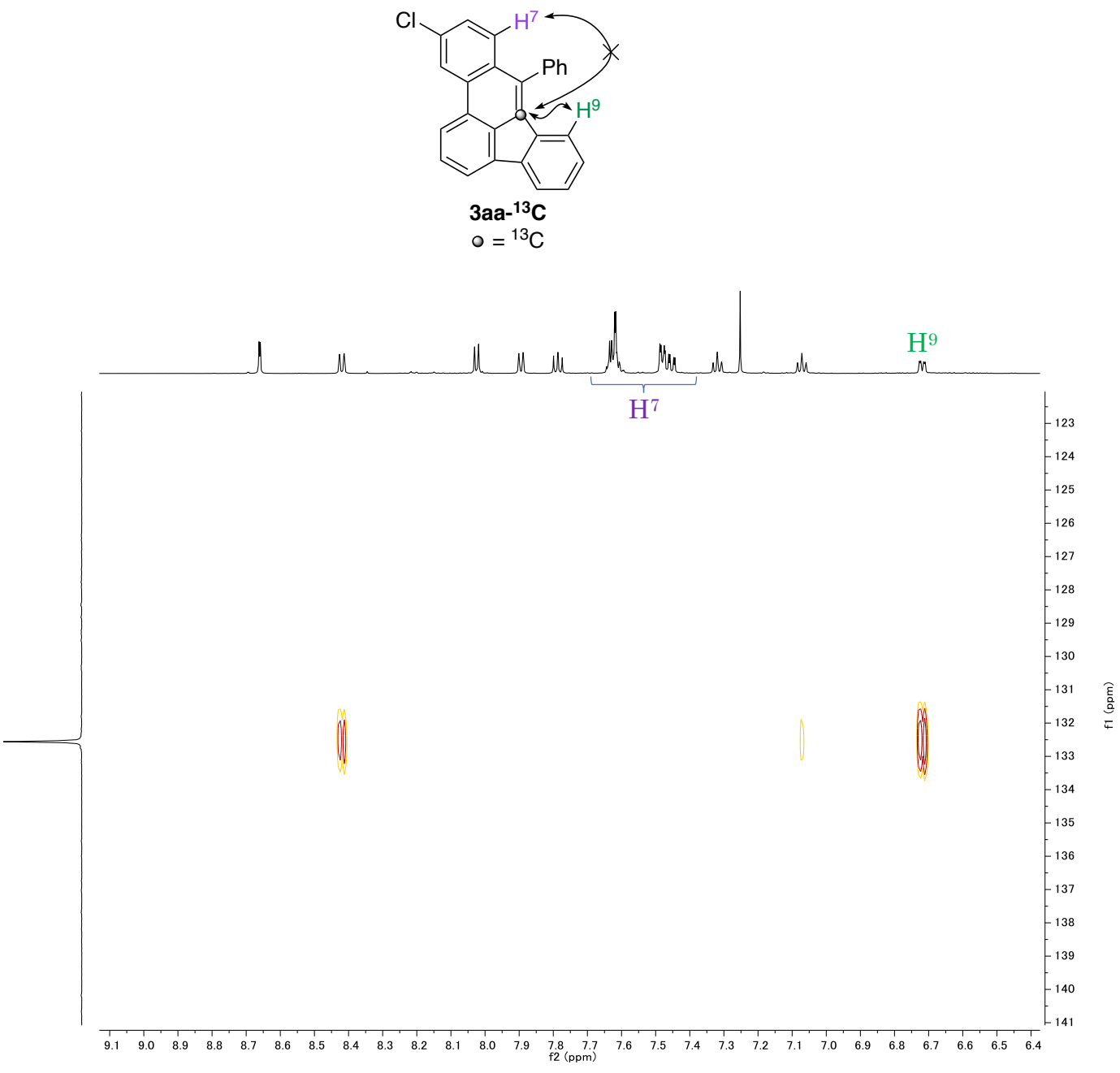


Figure S5. ^{1}H-^{13}C HMBC spectrum of **3aa-^{13}C**

4) Computational details

All calculations were performed using the Gaussian 16 package.[S4] Geometry optimizations was carried out at the M06[S5] level of theory with a mixed basis set of SDD[S6] for Au atom and 6-31G(d,p) for other atoms. Vibration frequency was computed at the same level of theory to confirm whether the structures are minima (no imaginary frequencies) or transition states (only one imaginary frequency). Energies of optimized structures were calculated by single point calculation at the same level of theory with solvation effects (dichloroethane, ε = 10.125000) with a mixed basis set of def2-TZVPPD[S7] for Au atom and 6-311G++(d,p) for other atoms using IEFPCM model.[S8] The molecular geometries of the transition states were first estimated by the Reaction plus Pro software package (Software to optimize reaction paths along the user's expected ones, HPC Systems Inc., http://www.hpc.co.jp/chem/react1.html (written in Japanese)), based on the nudged elastic band (NEB) method,[S9] and subsequently re-optimized by the Synchronous Transit-guided Quasi-Newton method with the keyword QST2 or QST3.[S10] Transition-state structures were confirmed to connect corresponding reactants and products through the use of intrinsic reaction coordination (IRC) calculations.[S11]

A) Total electronic energy and free energy with solvation effects (dichloroethane, ε = 10.125000) using SMD model

Table S1. Total energy *E* and Gibbs free energy *G* of 1ah at 298K

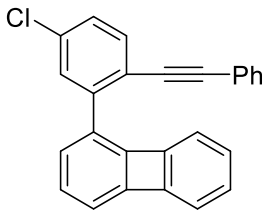
	E (Hartree)	*G* (Hartree)
1ab	-999.812361	-999.519261

Table S2. Total energies *E* and Gibbs free energies *G* of Au-P(OMe)$_3$ system at 298K

	E (Hartree)	*G* (Hartree)		*E* (Hartree)	*G* (Hartree)
Au[P(OMe)$_3$]$^+$	-822.315184	-822.229057	**Int1**	-1822.180108	-1821.784996
TS1	-1822.154653	-1821.758565	**TS1'**	-1822.146586	-1821.752862
Int2	-1822.170887	-1821.773799	**Int2'**	-1822.169774	-1821.772403
TS2	-1822.1492	-1821.752852	**TS2'**	-1822.152332	-1821.759749
Int3	-1822.25141	-1821.850651	**Int3'**	-1822.19304	-1821.794932
TS3	-1822.247893	-1821.848197	**TS3'**	-1822.179865	-1821.78605
Int4	-1822.317346	-1821.916377	**Int4'**	-1822.240667	-1821.843467

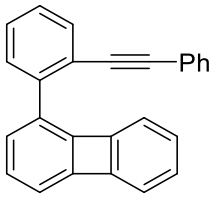
5) Characterization data for new compounds

1-(5-Chloro-2-(phenylethynyl)phenyl)biphenylene (1aa)



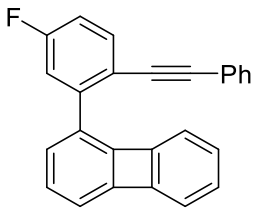
Isolated by flash column chromatography (hexane, Rf = 0.40). The title compound was obtained as a yellow solid (100.5 mg, 92%); mp 113-114 °C; ^{1}H NMR δ 7.56 (d, *J* = 8.3 Hz, 1H), 7.46 (d, *J* = 2.2 Hz, 1H), 7.32-7.22 (m, 6H), 7.05 (dd, *J* = 8.4, 0.6 Hz, 1H), 6.85 (dd, *J* = 8.4, 6.8 Hz, 1H), 6.77-6.73 (m, 1H), 6.70-6.66 (m, 3H), 6.60-6.58 (m, 1H); ^{13}C NMR δ 151.6, 151.2, 151.2, 150.1, 141.6, 134.4, 134.3, 131.6, 129.5, 129.3, 128.8, 128.6, 128.6, 128.5, 128.5, 128.4, 127.8, 123.2, 120.1, 119.1, 117.3, 116.8, 93.8, 88.1; HRMS (DART, positive): m/z calcd. for $C_{26}H_{19}ClN^{+}$ $[M+NH_4]^{+}$ 380.1201, found 380.1190.

1-(2-(Phenylethynyl)phenyl)biphenylene (1ab)



Isolated by PTLC (hexane/EtOAc = 9/1, Rf = 0.60). The title compound was obtained as yellow oil (152.8 mg, 93%); ^{1}H NMR δ 7.65-7.63 (m, 1H), 7.47-7.45 (m, 1H), 7.40-7.29 (m, 4H), 7.26-7.22 (m, 3H), 7.09-7.07 (m, 1H), 6.84 (dd, *J* = 8.4, 6.8 Hz, 1H), 6.74-6.64 (m, 4H), 6.58-6.57 (m, 1H); ^{13}C NMR δ 152.0, 151.3, 151.2, 149.9, 140.1, 133.1, 131.6, 130.8, 129.7, 128.8, 128.6, 128.4, 128.3, 128.3, 128.3, 128.2, 127.6, 123.5, 121.6, 119.0, 117.2, 116.4, 93.0, 89.1; HRMS (DART, positive): m/z calcd. for $C_{26}H_{20}N^{+}$ $[M+NH_4]^{+}$ 346.1590, found 346.1588.

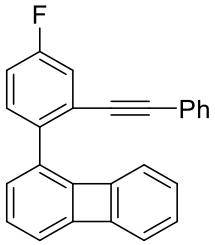
1-(5-Fluoro-2-(phenylethynyl)phenyl)biphenylene (1ac)



Isolated by PTLC (hexane/DCM = 9/1, Rf = 0.45). The title compound was obtained as a yellow solid (87.1 mg, 83%); mp 91-92 °C ; ^{1}H NMR δ 7.62 (dd, *J* = 8.6, 5.8 Hz, 1H), 7.28 (dd, *J* = 7.5, 2.2

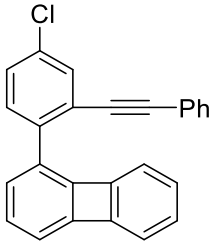
Hz, 2H), 7.26-7.23 (m, 3H), 7.18 (dd, *J* = 9.5, 2.7 Hz, 1H), 7.07-7.02 (m, 2H), 6.85 (dd, *J* = 8.4, 6.8 Hz, 1H), 6.76-6.73 (m, 1H), 6.70-6.66 (m, 3H), 6.61-6.59 (m, 1H); ^{13}C NMR δ 162.5 (d, *J* = 250.0 Hz), 151.6, 151.2, 151.2, 150.1, 142.4 (d, *J* = 8.3 Hz), 135.0 (d, *J* = 8.6 Hz), 131.5, 129.7, 129.7, 129.3, 128.6, 128.5, 128.3, 128.3, 123.4, 119.1, 117.8 (d, *J* = 3.3 Hz), 117.3, 116.8, 115.7 (d, *J* = 22.4 Hz), 115.0 (d, *J* = 22.0 Hz), 92.6 (d, *J* = 1.7 Hz), 88.1; ^{19}F NMR δ -111.0; HRMS (DART, positive): m/z calcd. for $C_{26}H_{16}F^+$ $[M + H]^+$ 347.1231, found 347.1227.

1-(4-Fluoro-2-(phenylethynyl)phenyl)biphenylene (1ad)



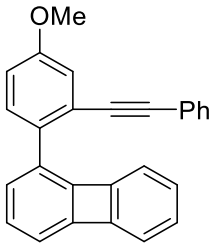
Isolated by PTLC (hexane/EtOAc = 9/1, Rf = 0.55). The title compound was obtained as a yellow solid (71.9 mg, 70%); mp 88-89 °C ; ^{1}H NMR δ 7.40 (dd, *J* = 8.6, 5.8 Hz, 1H), 7.33 (dd, *J* = 9.2, 2.6 Hz, 1H), 7.30-7.21 (m, 5H), 7.10-7.06 (m, 1H), 7.01 (d, *J* = 8.4 Hz, 1H), 6.83 (dd, *J* = 8.4, 6.8 Hz, 1H), 6.72 (dd, *J* = 7.0, 0.9 Hz, 1H), 6.68-6.64 (m, 3H), 6.56-6.54 (m, 1H); ^{13}C NMR δ 161.8 (d, *J* = 247.7 Hz), 151.8, 151.2, 151.2, 149.9, 136.4 (d, *J* = 3.3 Hz), 131.7, 130.4 (d, *J* = 8.6 Hz), 129.8, 129.6, 128.6, 128.5, 128.4, 128.4, 128.4, 123.3 (d, *J* = 9.8 Hz), 123.0, 119.4 (d, *J* = 22.7 Hz), 118.9, 117.3, 116.5, 116.0 (d, *J* = 21.5 Hz), 93.8, 88.0 (d, *J* = 3.0 Hz); ^{19}F NMR δ -114.6; HRMS (DART, positive): m/z calcd. for $C_{26}H_{19}FN^+$ $[M+NH_4]^+$ 364.1496, found 364.1492.

1-(4-Chloro-2-(phenylethynyl)phenyl)biphenylene (1ae)



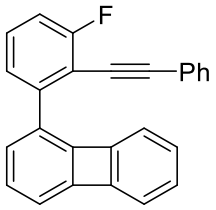
Isolated by flash column chromatography (hexane/DCM = 4/1, Rf = 0.50). The title compound was obtained as a yellow solid (96.1mg, 87%); mp 115-116 °C; ^{1}H NMR δ 7.63 (dd, *J* = 2.1, 0.4 Hz, 1H), 7.40-7.38 (m, 1H), 7.35 (dd, *J* = 8.3, 2.1 Hz, 1H), 7.30-7.22 (m, 5H), 7.02 (dd, *J* = 8.4, 0.7 Hz, 1H), 6.84 (dd, *J* = 8.5, 6.8 Hz, 1H), 6.75-6.72 (m, 1H), 6.69-6.65 (m, 3H), 6.57-6.55 (m, 1H); ^{13}C NMR δ 151.7, 151.2, 151.2, 150.0, 138.5, 133.4, 132.6, 131.7, 130.0, 129.7, 129.4, 128.8, 128.6, 128.5, 128.5, 128.4, 123.2, 123.0, 119.0, 117.3, 116.6, 94.1, 87.8; HRMS (DART, positive): m/z calcd. for $C_{26}H_{19}ClN^+$ $[M+NH_4]^+$ 380.1201, found 380.1198.

1-(4-Methoxy-2-(phenylethynyl)phenyl)biphenylene (1af)



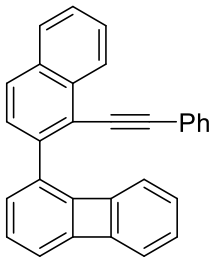
Isolated by flash column chromatography (hexane/EtOAc = 9/1, Rf = 0.65). The title compound was obtained as a yellow solid (160.8mg, 90%); mp 96-97 °C; ^{1}H NMR δ 7.38 (d, *J* = 8.6 Hz, 1H), 7.32-7.30 (m, 2H), 7.26-7.24 (m, 3H), 7.15 (d, *J* = 2.8 Hz, 1H), 7.06 (d, *J* = 8.4 Hz, 1H), 6.96 (dd, *J* = 8.7, 2.6 Hz, 1H), 6.82 (dd, *J* = 8.5, 6.8 Hz, 1H), 6.73-6.70 (m, 1H), 6.67-6.62 (m, 3H), 6.57 (d, *J* = 6.8 Hz, 1H), 3.87 (s, 3H); ^{13}C NMR δ 158.9, 152.1, 151.3, 151.1, 149.6, 132.9, 131.6, 130.6, 130.0, 129.8, 128.4, 128.3, 128.3, 128.2, 123.4, 122.5, 118.8, 117.2, 117.1, 116.1, 115.6, 92.7, 89.1, 55.6 (a pair of peaks at the aromatic region was overlapped); HRMS (DART, positive): m/z calcd. for $C_{27}H_{22}NO^{+}$ $[M+NH_4]^{+}$ 376.1696, found 376.1692.

1-(3-Fluoro-2-(phenylethynyl)phenyl)biphenylene (1ag)



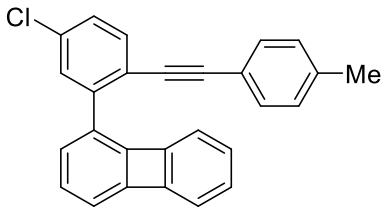
Isolated by PTLC (hexane/EtOAc = 9/1, Rf = 0.50). The title compound was obtained as a yellow solid (145.8 mg, 84%); mp 68-69 °C; ^{1}H NMR δ 7.37-7.32 (m, 3H), 7.27-7.23 (m, 4H), 7.13-7.09 (m, 1H), 7.06 (dd, *J* = 8.4, 0.6 Hz, 1H), 6.85 (dd, *J* = 8.4, 6.8 Hz, 1H), 6.76-6.73 (m, 1H), 6.70-6.66 (m, 3H), 6.59-6.58 (m, 1H); ^{13}C NMR δ 163.4 (d, *J* = 250.9 Hz), 151.7, 151.3, 151.2, 150.1, 142.3 (d, *J* = 1.2 Hz), 131.7, 129.7 (d, *J* = 2.7 Hz), 129.5, 129.4 (d, *J* = 8.8 Hz), 128.6, 128.5 (d, *J* = 2.1 Hz), 128.4, 128.3, 124.3 (d, *J* = 3.4 Hz), 123.2, 119.1, 117.3, 116.7, 114.5 (d, *J* = 21.5 Hz), 110.7 (d, *J* = 16.4 Hz), 98.4 (d, *J* = 4.1 Hz), 82.1 (a pair of peaks at the aromatic region was overlapped); ^{19}F NMR δ -108.4; HRMS (DART, positive): m/z calcd. for $C_{26}H_{16}F^{+}$ $[M+H]^{+}$ 347.1231, found 347.1225.

1-(1-(Phenylethynyl)naphthalen-2-yl)biphenylene (1ah)



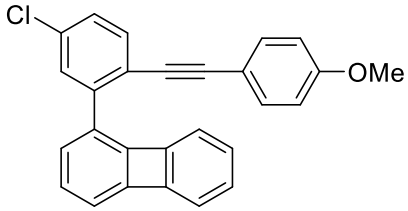
Isolated by flash column chromatography (hexane/EtOAc = 9/1, Rf = 0.60). The title compound was obtained as a yellow solid (95.0 mg, 83%); mp 123-125 °C; ^{1}H NMR δ 8.59 (d, *J* = 8.3 Hz, 1H), 7.88 (dd, *J* = 8.2, 2.2 Hz, 2H), 7.66-7.54 (m, 3H), 7.42-7.40 (m, 2H), 7.30-7.27 (m, 3H), 7.19 (d, *J* = 8.3 Hz, 1H), 6.89 (dd, *J* = 8.4, 6.8 Hz, 1H), 6.75-6.64 (m, 4H), 6.55 (d, *J* = 6.8 Hz, 1H); ^{13}C NMR δ 152.1, 151.4, 151.2, 150.5, 138.7, 133.8, 132.6, 131.6, 131.2, 129.9, 128.7, 128.5, 128.4, 128.4, 128.4, 128.3, 127.3, 126.9, 126.7, 126.6, 123.7, 119.2, 118.5, 117.2, 116.4, 98.6, 87.1 (a pair of peaks at the aromatic region was overlapped); HRMS (DART, positive): m/z calcd. for $C_{30}H_{22}N^{+}$ $[M+NH_4]^{+}$ 396.1747, found 396.1744.

1-(5-Chloro-2-(4-methylphenylethynyl)phenyl)biphenylene (1ba)



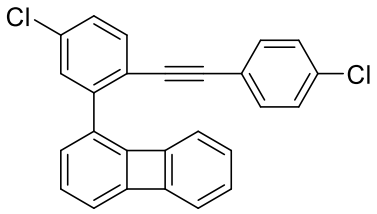
Isolated by flash column chromatography (hexane, Rf = 0.25). The title compound was obtained as a yellow solid (127.1 mg, 68%); mp 137-138 °C; ^{1}H NMR δ 7.54 (d, *J* = 8.3 Hz, 1H), 7.45 (d, *J* = 2.2 Hz, 1H), 7.29 (dd, *J* = 8.3, 2.2 Hz, 1H), 7.17 (d, *J* = 8.1 Hz, 2H), 7.08-7.02 (m, 3H), 6.83 (dd, *J* = 8.3, 6.8 Hz, 1H), 6.86-6.81 (m, 1H), 6.77-6.71 (m, 3H), 6.60-6.55 (m, 1H), 2.31 (s, 3H); ^{13}C NMR δ 151.6, 151.3, 151.2, 150.1, 141.4, 138.6, 134.2, 131.5, 129.5, 129.3, 129.1, 128.8, 128.6, 128.5, 128.5, 127.7, 120.3, 120.1, 119.1, 117.3, 116.8, 94.1, 87.5, 21.6 (a pair of peaks at the aromatic region was overlapped); HRMS (DART, positive): m/z calcd. For $C_{27}H_{21}ClN^{+}$ $[M+NH_4]^{+}$ 394.1357, found 394.1350.

1-(5-Chloro-2-(4-methoxyphenylethynyl)phenyl)biphenylene (1ca)



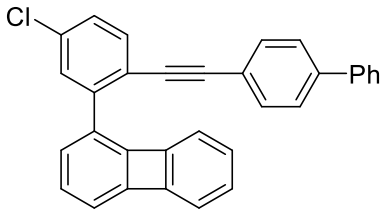
Isolated by flash column chromatography (hexane/EtOAc = 9/1, Rf = 0.60). The title compound was obtained as a yellow solid (126.1 mg, 68%); mp 129-130 °C; ^{1}H NMR δ 7.52 (d, *J* = 8.3 Hz, 1H), 7.44 (d, *J* = 2.2 Hz, 1H), 7.28 (dd, *J* = 8.3, 2.2 Hz, 1H), 7.21 (d, *J* = 8.9 Hz, 2H), 7.04 (d, *J* = 8.4 Hz, 1H), 6.83 (dd, *J* = 8.4, 6.9 Hz, 1H), 6.79-6.71 (m, 3H), 6.71-6.62 (m, 3H), 6.58 (d, *J* = 6.9 Hz, 1H), 3.77 (s, 3H); ^{13}C NMR δ 159.8, 151.7, 151.2, 151.2, 150.1, 141.3, 134.0, 134.0, 133.0, 129.6, 129.3, 128.7, 128.6, 128.5, 128.5, 127.7, 120.5, 119.1, 117.3, 116.7, 115.3, 114.0, 94.0, 86.9, 55.4; HRMS (DART, positive): m/z calcd. For $C_{27}H_{18}ClO^{+}$ $[M+H]^{+}$ 393.1041, found 393.1035.

1-(5-Chloro-2-(4-chlorophenylethynyl)phenyl)biphenylene (1da)



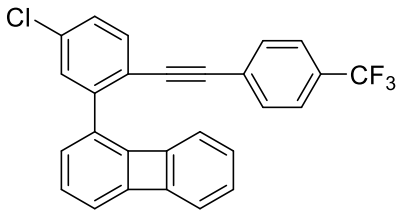
Isolated by flash column chromatography (hexane, Rf = 0.50). The title compound was obtained as a yellow solid (125.4 mg, 63%); mp 161-162 °C; ^{1}H NMR δ 7.55 (d, *J* = 8.3 Hz, 1H), 7.46 (d, *J* = 2.1 Hz, 1H), 7.31 (dd, *J* = 8.3, 2.2 Hz, 1H), 7.22-7.15 (m, 4 H), 6.99 (d, *J* = 8.4 Hz, 1H), 6.85 (dd, *J* = 8.4, 6.8 Hz, 1H), 6.77-6.73 (m, 1H), 6.72-6.64 (m, 3H), 6.59-6.54 (m, 1H); ^{13}C NMR δ 151.6, 151.2, 150.2, 141.7, 134.7, 134.5, 134.1, 132.8, 129.3, 129.2, 128.9, 128.7, 128.6, 128.6, 127.8, 121.7, 119.8, 119.2 117.4, 116.8, 92.7, 89.0 (two pairs of peaks at the aromatic region were overlapped); HRMS (DART, positive): m/z calcd. For $C_{26}H_{18}Cl_2N^{+}$ $[M+NH_4]^{+}$ 414.0811, found 414.0805.

1-(2-([1,1'-Biphenyl]-4-ylethynyl)-5-chlorophenyl)biphenylene (1ea)



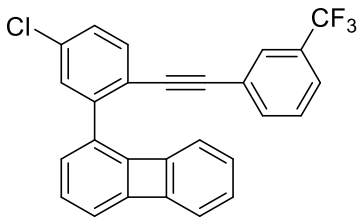
Isolated by flash column chromatography (hexane/DCM = 10/1, Rf = 0.20). The title compound was obtained as a yellow solid (72.4 mg, 33%); mp 136-137 °C; ^{1}H NMR δ 7.59-7.54 (m, 3H), 7.50-7.46 (m, 3H), 7.45-7.41 (m, 2H), 7.36-7.30 (m, 4H), 7.06 (d, *J* = 8.4 Hz, 1H), 6.87 (dd, *J* = 8.5, 6.8 Hz, 1H), 6.78-7.64 (m, 1H), 6.73-6.67 (m, 3H), 6.63-6.58 (m, 1H); ^{13}C NMR δ 151.7, 151.3, 151.2, 150.2, 141.6, 141.1, 140.5, 134.4, 134.2, 132.0, 129.5, 129.3, 129.0, 128.8, 128.6, 128.6, 128.6, 127.8, 127.8, 127.1, 127.0, 122.1, 120.2, 119.2, 117.4, 116.8, 93.8, 88.8; HRMS (DART, positive): m/z calcd. For $C_{32}H_{20}Cl^{+}$ $[M+H]^{+}$ 439.1248, found 439.1245.

1-(5-Chloro-2-(4-trifluoromethylphenylethynyl)phenyl)biphenylene (1fa)



Isolated by flash column chromatography (hexane, Rf = 0.25). The title compound was obtained as a yellow solid (166.7 mg, 78%); mp 129-130 °C; ^{1}H NMR δ 7.58 (d, *J* = 8.3 Hz, 1H), 7.51-7.45 (m, 3H), 7.35 (s, 1H), 7.35-7.30 (m, 2H), 6.98 (d, *J* = 8.4, 1H), 6.86 (dd, *J* = 8.4, 6.8 Hz, 1H), 6.80-6.73 (m, 1H), 6.73-6.65 (m, 3H), 6.60-6.52 (m, 1H); ^{13}C NMR δ 151.6, 151.2, 151,2, 150.2, 142.0, 135.1, 134.3, 131.7, 130.0 (q, *J* = 32.8 Hz), 129.2, 129.2, 129.0, 128.7, 128.7, 128.6, 127.9, 127.0 (q, *J* = 1.5 Hz), 125.3 (q, *J* = 3.7 Hz), 124.0 (q, *J* = 274.5 Hz), 119.4, 119.2, 117.4, 116.9, 92.3, 90.4; ^{19}F NMR δ -62.7; HRMS (DART, positive): m/z calcd. For $C_{27}H_{18}ClF_3N^{+}$ $[M+NH_4]^{+}$ 448.1074, found 448.1073.

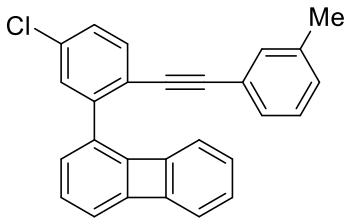
1-(5-Chloro-2-(3-trifluoromethylphenylethynyl)phenyl)biphenylene (1ga)



Isolated by flash column chromatography (hexane, Rf = 0.20). The title compound was obtained as a yellow solid (177.3 mg, 82%); mp 68-69 °C; ^{1}H NMR δ 7.57 (d, *J* = 8.3 Hz, 1H), 7.52-7.46 (m, 3H), 7.42 (d, *J* = 7.8 Hz, 1H), 7.38-7.31 (m, 2H), 6.97 (d, *J* = 8.4 Hz, 1H), 6.86 (dd, *J* = 8.4, 6.8 Hz, 1H), 6.78-6.73 (m, 1H), 6.72-6.64 (m, 3H), 6.57 (dd, *J* = 6.8, 0.8 Hz, 1H); ^{13}C NMR δ 151.6, 151.2, 151.2, 150.3, 142.0, 135.0, 134.5, 134.2, 131.0 (q, *J* = 32.7 Hz), 129.2, 129.1, 128.9, 128.8, 128.7, 128.7, 128.5, 128.4 (q, *J* = 3.8 Hz), 127.9, 124.9 (q, *J* = 3.8 Hz), 124.1, 123.8 (q, *J* = 277.0 Hz), 119.5,

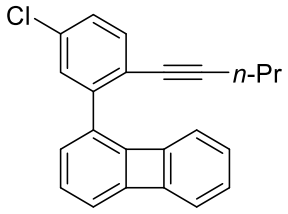
119.3, 117.5, 116.9, 92.1, 89.6; ^{19}F NMR δ -62.8; HRMS (DART, positive): m/z calcd. For $C_{27}H_{18}ClF_3N^+$ $[M+NH_4]^+$ 448.1074, found 448.1071.

1-(5-Chloro-2-(3-methylphenylethynyl)phenyl)biphenylene (1ha)



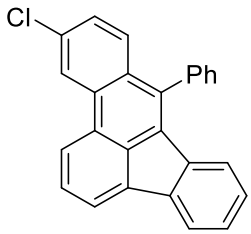
Isolated by PTLC (hexane, Rf = 0.30). The title compound was obtained as a yellow solid (85.4 mg, 76%); mp 98-99 °C; ^{1}H NMR δ 7.54 (d, *J* = 8.3 Hz, 1H), 7.45 (d, *J* = 2.2 Hz, 1H), 7.29 (dd, *J* = 8.3, 2.2 Hz, 1H), 7.14-7.05 (m, 4H), 7.04-7.01 (m, 1H), 6.84 (dd, *J* = 8.4, 6.8 Hz, 1H), 6.77-6.72 (m, 1H), 6.70-6.64 (m, 3H), 6.60-6.57 (m, 1H), 2.25 (s, 3H); ^{13}C NMR δ 151.7, 151.3, 151.2, 150.2, 141.6, 138.0, 134.3, 134.2, 132.3, 129.5, 129.3, 129.3, 128.8, 128.6, 128.6, 128.5, 128.2, 127.8, 123.0, 120.2, 119.2, 117.3, 116.8, 94.8, 94.0, 87.7, 21.3; HRMS (DART, positive): m/z calcd. For $C_{27}H_{21}ClN^+$ $[M+NH_4]^+$ 394.1357, found 394.1353.

1-(5-Chloro-2-(pent-1-yn-1-yl)phenyl)biphenylene (1ia)

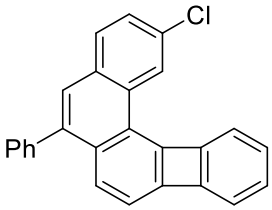


Isolated by PTLC (hexane, Rf = 0.45). The title compound was obtained as yellow oil (72.2 mg, 73%); ^{1}H NMR δ 7.44-7.38 (m, 2H), 7.23 (dd, *J* = 8.3, 2.2 Hz, 1H), 7.00 (d, *J* = 8.4 Hz, 1H), 6.80 (dd, *J* = 8.4, 6.8 Hz, 1H), 6.76-6.70 (m, 2H), 6.67-6.60 (m, 2H), 6.56-6.53 (m, 1H), 2.23 (t, *J* = 7.0 Hz, 2H), 1.49-1.39 (m, 2H), 0.90 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR δ 151.7, 151.3, 151.2, 150.0, 141.4, 134.3, 133.5, 130.0, 129.3, 128.6, 128.4, 128.4, 128.3, 127.6, 120.9, 119.0, 117.1, 116.6, 95.2, 79.1, 21.8, 21.8, 13.6; HRMS (DART, positive): m/z calcd. For $C_{23}H_{18}Cl^+$ $[M+H]^+$ 329.1092, found 329.1087.

5-Chloro-8-phenylbenzo[*b*]fluoranthene (3aa) and 2-chloro-6-phenylbenzo[3,4]cyclobuta[1,2-*c*]phenanthrene (4aa)



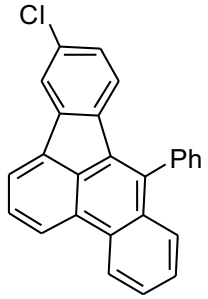
3aa



4aa

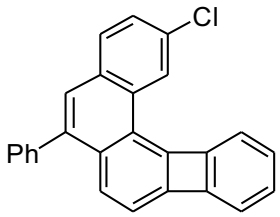
Separated by PTLC (hexane/toluene = 14/1, Rf = 0.40). The title compounds were obtained as a yellow solid (17.2 mg, **3aa**:**4aa** = 31:1 = 92%:3%); ^{1}H NMR (**3aa**) δ 8.64 (d, *J* = 2.2 Hz, 1H), 8.39 (d, *J* = 8.1 Hz, 1H), 8.00 (d, *J* = 7.1 Hz, 1H), 7.88 (d, *J* = 7.5 Hz, 1H), 7.76 (dd, *J* = 8.1, 7.1 Hz, 1H), 7.63-7.59 (m, 4H), 7.47-7.43 (m, 3H), 7.32-7.29 (m, 1H), 7.08-7.05 (m, 1H), 6.71 (d, *J* = 7.7 Hz, 1H); ^{13}C NMR (**3aa**) δ 140.8, 138.5, 137.8, 137.1, 135.9, 133.3, 132.8, 132.7, 132.2, 131.9, 130.0, 129.9, 129.1, 128.4, 128.4, 128.0, 127.5, 127.2, 126.5, 124.3, 122.8, 121.6, 121.3, 120.2; HRMS (DART, positive): m/z calcd. for $C_{26}H_{19}ClN^{+}$ $[M+NH_4]^{+}$ 380.1201, found 380.1195.

11-Chloro-8-phenylbenzo[*b*]fluoranthene (2aa)



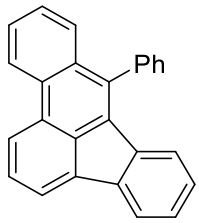
Isolated by short column (hexane/toluene = 14/1, Rf = 0.50). The title compound was obtained as a yellow solid (14.9 mg, 82%); mp 223-225 °C; ^{1}H NMR δ 8.74 (d, *J* = 8.1 Hz, 1H), 8.55 (d, *J* = 8.2 Hz, 1H), 8.00 (d, *J* = 7.1 Hz, 1H), 7.86 (d, *J* = 2.0 Hz, 1H), 7.82-7.79 (m, 1H), 7.72-7.68 (m, 2H), 7.65-7.60 (m, 3H), 7.55-7.52 (m, 1H), 7.50-7.48 (m, 2H), 7.04-7.02 (m, 1H), 6.62 (d, *J* = 8.2 Hz, 1H); ^{13}C NMR δ 142.5, 138.0, 137.0, 136.9, 135.9, 134.3, 133.8, 132.1, 131.4, 130.8, 130.0, 129.1, 128.6, 128.4, 128.2, 127.5, 127.3, 127.2, 127.0, 125.0, 123.2, 122.3, 121.5, 120.1; HRMS (DART, positive): m/z calcd. for $C_{26}H_{19}NCl^{+}$ $[M+NH_4]^{+}$ 380.1201, found 380.1198.

2-Chloro-6-phynylbenzo[3,4]cyclobuta[1,2-*c*]phenanthrene (4aa)

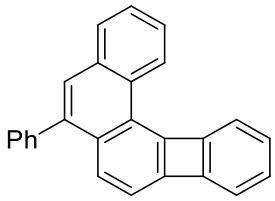


Isolated by PTLC (hexane/chloroform = 1/1, Rf = 0.50). The title compound was obtained as a yellow solid (17.2 mg, 95%); mp 244-246 °C; ^{1}H NMR δ 8.24 (d, *J* = 1.9 Hz, 1H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.51-7.42 (m, 6H), 7.32 (d, *J* = 7.7 Hz, 1H), 7.29 (s, 1H), 7.02 (d, *J* = 6.9 Hz, 1H), 6.90 (d, *J* = 7.7 Hz, 1H), 6.83-6.80 (m, 1H), 6.77-6.73 (m, 1H), 6.61 (s, 1H); ^{13}C NMR δ 151.7, 151.7, 150.6, 147.7, 140.5, 140.3, 132.9, 132.2, 130.7, 130.0, 129.9, 129.4, 128.9, 128.6, 128.6, 128.5, 128.5, 128.0, 127.7, 126.3, 125.3, 118.5, 117.0, 116.8; HRMS (DART, positive): m/z calcd. for $C_{26}H_{16}Cl^{+}$ $[M+H]^{+}$ 363.0935, found 363.0930.

8-Phenylbenzo[*b*]fluoranthene (3ab) and 6-phenylbenzo[3,4]cyclobuta[1,2-*c*]phenanthrene (4ab)



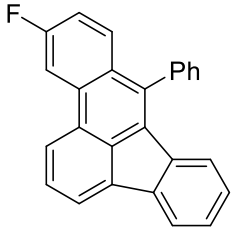
3ab



4ab

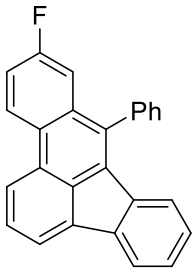
Separated by PTLC (hexane/toluene = 14/1, Rf = 0.60). The title compounds were obtained as a yellow solid (13.8 mg, **3ab**:**4ab** = 3:1 = 63%:21% ($P(OMe)_3$ was used as a ligand)); ^{1}H NMR δ 8.73 (d, *J* = 8.1 Hz, 1H (**major**)), 8.51 (d, *J* = 8.1 Hz, 1H (**major**)), 8.30 (d, *J* = 8.0 Hz, 1H (**minor**)), 8.01 (d, *J* = 7.1 Hz, 1H (**major**)), 7.90 (d, *J* = 7.5 Hz, 1H (**major**)), 7.78 (dd, *J* = 8.1, 7.2 Hz, 1H (**major**)), 7.72-7.69 (m, 1H (**major**) + 1H **(minor**)), 7.68-7.66 (m, 1H (**major**)), 7.65-7.40 (m, 7H (**major**) + 7H (**minor**)), 7.33-7.29 (m, 1H (**major**) + 2H (**minor**)), 7.08-7.05 (m, 1H (**major**)), 7.02 (d, *J* = 6.7 Hz, 1H **(minor**)), 6.88 (d, *J* = 7.8 Hz, 1H (**minor**)), 6.80-6.76 (m, 1H (**minor**)), 6.74-6.71 (m, 1H (**minor**)), 6.59 (d, *J* = 6.5 Hz, 1H (**minor**)); ^{13}C NMR (**3ab**) δ 140.9, 138.8, 138.3, 137.1, 136.5, 134.4, 132.4, 131.9, 130.8, 130.1, 129.0, 128.5, 128.2, 128.2, 127.8, 127.5, 127.4, 127.0, 126.8, 124.3, 123.2, 121.6, 121.2, 119.7; ^{13}C NMR (**4ab**) δ 152.3, 151.9, 150.4, 147.5, 140.9, 140.0, 132.9, 132.4, ,130.1, 130.0, 128.9, 128.7, 128.4, 128.4, 128.2, 127.7, 127.6, 127.2, 126.5, 125.6, 125.5, 118.3, 116.6, 116.6; HRMS (DART, positive): m/z calcd. For $C_{26}H_{17}^{+}$ $[M+H]^{+}$ 329.1325, found 329.1323.

5-Fluoro-8-phenylbenzo[*b*]fluoranthene (3ac)



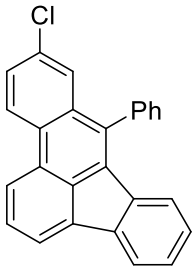
Isolated by PTLC (hexane, Rf = 0.30). The title compound was obtained as a yellow solid (14.4 mg, 83%); mp 194-195 °C; ^{1}H NMR δ 8.38 (d, *J* = 8.2 Hz, 1H), 8.31 (dd, *J* = 10.2, 2.6 Hz, 1H), 8.02 (d, *J* = 7.1 Hz, 1H), 7.90-7.88 (m, 1H), 7.77 (dd, *J* = 8.1, 7.2 Hz, 1H), 7.68 (dd, *J* = 9.1, 5.8 Hz, 1H), 7.64-7.60 (m, 3H), 7.49-7.47 (m, 2H), 7.33-7.29 (m, 1H), 7.26-7.22 (m, 1H), 7.09-7.05 (m, 1H), 6.72-6.70 (m, 1H); ^{13}C NMR δ 162.0 (d, *J* = 248.0 Hz), 140.6, 138.6, 138.1, 137.2, 136.1 (d, *J* = 1.2 Hz), 132.6 (d, *J* = 8.5 Hz), 132.3, 131.9 (d, *J* = 2.5 Hz), 131.2 (d, *J* = 1.8 Hz), 130.7 (d, *J* = 8.9 Hz), 130.0, 129.1, 128.4, 128.2, 127.9, 127.5, 126.9 (d, *J* = 4.1 Hz), 124.2, 121.6, 121.3, 120.2, 115.5 (d, *J* = 23.3 Hz), 108.4 (d, *J* = 22.1 Hz); ^{19}F NMR δ -113.3; HRMS (DART, positive): m/z calcd. for $C_{26}H_{15}F$ $[M]^{+}$ 346.1152, found 346.1147.

6-Fluoro-8-phenylbenzo[*b*]fluoranthene (3ad)



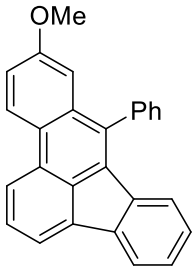
Isolated by PTLC (hexane/DCM = 4/1, Rf = 0.50). The title compound was obtained as a yellow solid (16.3 mg, 94%); mp 172-173 °C; ^{1}H NMR δ 8.69 (dd, *J* = 8.9, 5.7 Hz, 1H), 8.43 (d, *J* = 8.1 Hz, 1H), 8.00 (d, *J* = 7.1 Hz, 1H), 7.90 (d, *J* = 7.5 Hz, 1H), 7.80-7.77 (m, 1H), 7.66-7.60 (m, 3H), 7.49 (dd, *J* = 7.5, 1.7 Hz, 2H), 7.44-7.40 (m, 1H), 7.35-7.31 (m, 2H), 7.09-7.06 (m, 1H), 6.74 (d, *J* = 7.7 Hz, 1H); ^{13}C NMR δ 161.7 (d, *J* = 245.6 Hz), 141.0, 138.5, 137.7, 137.2, 136.2 (d, *J* = 8.2 Hz), 135.6 (d, *J* = 4.1 Hz), 133.6, 131.5 (d, *J* = 1.2 Hz), 130.0, 129.2, 128.6, 128.5, 128.2, 127.5, 127.3 (d, *J* = 1.9 Hz), 127.1, 125.1 (d, *J* = 8.9 Hz), 124.5, 121.4, 121.3, 119.5, 115.7 (*J* = 23.8 Hz), 113.2 (*J* = 22.5 Hz); ^{19}F NMR δ -114.6; HRMS (DART, positive): m/z calcd. for $C_{26}H_{15}F^{+}$ $[M]^{+}$ 346.1152, found 346.1142.

6-Chloro-8-phenylbenzo[*b*]fluoranthene (3ae)



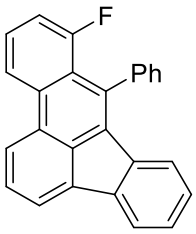
Isolated by PTLC (hexane/toluene = 4/1, Rf = 0.60). The title compound was obtained as a yellow solid (16.6 mg, 92%); mp 161-162 °C; ^{1}H NMR δ 8.61 (d, *J* = 8.6 Hz, 1H), 8.40 (d, *J* = 8.1 Hz, 1H), 7.99 (dd, *J* = 7.1, 0.6 Hz, 1H), 7.89-7.87 (m, 1H), 7.76 (dd, *J* = 8.2, 7.1 Hz, 1H), 7.65-7.60 (m, 5H), 7.48-7.46 (m, 2H), 7.33-7.30 (m, 1H), 7.08-7.05 (m, 1H), 6.70-6.68 (m, 1H); ^{13}C NMR δ 141.0, 138.5, 137.5, 137.2, 135.7, 135.4, 133.6, 132.9, 131.8, 130.0, 129.2, 129.1, 128.6, 128.5, 128.2, 127.6, 127.6, 127.4, 127.0, 124.6, 124.5, 121.5, 121.3, 119.9; HRMS (DART, positive): m/z calcd. for $C_{26}H_{19}ClN^{+}$ $[M+NH_4]^{+}$ 380.1201, found 380.1195.

6-Methoxy-8-phenylbenzo[*b*]fluoranthene (3af)

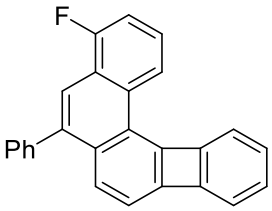


Isolated by PTLC (hexane/toluene = 4/1, Rf = 0.30). The title compound was obtained as a yellow solid (16.0 mg, 89%); mp 113-114 °C; ^{1}H NMR δ 8.63 (d, *J* = 8.9 Hz, 1H), 8.41 (d, *J* = 8.1 Hz, 1H), 7.95 (dd, *J* = 7.1, 0.6 Hz, 1H), 7.90-7.88 (m, 1H), 7.76 (dd, *J* = 8.1, 7.1 Hz, 1H), 7.64-7.57 (m, 3H), 7.52-7.50 (m, 2H), 7.32-7.29 (m, 2H), 7.11-7.04 (m, 2H), 6.72-6.70 (m, 1H), 3.77 (s, 3H); ^{13}C NMR δ 158.5, 141.1, 138.8, 138.4, 137.0, 136.0, 135.9, 133.0, 131.0, 130.0, 129.1, 128.3, 128.2, 127.9, 127.5, 127.3, 125.1, 124.6, 124.3, 121.2, 121.1, 118.8, 116.3, 110.2, 55.4; HRMS (DART, positive): m/z calcd. for $C_{27}H_{19}O$ $[M+H]^{+}$ 359.1430, found 364.1426.

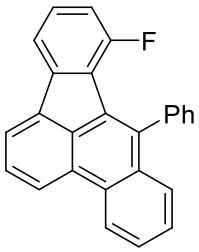
7-Fluoro-8-phenylbenzo[*b*]fluoranthene (3ag), 4-fluoro-6-phenylbenzo[3,4]cyclobuta[1,2-*c*]phenanthrene (4ag) and 9-fluoro-8-phenylbenzo[*b*]fluoranthene (2ag)



3ag



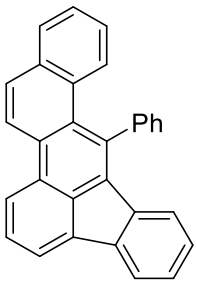
4ag



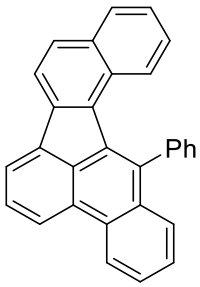
2ag

Separated by PTLC (hexane/toluene = 9/1, Rf = 0.45). The title compounds were obtained as a yellow solid (13.9 mg, **3ag**:**4ag:2ag** =15:4:1 = 61%:15%:4%); ^{1}H NMR (**3ag**) δ 8.55-8.53 (m, 1H), 8.46 (d, *J* = 8.1 Hz, 1H), 8.01 (dd, *J* = 7.1, 0.6 Hz, 1H), 7.88-7.86 (m, 1H), 7.78 (dd, *J* = 8.2, 7.1 Hz, 1H), 7.64-7.60 (m, 1H), 7.58-7.55 (m, 3H), 7.52-7.50 (m, 2H), 7.32-7.28 (m, 1H), 7.21-7.16 (m, 1H), 7.04-7.01 (m, 1H), 6.42-6.40 (m, 1H); ^{13}C NMR (**3ag**) δ 161.6 (d, *J* = 255.7 Hz), 141.1 (d, *J* = 4.5 Hz), 140.8, 138.7, 138.0, 137.2, 134.2, 133.2 (d, *J* = 3.8 Hz), 131.8, 128.7, 128.4 (d, *J* = 4.1 Hz), 128.1, 127.7, 127.6, 127.6, 127.6, 126.8 (d, *J* = 3.0 Hz), 124.8, 123.1, 122.0, 121.2, 120.1, 119.3 (d, *J* = 4.0 Hz), 113.7 (d, *J* = 23.2 Hz); ^{19}F NMR δ -105.0 (d, *J* = 13.6 Hz (**3ag**)), δ -105.6 (**4ag**); HRMS (DART, positive): m/z calcd. for $C_{26}H_{19}FN^{+}$ $[M+NH_4]^{+}$ 364.1496, found 364.1493.

10-Phenylnaphtho[1,2-*b*]fluoranthene (3ah) and 8-phenyldibenzo[*b*,*l*]fluoranthene (2ah)



3ah

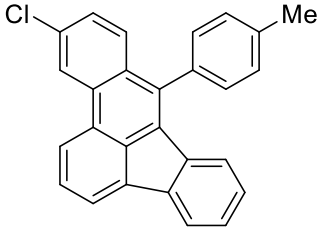


2ah

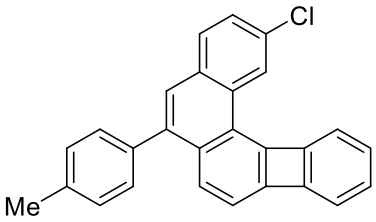
Separated by flash column chromatography (hexane/toluene = 4/1, Rf = 0.50). The title compounds were obtained as a yellow solid (11.7mg, **3ah**:**2ah** = 1.4:1 = 36%:26%); ^{1}H NMR δ 8.80 (d, *J* = 8.9 Hz, 1H (major)), 8.75-8.73 (m, 1H (minor)), 8.61 (d, *J* = 8.3 Hz, 1H (major)), 8.53 (d, *J* = 8.1 Hz, 1H (minor)), 8.07-8.03 (m, 2H (major) + 2H (minor)), 7.95-7.76 (m, 4H (major) + 4H (minor)), 7.71-7.65 (m, 3H (major) + 1H (minor)), 7.61-7.56 (m, 2H (major) + 5H (minor)), 7.53-7.50 (m, 1H (minor)), 7.47-7.44 (m, 1H (major)), 7.30-7.27 (m, 1H (major)), 7.22-7.19 (m, 1H (minor)), 7.15-7.11 (m, 1H (major)), 7.04-7.01 (m, 1H (major)), 6.84-6.78 (m, 2H (minor)), 6.38 (d, *J* = 7.8 Hz, 1H (major)); ^{13}C NMR δ 143.1, 141.4, 140.6, 140.4, 139.8, 138.6, 137.5, 137.1, 136.8, 135.3, 134.9, 134.8, 134.8, 134.6, 134.1, 132.5, 131.8, 131.7, 131.2, 130.9, 130.6, 130.3, 130.2, 129.9, 129.6, 129.6,

129.5, 129.3, 129.1, 129.0, 129.0, 128.4, 128.3, 128.2, 128.1, 127.9, 127.6, 127.5, 127.5, 127.4, 127.2, 126.8, 126.8, 125.7, 125.7, 125.4, 124.6, 124.6, 122.8, 122.6, 121.8, 121.7, 121.2, 119.8, 119.4, 119.3; HRMS (DART, positive): m/z calcd. for $C_{30}H_{22}N^+$ $[M+NH_4]^+$ 396.1747, found 396.1743.

5-Chloro-8-(4-methylphenyl)benzo[*b*]fluoranthene (3ba) and 2-chloro-6-(4-methylphenyl)benzo[3,4]cyclobuta[1,2-*c*]phenanthrene (4ba)



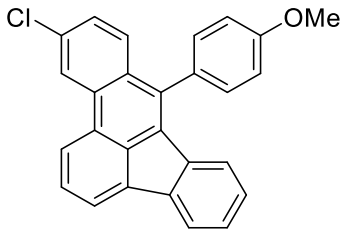
3ba



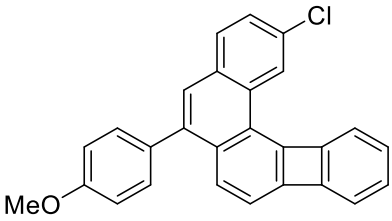
4ba

Separated by PTLC (hexane, Rf = 0.45). The title compounds were obtained as a yellow solid (12.1 mg, **3ba**:**4ba** = 32:1 = 64%:2%); ^{1}H NMR (**3ba**) δ 8.63 (d, *J* = 2.1 Hz, 1H), 8.39 (d, *J* = 8.3 Hz, 1H), 8.00 (d, *J* = 7.1 Hz, 1H), 7.92-7.84 (m, 1H), 7.80-7.72 (m, 1H), 7.64 (d, *J* = 8.8 Hz, 1H), 7.45-7.40 (m, 3H), 7.36-7.29 (m, 3H), 7.11-7.06 (m, 1H), 6.79 (d, *J* = 7.7 Hz, 1H), 2.55(s, 3H); ^{13}C NMR (**3ba**) δ 140.8, 138.6, 138.1, 137.1, 136.1, 134.7, 133.2, 133.0, 132.7, 132.2, 131.9, 129.9, 129.8, 129.8, 128.3, 128.0, 127.5, 127.1, 126.4, 124.4, 122.8, 121.5, 121.2, 120.2, 21.7; HRMS (DART, positive): m/z calcd. For $C_{27}H_{21}ClN^+$ $[M+NH_4]^+$ 394.1357, found 394.1352.

5-Chloro-8-(4-methoxyphenyl)benzo[*b*]fluoranthene (3ca) and 2-chloro-6-(4-methoxyphenyl)benzo[3,4]cyclobuta[1,2-*c*]phenanthrene (4ca)



3ca

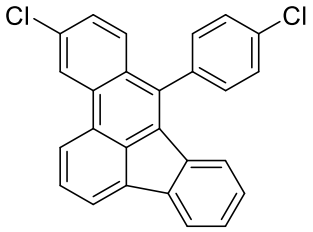


4ca

Separated by PTLC (hexane/toluene = 4/1, Rf = 0.55). The title compounds were obtained as a yellow solid (13.0 mg, **3ca**:**4ca** = 12:1 = 61%:5%); ^{1}H NMR (**3ca**) δ 8.62 (d, *J* = 2.1 Hz, 1H), 8.34 (d, *J* = 2.1 Hz, 1H), 7.99 (d, *J* = 7.1 Hz, 1H), 7.88 (d, *J* = 7.5 Hz, 1H), 7.75 (dd, *J* = 8.1, 7.2 Hz, 1H), 7.65 (d, *J* = 8.8 Hz, 1H), 7.44 (dd, *J* = 8.8, 2.1 Hz, 1H), 7.39-7.35 (m, 2H), 7.34-7.29 (m, 1H), 7.17-7.06 (m, 3H), 6.82 (d, *J* = 7.7 Hz, 1H), 3.97 (s, 3H); ^{13}C NMR (**3ca**) δ 159.7, 140.8, 138.6, 137.1, 135.8, 133.2, 133.2, 133.0, 132.2, 132.0, 131.2, 129.9, 129.8, 128.3, 128.0, 127.5, 127.1, 126.4, 124.4, 122.8,

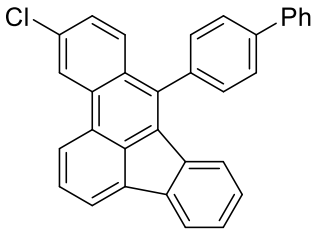
121.5, 121.3, 120.2, 114.5, 55.5; HRMS (DART, positive): m/z calcd. For $C_{27}H_{21}ClNO^+$ $[M+NH_4]^+$ 410.1306, found 410.1301.

5-Chloro-8-(4-chlorophenyl)benzo[*b*]fluoranthene (3da)



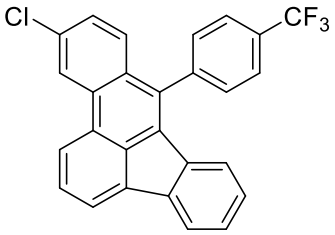
Isolated by PTLC (hexane/toluene = 4/1, Rf = 0.75). The title compound was obtained as a yellow solid (15.5 mg, 77 %); mp 156-157 °C; ^{1}H NMR δ 8.63 (d, *J* = 2.1 Hz, 1H), 8.38 (d, *J* = 8.1 Hz, 1H), 7.99 (d, *J* = 7.2 Hz, 1H), 7.88 (d, *J* = 7.5 Hz, 1H), 7.76 (dd, *J* = 8.1, 7.2 Hz, 1H), 7.62-7.57 (m, 2H), 7.55 (d, *J* = 8.8 Hz, 1H), 7.44 (dd, *J* = 8.8, 2.1 Hz, 1H), 7.42-7.37 (m, 2H), 7.37-7.31 (m, 1H), 7.11 (m, 1H), 6.76 (d, *J* = 7.7 Hz, 1H); ^{13}C NMR δ 140.9, 138.2, 137.1, 136.3, 134.5, 134.4, 133.4, 132.9, 132.5, 132.1, 131.9, 131.5, 129.5, 127.5, 128.6, 128.3, 127.6, 127.3, 126.6, 124.2, 122.9, 121.6, 121.4, 120.3; HRMS (DART, positive): m/z calcd. For $C_{26}H_{14}Cl_2^+$ $[M]^+$ 396.0467, found 396.0457.

8-([1,1'-Biphenyl]-4-yl)-5-chlorobenzo[*b*]fluoranthene (3ea)

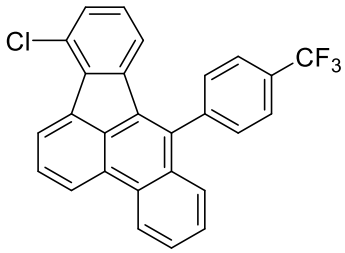


Isolated by PTLC (hexane/toluene = 9/1, Rf = 0.50). The title compound was obtained as a yellow solid (16.5 mg, 75 %); mp 249-250 °C; ^{1}H NMR δ 8.68 (d, *J* = 2.2 Hz, 1H), 8.44 (d, *J* = 8.1 Hz, 1H), 8.04 (d, *J* = 7.0 Hz, 1H), 7.92-7.87 (m, 3H), 7.82-7.79 (m, 3H), 7.72 (d, *J* = 8.8 Hz, 1H), 7.57-7.53 (m, 4H), 7.49-7.42 (m, 2H), 7.35-7.32 (m, 1H), 7.11-7.07 (m, 1H), 6.87 (d, *J* = 7.7 Hz, 1H); ^{13}C NMR δ 141.1, 140.9, 140.7, 138.5, 137.2, 136.8, 135.6, 133.4, 132.8, 132.8, 132.3, 132.0, 130.5, 129.9, 129.1, 128.5, 128.1, 127.8, 127.7, 127.6, 127.3, 127.3, 126.6, 124.4, 122.9, 121.6, 121.3, 120.3; HRMS (DART, positive): m/z calcd. for $C_{32}H_{23}ClN^+$ $[M + NH_4]^+$ 456.1514, found 456.1510.

5-Chloro-8-(4-trifluoromethylphenyl)benzo[*b*]fluoranthene (3fa) and 11-chloro-8-(4-trifluoromethylphenyl)benzo[*b*]fluoranthene (2fa)



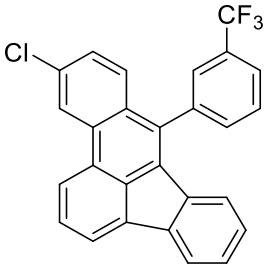
3fa



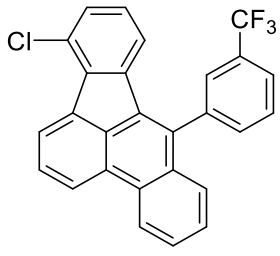
2fa

Separated by PTLC (hexane/toluene = 14/1, Rf = 0.45). The title compounds were obtained as a yellow solid (14.8 mg, **3fa**:**2fa** = 4.3:1 = 55%:13%); ^{1}H NMR δ 8.74 (d, *J* = 8.0 Hz, 1H (minor)), 8.67 (d, *J* = 2.0 Hz, 1H (major)), 8.54 (d, *J* = 8.2 Hz, 1H (minor)), 8.42 (d, *J* = 8.2 Hz, 1H (major)), 8.03 (d, *J* = 7.0 Hz, 1H (major)), 8.00 (d, *J* = 7.1 Hz, 1H (minor)), 7.94-7.88 (m, 3H (major) + 2H (minor)), 7.86 (d, *J* = 1.9 Hz, 1H (minor)), 7.83-7.78 (m, 1H (major) + 1H (minor)), 7.76-7.68 (m, 1H (minor)), 7.64-7.61 (m, 2H (major) + 2H (minor)), 7.58-7.54 (m, 2H (minor)), 7.50-7.45 (m, 2H (major)), 7.36-7.33 (m, 1H (major)), 7.12-7.08 (m, 1H (major)), 7.06 (dd, *J* = 8.2, 2.0 Hz, 1H (minor)), 6.66 (d, *J* = 7.7 Hz, 1H (major)), 6.56 (d, *J* = 8.2 Hz, 1H (minor)); ^{13}C NMR (**3fa**) δ 141.8, 140.9, 138.0, 137.2, 134.0, 133.6, 132.8, 132.0, 132.0 (q, *J* = 35.0 Hz), 131.9, 130.6, 129.3, 128.8, 128.4, 127.7, 127.4, 126.8, 126.6, 126.2 (q, *J* = 3.5 Hz), 124.4 (q, *J* = 274.2 Hz), 124.1, 123.0, 121.7, 121.5, 120.4; ^{19}F NMR (**3fa**) δ -62.2; HRMS (DART, positive): m/z calcd. For $C_{27}H_{15}ClF_3^+$ $[M+H]^+$ 430.0731, found 430.0727.

5-Chloro-8-(3-trifluoromethylphenyl)benzo[*b*]fluoranthene (3ga) and 11-chloro-8-(3-trifluoromethylphenyl)benzo[*b*]fluoranthene (2ga)



3ga

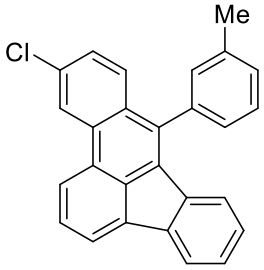


2ga

Separated by PTLC (hexane/toluene = 4/1, Rf = 0.50). The title compounds were obtained as a yellow solid (20.0 mg, **3ga**:**2ga** = 6.7:1 = 80%:11%); ^{1}H NMR δ 8.74 (d, *J* = 8.5 Hz, 1H (minor)), 8.67 (d, *J* = 2.0 Hz, 1H (major)), 8.54 (d, *J* = 8.1 Hz, 1H (minor)), 8.42 (d, *J* = 8.1 Hz, 1H (major)), 8.04-8.01 (m, 1H (major)), 7.99 (d, *J* = 7.1 Hz, 1H (minor)), 7.92-7.88 (m, 2H (major)), 7.86 (d, *J* = 1.9 Hz, 1H (minor)), 7.84-7.74 (m, 3H (major) + 3H (minor)), 7.73 (s, 1H (minor)), 7.70-7.67 (m, 1H (major) +

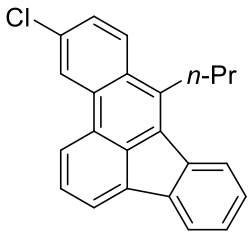
1H (minor)), 7.64-7.53 (m, 3H (minor)), 7.53-7.46 (m, 2H (major)), 7.36-7.32 (m, 1H (major)), 7.11-7.06 (m, 1H (major)), 7.05 (dd, J = 8.2, 2.0 Hz, 1H (minor)), 6.62 (d, J = 7.7 Hz, 1H (major)), 6.52 (d, J = 8.2 Hz, 1H (minor)); ^{13}C NMR (**3ga**) δ 141.0, 138.8, 138.0, 137.2, 133.8, 133.6 (q, J = 1.2 Hz), 133.6, 133.1, 132.3, 132.0, 131.9, 131.7 (q, J = 32.8Hz), 129.7, 129.3, 128.8, 128.4, 127.7, 127.5, 127.0 (q, J = 3.7 Hz), 126.7, 125.4 (q, J = 3.7 Hz), 124.2 (q, J = 272.9 Hz), 124.0, 123.0, 121.7, 121.5, 120.4; ^{19}F NMR (**3ga**) δ -62.3; HRMS (DART, positive): m/z calcd. For $C_{27}H_{18}ClF_3N^+$ $[M+NH_4]^+$ 448.1074, found 448.1072.

5-Chloro-8-(3-methylphenyl)benzo[*b*]fluoranthene (3ha)

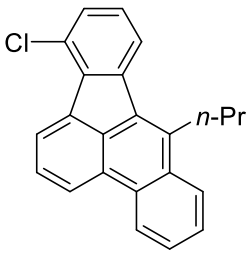


Isolated by PTLC (hexane/toluene = 9/1, Rf = 0.30). The title compound was obtained as a yellow solid (5.9 mg, 31%); mp 47-48 °C; ^{1}H NMR δ 8.66 (d, J = 2.1 Hz, 1H), 8.43 (d, J = 8.1 Hz, 1H), 8.03 (d, J = 7.1 Hz, 1H), 7.90 (d, J = 7.5 Hz, 1H), 7.79 (dd, J = 8.1, 7.2 Hz, 1H), 7.66 (d, J = 8.8 Hz, 1H), 7.53 -7.41 (m, 3H), 7.34-7.27 (m, 3H), 7.11-7.07 (m, 1H), 6.76 (d, J = 7.7 Hz, 1H), 2.48 (s, 3H); ^{13}C NMR δ 140.8, 138.8, 138.6, 137.7, 137.2, 136.2, 133.3, 132.9, 132.6, 131.9, 130.6, 130.0, 129.1, 129.0, 128.4, 128.0, 127.6, 127.2, 127.0, 126.5, 124.4, 122.8, 121.6, 121.3, 120.2, 21.7 (a pair of peaks at the aromatic region was overlapped); HRMS (DART, positive): m/z calcd. for $C_{27}H_{21}ClN^+$ $[M+NH_4]^+$ 394.1357, found 394.1353.

5-Chloro-8-propylbenzo[*b*]fluoranthene (3ia), and 11-chloro-8-propylbenzo[*b*]fluoranthene (2ia)



3ia

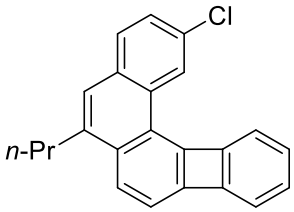


2ia

Separated by PTLC (hexane/toluene = 14/1, Rf = 0.40). The title compounds were obtained as a yellow solid (13.0 mg, **3ia**:**2ia** = 12:1 = 72%:6%); ^{1}H NMR δ 8.71-8.69 (m, 1H (minor)), 8.63 (d, J = 2.2 Hz, 1H (major)), 8.48 (d, J = 8.4 Hz, 1H (minor)), 8.36-8.34 (m, 1H (major)), 8.31-8.29 (m,

1H (minor)), 8.21 (d, *J* = 8.9 Hz, 1H (major)), 8.07-8.05 (m, 1H (major) + 1H (minor)), 8.00-7.96 (m, 2H (major) + 2H (minor)), 7.92 (d, *J* = 2.0 Hz, 1H (minor)), 7.74-7.68 (m, 1H (major) + 1H (minor)), 7.61 (dd, *J* = 8.9, 2.2 Hz, 1H (major)), 7.45-7.43 (m, 2H (major) +2H (minor)), 3.55-3.52 (m, 2H (major) +2H (minor)), 1.96-1.88 (m, 2H (major)+ 2H (minor)), 1.25-1.21 (m, 3H (major) + 3H (minor)); ^{13}C NMR (**3ia**) δ 140.9, 136.9, 136.5, 133.1, 132.4, 132.4, 132.3, 132.1, 127.8, 127.7, 127.7, 127.3, 127.2, 124.7, 123.2, 121.5, 121.5, 119.8, 31.3, 23.7, 14.8 (two pairs of peaks at the aromatic region were overlapped); HRMS (DART, positive): m/z calcd. for $C_{23}H_{18}Cl^+$ $[M+H]^+$ 329.1092, found 329.1087.

2-Chloro-6-propylbenzo[3,4]cyclobuta[1,2-*c*]phenanthrene (4ia)



Isolated by PTLC (hexane/toluene = 14/1, Rf = 0.45). The title compound was obtained as a yellow solid (3.3 mg, 20%); mp 125-126 °C; ^{1}H NMR δ 8.15 (d, *J* = 2.0 Hz, 1H), 7.58-7.53 (m, 2H), 7.45-7.43 (m, 1H), 7.21 (s, 1H), 7.00-6.97 (m, 2H), 6.81-6.72 (m, 2H), 6.60-6.58 (m, 1H), 2.88-2.85 (m, 2H), 1.80-1.73 (m, 2H), 1.05-1.03 (m, 3H); ^{13}C NMR δ 151.9, 151.8, 150.1, 147.9, 138.2, 132.8, 131.4, 131.0, 129.7, 128.8, 128.8, 128.5, 127.7, 125.4, 125.1, 125.0, 124.7, 118.5, 116.9, 116.6, 35.8, 23.2, 14.4; m/z calcd. for $C_{23}H_{21}ClN^+$ $[M+NH_4]^+$ 346.1357, found 346.1353.

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7) Cartesian coordinates of stationary points optimized at M06/SDD for Au and M06/6-31G(d,p) for other atoms

1ab (NIMGA = 0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.717536	1.362164	-1.678192
2	6	0	-2.239281	2.551176	-2.199942
3	6	0	-1.096963	3.196527	-1.668455
4	6	0	-0.503057	2.561757	-0.610591
5	6	0	-0.990407	1.340275	-0.076944
6	6	0	-2.099627	0.697917	-0.580742
7	6	0	0.582341	2.579944	0.425222
8	6	0	0.085194	1.367169	0.968726
9	6	0	1.682916	3.216588	0.937578
10	6	0	2.289946	2.590712	2.052953
11	6	0	1.796193	1.410777	2.590943
12	6	0	0.662062	0.757965	2.052721
13	6	0	-2.665351	-0.558104	-0.052057
14	6	0	-1.866347	-1.699072	0.193766
15	6	0	-2.468860	-2.870476	0.682190
16	6	0	-3.833301	-2.925929	0.922152
17	6	0	-4.624350	-1.806147	0.672527
18	6	0	-4.040368	-0.641857	0.189004
19	6	0	-0.469007	-1.702581	-0.076259
20	6	0	0.726867	-1.715339	-0.292465
21	6	0	2.129583	-1.660257	-0.531687
22	6	0	2.758789	-0.418001	-0.713319
23	6	0	4.128198	-0.354435	-0.932206
24	6	0	4.887279	-1.522567	-0.979246
25	6	0	4.269313	-2.759391	-0.804673
26	6	0	2.900034	-2.831827	-0.581737
27	1	0	-3.587243	0.895439	-2.138249
28	1	0	-2.753886	2.996373	-3.048506
29	1	0	-0.736925	4.132871	-2.086269
30	1	0	2.082225	4.142705	0.531819
31	1	0	3.168693	3.047725	2.502605
32	1	0	2.301473	0.970241	3.447402
33	1	0	0.296878	-0.174960	2.474872
34	1	0	-1.840412	-3.740260	0.859300
35	1	0	-4.280638	-3.841798	1.300301
36	1	0	-5.694839	-1.837500	0.860259
37	1	0	-4.655090	0.238775	0.010704
38	1	0	2.159823	0.490314	-0.668219
39	1	0	4.605838	0.613612	-1.064736
40	1	0	5.959736	-1.469276	-1.151116
41	1	0	4.858111	-3.672921	-0.842067
42	1	0	2.410704	-3.793268	-0.443704

Au[P(OMe)$_3$] (NIMGA = 0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	1.332594	-0.000249	0.000719
2	15	0	-1.031793	0.000281	-0.000582
3	8	0	-1.714397	1.523830	0.109883
4	8	0	-1.714647	-0.857963	1.262851
5	8	0	-1.712766	-0.665686	-1.376218
6	6	0	-1.797254	-0.316853	2.632633
7	1	0	-2.385855	0.602322	2.628658
8	1	0	-2.298250	-1.100708	3.197241
9	1	0	-0.792211	-0.146022	3.032478
10	6	0	-1.790147	2.441086	-1.042819
11	1	0	-2.374384	1.979447	-1.840917
12	1	0	-2.293012	3.321690	-0.648022

13	1	0	-0.782981	2.701968	-1.384524
14	6	0	-1.792214	-2.122765	-1.592130
15	1	0	-2.379176	-2.579996	-0.793491
16	1	0	-2.293700	-2.221197	-2.552865
17	1	0	-0.786282	-2.552316	-1.644844

Int1 (NIMGA = 0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.029738	-1.642080	-0.699488
2	6	0	2.669378	-2.871195	-0.166549
3	6	0	1.933715	-2.986699	1.044941
4	6	0	1.592999	-1.805366	1.650238
5	6	0	1.948138	-0.533467	1.096538
6	6	0	2.677690	-0.404505	-0.073753
7	6	0	0.967575	-1.105899	2.836102
8	6	0	1.335138	0.160334	2.290590
9	6	0	0.316464	-1.219830	4.038553
10	6	0	0.023554	0.000800	4.701032
11	6	0	0.383360	1.233832	4.167897
12	6	0	1.062668	1.345343	2.926366
13	6	0	3.115566	0.889486	-0.633519
14	6	0	2.223584	1.970554	-0.828142
15	6	0	2.705928	3.193518	-1.329590
16	6	0	4.049063	3.346476	-1.648408
17	6	0	4.928733	2.276700	-1.475207
18	6	0	4.462522	1.064519	-0.973373
19	6	0	0.807176	1.867112	-0.582156
20	6	0	-0.351141	2.290942	-0.376228
21	6	0	-1.676119	2.754871	-0.139448
22	6	0	-2.294340	2.528230	1.107894
23	6	0	-3.595814	2.966121	1.320766
24	6	0	-4.285533	3.634419	0.304689
25	6	0	-3.676256	3.865725	-0.931326
26	6	0	-2.377857	3.424766	-1.161089
27	1	0	3.596678	-1.604022	-1.627218
28	1	0	2.968753	-3.777440	-0.685871
29	1	0	1.683910	-3.962513	1.447778
30	1	0	0.046125	-2.170757	4.487487
31	1	0	-0.485780	-0.031637	5.659626
32	1	0	0.150459	2.137833	4.723205
33	1	0	1.349957	2.316366	2.532932
34	1	0	2.008657	4.012970	-1.478343
35	1	0	4.407537	4.294653	-2.035356
36	1	0	5.979102	2.389478	-1.724083
37	1	0	5.154068	0.241749	-0.812233
38	1	0	-1.741420	2.011059	1.890121
39	1	0	-4.074335	2.793547	2.279397
40	1	0	-5.300528	3.978417	0.478216
41	1	0	-4.215593	4.389061	-1.714209
42	1	0	-1.894726	3.592238	-2.119612
43	79	0	-0.242204	-0.147098	-0.596035
44	15	0	-1.533203	-2.120129	-0.883881
45	8	0	-1.268261	-3.477697	0.086002
46	8	0	-1.451627	-2.797432	-2.432842
47	8	0	-3.199334	-1.896615	-0.687470
48	6	0	-1.704126	-3.481770	1.482489
49	6	0	-0.198227	-3.398588	-2.888622
50	6	0	-3.880099	-0.844412	-1.438399
51	1	0	-2.794734	-3.440595	1.529019
52	1	0	-1.340894	-4.426094	1.886319
53	1	0	-1.260168	-2.641129	2.032512
54	1	0	0.009644	-4.301914	-2.309097
55	1	0	-0.367484	-3.647009	-3.934852
56	1	0	0.632004	-2.684772	-2.802120
57	1	0	-3.855016	-1.074590	-2.507205
58	1	0	-4.905782	-0.854962	-1.073481

59	1	0	-3.425333	0.137066	-1.240231

TS1 (NIMGA = 1, 410.90*i* cm^{-1})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.787352	1.365150	-2.113574
2	6	0	4.482437	0.239607	-2.547245
3	6	0	4.653683	-0.921181	-1.744369
4	6	0	4.033003	-0.898929	-0.525779
5	6	0	3.211077	0.216103	-0.095140
6	6	0	3.173343	1.410225	-0.840286
7	6	0	3.974082	-1.485137	0.844363
8	6	0	3.268914	-0.346149	1.316430
9	6	0	4.342823	-2.515666	1.681779
10	6	0	3.966168	-2.366491	3.034394
11	6	0	3.278561	-1.241078	3.492528
12	6	0	2.908612	-0.181188	2.630178
13	6	0	2.421570	2.564679	-0.346738
14	6	0	1.087137	2.350040	0.082153
15	6	0	0.347291	3.431827	0.565045
16	6	0	0.913625	4.705437	0.632116
17	6	0	2.220077	4.914261	0.194540
18	6	0	2.970761	3.845976	-0.300920
19	6	0	0.523700	1.012882	-0.094168
20	6	0	1.173870	-0.075587	-0.428074
21	79	0	-1.513466	0.555967	0.061160
22	6	0	1.041135	-1.469366	-0.765270
23	6	0	0.914082	-2.439444	0.248589
24	6	0	0.755285	-3.780668	-0.090843
25	6	0	0.731897	-4.165011	-1.433521
26	6	0	0.860304	-3.207507	-2.445435
27	6	0	1.016998	-1.865283	-2.116981
28	1	0	3.704921	2.233411	-2.761600
29	1	0	4.943467	0.262987	-3.530998
30	1	0	5.293942	-1.730451	-2.076847
31	1	0	4.891443	-3.390522	1.349609
32	1	0	4.224831	-3.147659	3.742741
33	1	0	3.017840	-1.177840	4.544880
34	1	0	2.373126	0.686770	3.002151
35	1	0	-0.682235	3.273849	0.878383
36	1	0	0.328309	5.536220	1.012959
37	1	0	2.656692	5.907006	0.235021
38	1	0	3.995450	4.001033	-0.629175
39	1	0	0.928739	-2.125097	1.289918
40	1	0	0.652446	-4.526753	0.691080
41	1	0	0.613420	-5.212617	-1.693970
42	1	0	0.837412	-3.511453	-3.487348
43	1	0	1.116578	-1.108121	-2.891015
44	15	0	-3.785286	-0.157002	0.181483
45	8	0	-4.155203	-1.444246	-0.892448
46	8	0	-5.107422	0.842061	-0.171681
47	8	0	-4.195407	-0.698830	1.719916
48	6	0	-3.197186	-2.535947	-1.022891
49	6	0	-5.320439	1.319972	-1.536202
50	6	0	-5.567630	-1.113145	2.041343
51	1	0	-3.092959	-3.069793	-0.071547
52	1	0	-3.614616	-3.199775	-1.778976
53	1	0	-2.217163	-2.166062	-1.355796
54	1	0	-5.552634	0.479854	-2.194930
55	1	0	-6.168615	1.999318	-1.468140
56	1	0	-4.438842	1.862644	-1.898440
57	1	0	-5.924435	-1.843490	1.308914
58	1	0	-5.494517	-1.563253	3.029961
59	1	0	-6.220477	-0.238762	2.056805

Int2 (NIMGA = 0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.150104	1.739357	-1.760152
2	6	0	4.807658	0.667513	-2.383754
3	6	0	4.698421	-0.666377	-1.947736
4	6	0	3.832526	-0.904726	-0.907085
5	6	0	2.875699	0.155960	-0.366506
6	6	0	3.195663	1.540754	-0.764206
7	6	0	3.898977	-1.616978	0.362019
8	6	0	3.363917	-0.478283	0.990590
9	6	0	4.421699	-2.682424	1.084744
10	6	0	4.372411	-2.537026	2.475268
11	6	0	3.869180	-1.375621	3.090346
12	6	0	3.368361	-0.286940	2.354839
13	6	0	2.367955	2.591066	-0.232331
14	6	0	1.032812	2.260588	0.148970
15	6	0	0.222677	3.290913	0.642031
16	6	0	0.701141	4.592163	0.767598
17	6	0	2.007561	4.911215	0.377081
18	6	0	2.828305	3.918296	-0.135321
19	6	0	0.507164	0.905106	-0.062684
20	6	0	1.351298	-0.107852	-0.377503
21	79	0	-1.517666	0.470466	0.021811
22	6	0	0.935291	-1.523620	-0.512128
23	6	0	0.364565	-2.208137	0.572700
24	6	0	-0.042777	-3.536047	0.437023
25	6	0	0.116447	-4.194628	-0.783346
26	6	0	0.689516	-3.523641	-1.866979
27	6	0	1.105032	-2.199957	-1.729254
28	1	0	4.330539	2.744126	-2.129953
29	1	0	5.501573	0.893790	-3.189523
30	1	0	5.390729	-1.420639	-2.306831
31	1	0	4.842769	-3.569079	0.624493
32	1	0	4.745414	-3.337903	3.105760
33	1	0	3.855800	-1.327369	4.175286
34	1	0	2.982637	0.604607	2.838166
35	1	0	-0.802935	3.055836	0.918104
36	1	0	0.051627	5.367919	1.161520
37	1	0	2.375766	5.926804	0.476698
38	1	0	3.852102	4.153206	-0.416077
39	1	0	0.253209	-1.690594	1.523979
40	1	0	-0.478299	-4.056880	1.284982
41	1	0	-0.197910	-5.228779	-0.889342
42	1	0	0.808740	-4.031616	-2.819515
43	1	0	1.542046	-1.674227	-2.576715
44	15	0	-3.817769	-0.214850	0.027008
45	8	0	-4.196246	-1.400229	-1.131159
46	8	0	-5.055718	0.910500	-0.261212
47	8	0	-4.403708	-0.959277	1.438862
48	6	0	-3.408024	-2.628381	-1.157967
49	6	0	-5.173101	1.525117	-1.580528
50	6	0	-4.653023	-0.146233	2.625113
51	1	0	-3.560132	-3.190974	-0.231379
52	1	0	-3.788112	-3.194264	-2.007306
53	1	0	-2.340601	-2.411276	-1.302015
54	1	0	-5.460664	0.770753	-2.317080
55	1	0	-5.956440	2.274589	-1.478634
56	1	0	-4.232022	2.008131	-1.872549
57	1	0	-5.470397	0.553284	2.432647
58	1	0	-4.935624	-0.853500	3.403382
59	1	0	-3.747061	0.394994	2.926736

TS2 (NIMGA = 1, 463.72*i* cm^{-1})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	4.634642	1.505747	-1.426150
2	6	0	5.383208	0.409051	-1.787605
3	6	0	5.084847	-0.897505	-1.282111
4	6	0	3.916936	-1.071770	-0.609172
5	6	0	2.962805	0.045528	-0.441828
6	6	0	3.417382	1.378086	-0.690414
7	6	0	3.558145	-1.801409	0.624119
8	6	0	2.756826	-0.780674	1.151294
9	6	0	3.944497	-2.851373	1.435098
10	6	0	3.486058	-2.820841	2.768315
11	6	0	2.731758	-1.758022	3.267795
12	6	0	2.342140	-0.670282	2.451246
13	6	0	2.589549	2.459719	-0.280686
14	6	0	1.241642	2.182215	0.154182
15	6	0	0.447513	3.279374	0.582426
16	6	0	0.935968	4.565033	0.586007
17	6	0	2.250659	4.830505	0.137609
18	6	0	3.052239	3.800962	-0.295281
19	6	0	0.666948	0.876370	0.031455
20	6	0	1.487475	-0.212042	-0.287232
21	79	0	-1.376293	0.532400	0.075198
22	6	0	0.911971	-1.523509	-0.691536
23	6	0	0.116737	-2.277728	0.184734
24	6	0	-0.496601	-3.449587	-0.253984
25	6	0	-0.316317	-3.881954	-1.570549
26	6	0	0.482437	-3.142021	-2.443913
27	6	0	1.100300	-1.970262	-2.005908
28	1	0	4.951095	2.490887	-1.752890
29	1	0	6.277875	0.550160	-2.386052
30	1	0	5.839580	-1.676935	-1.318623
31	1	0	4.598132	-3.645428	1.089704
32	1	0	3.746545	-3.637347	3.434232
33	1	0	2.409337	-1.772431	4.304430
34	1	0	1.725144	0.141093	2.823051
35	1	0	-0.570900	3.073602	0.905010
36	1	0	0.310170	5.383942	0.926661
37	1	0	2.626859	5.848360	0.143128
38	1	0	4.069834	4.012257	-0.609412
39	1	0	-0.009331	-1.947604	1.214589
40	1	0	-1.109279	-4.027524	0.431810
41	1	0	-0.789592	-4.798140	-1.911282
42	1	0	0.626223	-3.476669	-3.466777
43	1	0	1.718269	-1.390437	-2.687986
44	15	0	-3.698728	-0.059593	0.005944
45	8	0	-4.213668	-0.720322	-1.472680
46	8	0	-4.911403	1.095326	0.272835
47	8	0	-4.179877	-1.279806	1.087595
48	6	0	-3.533424	-1.904284	-1.989062
49	6	0	-5.154179	2.132688	-0.727380
50	6	0	-4.420331	-0.949514	2.489763
51	1	0	-3.741638	-2.762573	-1.343166
52	1	0	-3.951717	-2.066398	-2.981357
53	1	0	-2.449429	-1.737907	-2.062826
54	1	0	-5.544690	1.681022	-1.642388
55	1	0	-5.896738	2.791643	-0.280309
56	1	0	-4.235714	2.694800	-0.937668
57	1	0	-5.268602	-0.265943	2.571763
58	1	0	-4.648966	-1.898695	2.971968
59	1	0	-3.525799	-0.506026	2.945237

Int3 (NIMGA = 0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.044171	-0.790270	-1.050663
2	6	0	5.667059	0.444156	-1.221644
3	6	0	4.963852	1.649049	-1.069310
4	6	0	3.630178	1.595460	-0.674103

5	6	0	3.053546	0.353919	-0.399281
6	6	0	3.693830	-0.851433	-0.647542
7	6	0	2.555695	2.594265	-0.636414
8	6	0	1.331918	1.943327	-0.347211
9	6	0	2.586313	3.951550	-0.936156
10	6	0	1.385278	4.663607	-0.972499
11	6	0	0.173692	4.018578	-0.723259
12	6	0	0.141325	2.655258	-0.402960
13	6	0	2.869469	-2.056682	-0.610975
14	6	0	1.432958	-1.929945	-0.502343
15	6	0	0.642962	-3.108877	-0.596344
16	6	0	1.212971	-4.356188	-0.750529
17	6	0	2.609820	-4.463594	-0.819382
18	6	0	3.418502	-3.333240	-0.755953
19	6	0	0.779795	-0.676939	-0.296680
20	6	0	1.633799	0.494686	0.047920
21	79	0	-1.274504	-0.459564	-0.275181
22	6	0	1.507419	0.327961	1.628208
23	6	0	0.433786	0.923029	2.307606
24	6	0	0.315297	0.791281	3.690620
25	6	0	1.255366	0.053715	4.408784
26	6	0	2.319178	-0.548382	3.735512
27	6	0	2.440906	-0.422037	2.353509
28	1	0	5.600745	-1.696236	-1.271041
29	1	0	6.706534	0.472680	-1.532861
30	1	0	5.448454	2.594363	-1.296166
31	1	0	3.526878	4.449622	-1.155632
32	1	0	1.392940	5.722517	-1.211109
33	1	0	-0.756290	4.576951	-0.777492
34	1	0	-0.820170	2.176936	-0.217788
35	1	0	-0.437922	-3.004993	-0.524969
36	1	0	0.592698	-5.243494	-0.810945
37	1	0	3.068752	-5.441604	-0.930017
38	1	0	4.495499	-3.450297	-0.821280
39	1	0	-0.289991	1.529595	1.772432
40	1	0	-0.506263	1.279542	4.206523
41	1	0	1.164485	-0.046876	5.485703
42	1	0	3.063227	-1.114318	4.287267
43	1	0	3.280860	-0.892269	1.852771
44	15	0	-3.629356	0.016775	-0.236717
45	8	0	-4.469814	-0.382035	1.182417
46	8	0	-4.660230	-0.617893	-1.417550
47	8	0	-3.949387	1.677750	-0.369283
48	6	0	-4.109173	0.271815	2.438800
49	6	0	-5.069842	-2.021824	-1.368920
50	6	0	-3.958979	2.330638	-1.679559
51	1	0	-4.369380	1.332318	2.391510
52	1	0	-4.700339	-0.230930	3.202489
53	1	0	-3.039565	0.143151	2.653621
54	1	0	-5.669850	-2.201559	-0.473986
55	1	0	-5.666635	-2.172034	-2.266870
56	1	0	-4.194471	-2.682013	-1.388650
57	1	0	-4.744198	1.900018	-2.304669
58	1	0	-4.169547	3.378324	-1.470209
59	1	0	-2.981410	2.234690	-2.168634

TS3 (NIMGA = 1, 207.84*i* cm^{-1})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.907264	-0.949476	-1.398048
2	6	0	5.584084	0.247175	-1.619676
3	6	0	4.984278	1.498618	-1.387327
4	6	0	3.695938	1.520307	-0.876089
5	6	0	3.060142	0.305632	-0.583449
6	6	0	3.594625	-0.940849	-0.881030
7	6	0	2.702003	2.588828	-0.689055
8	6	0	1.465667	2.005323	-0.309994

9	6	0	2.794287	3.952527	-0.930884
10	6	0	1.643182	4.738027	-0.813342
11	6	0	0.416949	4.159488	-0.482947
12	6	0	0.319686	2.786152	-0.229523
13	6	0	2.727856	-2.108904	-0.693903
14	6	0	1.380679	-1.924854	-0.256428
15	6	0	0.565319	-3.057362	-0.093220
16	6	0	1.035898	-4.336738	-0.353358
17	6	0	2.352409	-4.511061	-0.789495
18	6	0	3.181802	-3.409766	-0.956215
19	6	0	0.805410	-0.587028	0.030083
20	6	0	1.696638	0.537163	-0.093635
21	79	0	-1.264427	-0.339893	-0.107337
22	6	0	1.460034	0.065298	1.574298
23	6	0	0.582611	0.847530	2.352143
24	6	0	0.722930	0.899763	3.732069
25	6	0	1.743934	0.180301	4.359095
26	6	0	2.624300	-0.592815	3.597807
27	6	0	2.485919	-0.651919	2.217619
28	1	0	5.398016	-1.884187	-1.650666
29	1	0	6.592894	0.213131	-2.019764
30	1	0	5.514529	2.412974	-1.636856
31	1	0	3.738528	4.401850	-1.226007
32	1	0	1.699343	5.805411	-1.003163
33	1	0	-0.474421	4.776658	-0.431709
34	1	0	-0.655373	2.353027	-0.006012
35	1	0	-0.457649	-2.914636	0.251262
36	1	0	0.385737	-5.195105	-0.219045
37	1	0	2.729795	-5.507265	-0.997899
38	1	0	4.202374	-3.563977	-1.293304
39	1	0	-0.206816	1.420354	1.877138
40	1	0	0.039007	1.503788	4.319057
41	1	0	1.854346	0.223730	5.438122
42	1	0	3.420185	-1.149565	4.081039
43	1	0	3.173811	-1.262472	1.642655
44	15	0	-3.601391	0.073188	-0.394066
45	8	0	-3.940843	1.638351	0.130376
46	8	0	-4.741275	-0.943461	0.385610
47	8	0	-4.311750	0.083568	-1.931407
48	6	0	-5.265508	2.238468	-0.076125
49	6	0	-4.607456	-1.187553	1.816779
50	6	0	-4.492170	-1.168756	-2.665002
51	1	0	-6.048338	1.564199	0.285153
52	1	0	-5.249547	3.156363	0.509259
53	1	0	-5.410097	2.452798	-1.136452
54	1	0	-4.783475	-0.263217	2.377667
55	1	0	-5.373541	-1.922484	2.060022
56	1	0	-3.616834	-1.593152	2.058060
57	1	0	-5.202350	-1.810494	-2.138143
58	1	0	-4.889522	-0.872789	-3.634443
59	1	0	-3.531319	-1.679972	-2.798859

Int4 (NIMGA = 0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.804342	-2.923632	-1.550319
2	6	0	-2.440020	-4.072249	-0.857524
3	6	0	-1.724338	-4.026438	0.358939
4	6	0	-1.365465	-2.788449	0.861400
5	6	0	-1.725717	-1.635051	0.134835
6	6	0	-2.453008	-1.646685	-1.053022
7	6	0	-0.665690	-2.333447	2.070475
8	6	0	-0.627839	-0.907542	2.074051
9	6	0	-0.088134	-3.051729	3.110435
10	6	0	0.533615	-2.354217	4.151012
11	6	0	0.580807	-0.957119	4.149404
12	6	0	0.003393	-0.219943	3.110694

13	6	0	-2.791734	-0.357644	-1.631201
14	6	0	-2.403762	0.849415	-0.955603
15	6	0	-2.800243	2.090767	-1.503323
16	6	0	-3.520854	2.156180	-2.681030
17	6	0	-3.874464	0.976491	-3.353359
18	6	0	-3.517979	-0.254658	-2.830898
19	6	0	-1.640685	0.817994	0.290756
20	6	0	-1.283297	-0.439987	0.817951
21	79	0	0.658880	0.038166	-0.319959
22	6	0	-1.395349	2.064523	1.068509
23	6	0	-2.089148	2.259883	2.270505
24	6	0	-1.863875	3.406206	3.031874
25	6	0	-0.943410	4.363783	2.603605
26	6	0	-0.257178	4.182024	1.401720
27	6	0	-0.488373	3.042285	0.632991
28	1	0	-3.372560	-3.023078	-2.469982
29	1	0	-2.728181	-5.039353	-1.258169
30	1	0	-1.482643	-4.948044	0.880769
31	1	0	-0.122441	-4.137945	3.120589
32	1	0	0.982214	-2.904303	4.972553
33	1	0	1.066375	-0.435391	4.968167
34	1	0	0.044862	0.866628	3.121568
35	1	0	-2.542042	3.006175	-0.980247
36	1	0	-3.818697	3.119979	-3.080929
37	1	0	-4.439189	1.028248	-4.278884
38	1	0	-3.813563	-1.159032	-3.353936
39	1	0	-2.798697	1.507760	2.608218
40	1	0	-2.407752	3.551176	3.960104
41	1	0	-0.767030	5.252975	3.200722
42	1	0	0.449922	4.931914	1.059482
43	1	0	0.031633	2.908590	-0.316665
44	15	0	2.882254	0.040796	-1.114914
45	8	0	3.572313	1.533802	-1.494866
46	8	0	3.232927	-0.867983	-2.491004
47	8	0	3.978549	-0.573899	0.013602
48	6	0	3.900799	2.485351	-0.430679
49	6	0	2.811267	-0.405694	-3.816491
50	6	0	3.752347	-1.899941	0.590108
51	1	0	4.699228	2.078722	0.193825
52	1	0	4.237349	3.380549	-0.950587
53	1	0	3.013967	2.712663	0.174925
54	1	0	3.333449	0.520485	-4.066867
55	1	0	3.102184	-1.205360	-4.495114
56	1	0	1.724452	-0.263137	-3.849552
57	1	0	3.865741	-2.664139	-0.183616
58	1	0	4.523204	-2.012117	1.350357
59	1	0	2.758637	-1.959236	1.057037

TS1' (NIMGA = 1, 398.84*i* cm^{-1})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.447836	0.880315	-1.761772
2	6	0	3.014648	2.161677	-1.580168
3	6	0	4.084398	2.400476	-0.704402
4	6	0	4.601638	1.281474	-0.080172
5	6	0	4.069801	-0.032939	-0.280438
6	6	0	3.004786	-0.280075	-1.101413
7	6	0	5.594540	0.735606	0.896093
8	6	0	5.065561	-0.576970	0.711226
9	6	0	6.631236	0.998517	1.759333
10	6	0	7.145427	-0.121654	2.452968
11	6	0	6.625846	-1.402249	2.273729
12	6	0	5.553558	-1.666479	1.385694
13	6	0	2.349190	-1.578946	-1.257746
14	6	0	0.937557	-1.655094	-1.145669
15	6	0	0.315219	-2.903843	-1.262523
16	6	0	1.061641	-4.057210	-1.491652

17	6	0	2.451222	-3.980031	-1.585600
18	6	0	3.089219	-2.746804	-1.461354
19	6	0	0.175358	-0.449112	-0.829742
20	6	0	0.524239	0.807703	-0.860936
21	79	0	-1.795439	-0.499911	-0.080458
22	6	0	0.090258	2.171959	-0.687321
23	6	0	-0.685646	2.795586	-1.682549
24	6	0	-1.130988	4.102256	-1.499510
25	6	0	-0.801767	4.795417	-0.331582
26	6	0	-0.028594	4.181964	0.659401
27	6	0	0.421496	2.877604	0.484169
28	1	0	1.871666	0.717527	-2.675496
29	1	0	2.591343	2.993876	-2.138194
30	1	0	4.478368	3.400076	-0.561180
31	1	0	7.046928	1.988163	1.915901
32	1	0	7.969590	0.019976	3.145230
33	1	0	7.059213	-2.226681	2.832166
34	1	0	5.163488	-2.671970	1.267208
35	1	0	-0.766805	-2.965710	-1.165479
36	1	0	0.560950	-5.015368	-1.586798
37	1	0	3.036800	-4.877590	-1.757856
38	1	0	4.170869	-2.675861	-1.551131
39	1	0	-0.937411	2.241829	-2.584266
40	1	0	-1.730943	4.581993	-2.266592
41	1	0	-1.145771	5.816030	-0.193729
42	1	0	0.221514	4.723915	1.566065
43	1	0	1.029770	2.388375	1.241267
44	15	0	-4.023334	-0.387392	0.774018
45	8	0	-4.568482	-1.569845	1.854895
46	8	0	-5.289065	-0.364126	-0.351282
47	8	0	-4.333114	1.034219	1.646133
48	6	0	-3.984232	-1.662130	3.192511
49	6	0	-5.665028	-1.590025	-1.054500
50	6	0	-4.206313	2.322491	0.968334
51	1	0	-4.239715	-0.770505	3.769952
52	1	0	-4.435376	-2.547294	3.637657
53	1	0	-2.895990	-1.787733	3.134764
54	1	0	-6.054530	-2.321665	-0.342634
55	1	0	-6.442650	-1.287750	-1.753849
56	1	0	-4.809639	-2.001214	-1.604527
57	1	0	-4.341856	3.069821	1.748432
58	1	0	-3.210467	2.434181	0.515644
59	1	0	-4.986998	2.418510	0.208961

Int2' (NIMGA = 0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.489834	-2.827405	-0.531963
2	6	0	1.044420	-1.537976	-0.494463
3	6	0	2.458911	-1.420714	-0.619251
4	6	0	3.251065	-2.572802	-0.792469
5	6	0	2.671736	-3.829209	-0.842456
6	6	0	1.282597	-3.954598	-0.702286
7	6	0	0.194375	-0.359916	-0.320358
8	6	0	0.716874	0.891004	-0.423456
9	6	0	2.204483	1.094409	-0.743010
10	6	0	3.059995	-0.120688	-0.498761
11	6	0	2.790113	2.416640	-0.386217
12	6	0	4.100572	2.606895	-0.032161
13	6	0	4.875855	1.441986	0.060690
14	6	0	4.365688	0.131418	-0.172913
15	6	0	6.199627	0.898713	0.425571
16	6	0	5.714471	-0.431759	0.232251
17	6	0	7.480140	1.175138	0.850455
18	6	0	8.295241	0.047066	1.085450
19	6	0	7.819390	-1.251787	0.906481
20	6	0	6.497239	-1.530053	0.473287

21	79	0	-1.850795	-0.520640	0.007606
22	1	0	-2.136013	3.794305	1.832103
23	6	0	-0.126482	2.110755	-0.353124
24	6	0	-0.291645	2.945906	-1.469838
25	6	0	-1.114106	4.070649	-1.400155
26	6	0	-1.780257	4.379900	-0.212432
27	6	0	-1.621618	3.558737	0.904898
28	6	0	-0.797490	2.434696	0.837826
29	1	0	-0.662052	1.799807	1.710579
30	1	0	-2.417955	5.257261	-0.158573
31	1	0	-1.241264	4.700731	-2.275596
32	1	0	0.200846	2.696250	-2.408959
33	1	0	-0.588484	-2.927347	-0.428349
34	1	0	0.823426	-4.937910	-0.731232
35	1	0	3.286437	-4.710263	-0.995166
36	1	0	4.322749	-2.461641	-0.934867
37	1	0	2.175246	1.180641	-1.865420
38	1	0	2.122395	3.271325	-0.472369
39	1	0	4.492330	3.593458	0.185508
40	1	0	7.859543	2.179879	1.001922
41	1	0	6.159598	-2.554828	0.361070
42	1	0	9.318197	0.192427	1.416896
43	1	0	8.486541	-2.084309	1.108973
44	15	0	-4.227980	-0.503780	0.342526
45	8	0	-4.908096	-1.306859	1.676118
46	8	0	-5.231177	-1.076978	-0.903050
47	8	0	-4.862260	1.059838	0.555476
48	6	0	-4.614160	-0.835136	3.025258
49	6	0	-5.262745	-2.506330	-1.195694
50	6	0	-4.727431	2.016809	-0.539229
51	1	0	-5.068633	0.146350	3.182499
52	1	0	-5.061802	-1.571558	3.690956
53	1	0	-3.531235	-0.789701	3.197829
54	1	0	-5.708442	-3.047846	-0.357274
55	1	0	-5.885360	-2.604151	-2.083616
56	1	0	-4.254629	-2.885334	-1.406875
57	1	0	-5.361616	1.711909	-1.376121
58	1	0	-5.065933	2.969708	-0.133854
59	1	0	-3.679306	2.106011	-0.858761

TS2' (NIMGA = 1, 983.08*i* cm^{-1})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.460847	-2.839154	0.375305
2	6	0	-1.028721	-1.545135	0.338484
3	6	0	-2.452612	-1.427034	0.324107
4	6	0	-3.236681	-2.594819	0.375254
5	6	0	-2.649155	-3.846332	0.422847
6	6	0	-1.250076	-3.971764	0.416998
7	6	0	-0.173789	-0.386203	0.287572
8	6	0	-0.716264	0.892394	0.366212
9	6	0	-2.250566	1.071879	0.420627
10	6	0	-3.071223	-0.123727	0.258093
11	6	0	-2.823748	2.379640	0.423087
12	6	0	-4.187746	2.582441	0.251400
13	6	0	-4.956251	1.442364	0.067119
14	6	0	-4.417885	0.130559	0.074370
15	6	0	-6.327751	0.899846	-0.181348
16	6	0	-5.805055	-0.427271	-0.190665
17	6	0	-7.654343	1.178345	-0.385570
18	6	0	-8.486167	0.053905	-0.613514
19	6	0	-7.979380	-1.240108	-0.633434
20	6	0	-6.603259	-1.517689	-0.421283
21	79	0	1.883229	-0.499033	0.037739
22	1	0	0.963027	4.594670	-1.885533
23	6	0	0.130246	2.115204	0.297905
24	6	0	0.997828	2.451338	1.346615

25	6	0	1.846231	3.553525	1.232587
26	6	0	1.833629	4.325817	0.069931
27	6	0	0.972535	3.995417	-0.980059
28	6	0	0.120407	2.898026	-0.865675
29	1	0	-0.551741	2.635586	-1.680404
30	1	0	2.489121	5.187342	-0.016634
31	1	0	2.511324	3.810420	2.051446
32	1	0	1.011316	1.841083	2.248052
33	1	0	0.624031	-2.922535	0.376531
34	1	0	-0.793244	-4.955439	0.449585
35	1	0	-3.271541	-4.734376	0.469193
36	1	0	-4.317030	-2.505789	0.409197
37	1	0	-1.541862	0.953800	1.455479
38	1	0	-2.162351	3.230144	0.560411
39	1	0	-4.603956	3.583085	0.252206
40	1	0	-8.065331	2.182105	-0.381832
41	1	0	-6.245424	-2.541735	-0.459593
42	1	0	-9.547434	0.208548	-0.781048
43	1	0	-8.656093	-2.068414	-0.820056
44	15	0	4.261269	-0.475908	-0.266200
45	8	0	5.076213	-1.896274	-0.702305
46	8	0	5.179265	0.020906	1.072344
47	8	0	4.822086	0.595018	-1.458541
48	6	0	4.913014	-2.444592	-2.047365
49	6	0	5.377959	-0.892883	2.195478
50	6	0	4.460803	2.006289	-1.359155
51	1	0	5.350355	-1.763200	-2.780858
52	1	0	5.452417	-3.390258	-2.036200
53	1	0	3.853679	-2.622556	-2.270526
54	1	0	5.957053	-1.760676	1.870955
55	1	0	5.934869	-0.318793	2.934225
56	1	0	4.415381	-1.207930	2.617423
57	1	0	4.917391	2.446197	-0.467259
58	1	0	4.865208	2.469378	-2.257952
59	1	0	3.369384	2.132686	-1.332686

Int3' (NIMGA = 0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.500967	-2.876853	0.143940
2	6	0	1.042617	-1.578396	-0.103885
3	6	0	2.474054	-1.407506	-0.128335
4	6	0	3.275561	-2.546007	0.034616
5	6	0	2.711973	-3.795016	0.251851
6	6	0	1.315357	-3.969496	0.320804
7	6	0	0.174756	-0.502896	-0.341843
8	6	0	0.722108	0.830643	-0.740433
9	6	0	2.212545	1.034490	-0.593564
10	6	0	3.055798	-0.092927	-0.305454
11	6	0	2.742091	2.302747	-0.784916
12	6	0	4.128850	2.567717	-0.694441
13	6	0	4.928980	1.494275	-0.400281
14	6	0	4.413193	0.184487	-0.202065
15	6	0	6.321308	0.995411	-0.122119
16	6	0	5.810645	-0.319278	0.091818
17	6	0	7.650820	1.300353	-0.005215
18	6	0	8.500622	0.220868	0.347279
19	6	0	8.008403	-1.059891	0.566215
20	6	0	6.629217	-1.364596	0.444486
21	79	0	-1.890062	-0.551837	-0.183639
22	1	0	-0.750149	3.328185	2.928949
23	6	0	-0.122851	1.935439	-0.114307
24	6	0	-1.060668	2.642136	-0.873946
25	6	0	-1.891883	3.586315	-0.266299
26	6	0	-1.784468	3.830706	1.103224
27	6	0	-0.843921	3.131343	1.864909
28	6	0	-0.016572	2.186166	1.259601

29	1	0	0.723125	1.645653	1.848539
30	1	0	-2.422555	4.572545	1.574456
31	1	0	-2.612821	4.136158	-0.863963
32	1	0	-1.142691	2.453624	-1.943945
33	1	0	-0.582510	-2.975018	0.167111
34	1	0	0.897093	-4.953848	0.498294
35	1	0	3.362242	-4.656930	0.370290
36	1	0	4.352601	-2.449305	-0.028686
37	1	0	0.494523	0.851098	-1.831297
38	1	0	2.062911	3.124573	-0.999149
39	1	0	4.509275	3.572567	-0.840766
40	1	0	8.054028	2.294776	-0.163112
41	1	0	6.285046	-2.376227	0.638588
42	1	0	9.565925	0.402442	0.452754
43	1	0	8.698012	-1.852271	0.840801
44	15	0	-4.273866	-0.340411	0.045321
45	8	0	-4.959879	0.919651	-0.859893
46	8	0	-4.829111	0.041714	1.600380
47	8	0	-5.292413	-1.628461	-0.365201
48	6	0	-4.924141	0.859629	-2.318310
49	6	0	-4.431555	1.313184	2.204184
50	6	0	-5.415954	-2.786072	0.519897
51	1	0	-5.504718	0.003456	-2.672385
52	1	0	-5.382202	1.788655	-2.653968
53	1	0	-3.889403	0.802892	-2.681313
54	1	0	-4.896915	2.140289	1.661425
55	1	0	-4.801594	1.270153	3.227286
56	1	0	-3.338334	1.424883	2.204096
57	1	0	-5.861423	-2.480821	1.469450
58	1	0	-6.073713	-3.474964	-0.007320
59	1	0	-4.438793	-3.256321	0.684803

TS3' (NIMGA = 1, 938.85*i* cm^{-1})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.471484	-2.845173	-0.137183
2	6	0	1.048356	-1.559571	-0.130058
3	6	0	2.463334	-1.425347	-0.062968
4	6	0	3.240271	-2.592117	0.009015
5	6	0	2.650818	-3.847499	0.011048
6	6	0	1.257626	-3.981112	-0.064076
7	6	0	0.187578	-0.394017	-0.159032
8	6	0	0.796874	0.915509	-0.200762
9	6	0	2.245715	1.079550	-0.118415
10	6	0	3.075212	-0.105322	-0.067507
11	6	0	2.800633	2.366481	-0.083112
12	6	0	4.184900	2.585064	-0.006180
13	6	0	4.969591	1.455118	0.021237
14	6	0	4.436641	0.138125	-0.009229
15	6	0	6.363512	0.907609	0.085208
16	6	0	5.848563	-0.421392	0.052438
17	6	0	7.703323	1.186204	0.148772
18	6	0	8.562751	0.059932	0.177772
19	6	0	8.068076	-1.238066	0.142450
20	6	0	6.678273	-1.514772	0.077546
21	79	0	-1.897741	-0.497374	-0.071787
22	1	0	-2.122789	3.628271	2.196226
23	6	0	-0.098958	2.107306	-0.081636
24	6	0	-0.277145	2.987223	-1.155623
25	6	0	-1.125498	4.087393	-1.026085
26	6	0	-1.789908	4.318353	0.179930
27	6	0	-1.611440	3.446067	1.255973
28	6	0	-0.771062	2.340386	1.126984
29	1	0	-0.620991	1.661848	1.964344
30	1	0	-2.441471	5.180915	0.283576
31	1	0	-1.261471	4.765710	-1.862699
32	1	0	0.252766	2.811178	-2.090509

33	1	0	-0.612366	-2.927214	-0.196484
34	1	0	0.802285	-4.965681	-0.065749
35	1	0	3.275360	-4.733469	0.070382
36	1	0	4.318191	-2.506998	0.070354
37	1	0	0.428636	0.337518	-1.307128
38	1	0	2.134498	3.223207	-0.104288
39	1	0	4.587085	3.590998	0.029324
40	1	0	8.105744	2.193165	0.175054
41	1	0	6.339368	-2.545926	0.048462
42	1	0	9.635984	0.215932	0.227592
43	1	0	8.765739	-2.069820	0.164391
44	15	0	-4.286394	-0.480075	0.059647
45	8	0	-4.930988	1.043025	0.435209
46	8	0	-5.052617	-1.461664	1.206100
47	8	0	-5.157659	-0.868173	-1.340297
48	6	0	-4.765366	2.135267	-0.522603
49	6	0	-4.950578	-1.148606	2.630791
50	6	0	-5.235772	-2.256558	-1.793171
51	1	0	-5.370220	1.939629	-1.411694
52	1	0	-5.122336	3.025475	-0.006368
53	1	0	-3.707652	2.265180	-0.792302
54	1	0	-5.456530	-0.203051	2.839182
55	1	0	-5.453256	-1.970520	3.137746
56	1	0	-3.900687	-1.103807	2.945664
57	1	0	-5.780376	-2.855692	-1.059553
58	1	0	-5.781841	-2.217181	-2.734120
59	1	0	-4.232914	-2.667732	-1.962181

Int4’ (NIMGA = 0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.039302	-0.246791	3.629769
2	6	0	-0.356689	0.337213	2.389595
3	6	0	-1.646813	0.159976	1.832453
4	6	0	-2.597608	-0.574976	2.562387
5	6	0	-2.275361	-1.138730	3.786969
6	6	0	-0.987938	-0.980466	4.322541
7	6	0	0.625624	1.163961	1.690426
8	6	0	0.262727	1.916171	0.546089
9	6	0	-0.998572	1.645667	-0.105272
10	6	0	-1.945681	0.745517	0.535683
11	6	0	-1.268824	2.197644	-1.375673
12	6	0	-2.452018	1.940671	-2.078562
13	6	0	-3.346696	1.095040	-1.456473
14	6	0	-3.098155	0.502919	-0.189361
15	6	0	-4.655154	0.370962	-1.557376
16	6	0	-4.414962	-0.246628	-0.294237
17	6	0	-5.779494	0.127220	-2.302411
18	6	0	-6.700745	-0.791162	-1.739782
19	6	0	-6.466208	-1.404654	-0.515046
20	6	0	-5.298513	-1.145303	0.248597
21	79	0	1.499144	-0.400270	0.360675
22	1	0	4.429377	3.770515	-0.453691
23	6	0	1.149477	3.017919	0.110067
24	6	0	0.608967	4.302875	-0.078867
25	6	0	1.436222	5.378838	-0.391148
26	6	0	2.811561	5.192419	-0.528377
27	6	0	3.360230	3.922762	-0.342725
28	6	0	2.537813	2.847235	-0.020436
29	1	0	2.973791	1.855562	0.108711
30	1	0	3.453112	6.031259	-0.778905
31	1	0	1.004526	6.366199	-0.521439
32	1	0	-0.458062	4.461722	0.052999
33	1	0	0.955848	-0.097707	4.044243
34	1	0	-0.742151	-1.418099	5.284822
35	1	0	-3.025366	-1.695625	4.339548
36	1	0	-3.604642	-0.673578	2.172052

37	1	0	1.467905	1.527633	2.282179
38	1	0	-0.513924	2.829398	-1.833894
39	1	0	-2.624703	2.377035	-3.055748
40	1	0	-5.975877	0.592844	-3.262322
41	1	0	-5.149495	-1.653632	1.196201
42	1	0	-7.612754	-1.022525	-2.281369
43	1	0	-7.199179	-2.105499	-0.126841
44	15	0	2.211482	-2.198386	-1.018679
45	8	0	3.175290	-3.419616	-0.366106
46	8	0	3.083854	-1.779281	-2.403416
47	8	0	0.921334	-3.077419	-1.671044
48	6	0	2.623152	-4.357382	0.614781
49	6	0	4.468265	-1.317053	-2.290106
50	6	0	-0.102126	-2.375957	-2.445460
51	1	0	1.857750	-4.976404	0.141524
52	1	0	3.470139	-4.965601	0.926911
53	1	0	2.211009	-3.819305	1.476977
54	1	0	5.096341	-2.120115	-1.897319
55	1	0	4.763381	-1.063959	-3.306794
56	1	0	4.529085	-0.426681	-1.651515
57	1	0	0.331824	-1.996326	-3.374293
58	1	0	-0.860079	-3.127456	-2.659261
59	1	0	-0.545397	-1.557467	-1.859689

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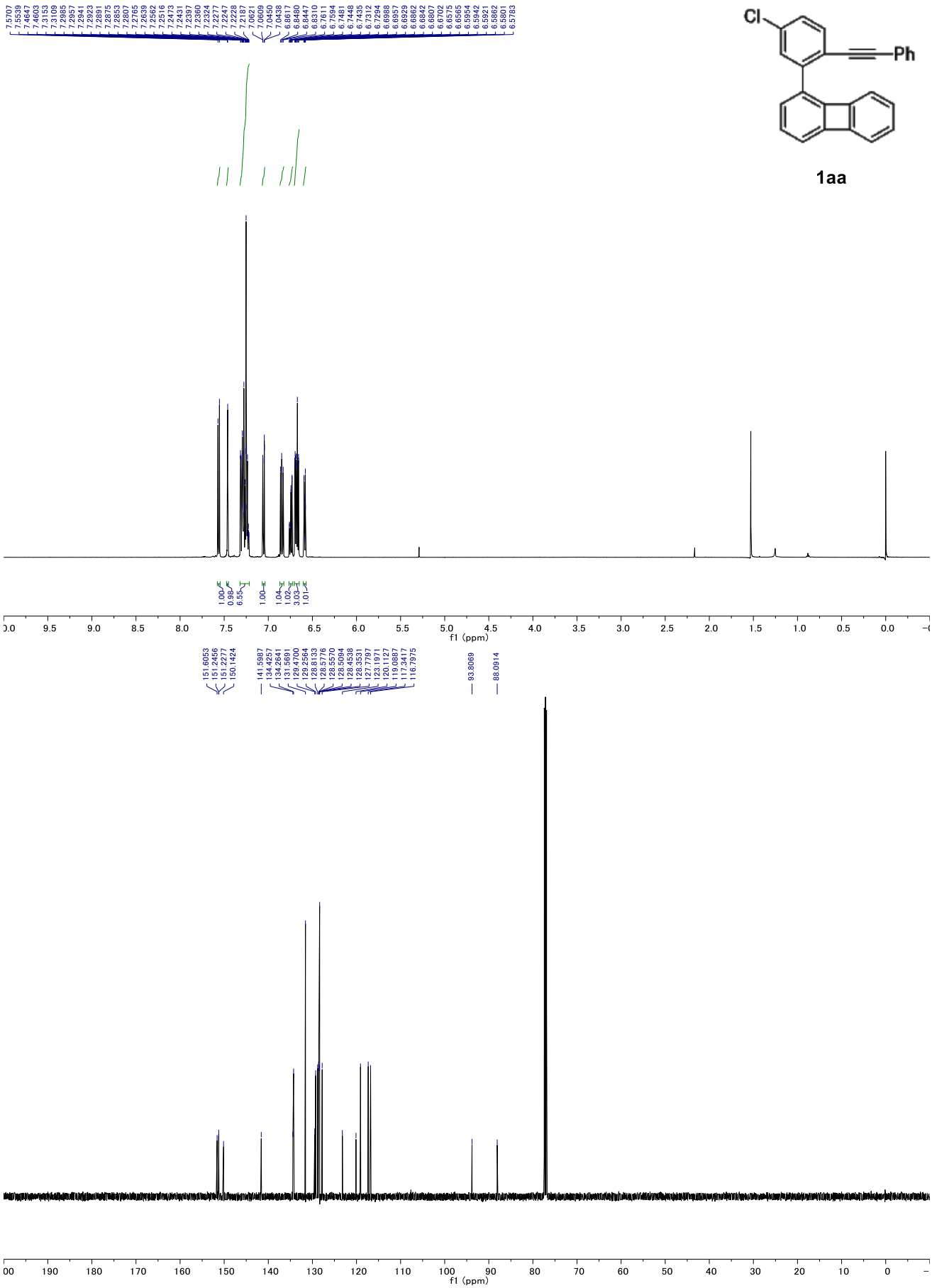
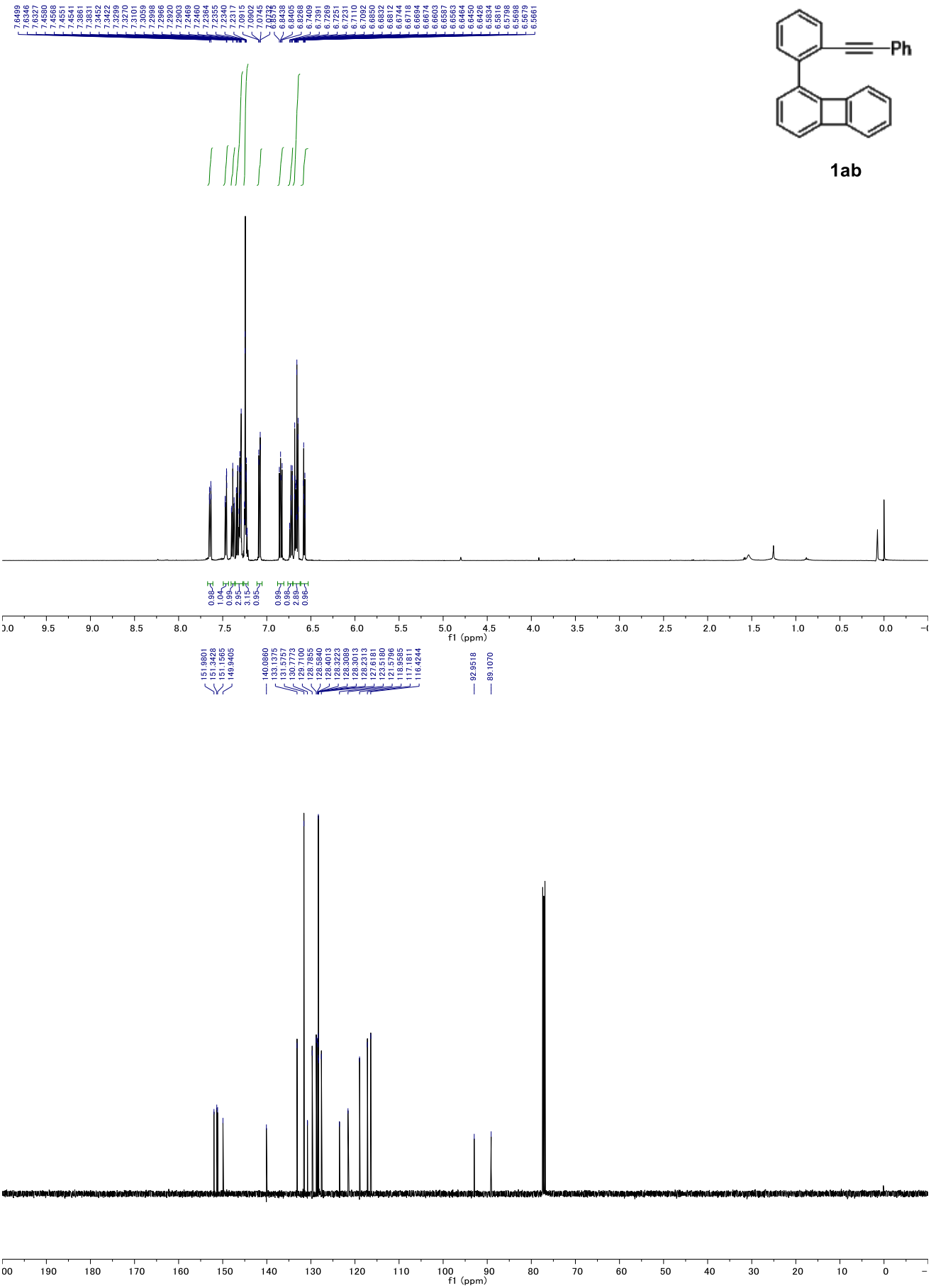
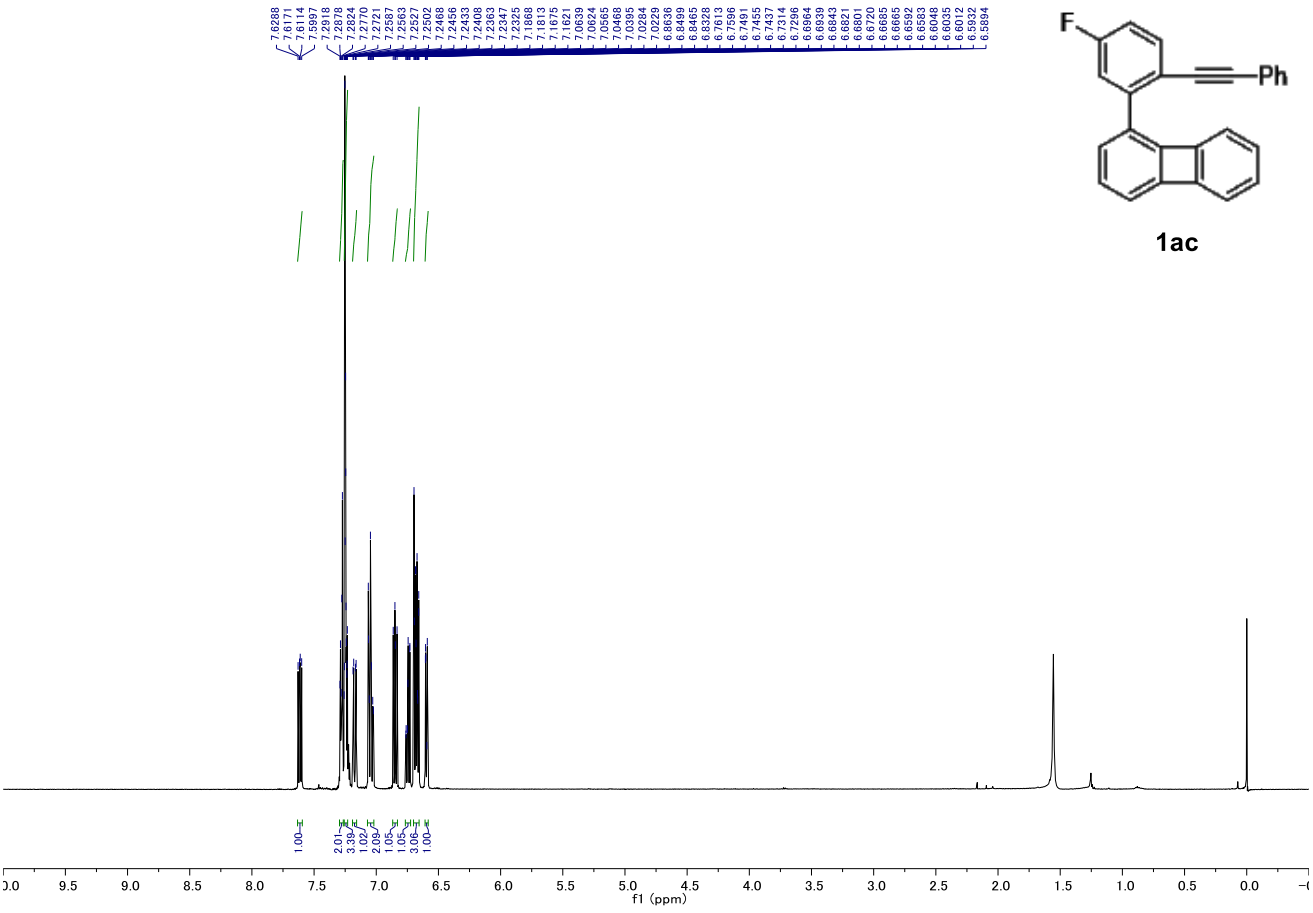
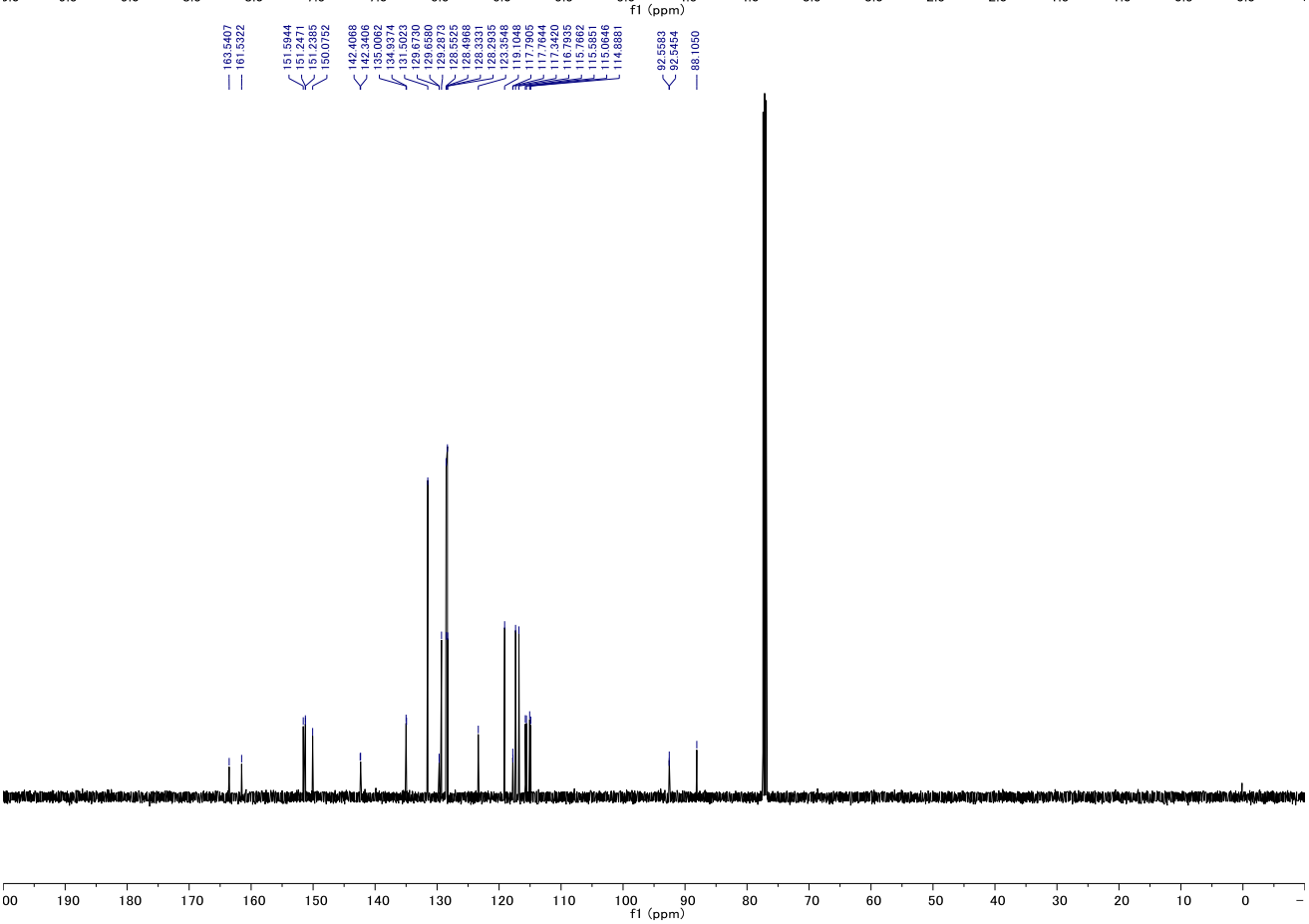
8) ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra for new compounds

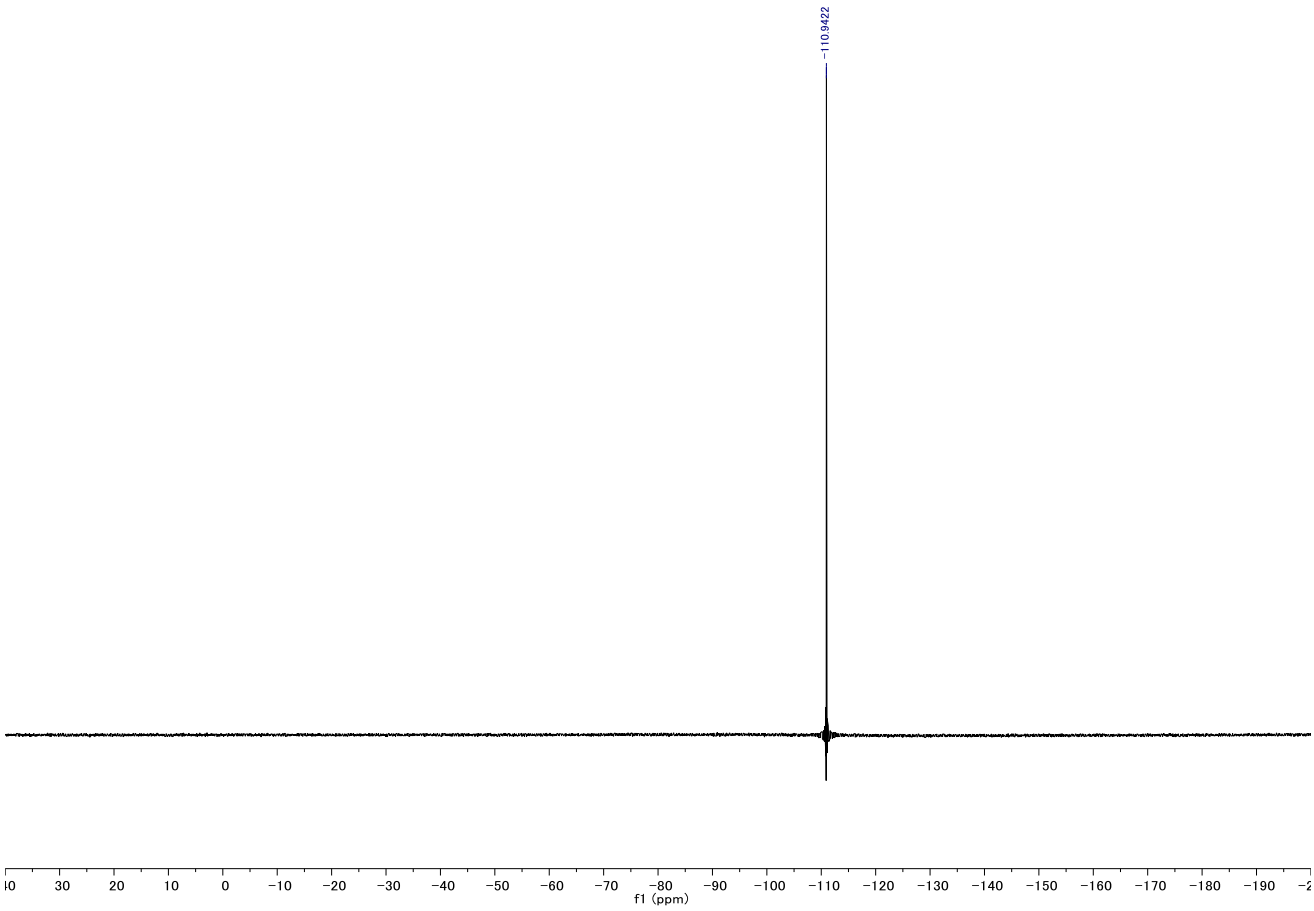



Ph
1ab
f1 (ppm)
f1 (ppm)



1ac

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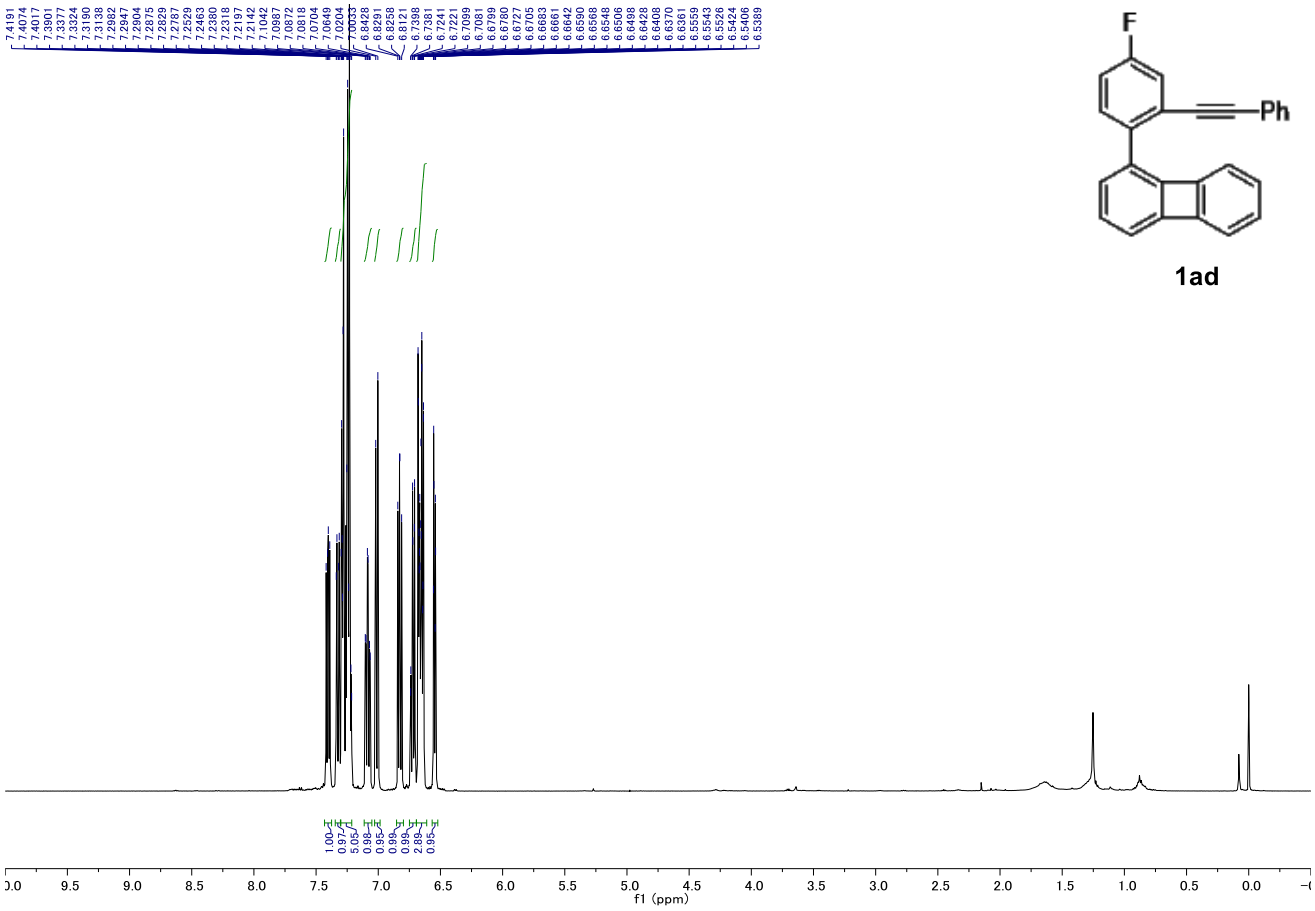
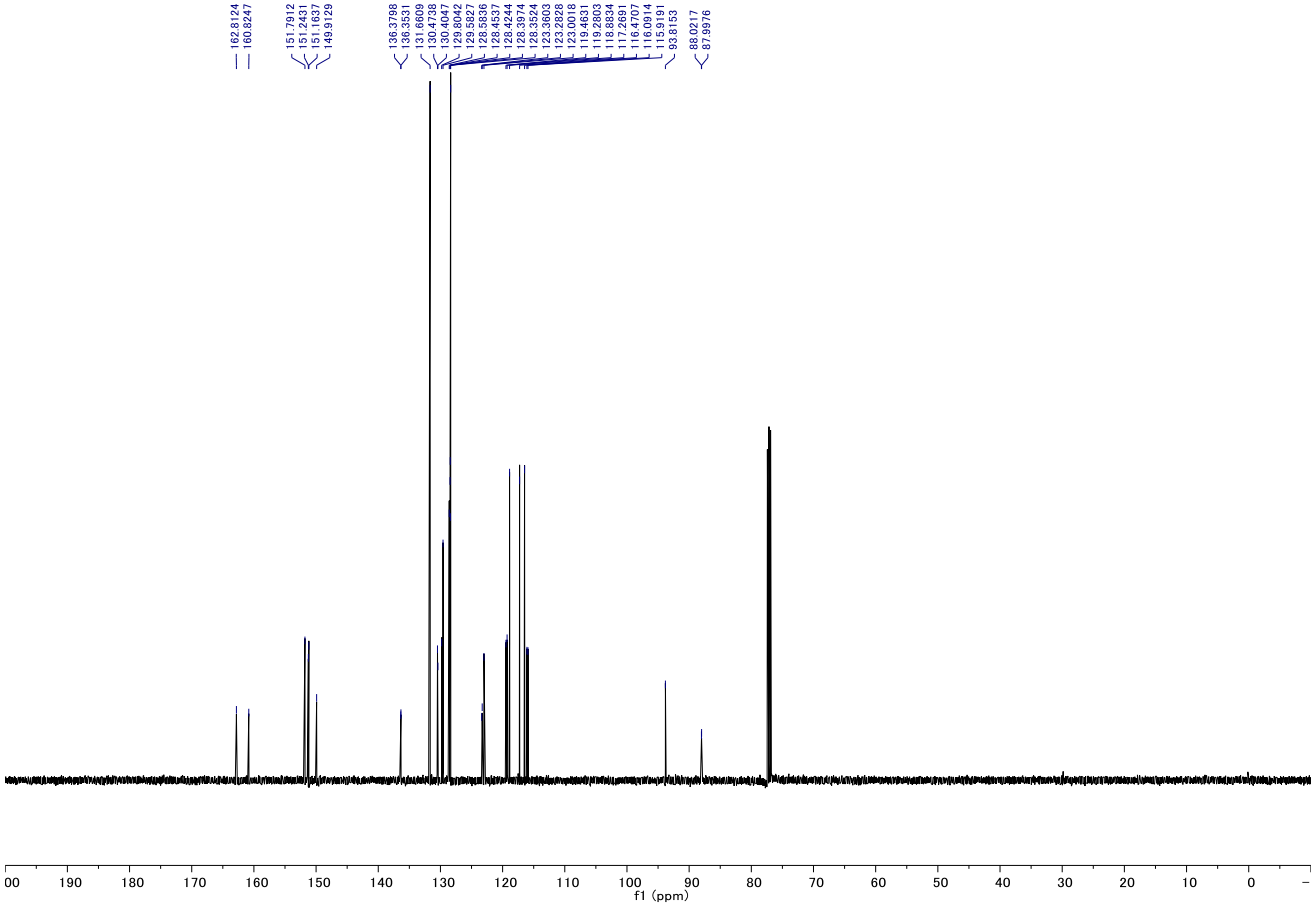
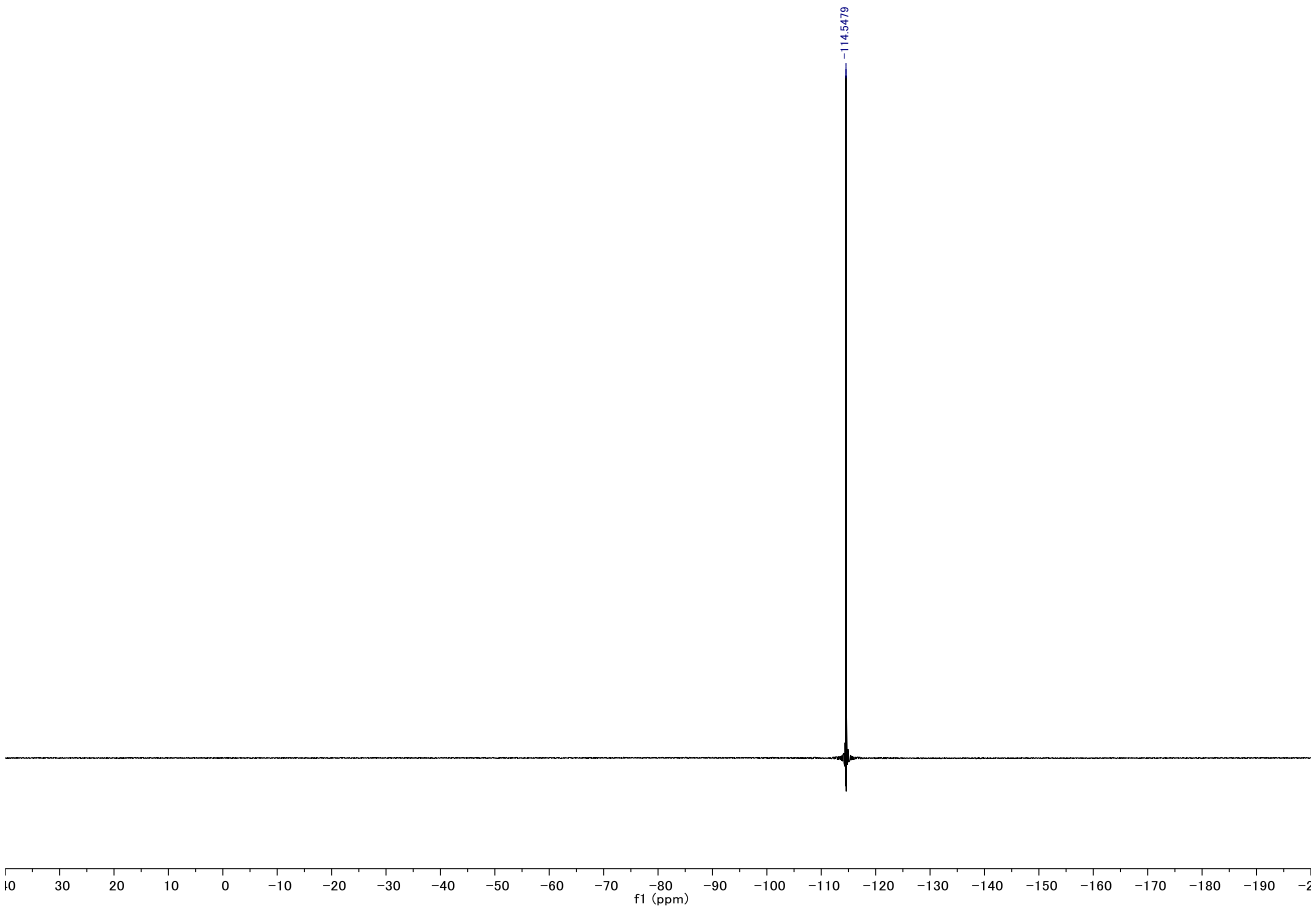
f1 (ppm)



1ad

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−40
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−80
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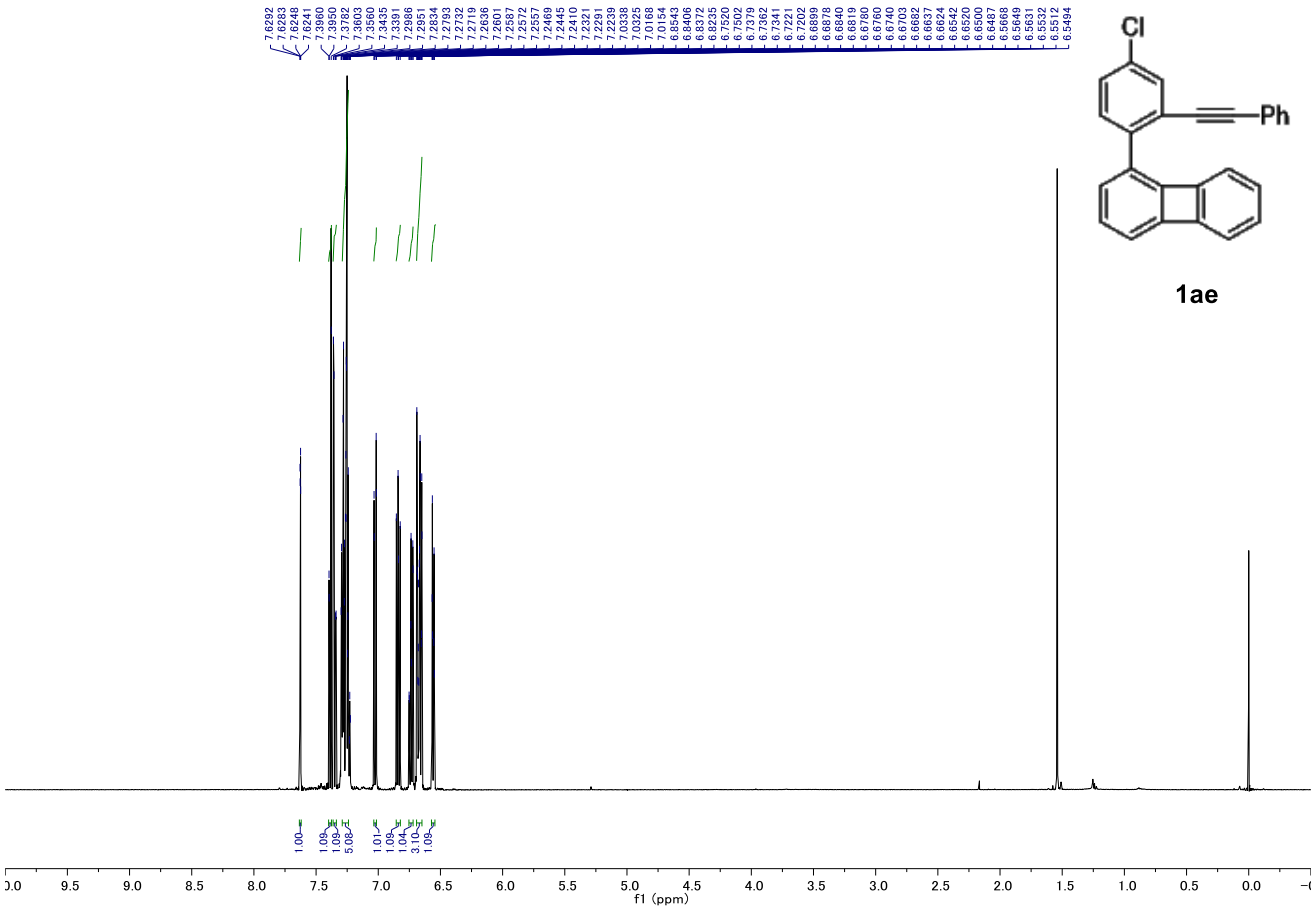
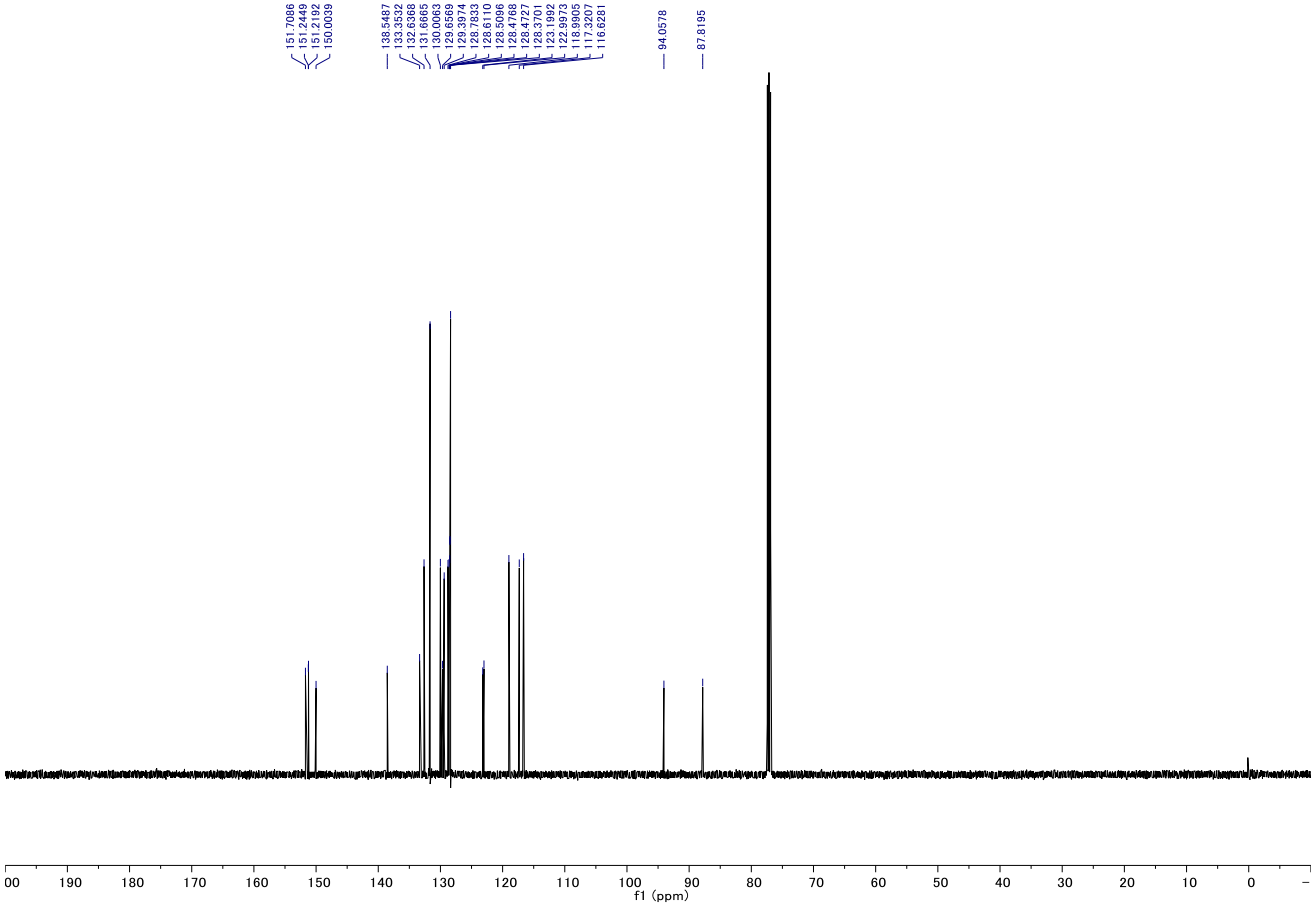
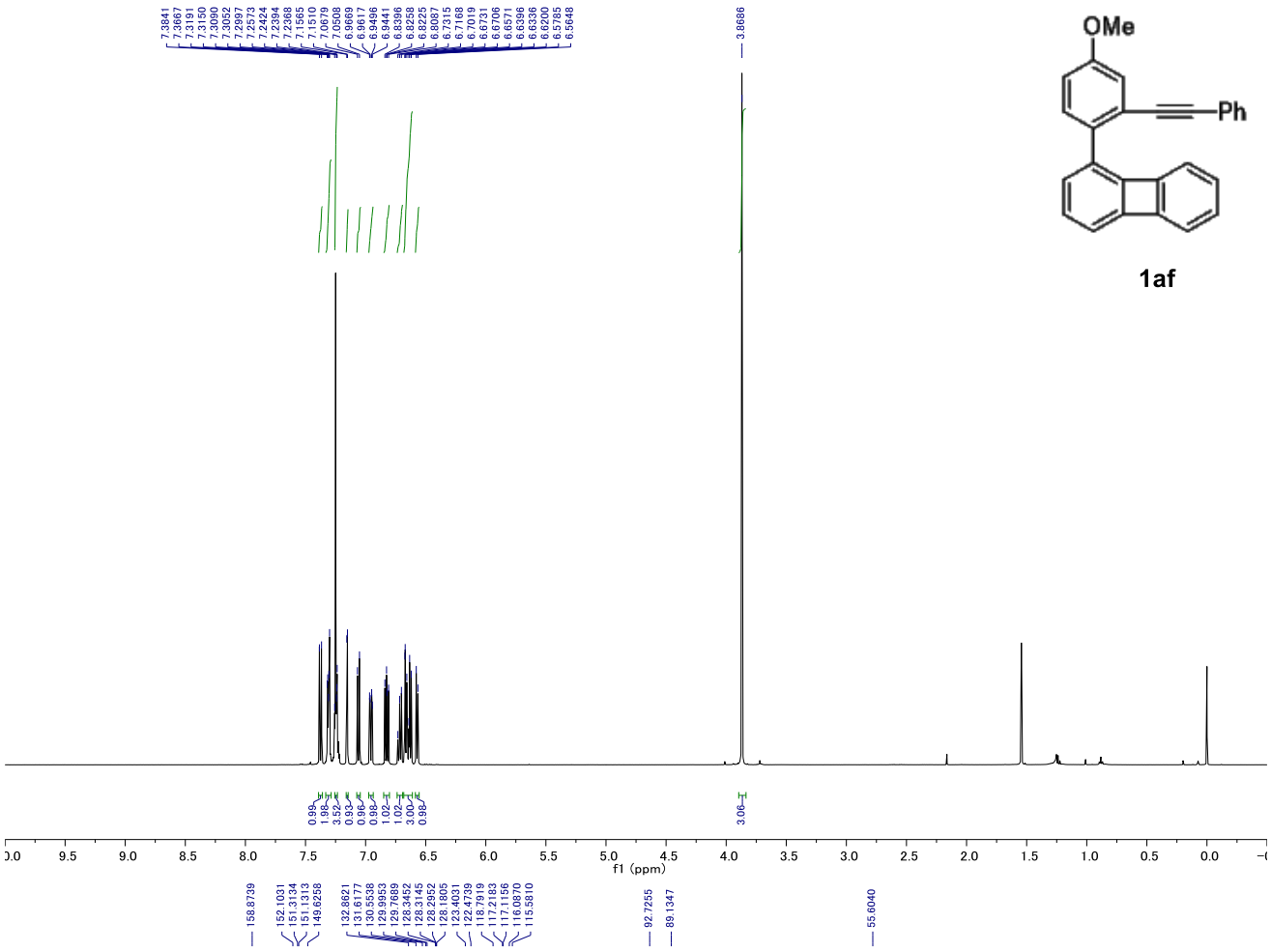
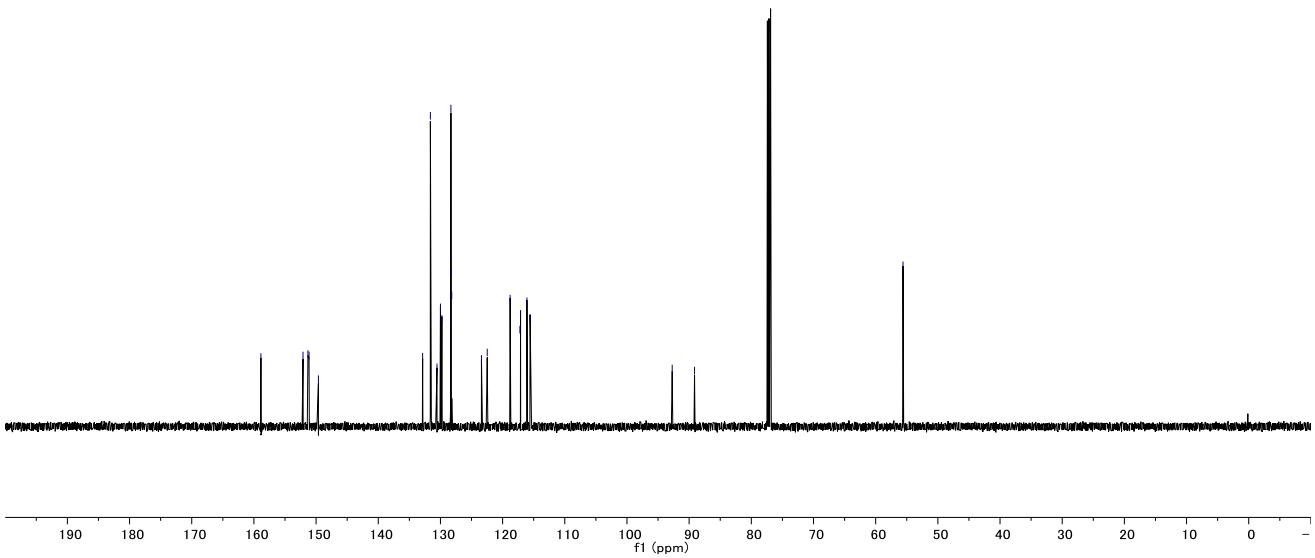
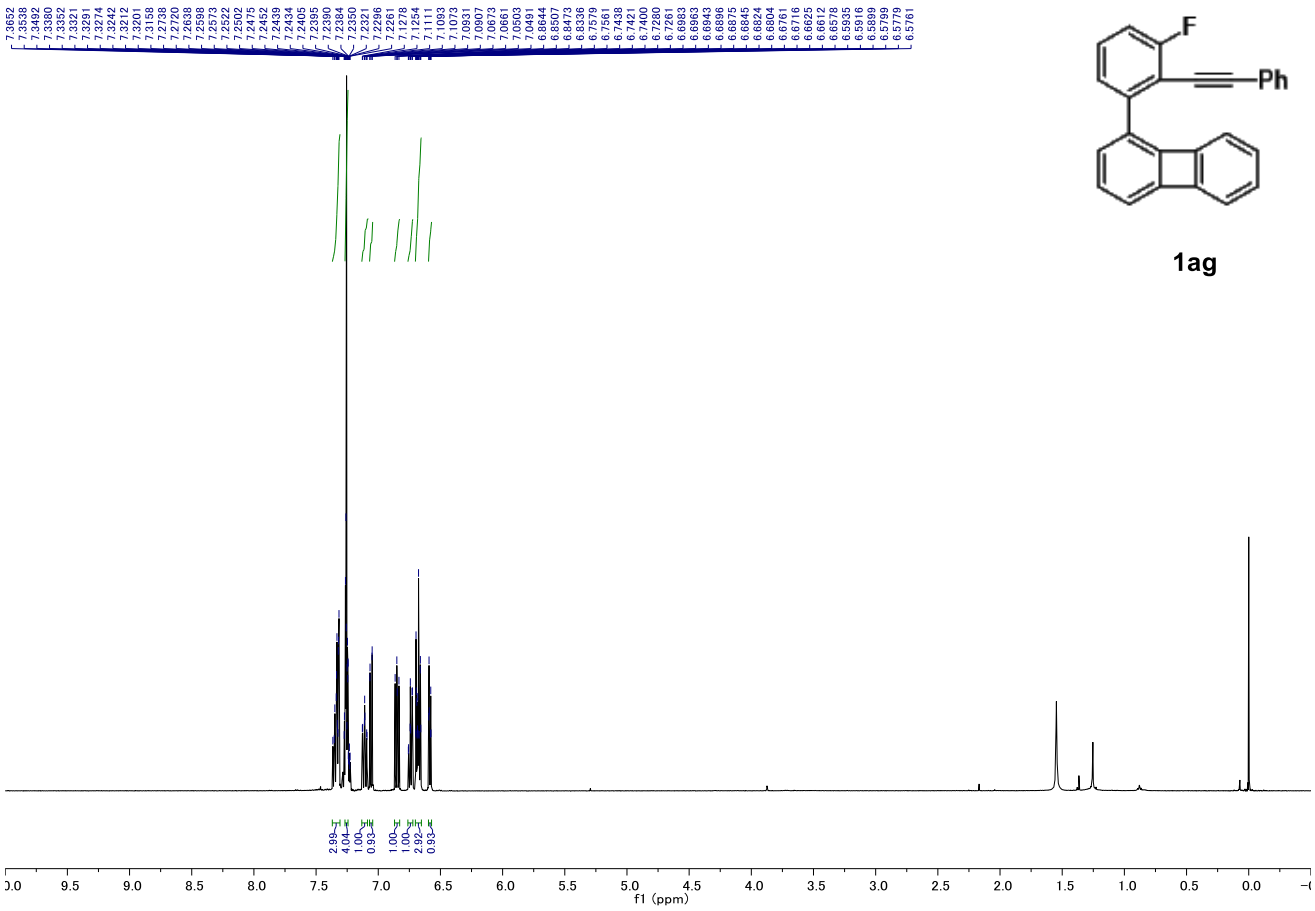
−140
−150
−160
−170
−180
−190
f1 (ppm)


Cl
Ph
1ae
f1 (ppm)


f1 (ppm)


OMe
Ph
1af
f1 (ppm)


f1 (ppm)



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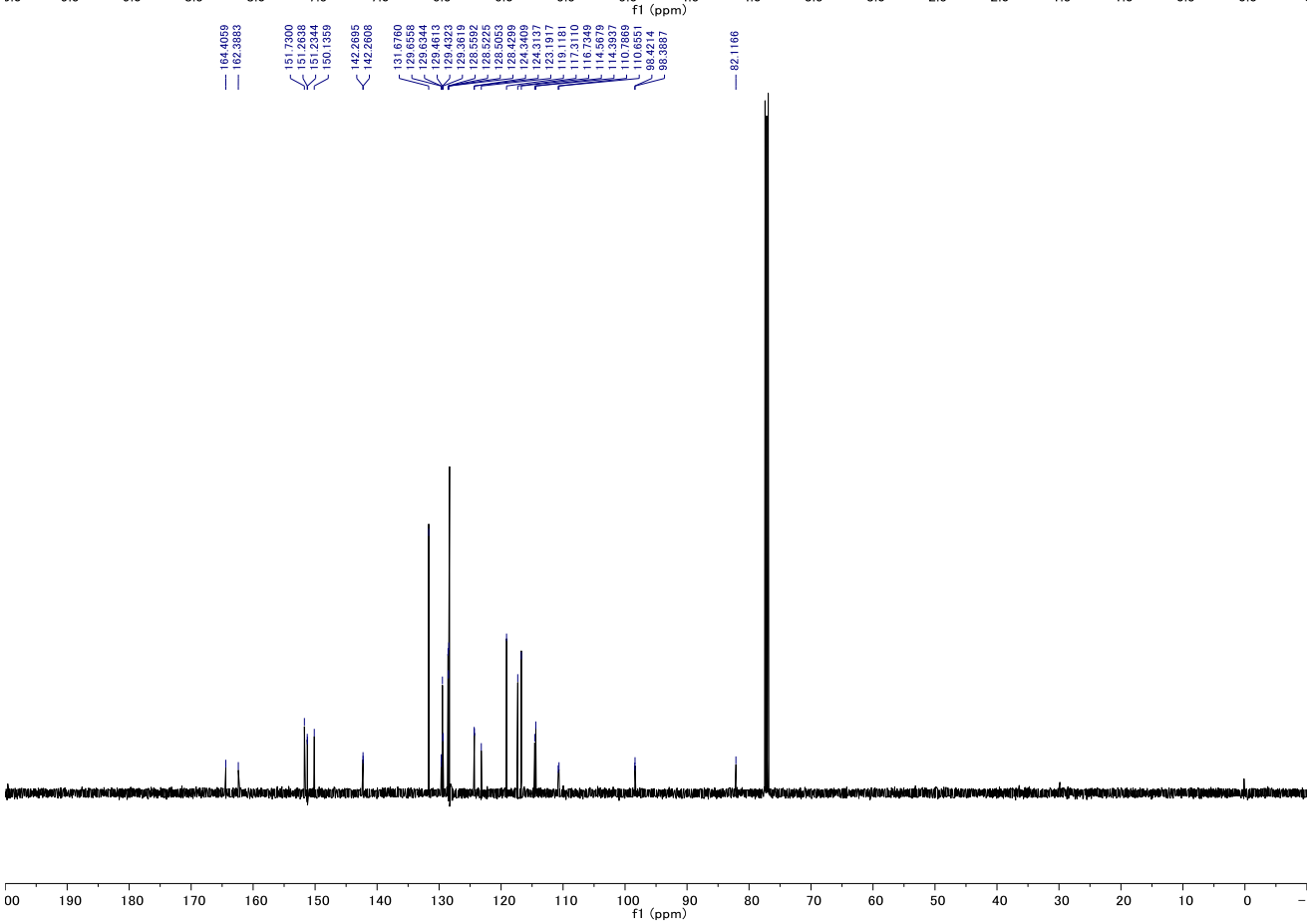

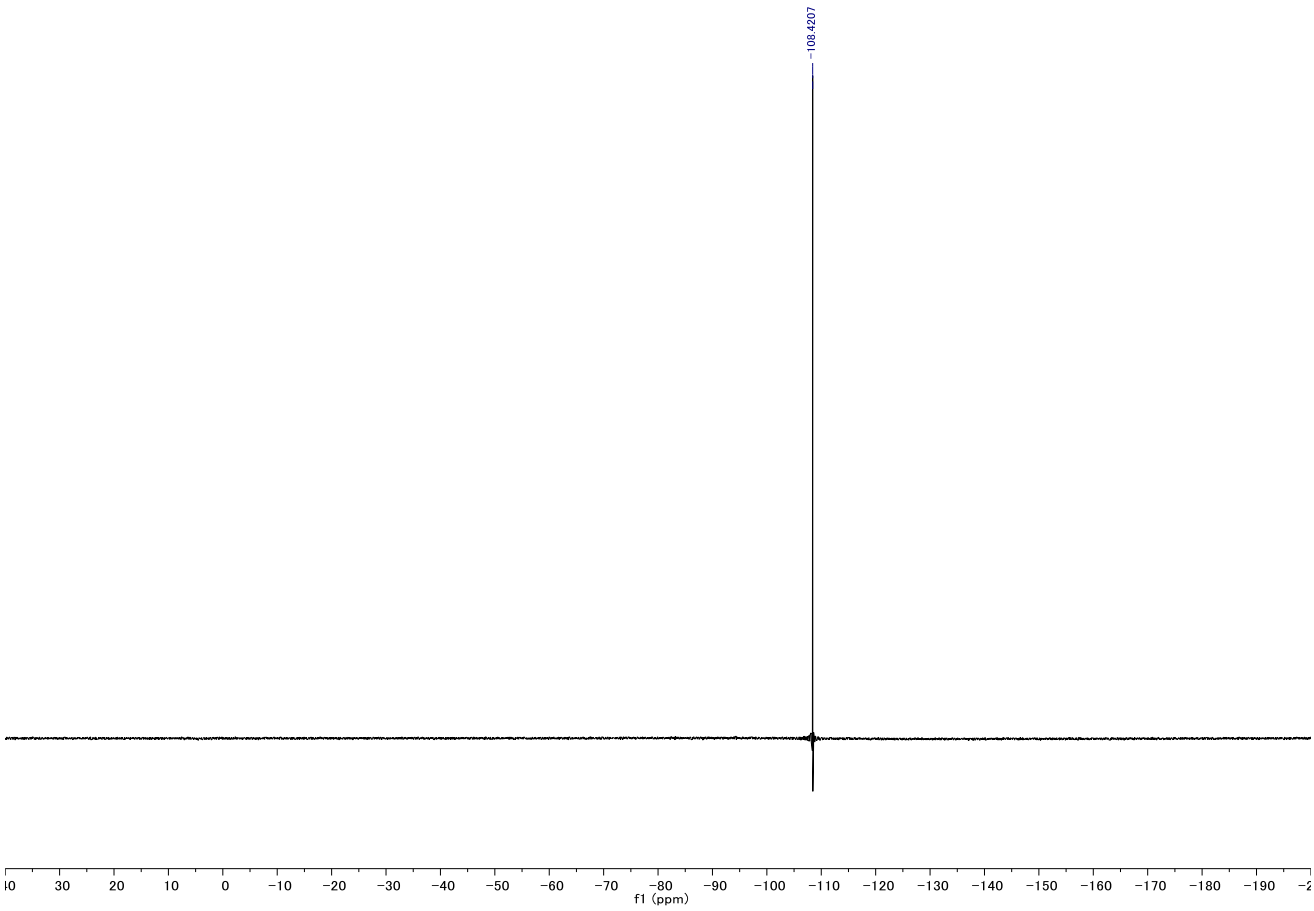
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−20
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−40
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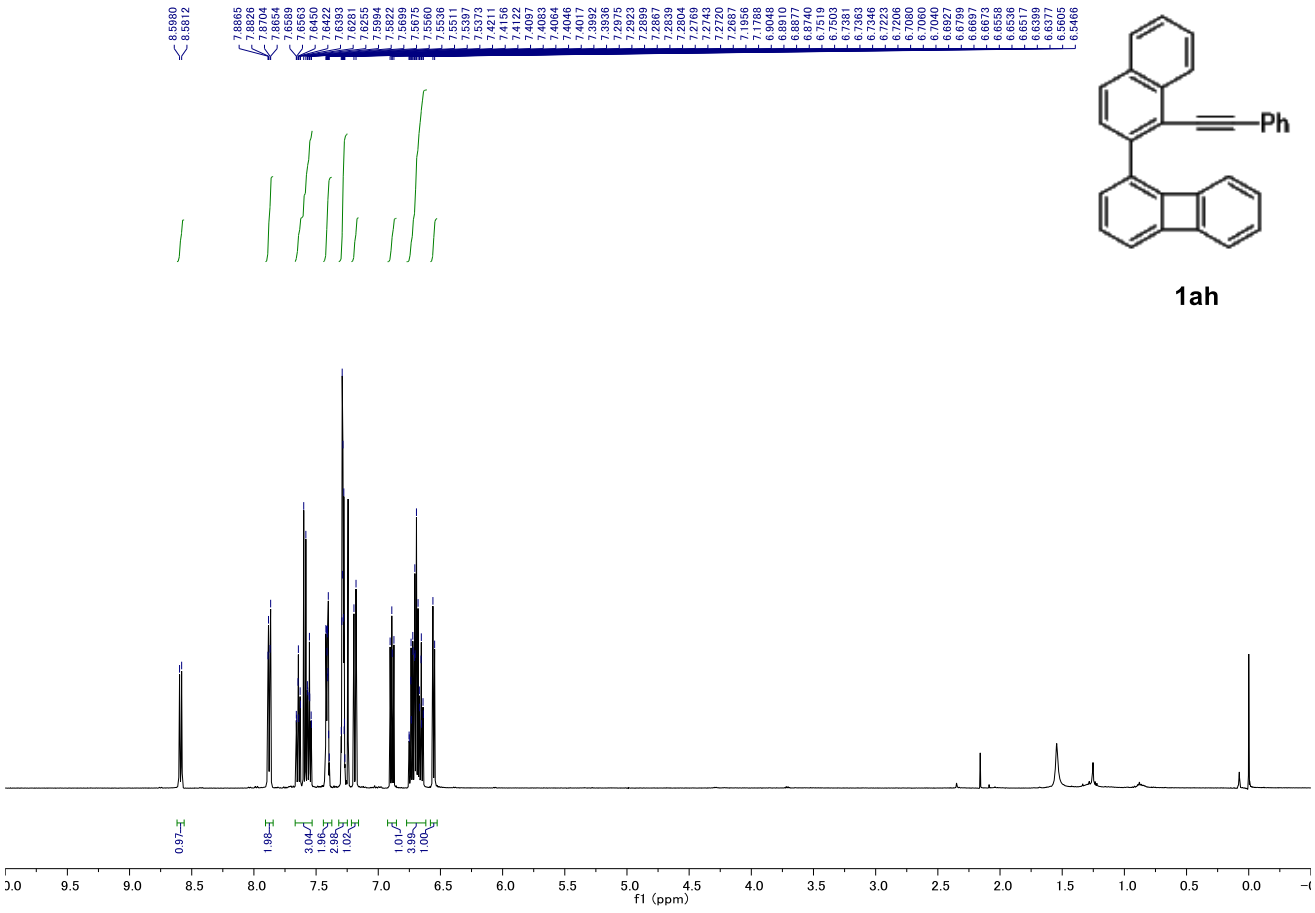
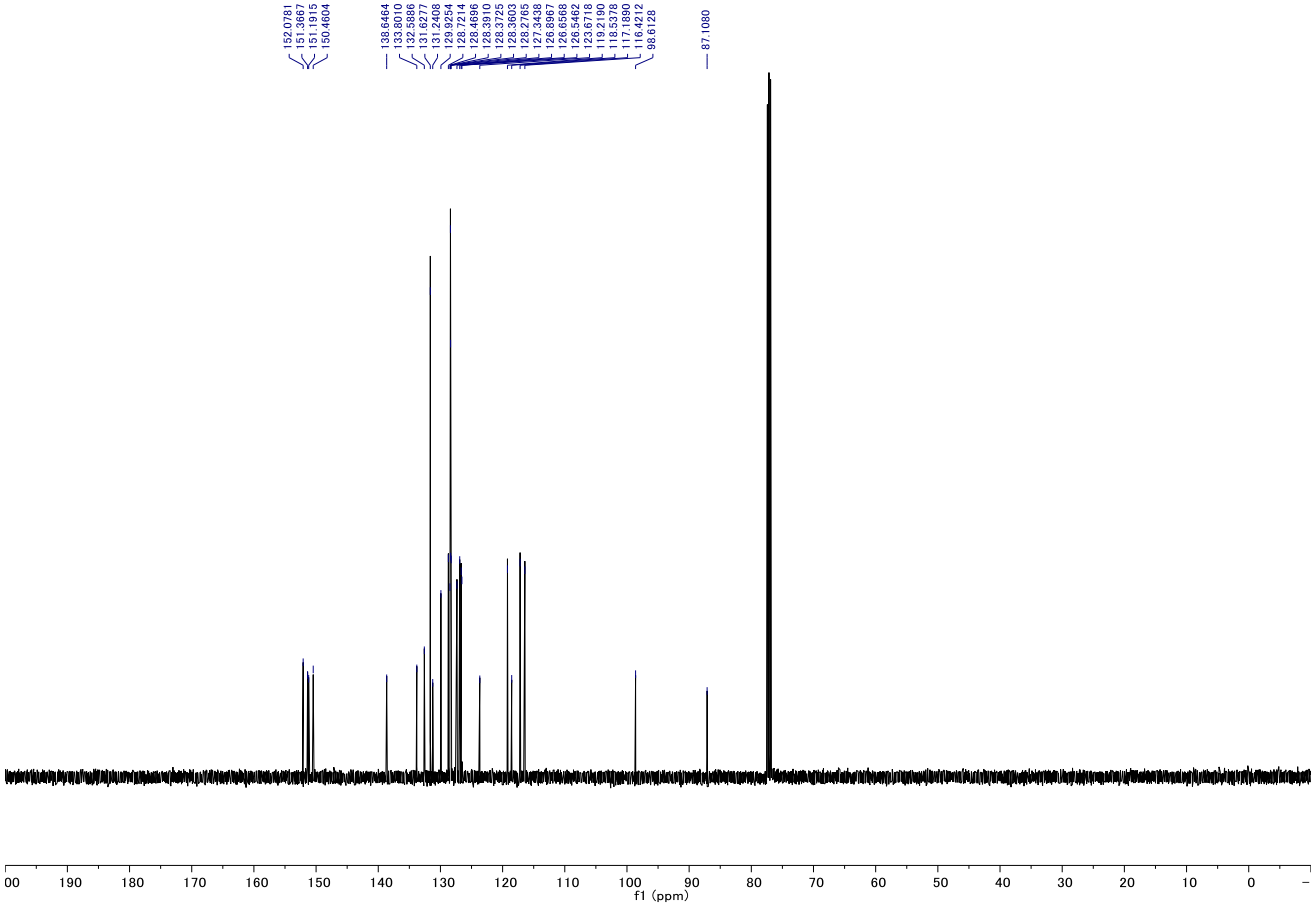
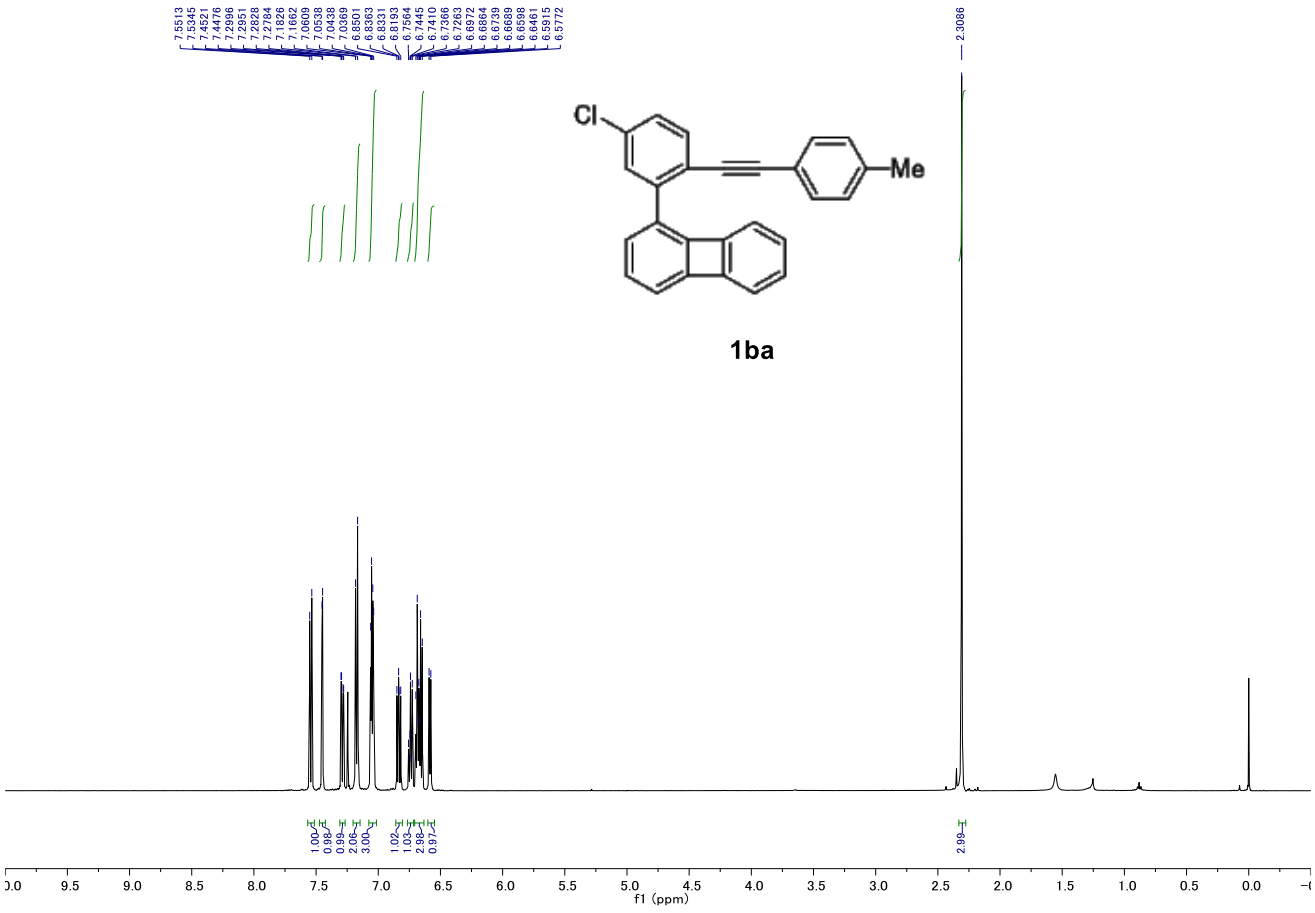
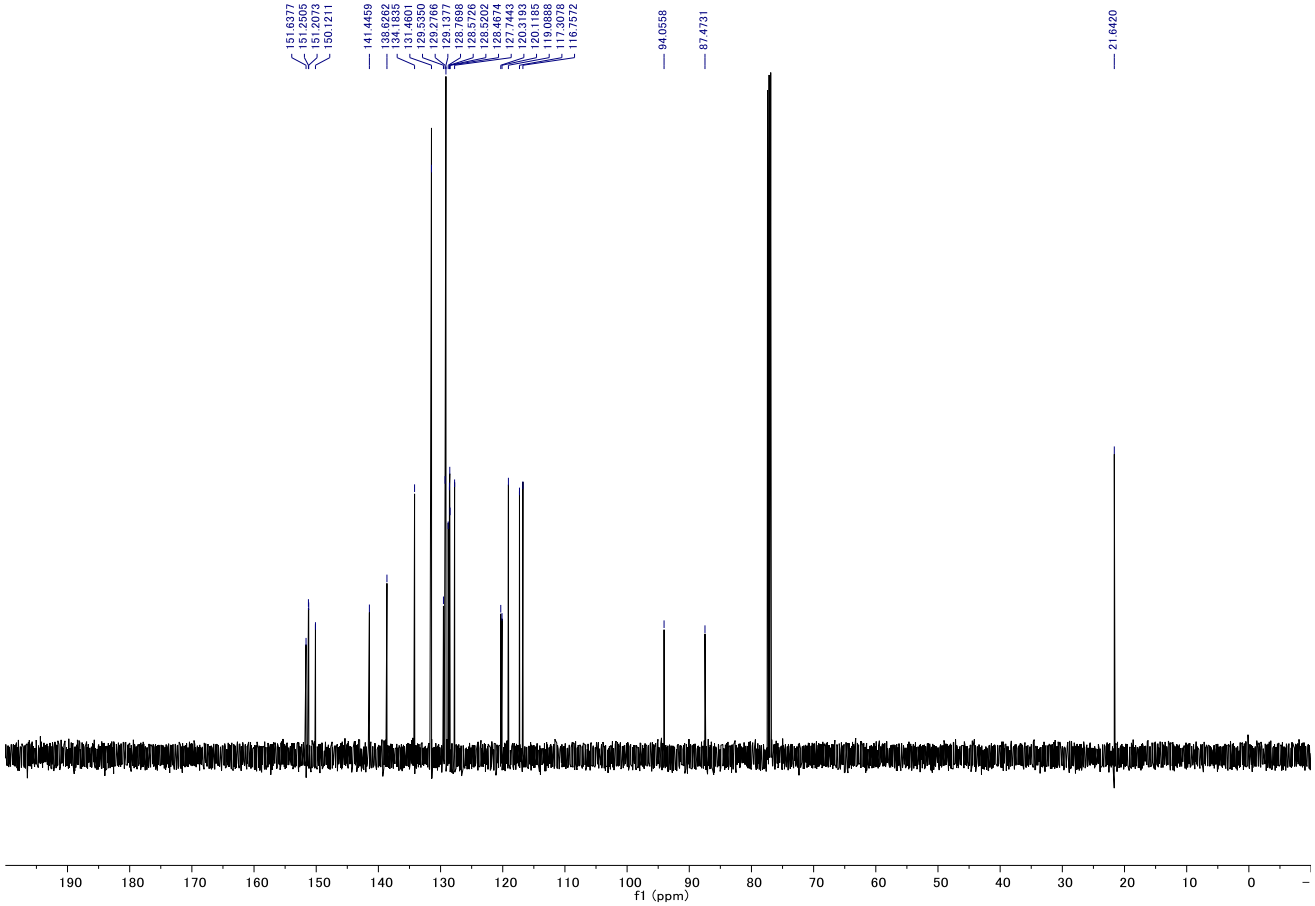
−110
−120
−130
−140
−150
−160
−170
−180
−190
f1 (ppm)


Ph
1ah
f1 (ppm)


f1 (ppm)


Cl
Me
2.3086
1ba
f1 (ppm)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141.4459
138.6262
134.1835
131.4661
129.5550
129.2786
129.1377
128.7698
128.5726
128.5202
128.4674
127.7443
120.3193
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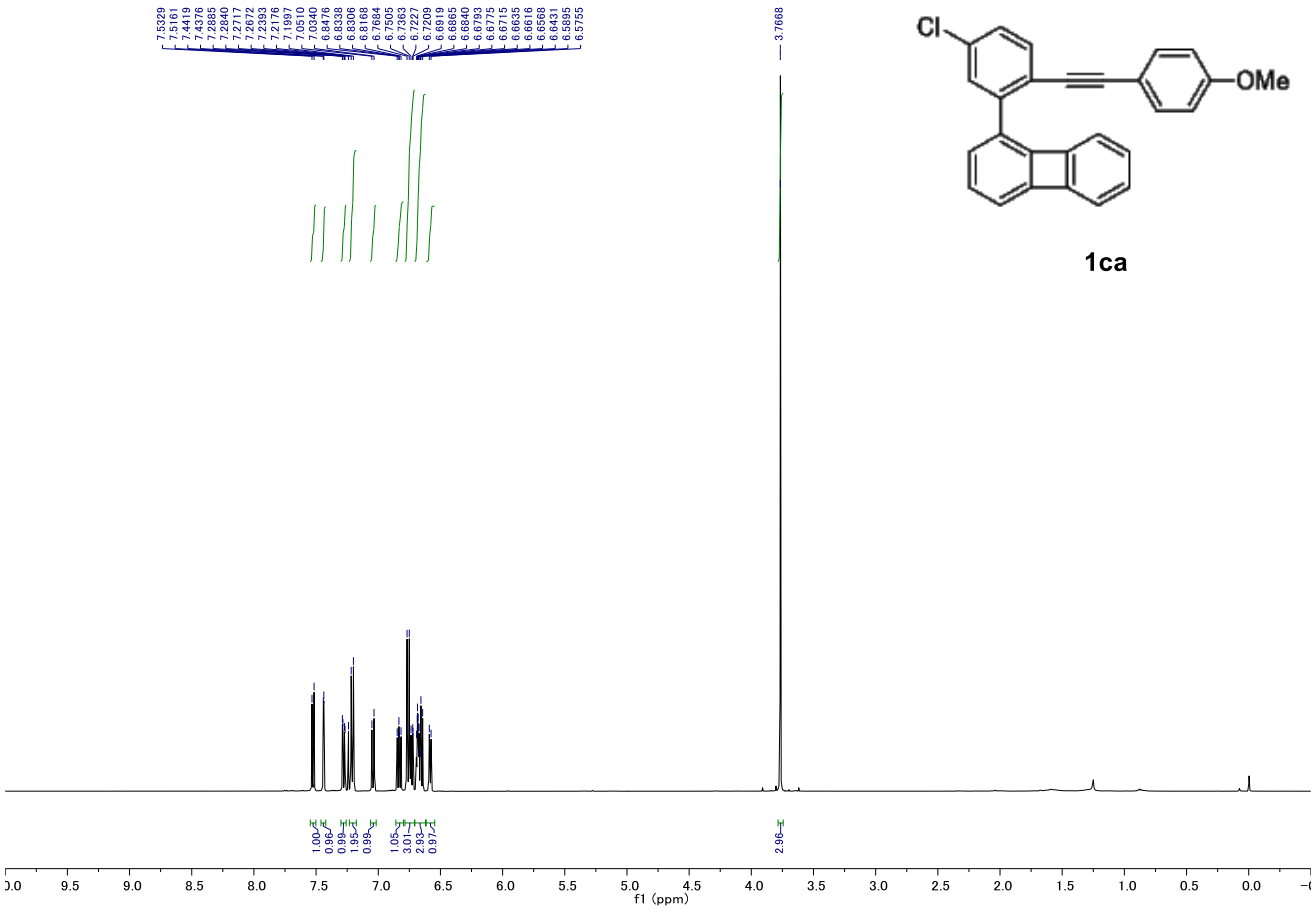
119.0088
117.2078
116.7572
94.0558
87.4731
21.6420
f1 (ppm)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7.2885
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7.2717
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7.2393
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7.1997
7.0510
7.0340
6.8476
6.8338
6.8186
6.8136
6.7684
6.7505
6.7363
6.7227
6.7209
6.6919
6.6885
6.6840
6.6793
6.6775
6.6715
6.6635
6.6616
6.6568
6.6431
6.5895
6.5755
3.7668
Cl
OMe
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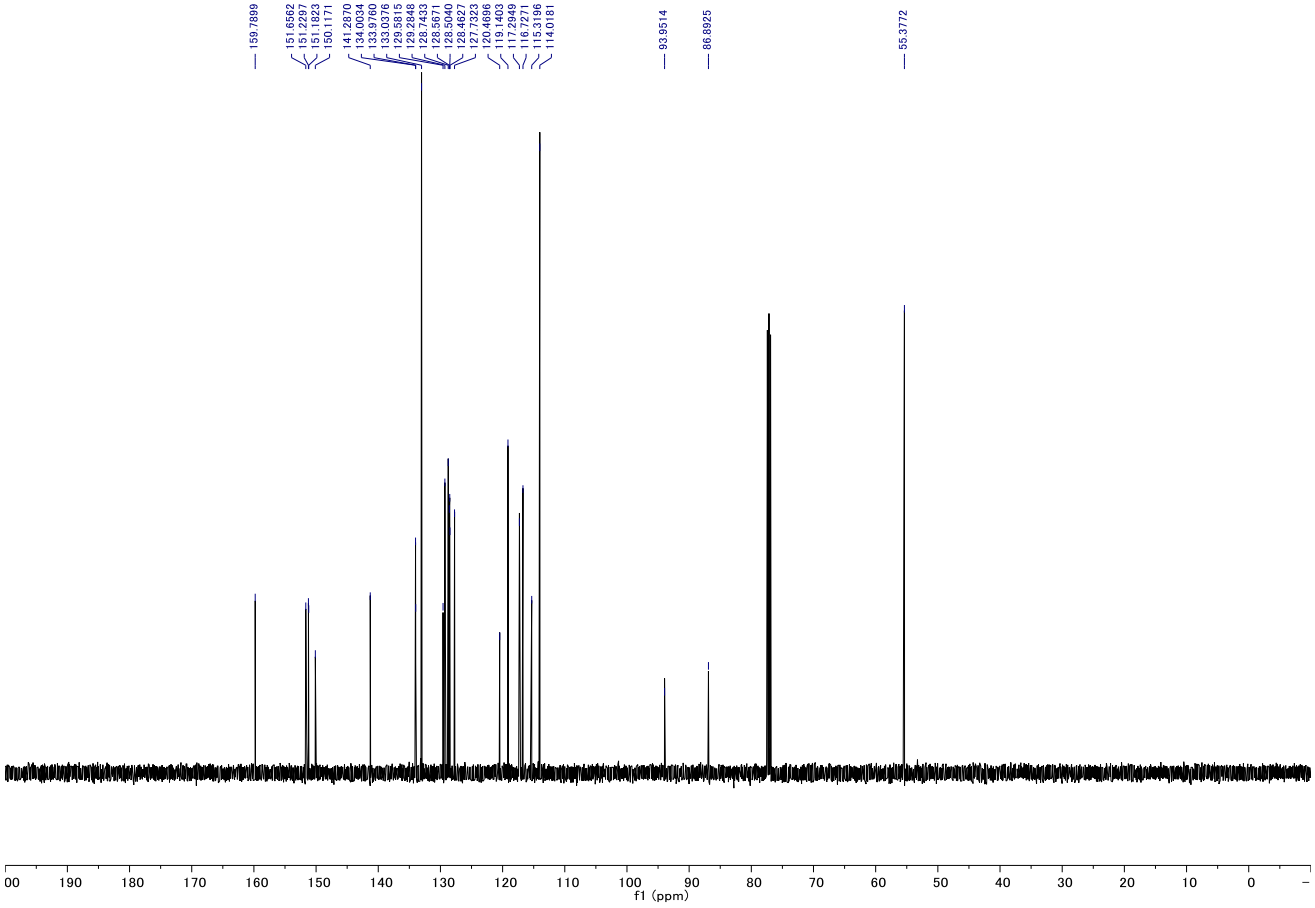
0.99
1.95
0.99
1.05
3.01
2.01
0.97
2.96
f1 (ppm)

1ca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128.7433
128.5071
128.5040
128.4621
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115.3196
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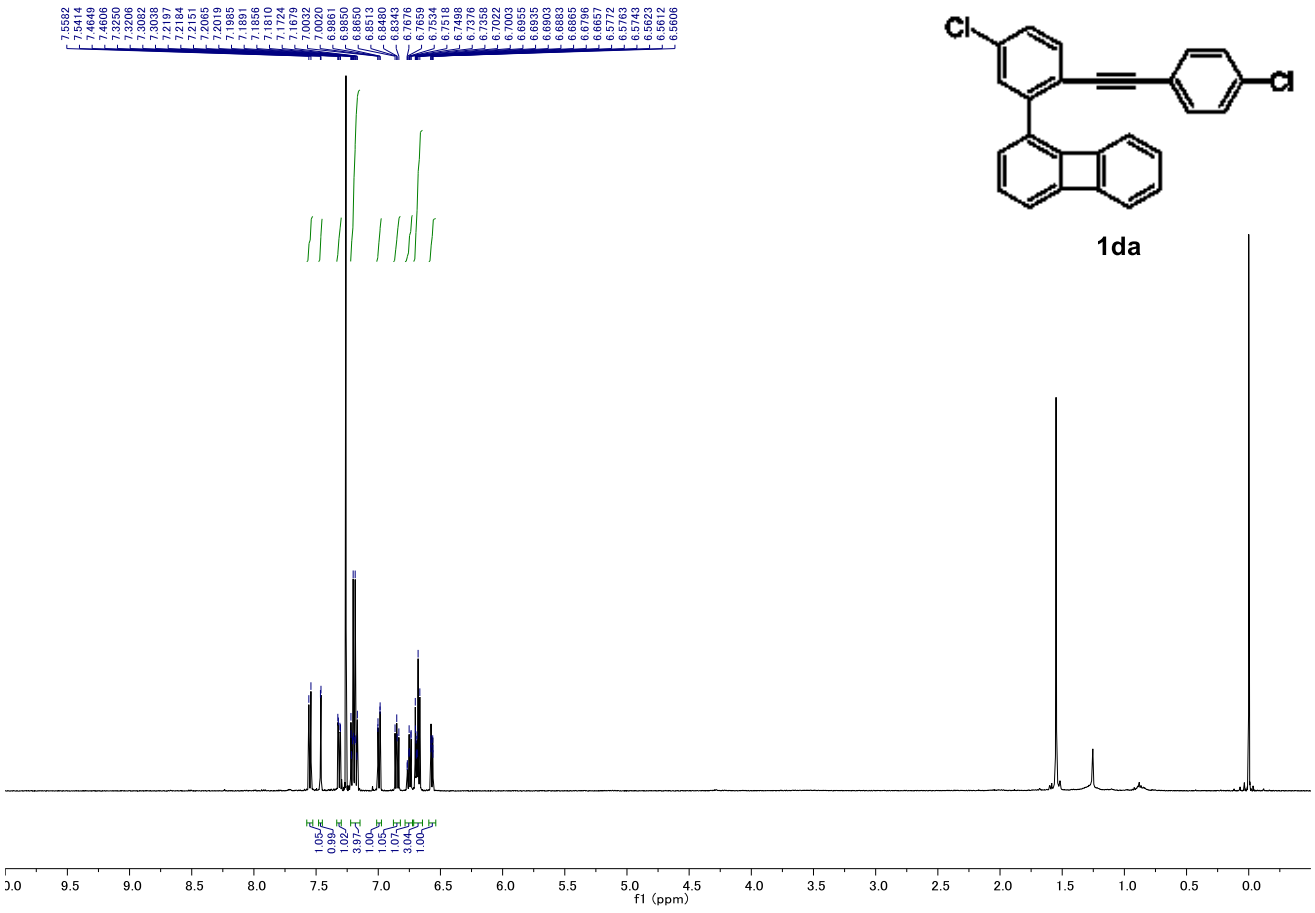
93.9514
86.8925
55.3772
f1 (ppm)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7.2065
7.2019
7.1985
7.1891
7.1856
7.1810
7.1724
7.1679
7.0032
7.0020
6.9861
6.9850
6.8650
6.8513
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6.7659
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6.7518
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6.7376
6.7358
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6.6903
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6.6865
6.6796
6.6657
6.5772
6.5763
6.5743
6.5623
6.5612
6.5606
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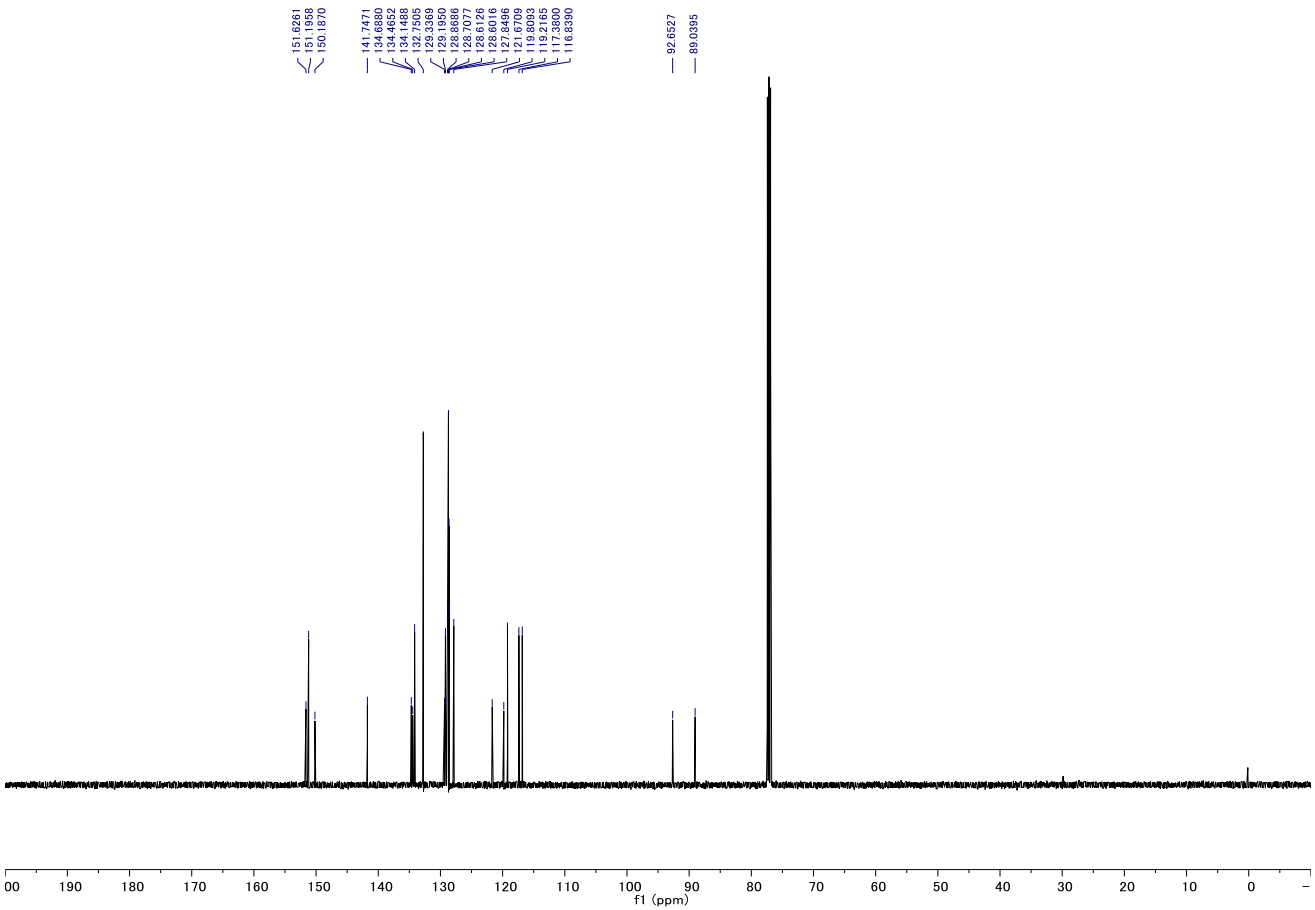
1.00
1.05
1.07
3.04
1.00
f1 (ppm)

Cl
Cl

1da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129.1950
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116.8390
92.6527
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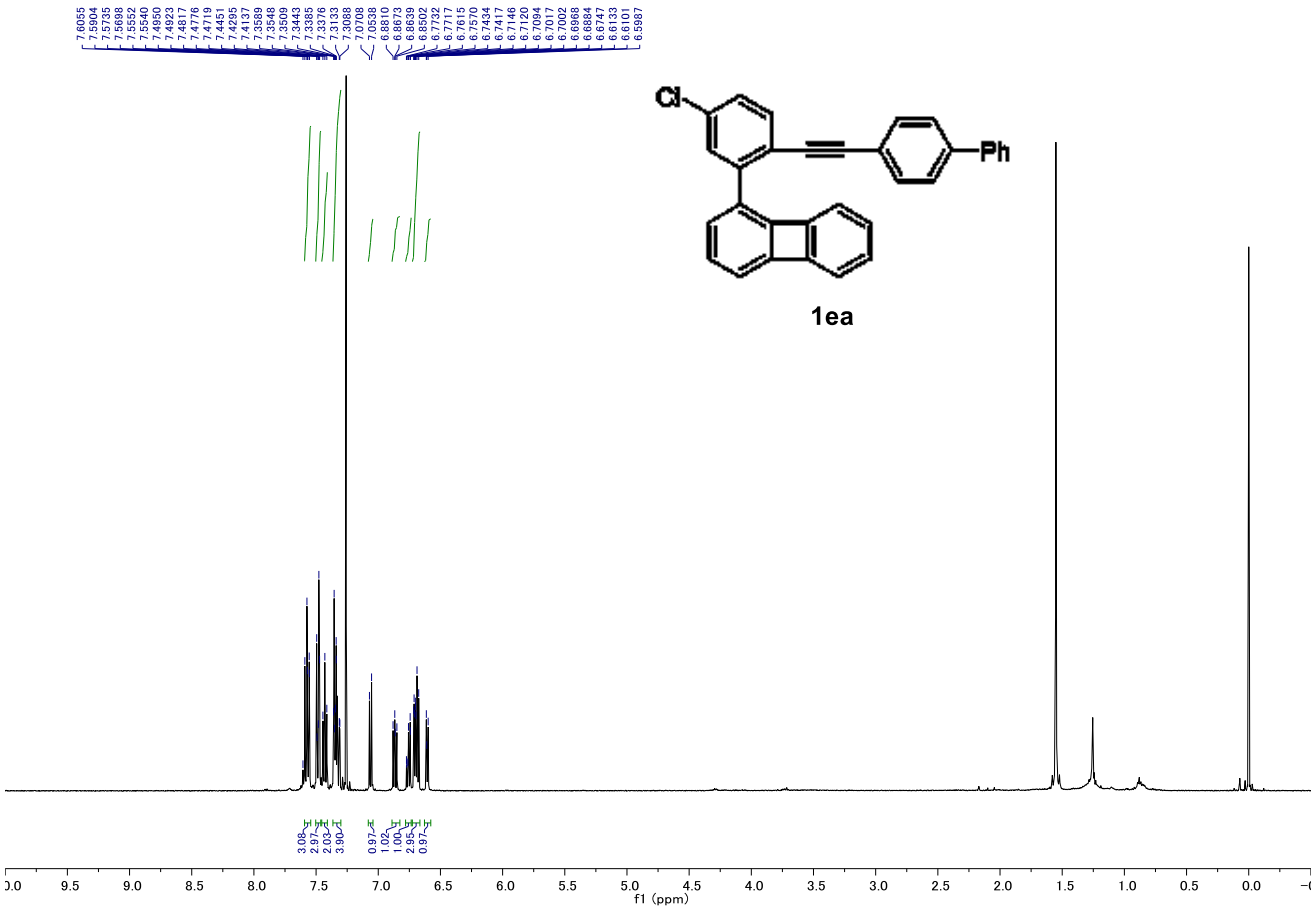
f1 (ppm)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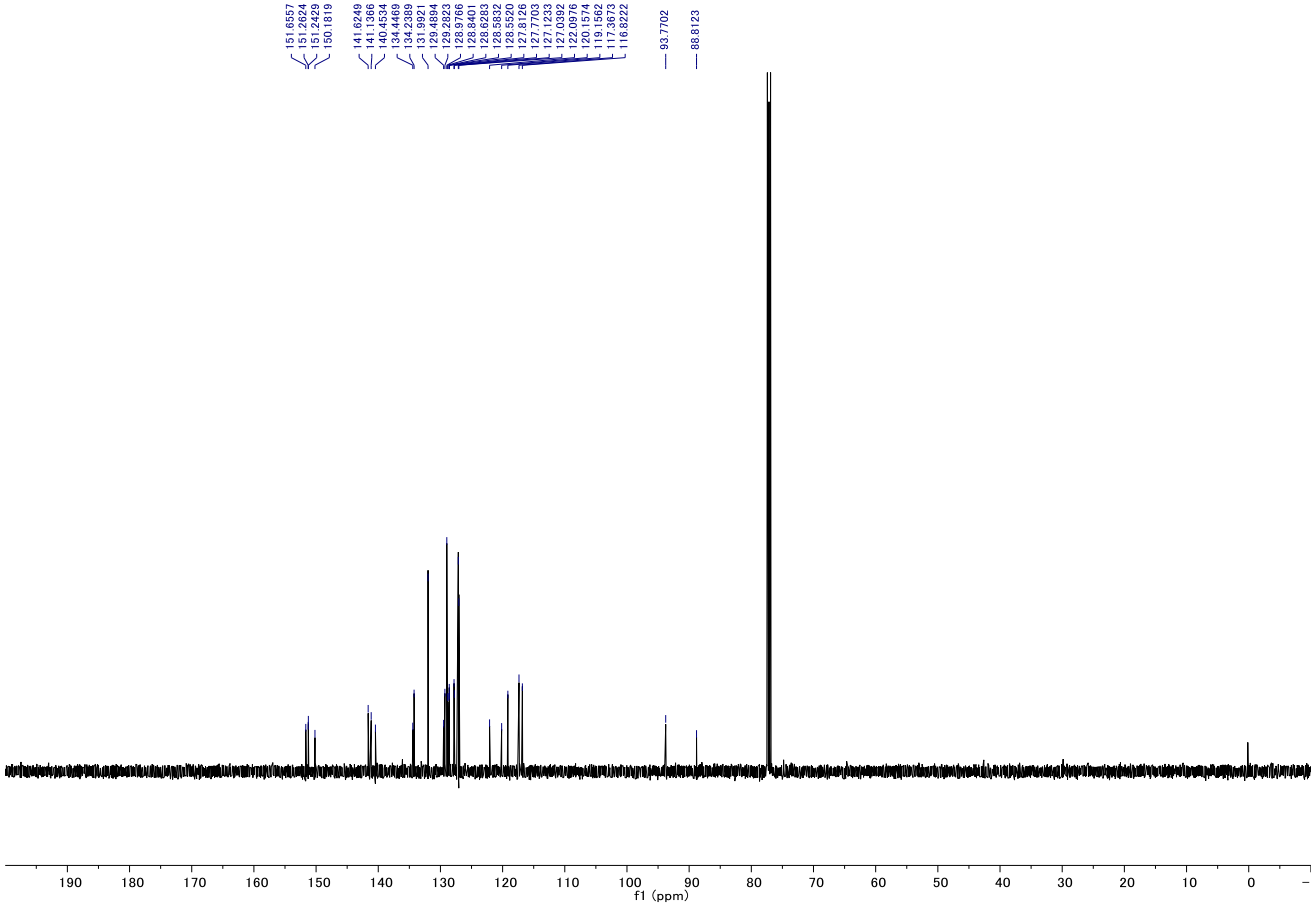
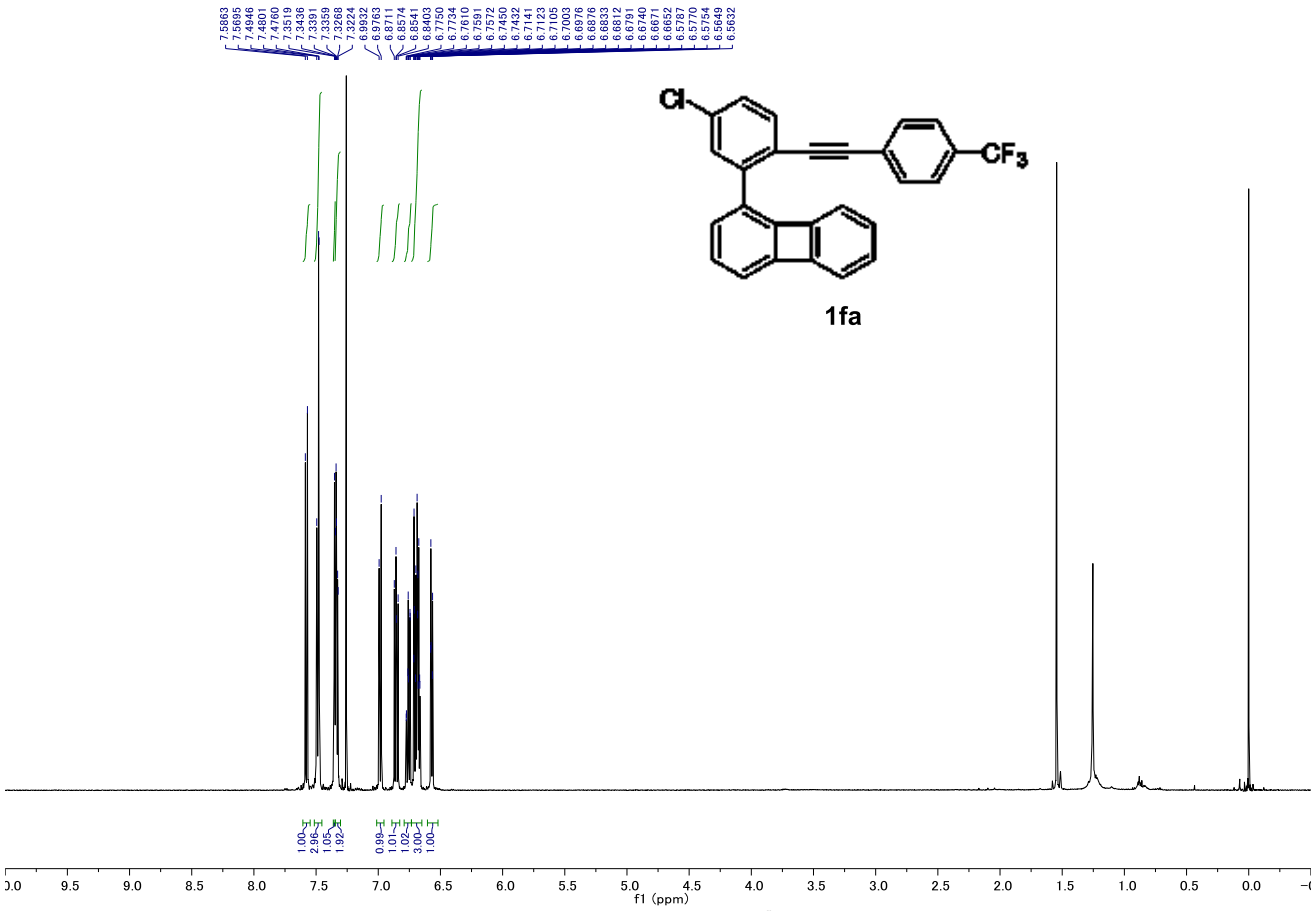
Ph
1ea
f1 (ppm)


f1 (ppm)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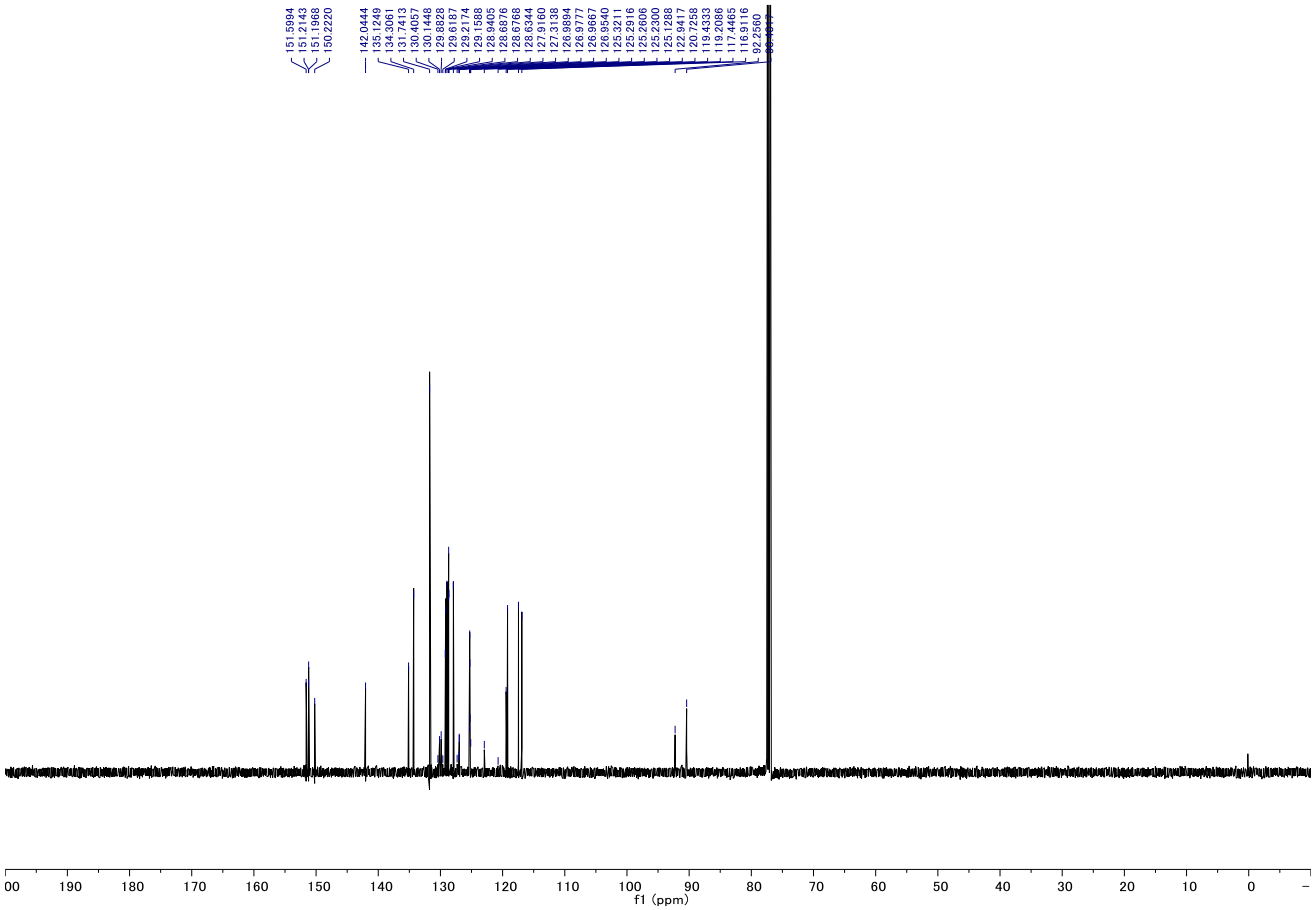
f1 (ppm)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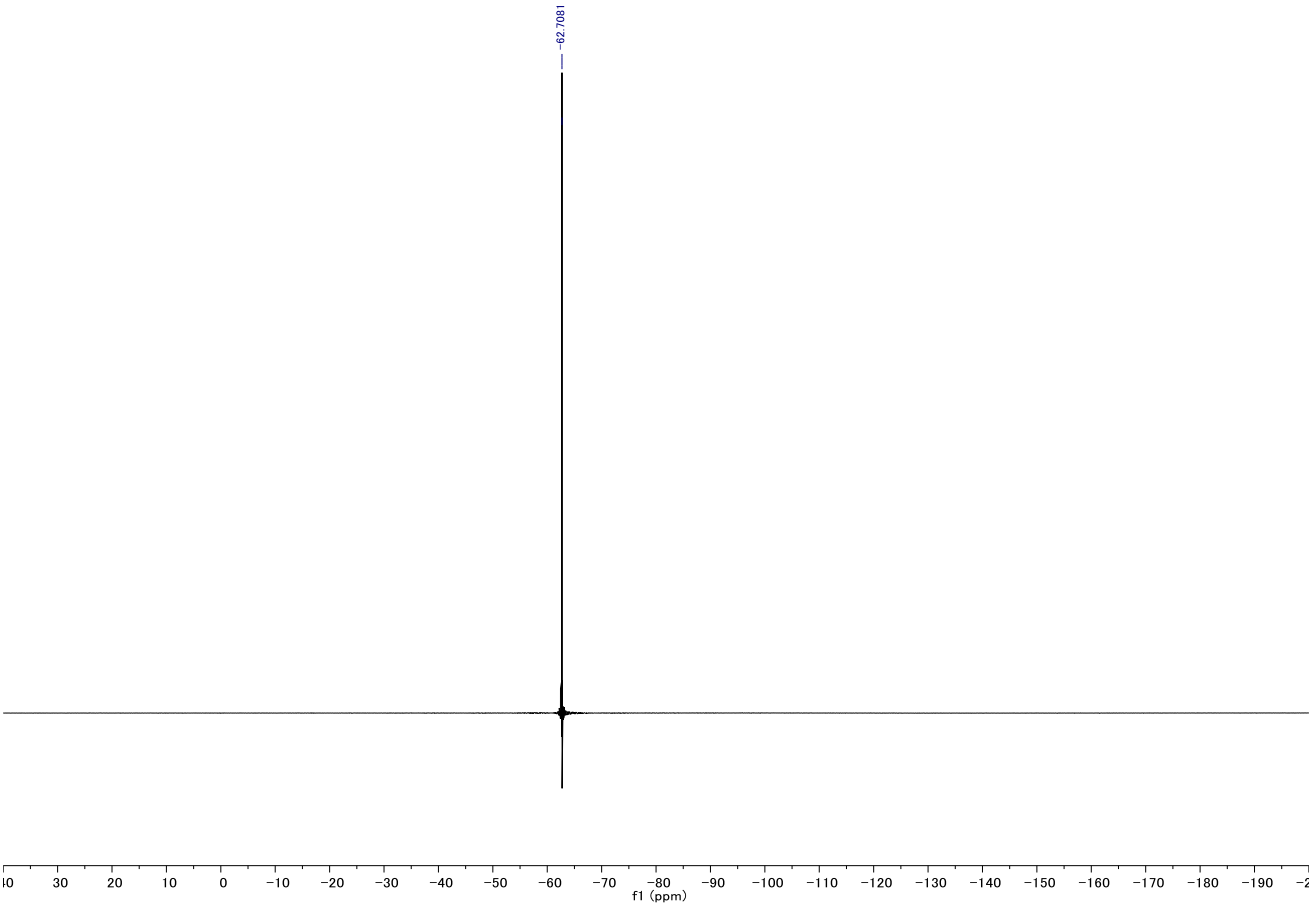
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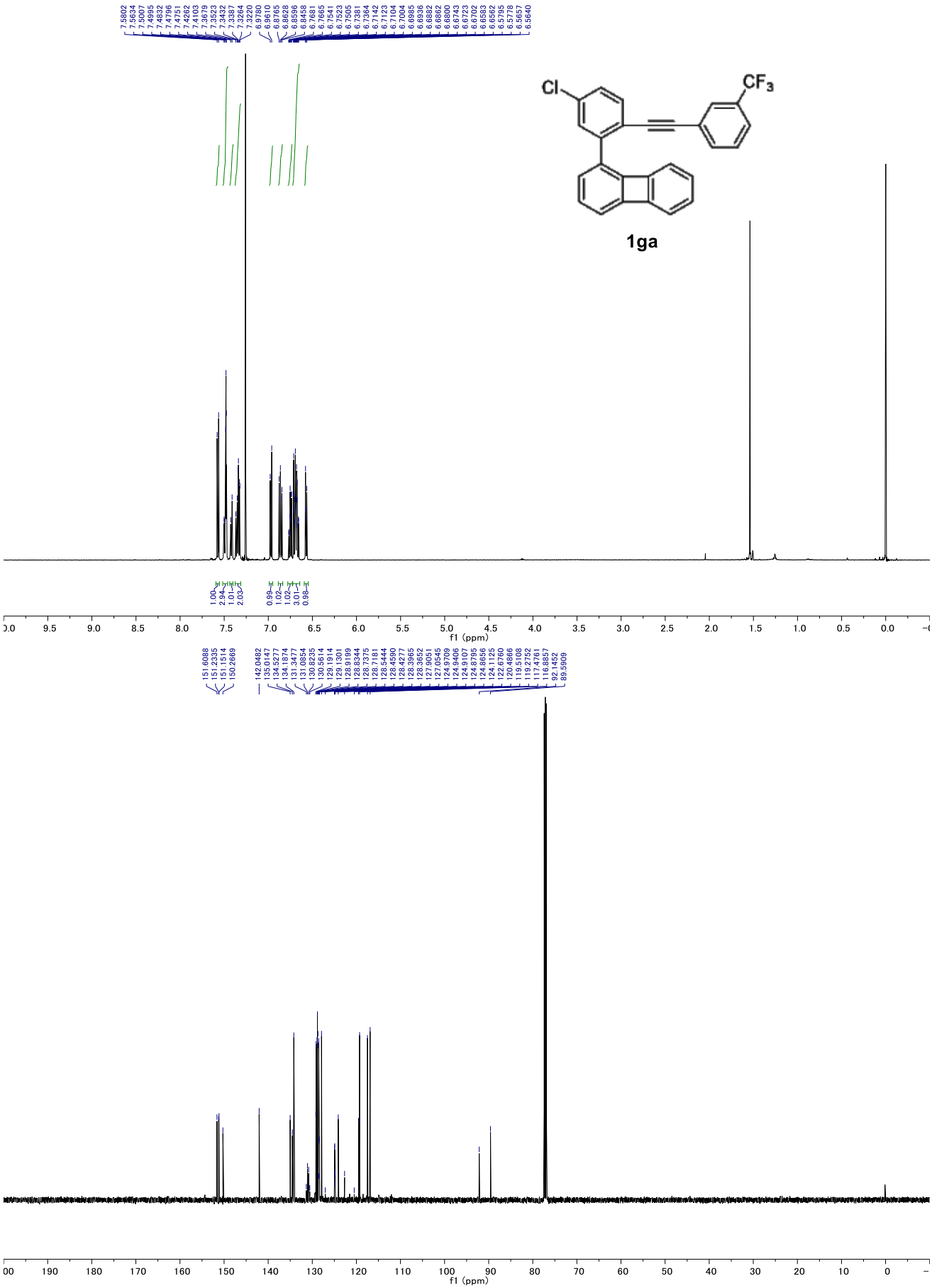
f1 (ppm)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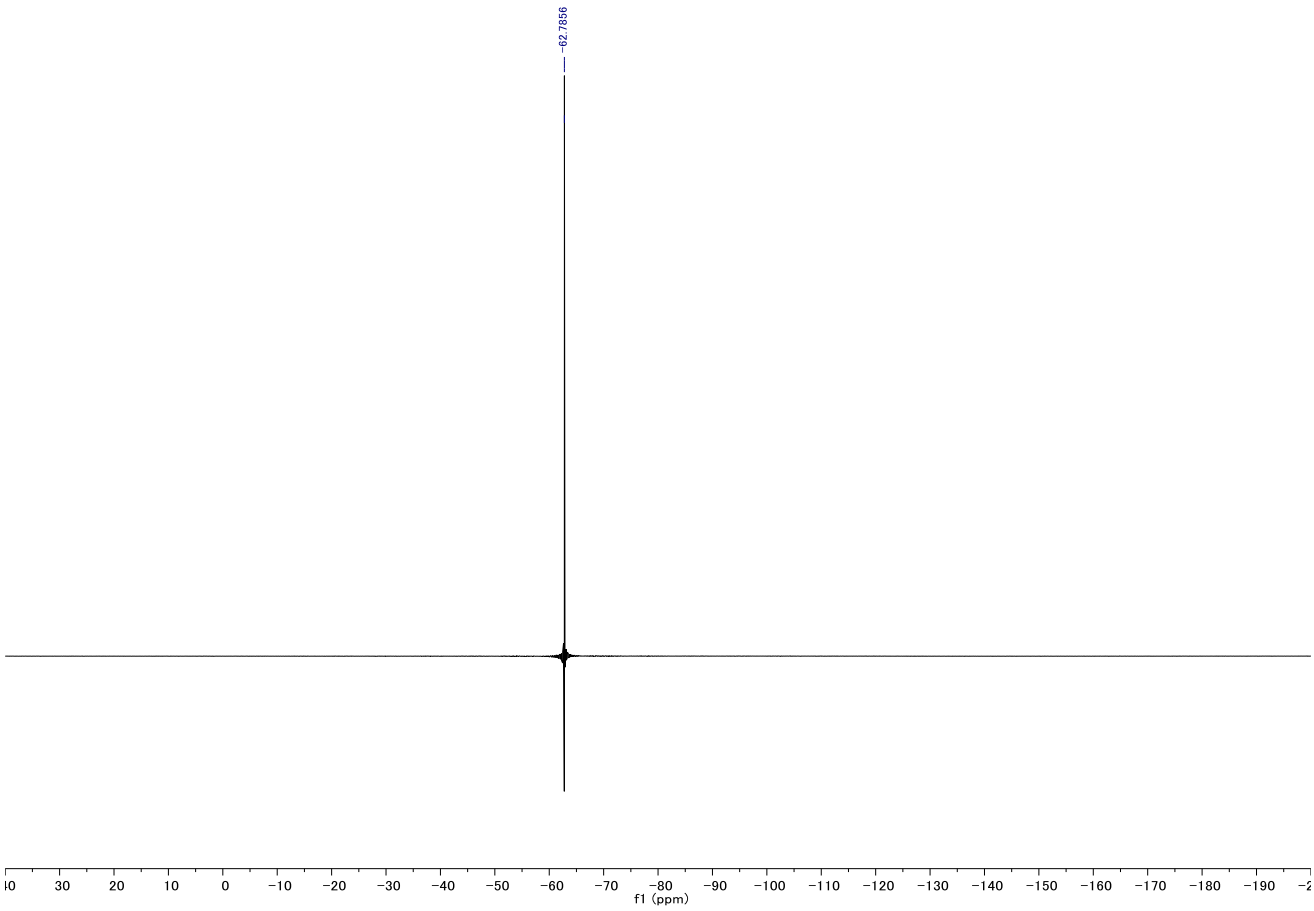
f1 (ppm)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−150
−160
−170
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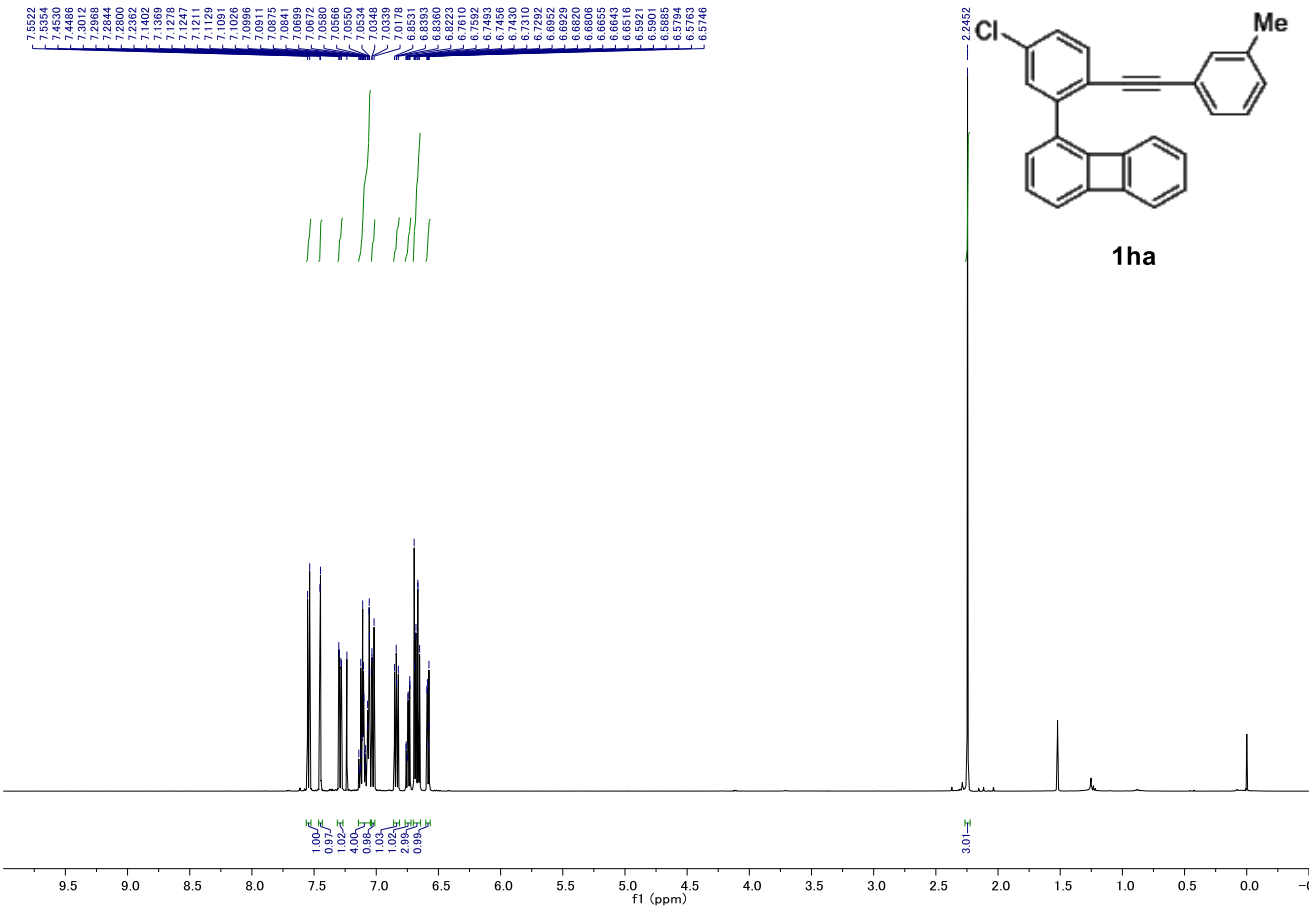
−190
f1 (ppm)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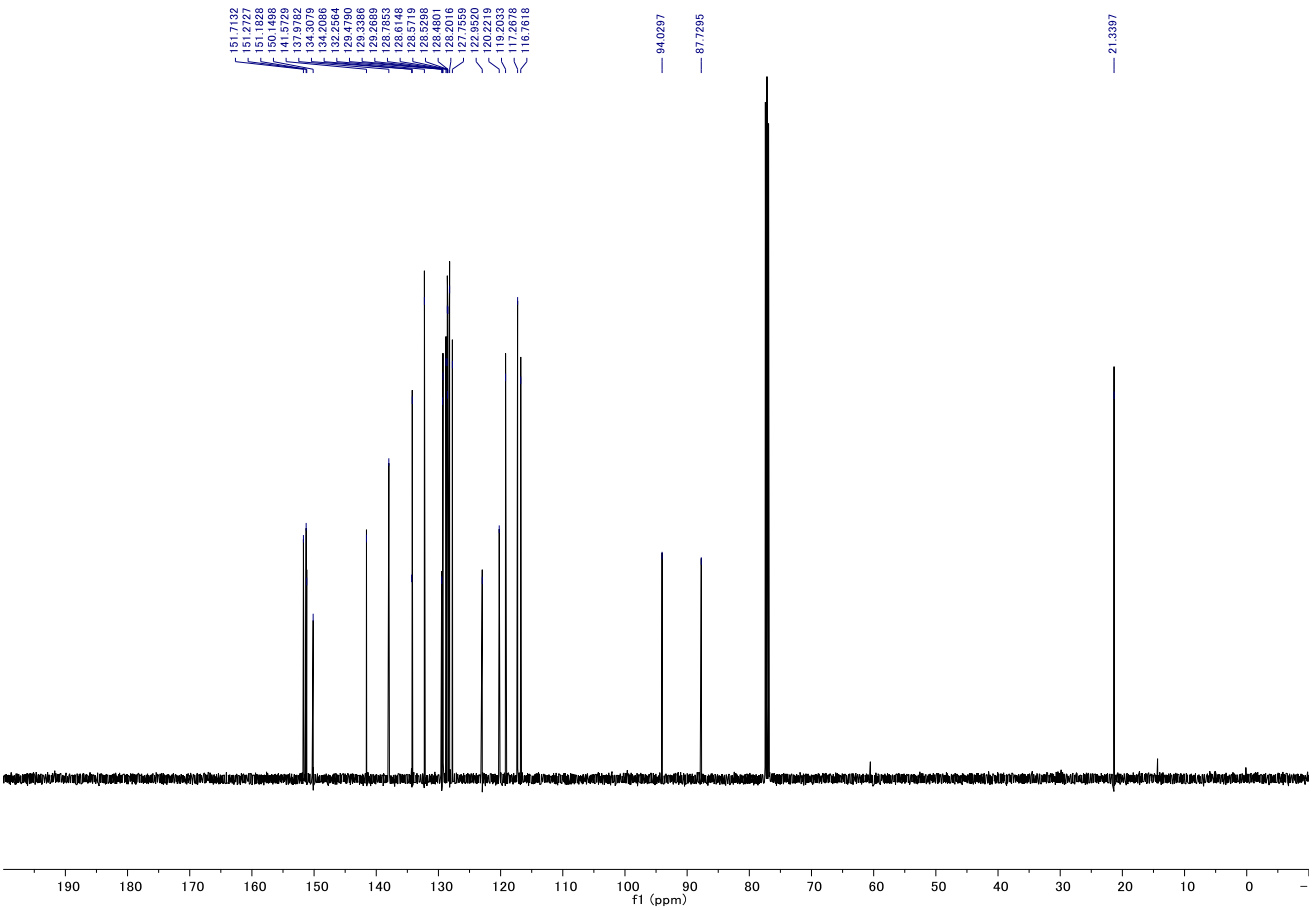
Me
1ha
f1 (ppm)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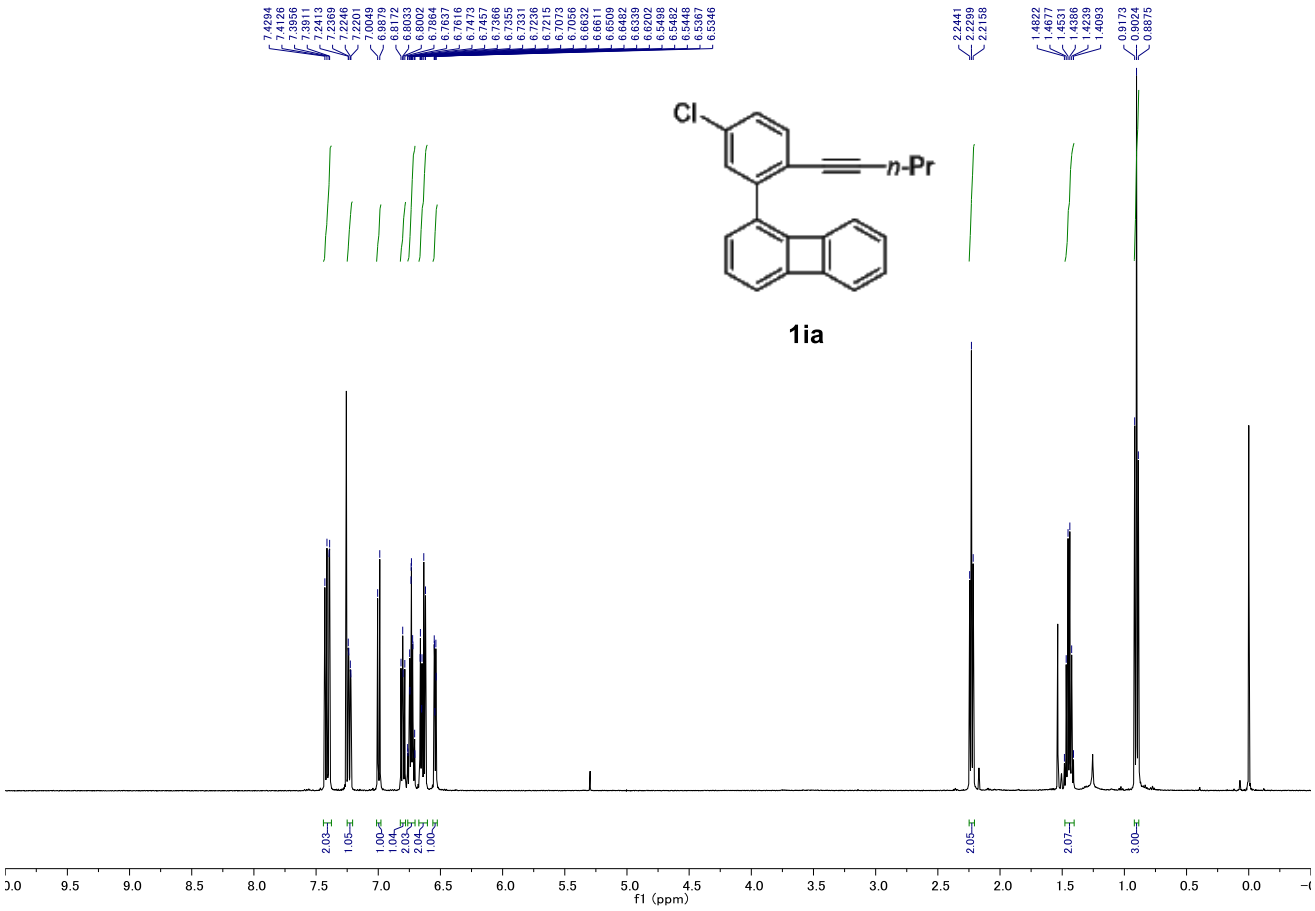
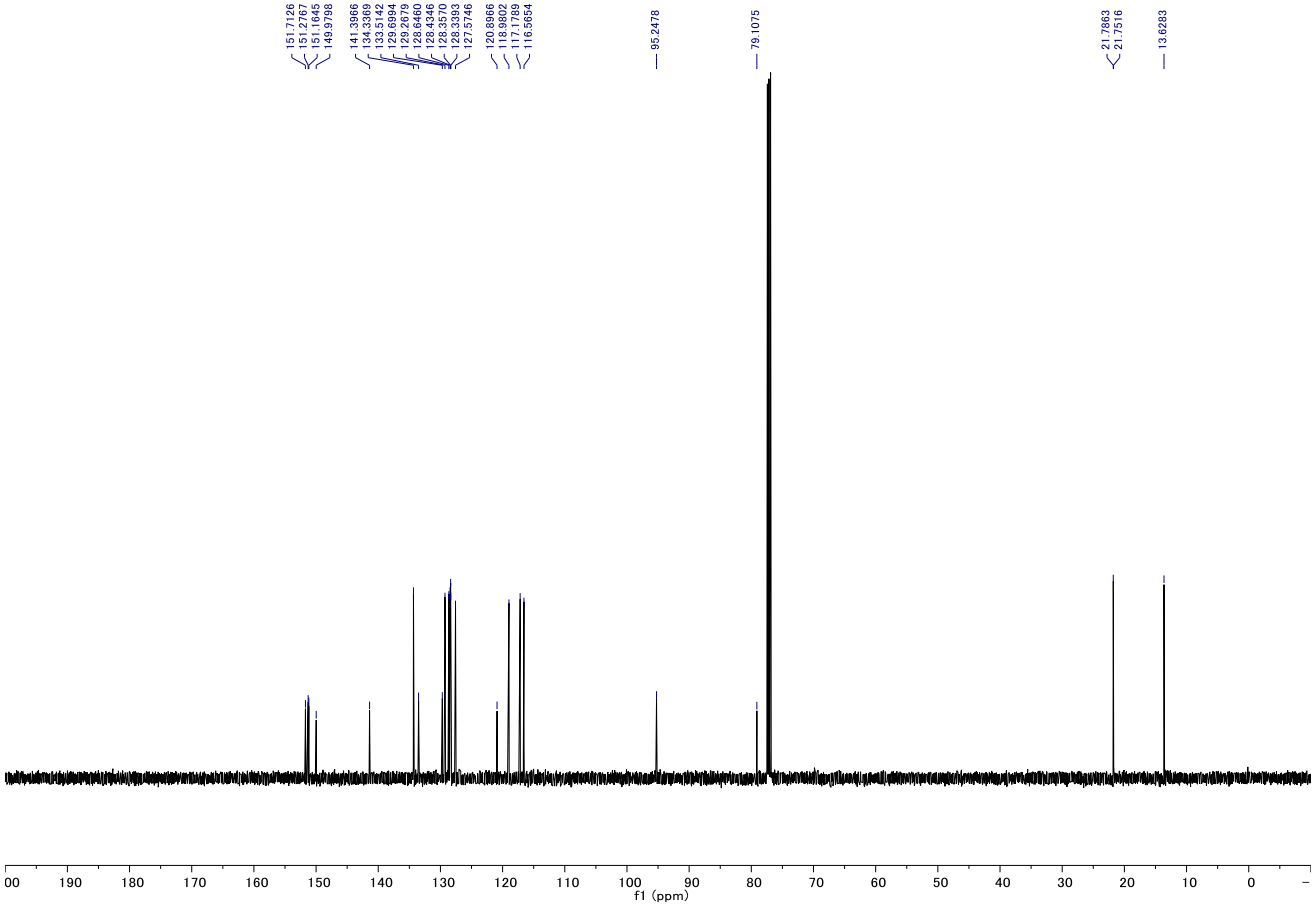

Cl
n-Pr
1ia
f1 (ppm)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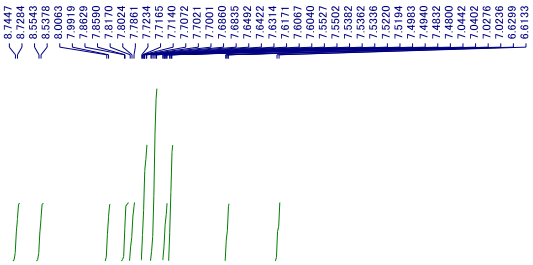
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7.7234
7.7165
7.7140
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7.7021
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7.6860
7.6835
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7.6422
7.6314
7.6171
7.6067
7.6040
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7.5502
7.5382
7.5332
7.5256
7.5220
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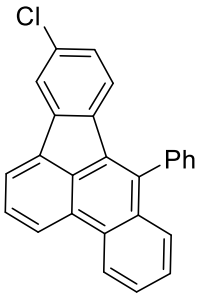
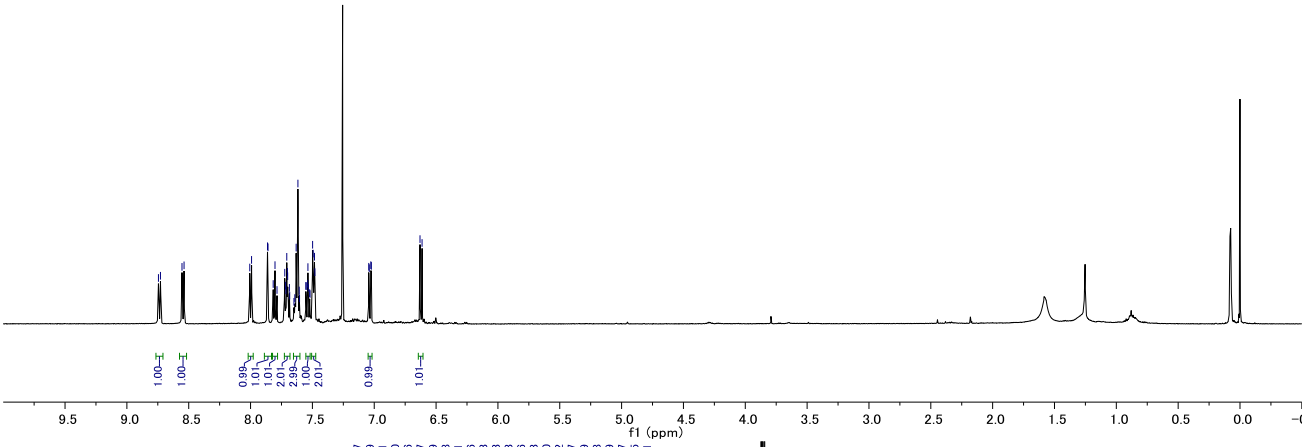
6.6299
6.6133


Cl
Ph

2aa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2.01
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1.00
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0.99
1.01
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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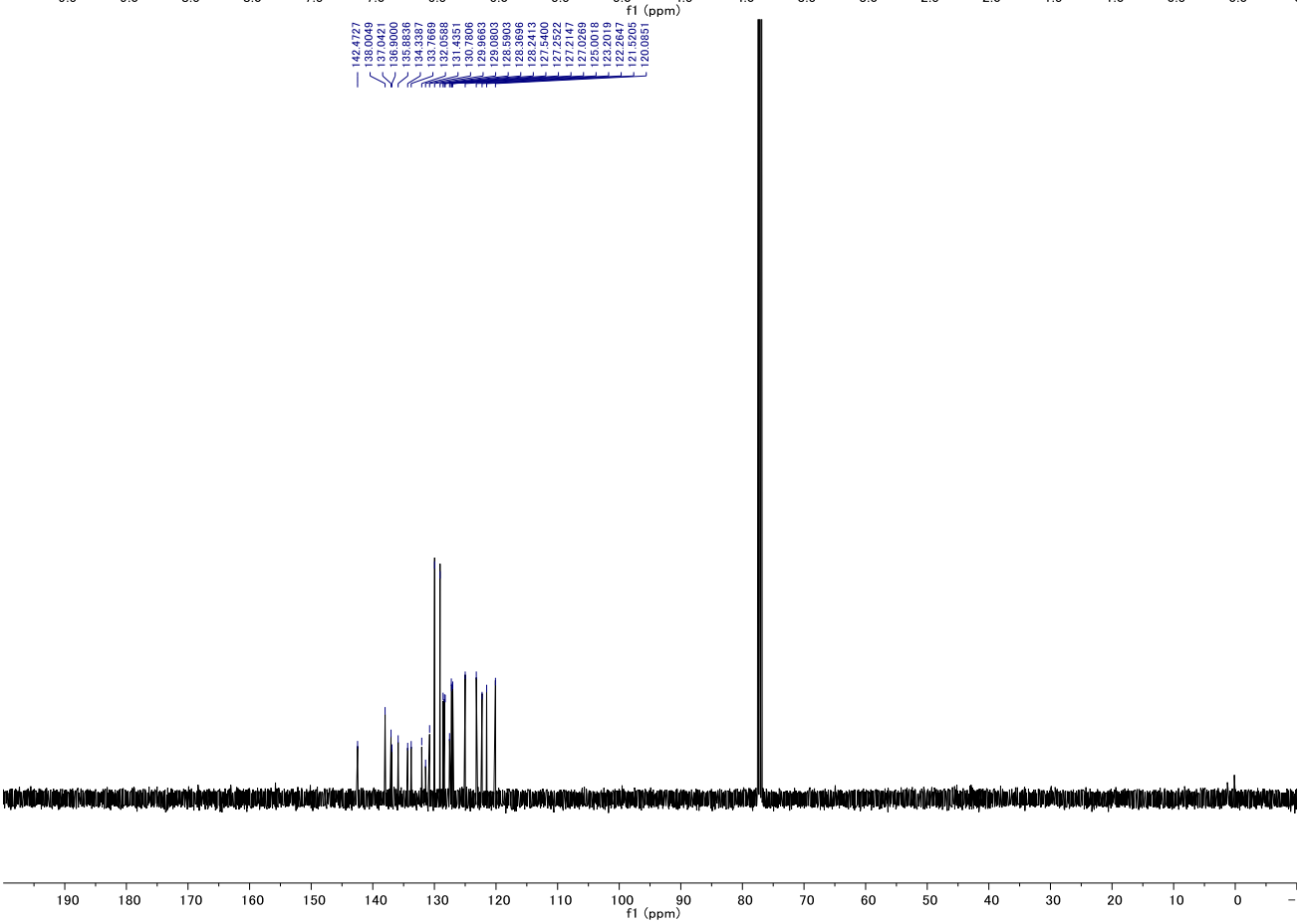
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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128.2413
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122.2647
121.5205
120.0851
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180
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130
120
110
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90
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70
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50
40
30
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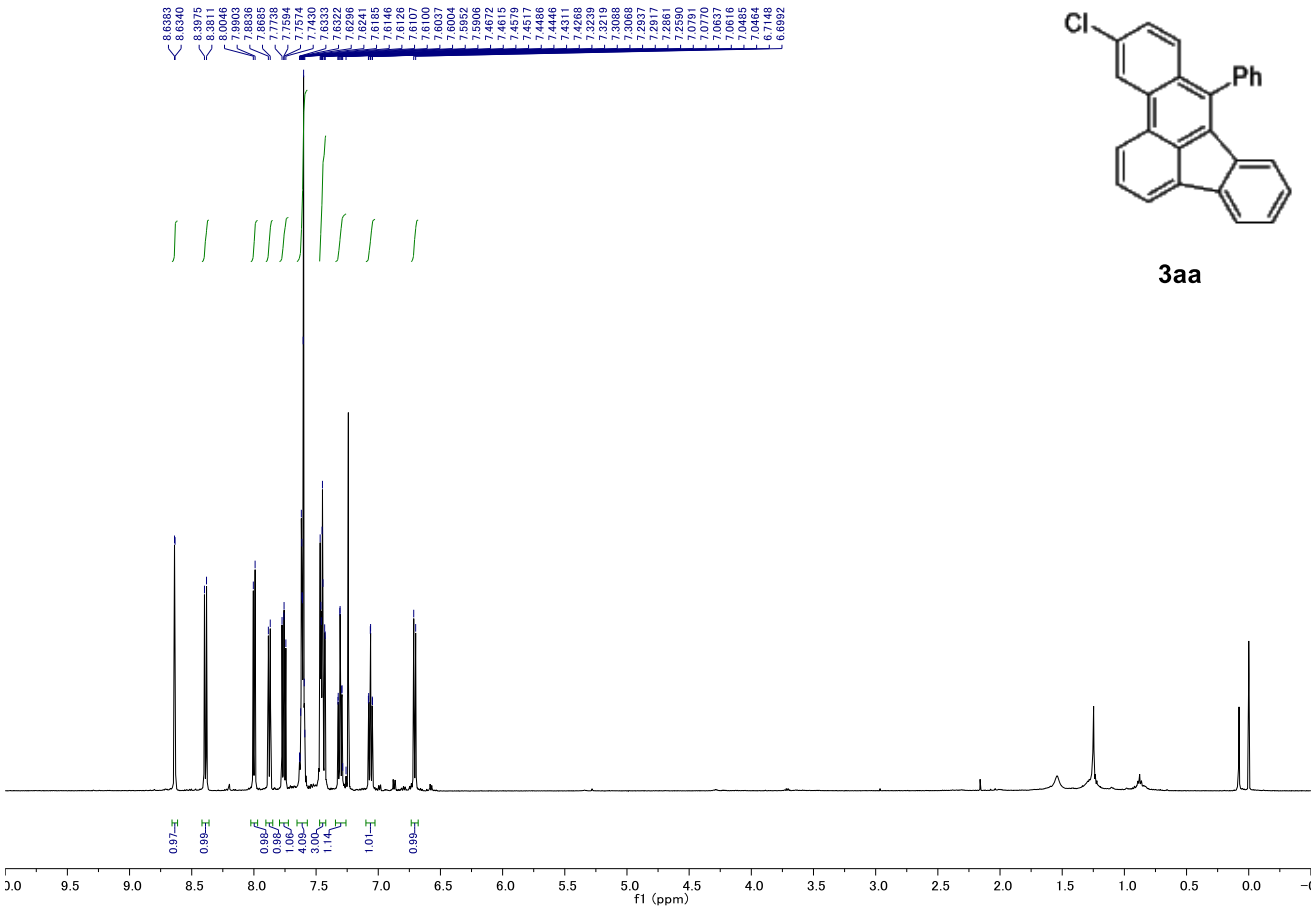
f1 (ppm)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8.0046
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7.7430
7.6333
7.6222
7.6266
7.6241
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7.6146
7.6126
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7.6037
7.6004
7.5952
7.5696
7.4672
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7.4517
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7.4446
7.4311
7.4268
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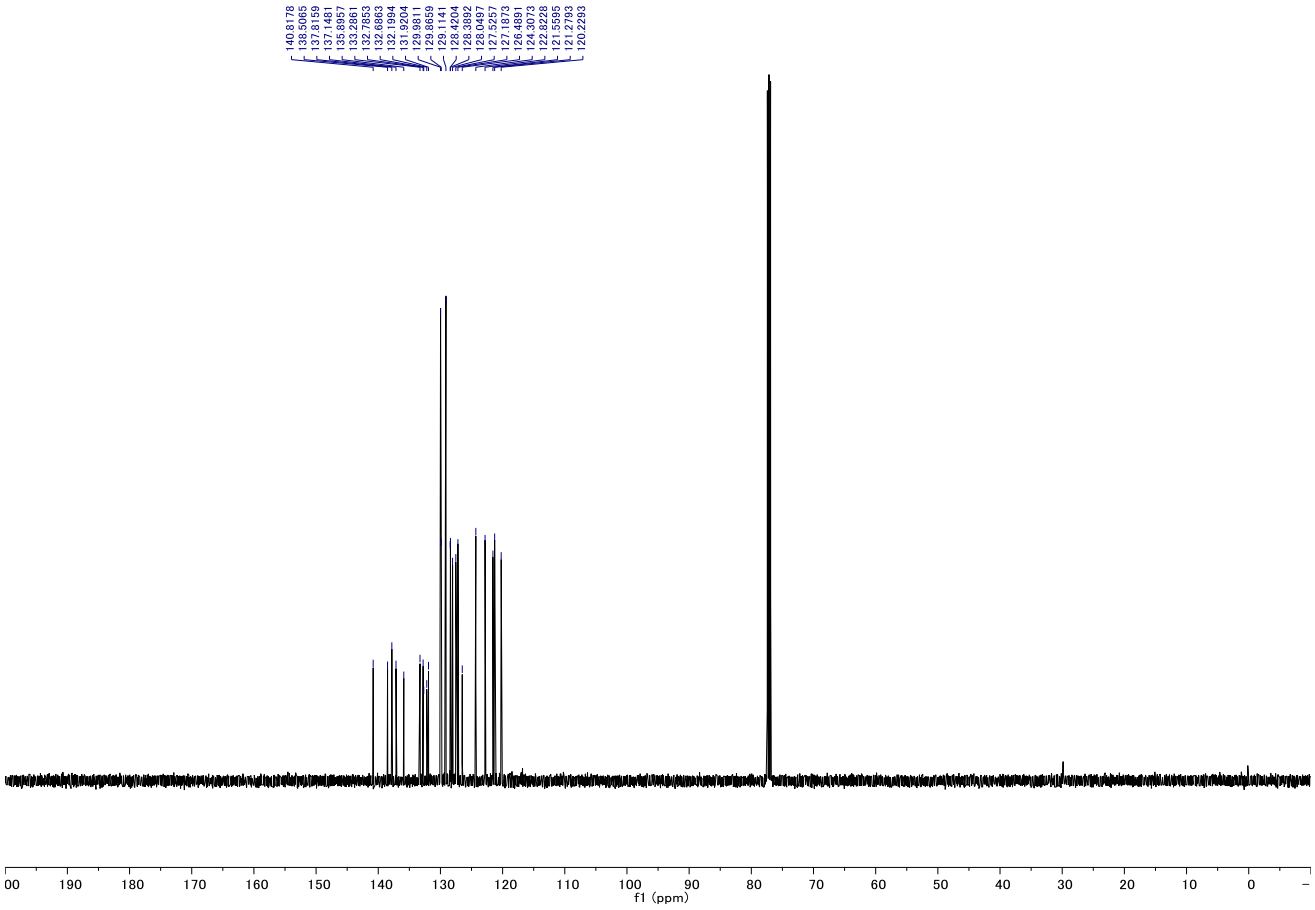
7.3219
7.3088
7.3068
7.2937
7.2917
7.2861
7.2590
7.0791
7.0770
7.0637
7.0616
7.0485
7.0464
6.7148
6.6992
0.97
0.89
0.98
0.98
1.06
4.09
3.00
1.14
1.01
0.99
f1 (ppm)

Cl
Ph

3aa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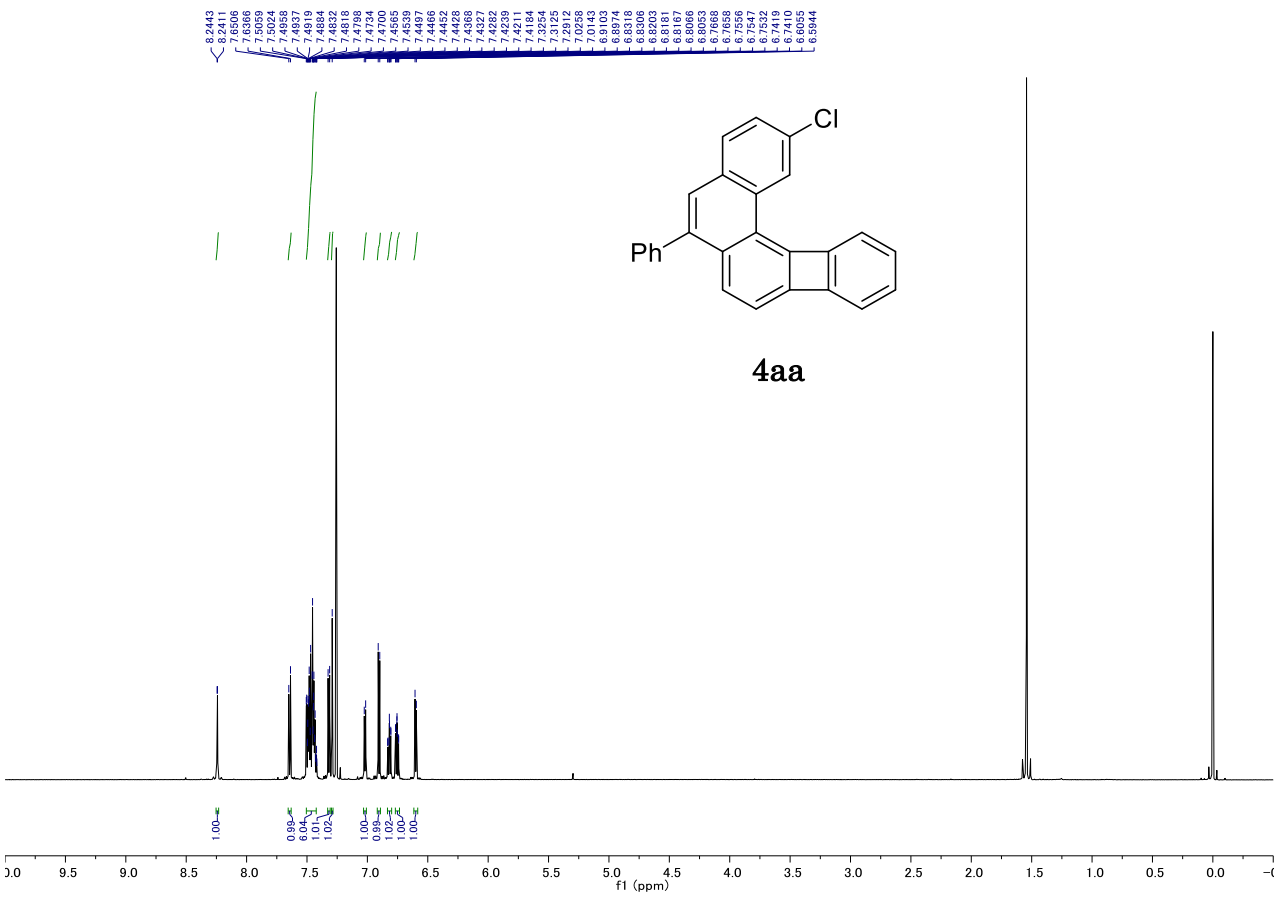
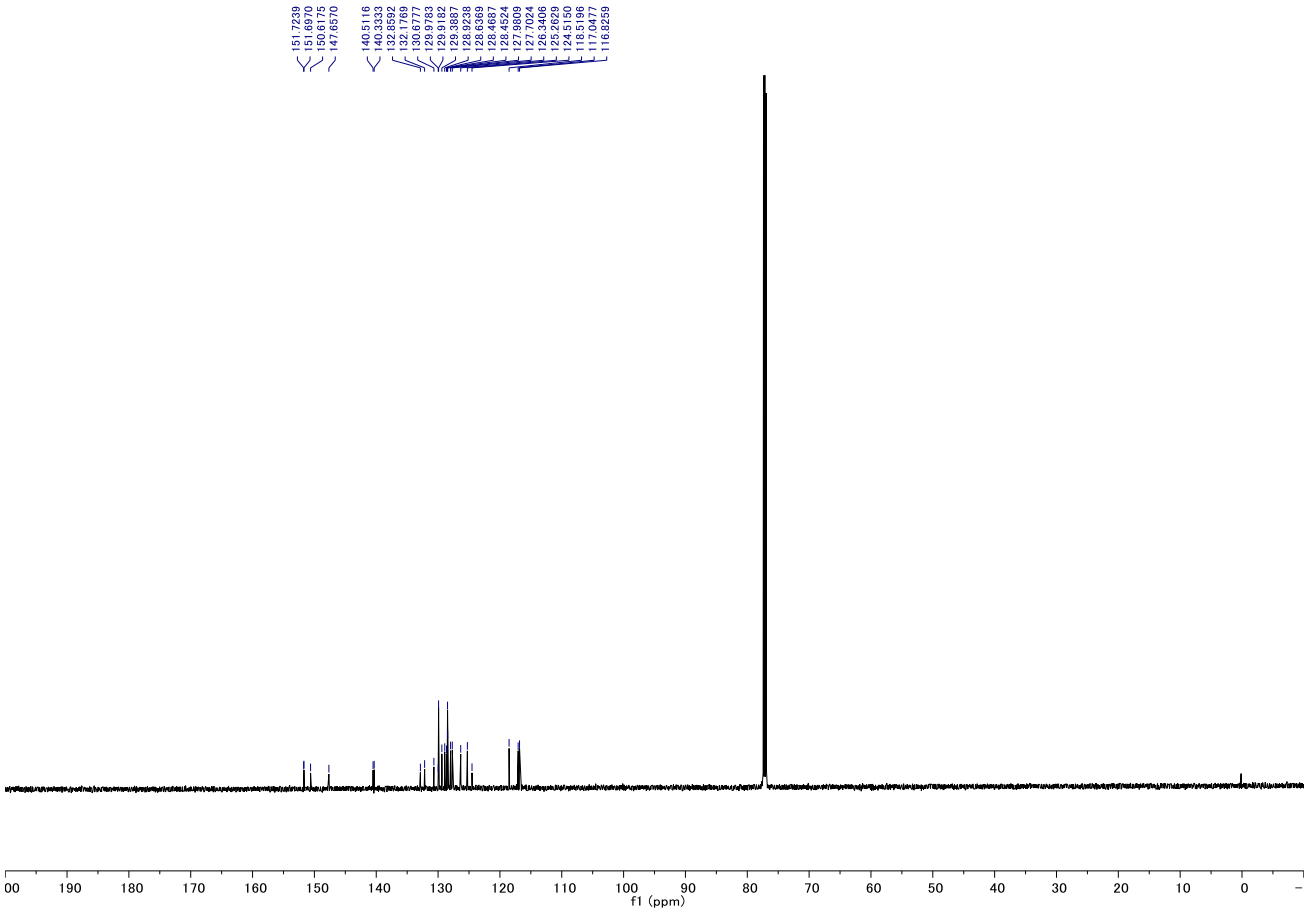
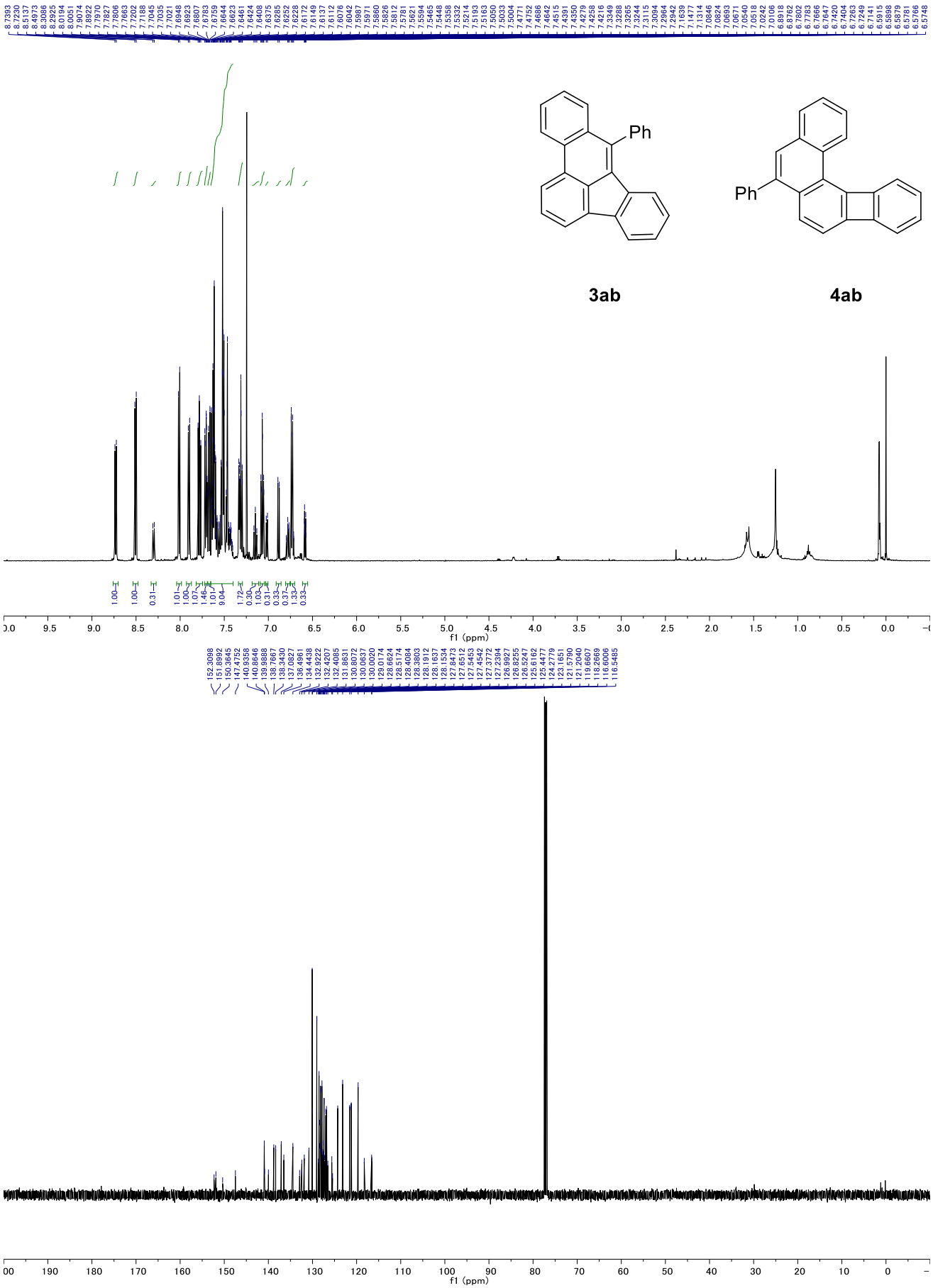
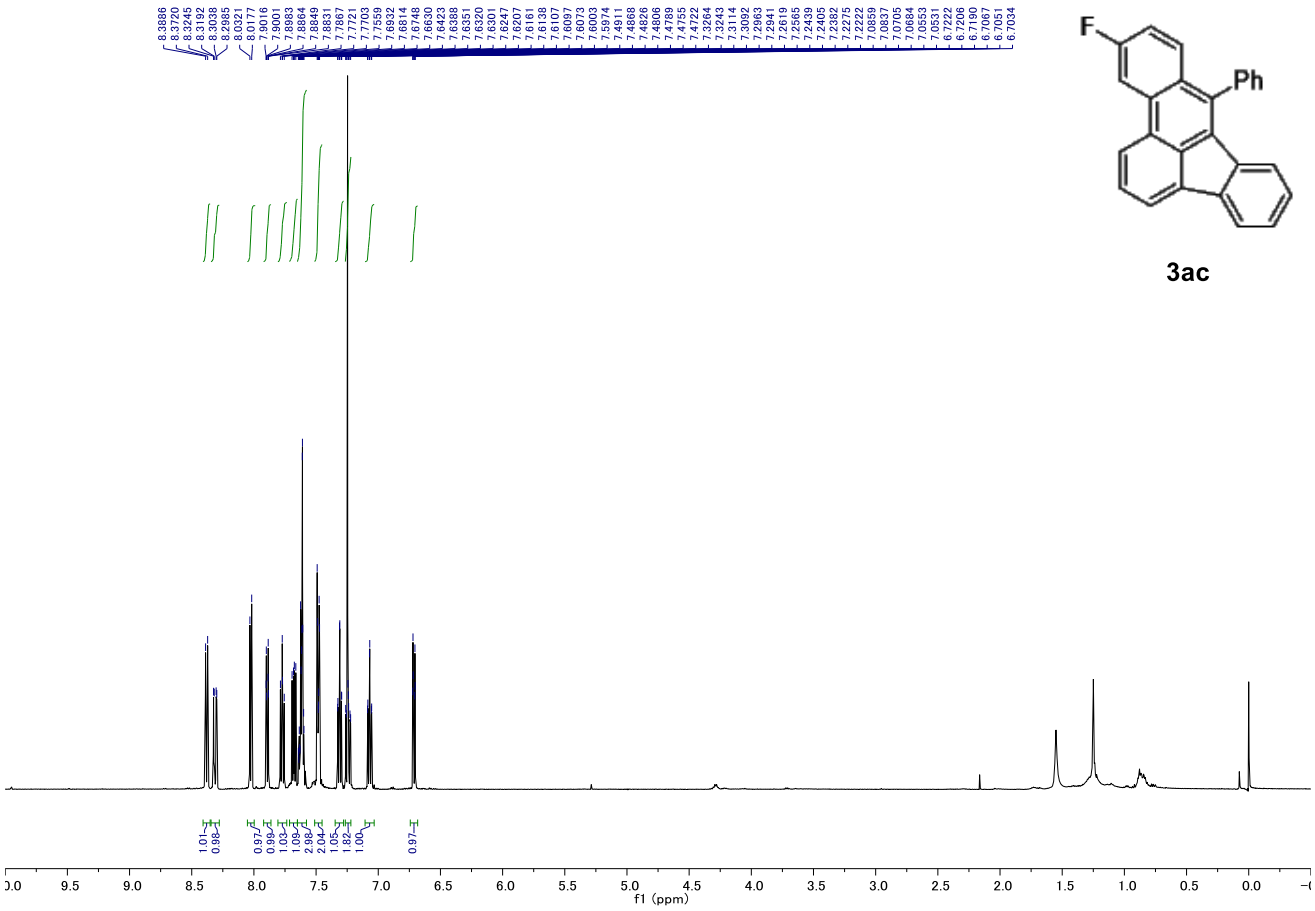
127.5257
127.1373
126.4891
124.3073
122.8228
121.5595
121.2793
120.2293
f1 (ppm)

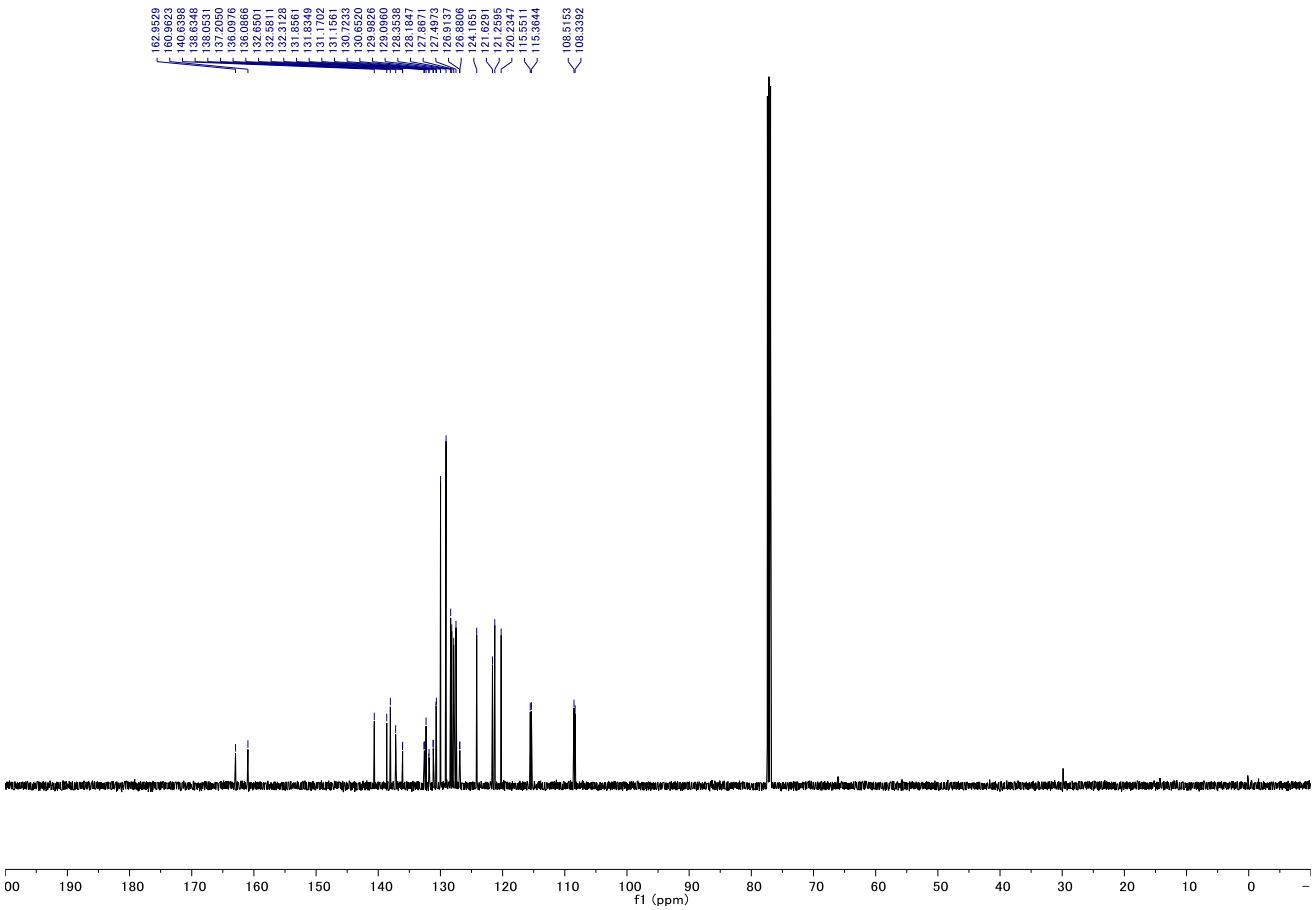


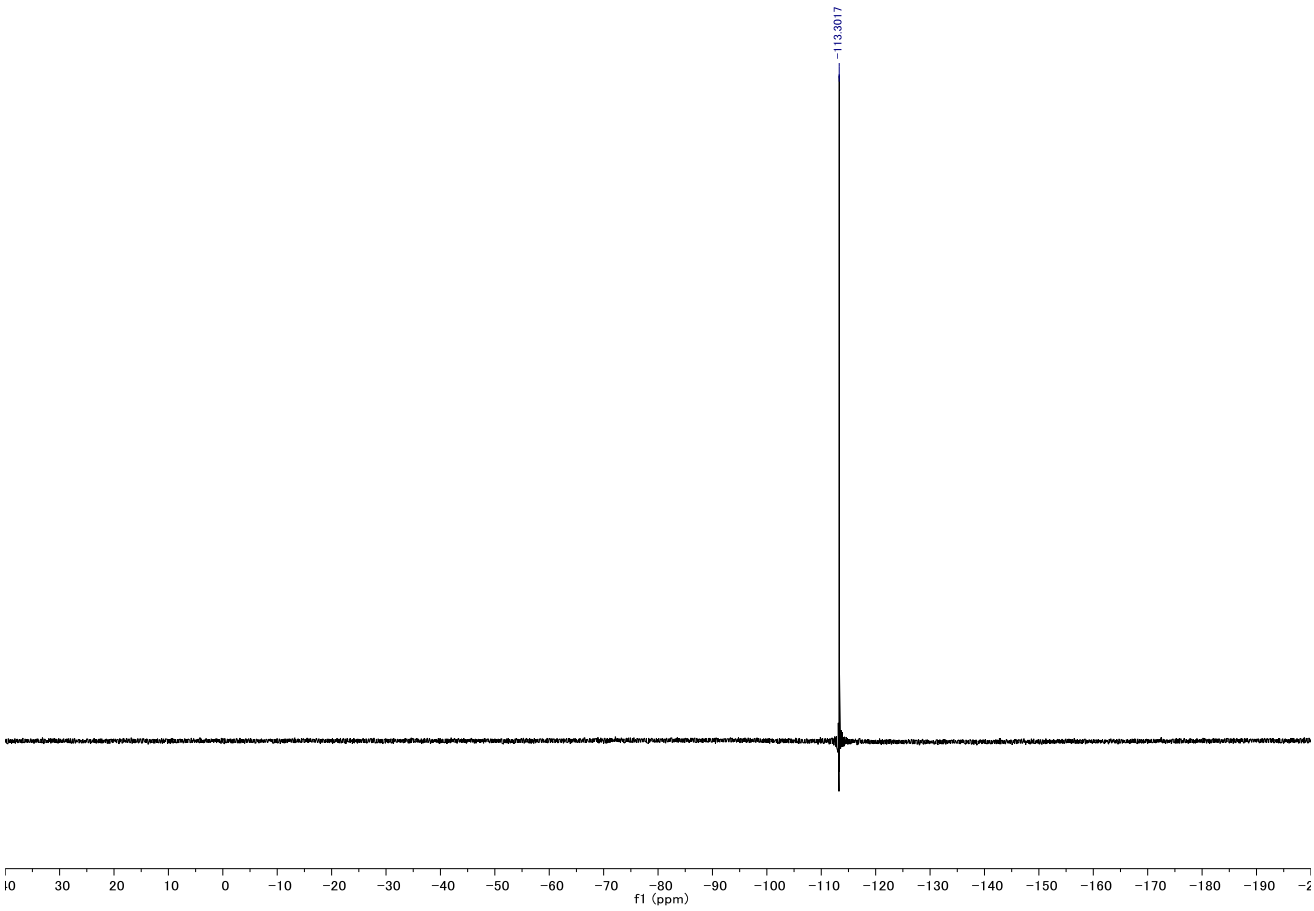
4aa

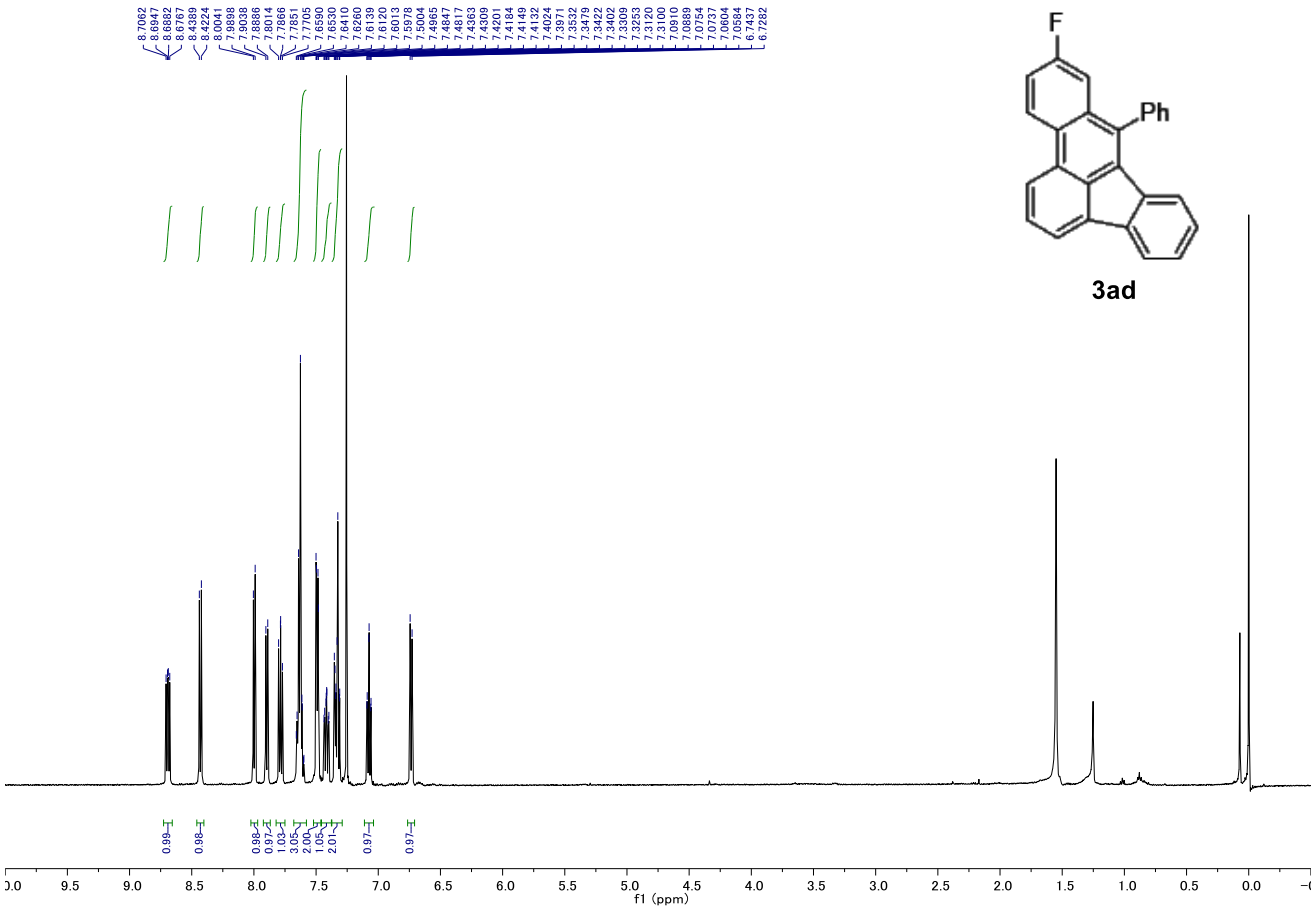


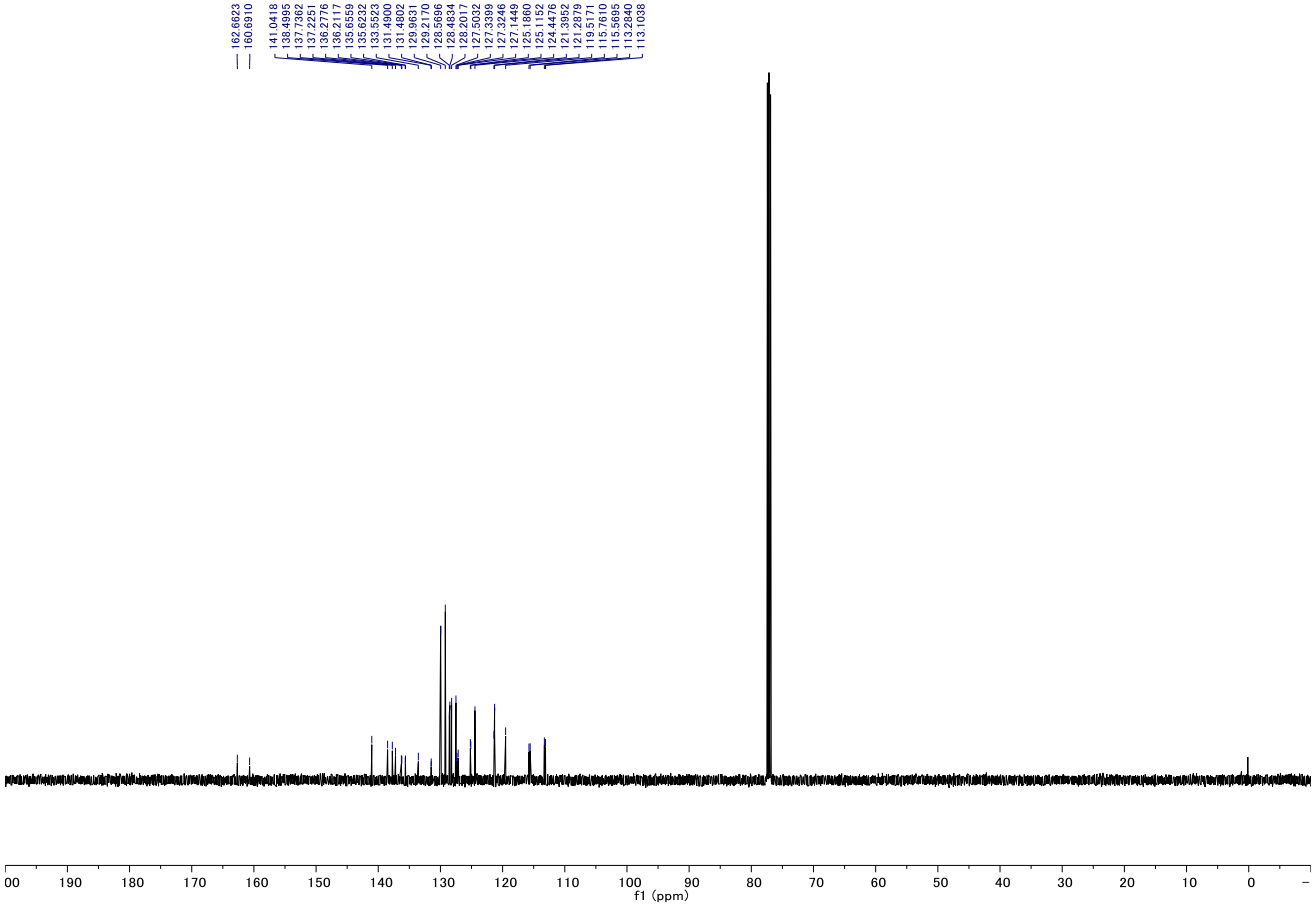

Ph
Ph
3ab
4ab
f1 (ppm)
f1 (ppm)

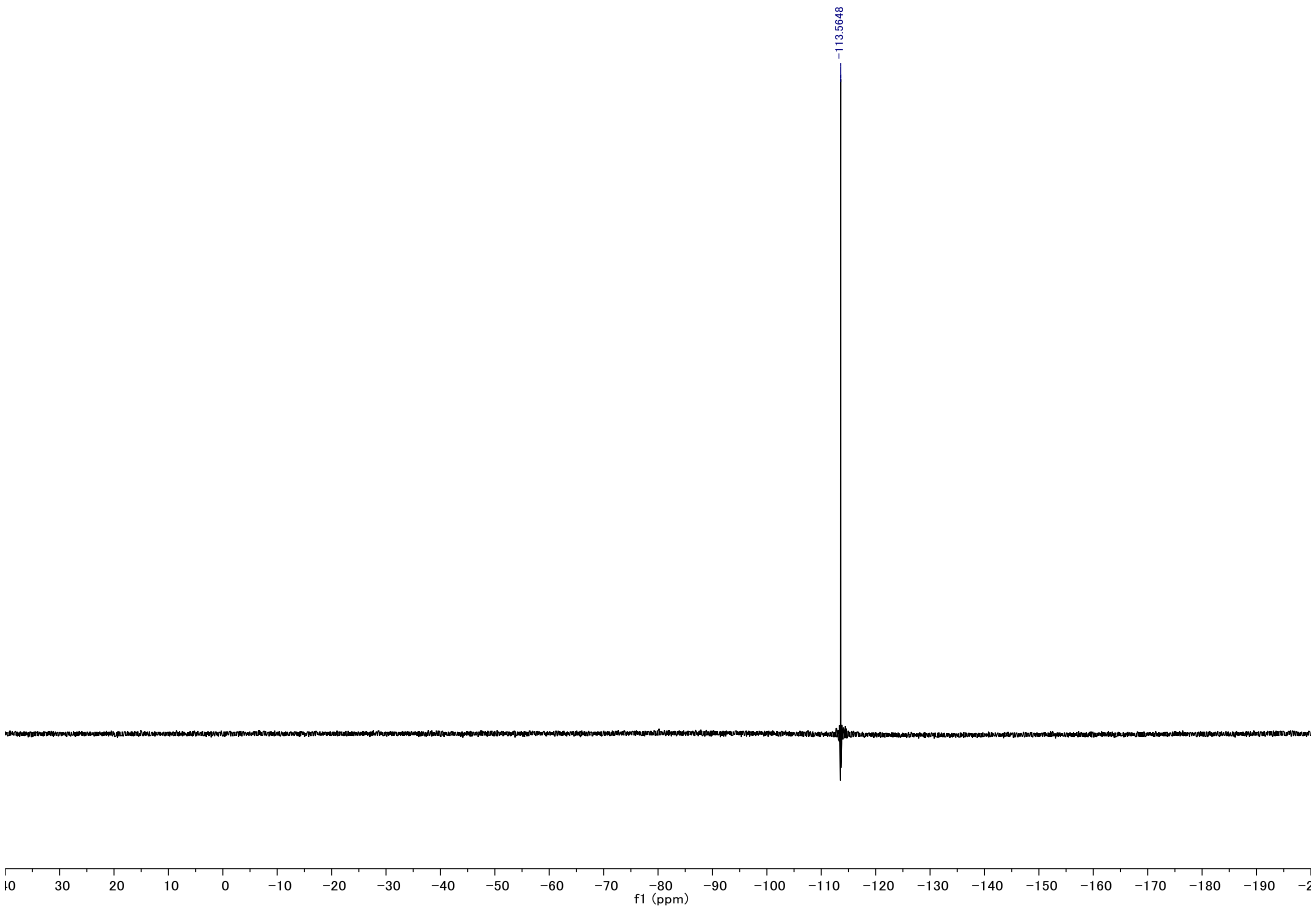

F
Ph
3ac
f1 (ppm)


f1 (ppm)


-113.3017
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
f1 (ppm)


F
Ph
3ad
f1 (ppm)


f1 (ppm)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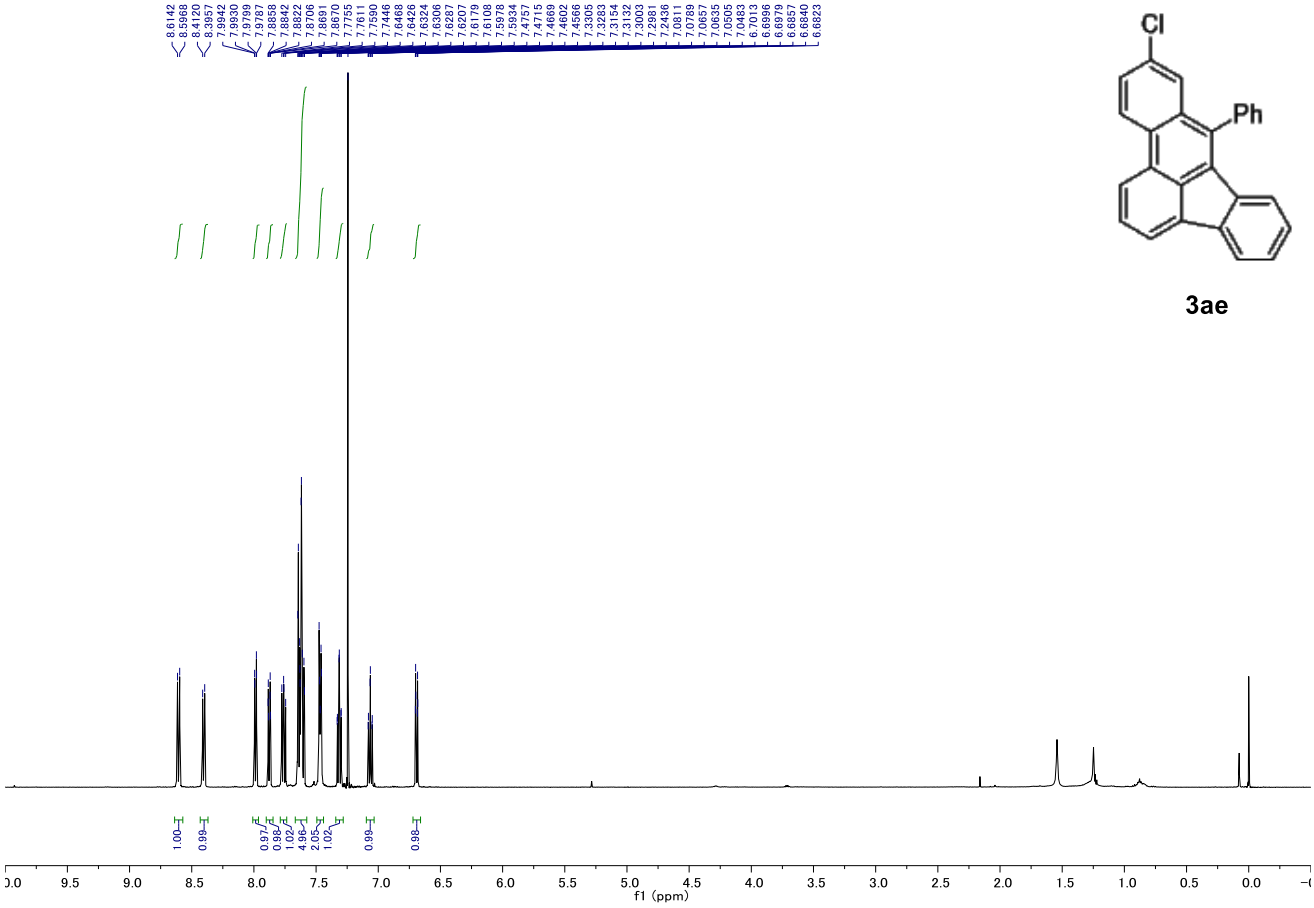
f1 (ppm)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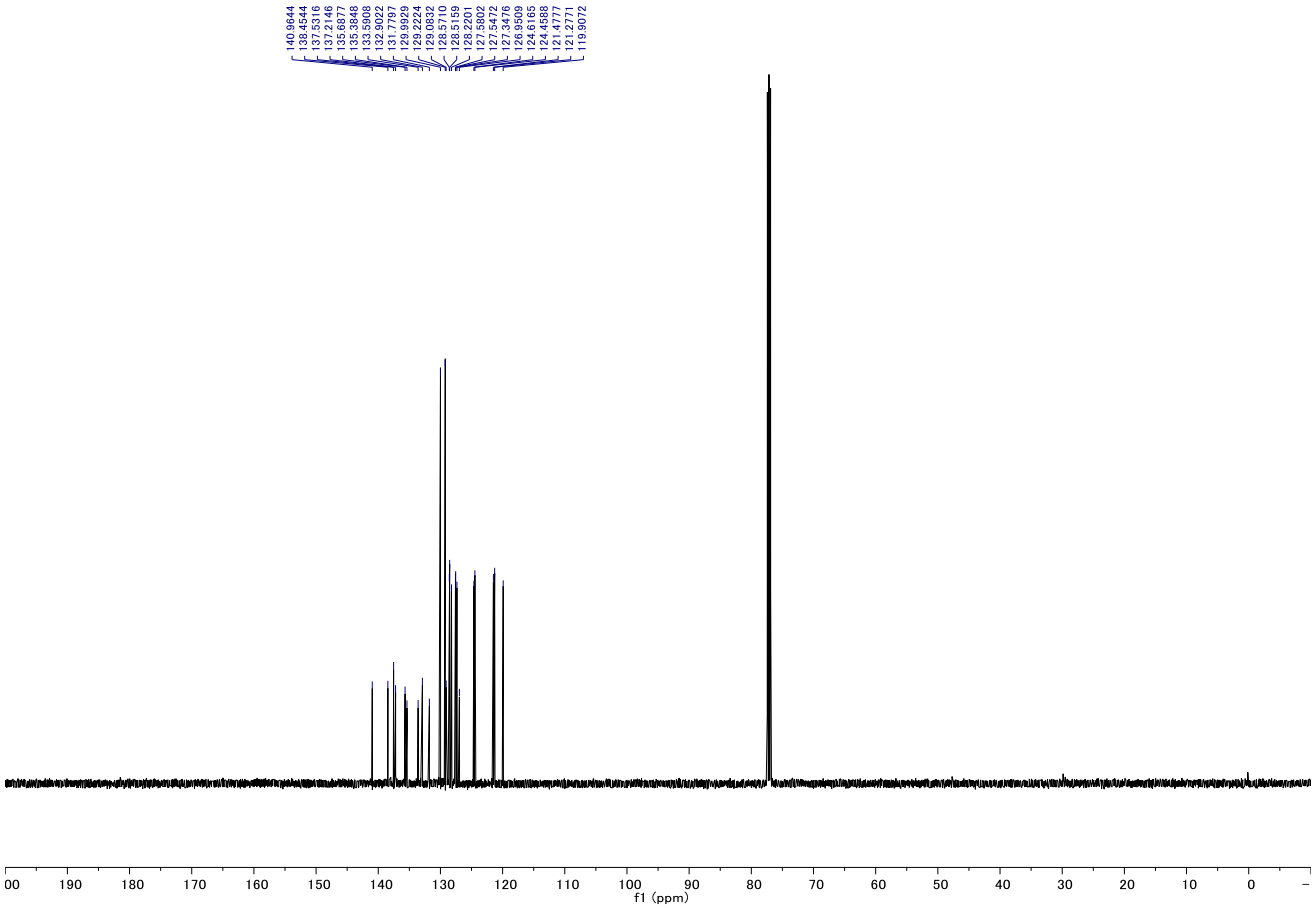
8.4400
8.3957
7.9942
7.9930
7.9799
7.9787
7.8858
7.8842
7.8822
7.8706
7.8691
7.8670
7.7755
7.7611
7.7590
7.7446
7.6468
7.6426
7.6324
7.6306
7.6287
7.6207
7.6179
7.6108
7.5978
7.5934
7.4757
7.4715
7.4669
7.4602
7.4566
7.4395
7.3283
7.3154
7.3132
7.3003
7.2981
7.2436
7.0811
7.0789
7.0657
7.0635
7.0555
7.0483
6.7013
6.6996
6.6979
6.6857
6.6840
6.6823
1.00
0.99
0.97
0.98
1.02
4.96
2.05
1.02
0.99
0.98
f1 (ppm)

Cl
Ph

3ae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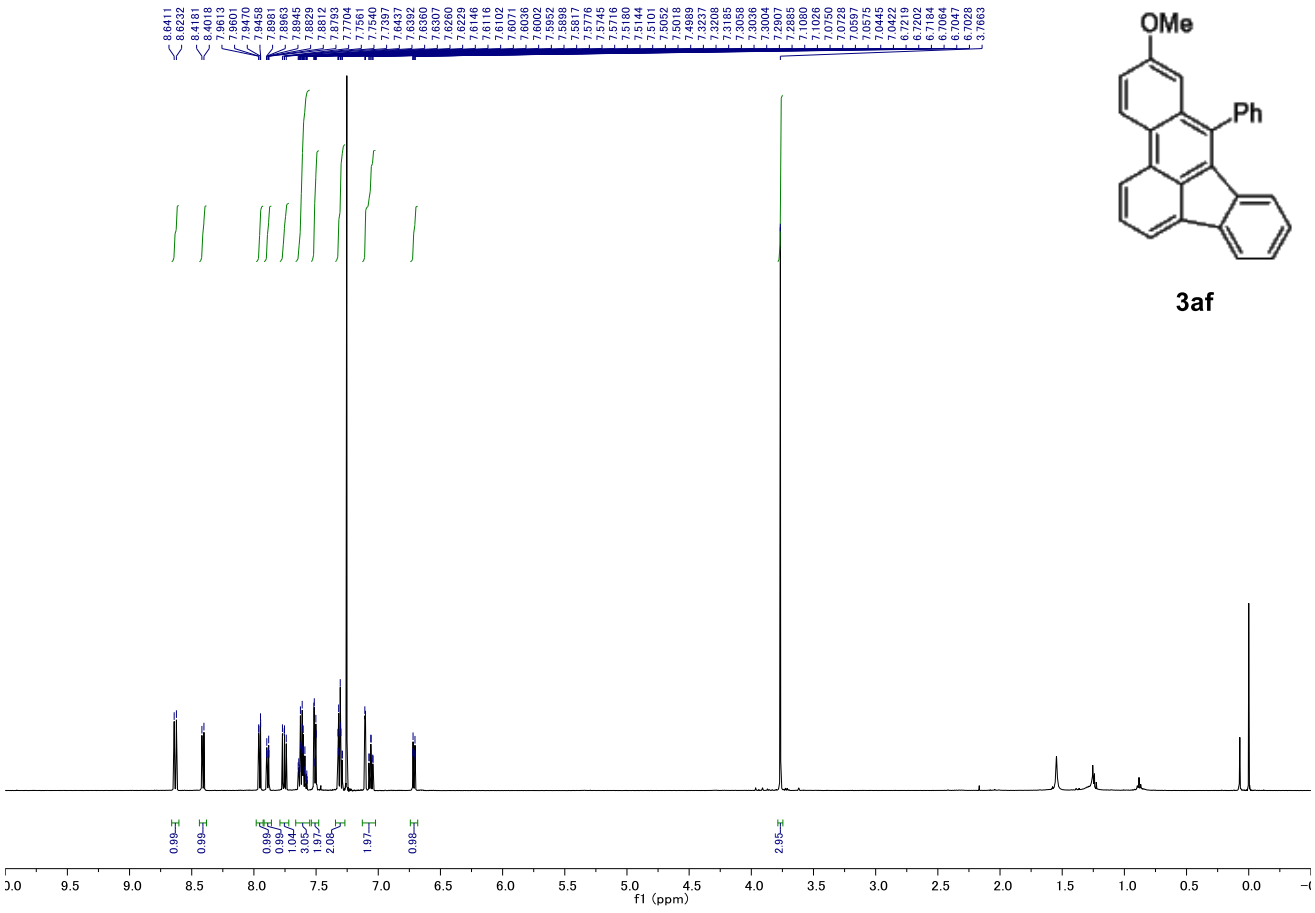
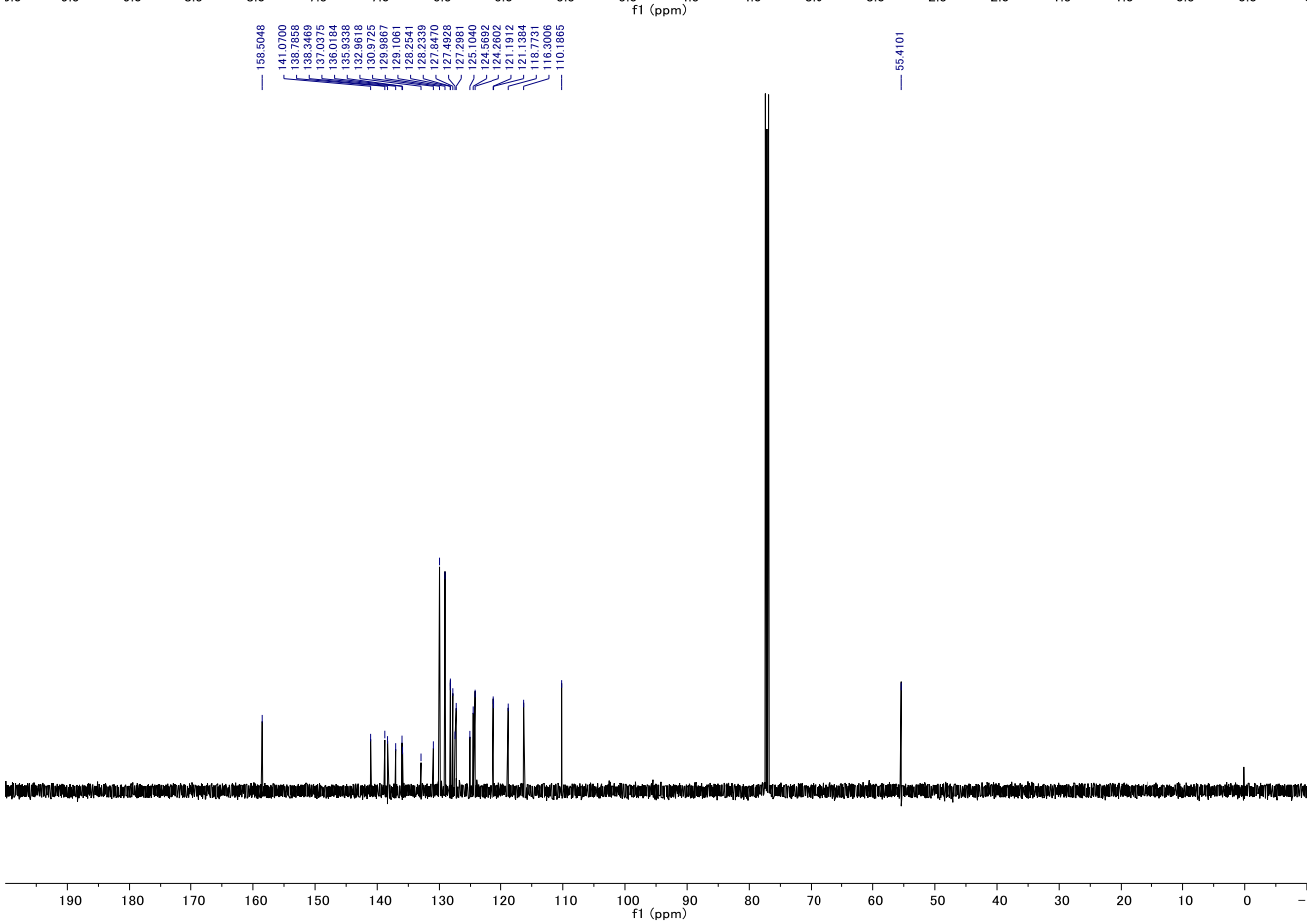
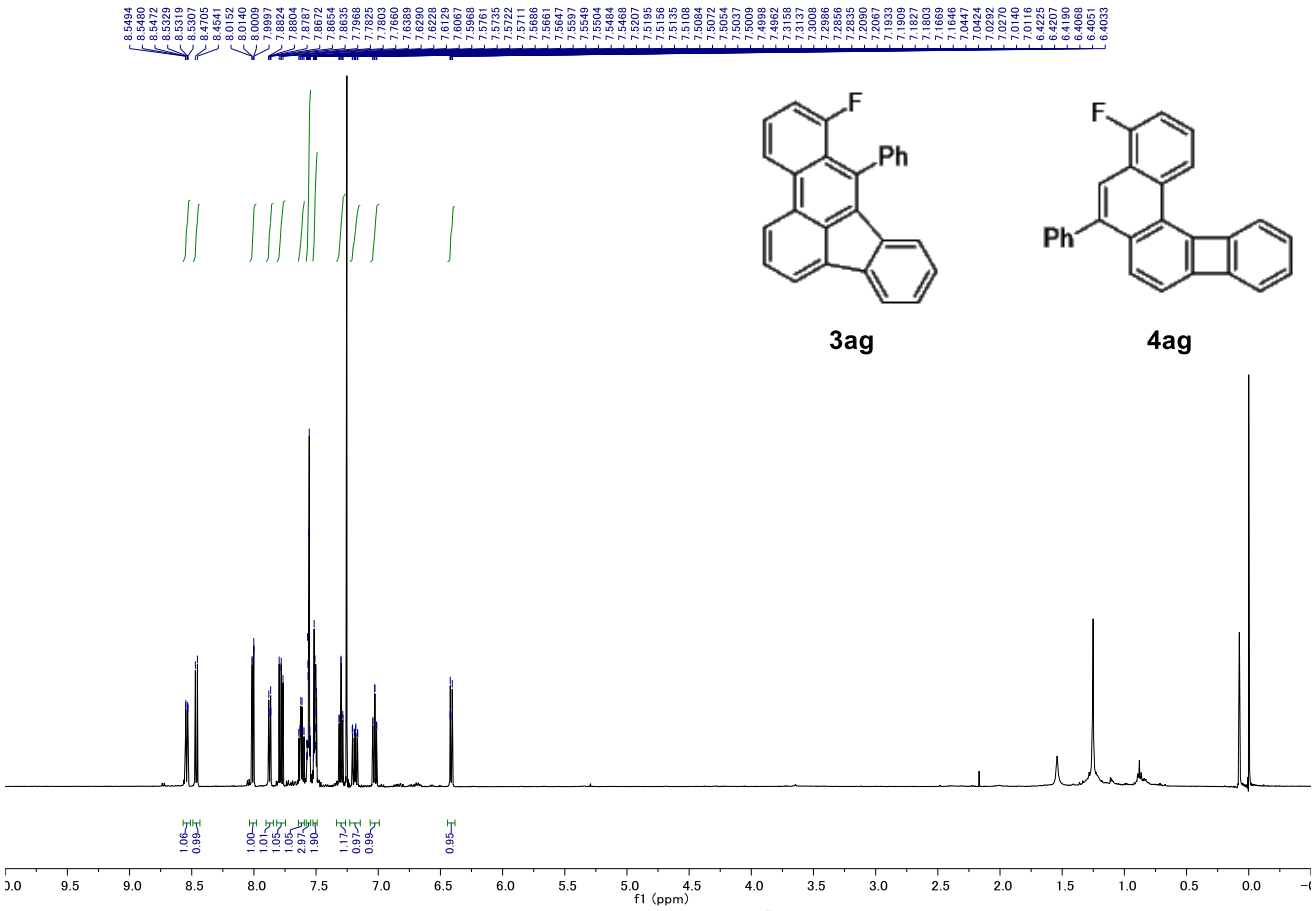
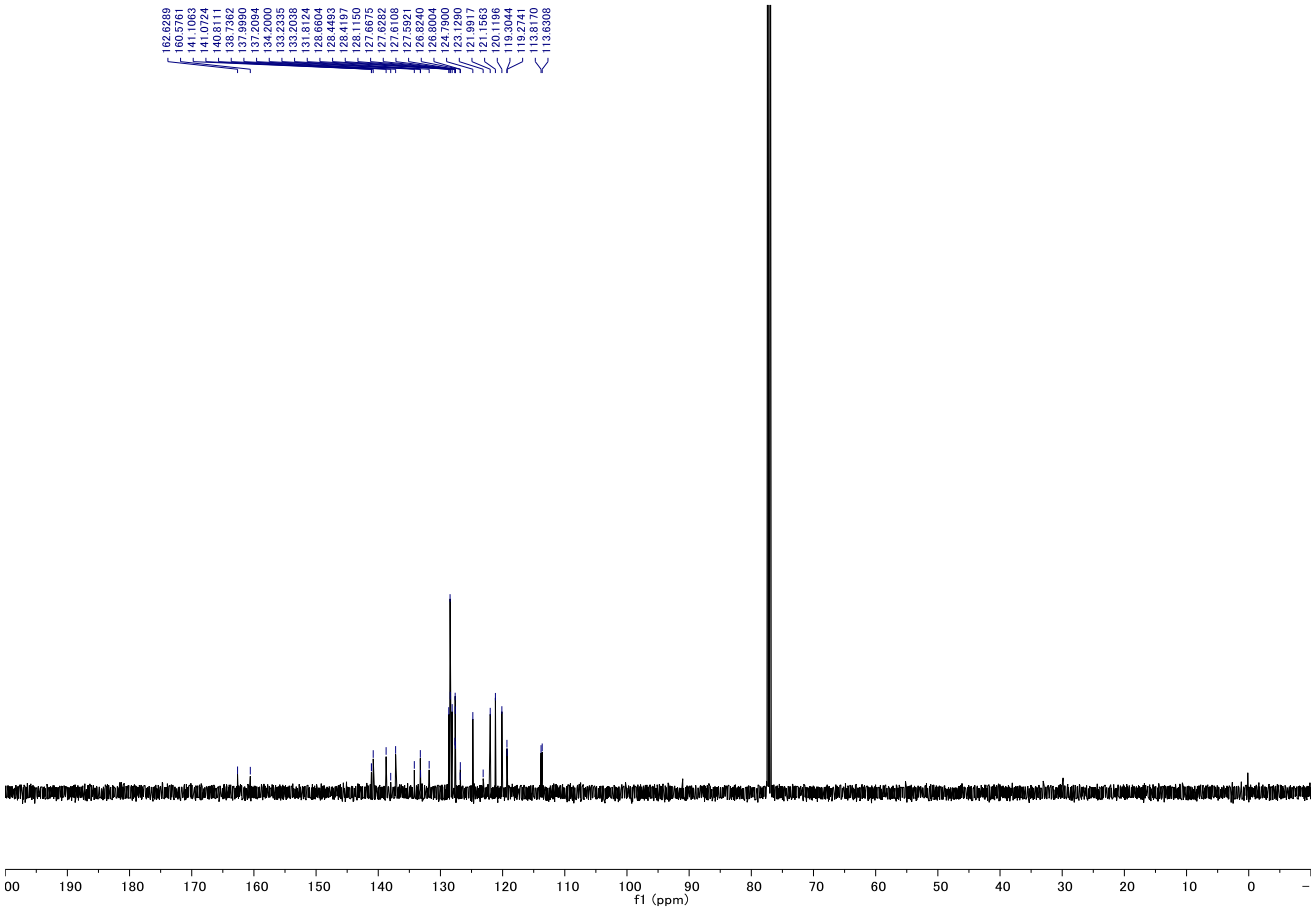
137.2146
135.6877
135.3848
133.5908
132.6092
131.7792
129.9929
129.2224
129.0832
128.5710
128.5159
128.2201
127.5802
127.5472
127.3476
126.8698
124.6165
124.4588
121.4777
121.2771
119.9072
f1 (ppm)



3af




F
Ph
3ag
F
Ph
4ag
f1 (ppm)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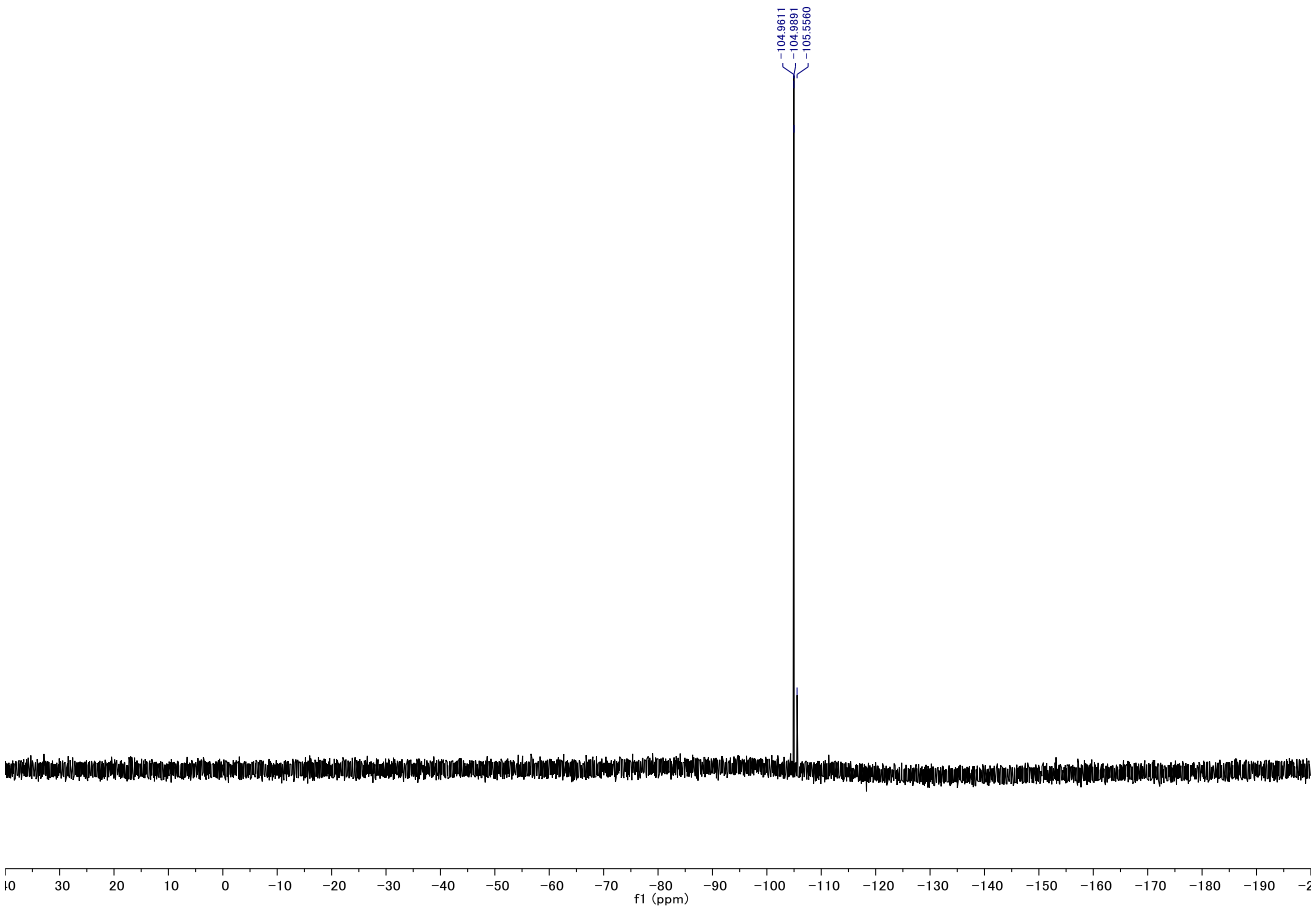
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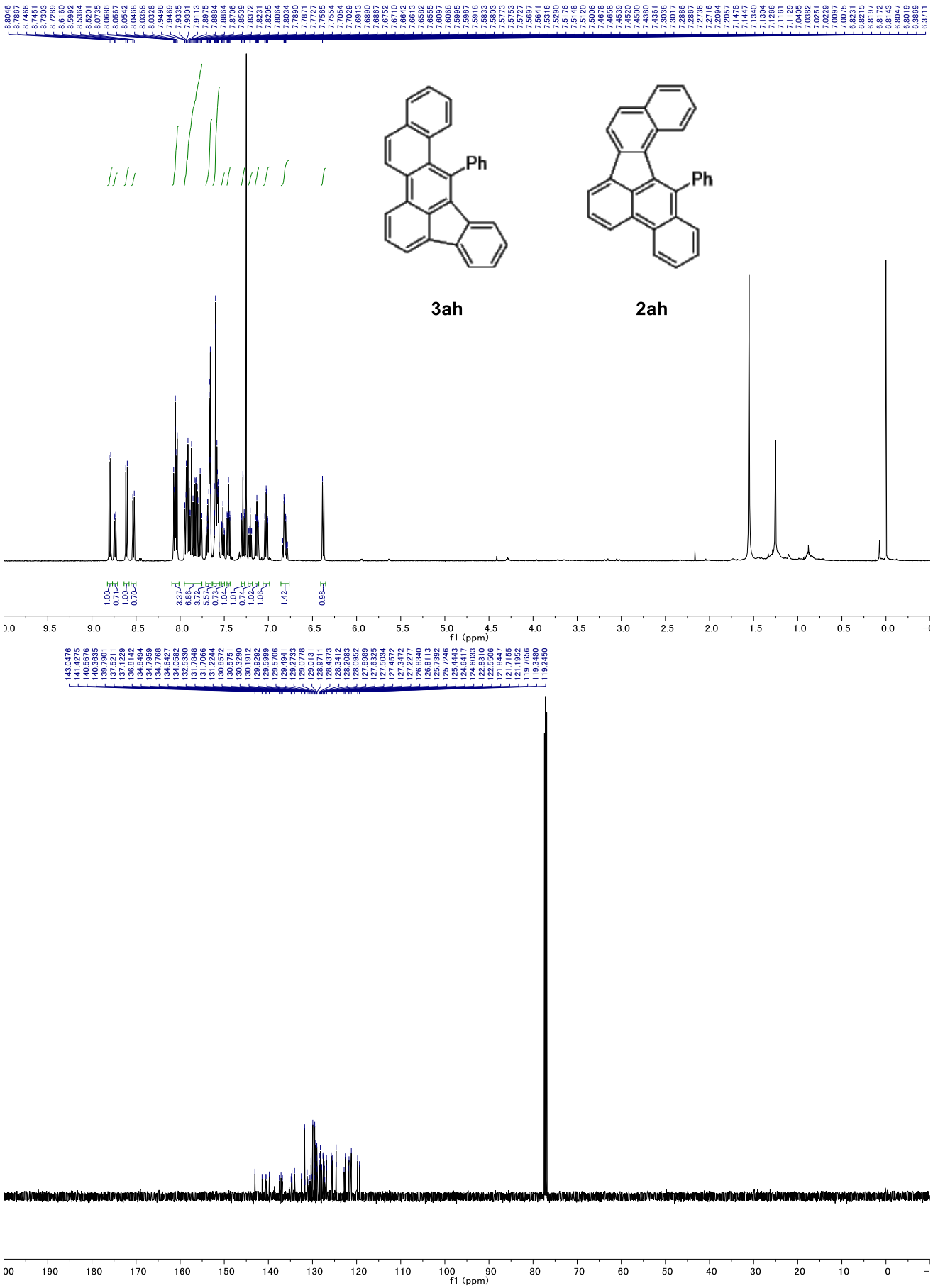
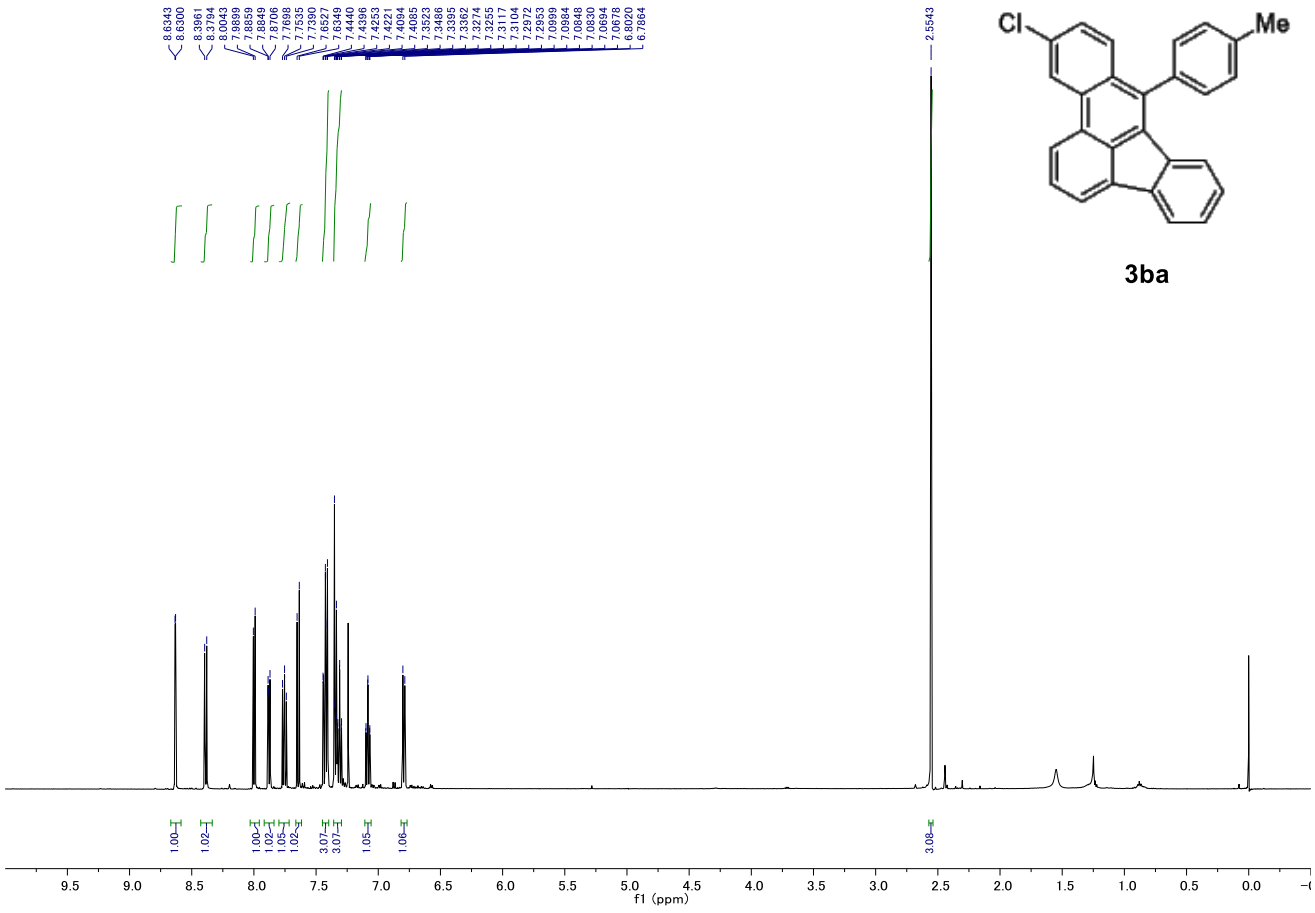
-104.9891
-105.5560
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
f1 (ppm)


Ph
3ah
Ph
2ah
f1 (ppm)
f1 (ppm)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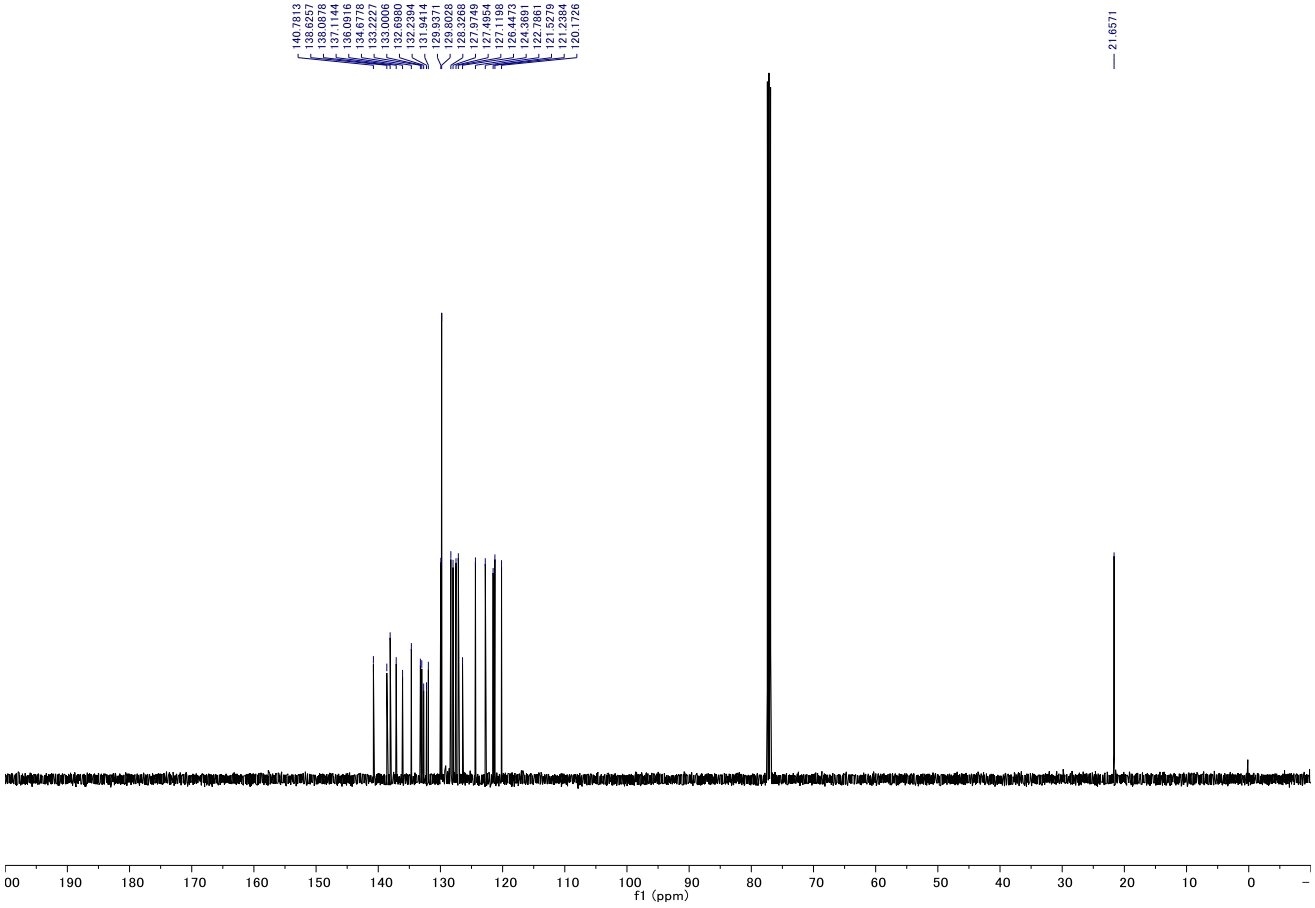
8.3961
8.3744
8.0043
7.9899
7.8859
7.8849
7.8706
7.7698
7.7535
7.7390
7.6527
7.6449
7.4440
7.4436
7.4253
7.4221
7.4094
7.4085
7.3523
7.3486
7.3395
7.3392
7.3274
7.3255
7.3117
7.3104
7.2972
7.2953
7.0999
7.0984
7.0848
7.0830
7.0674
7.0673
6.8020
6.7864
2.5543
1.00
1.02
1.00
1.02
1.05
1.02
3.07
3.07
1.05
1.06
3.08
f1 (ppm)

Cl
Me

3ba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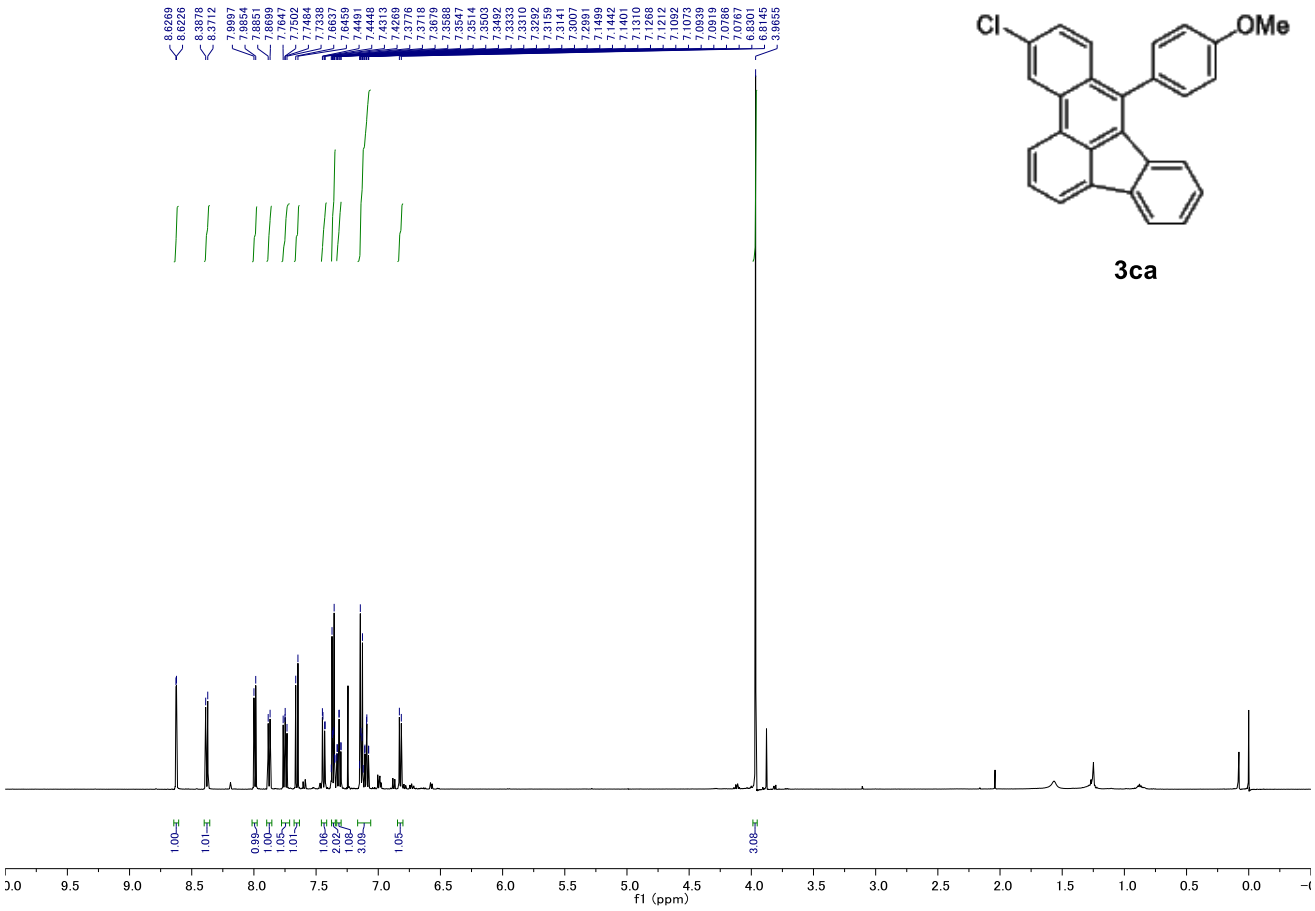
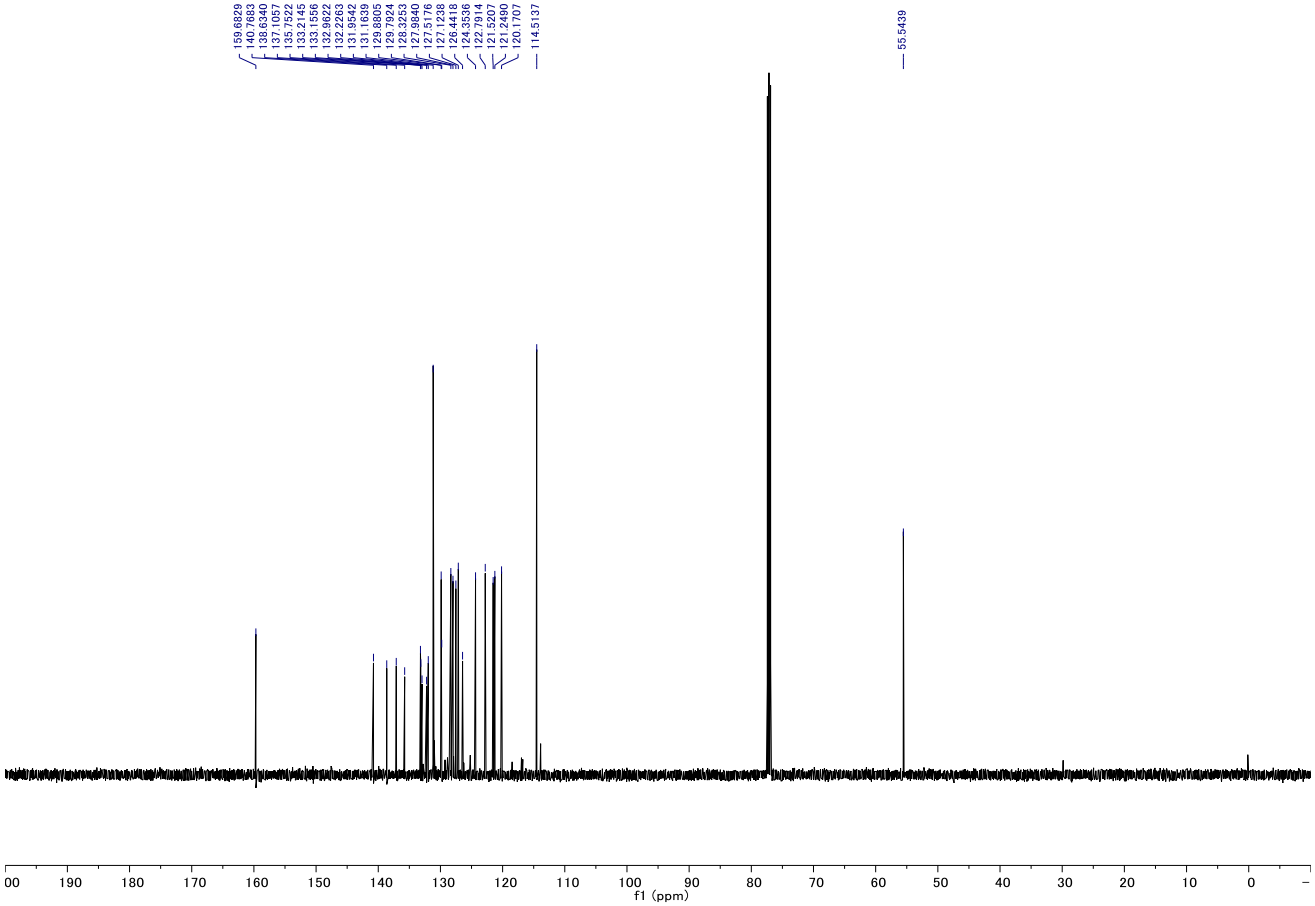
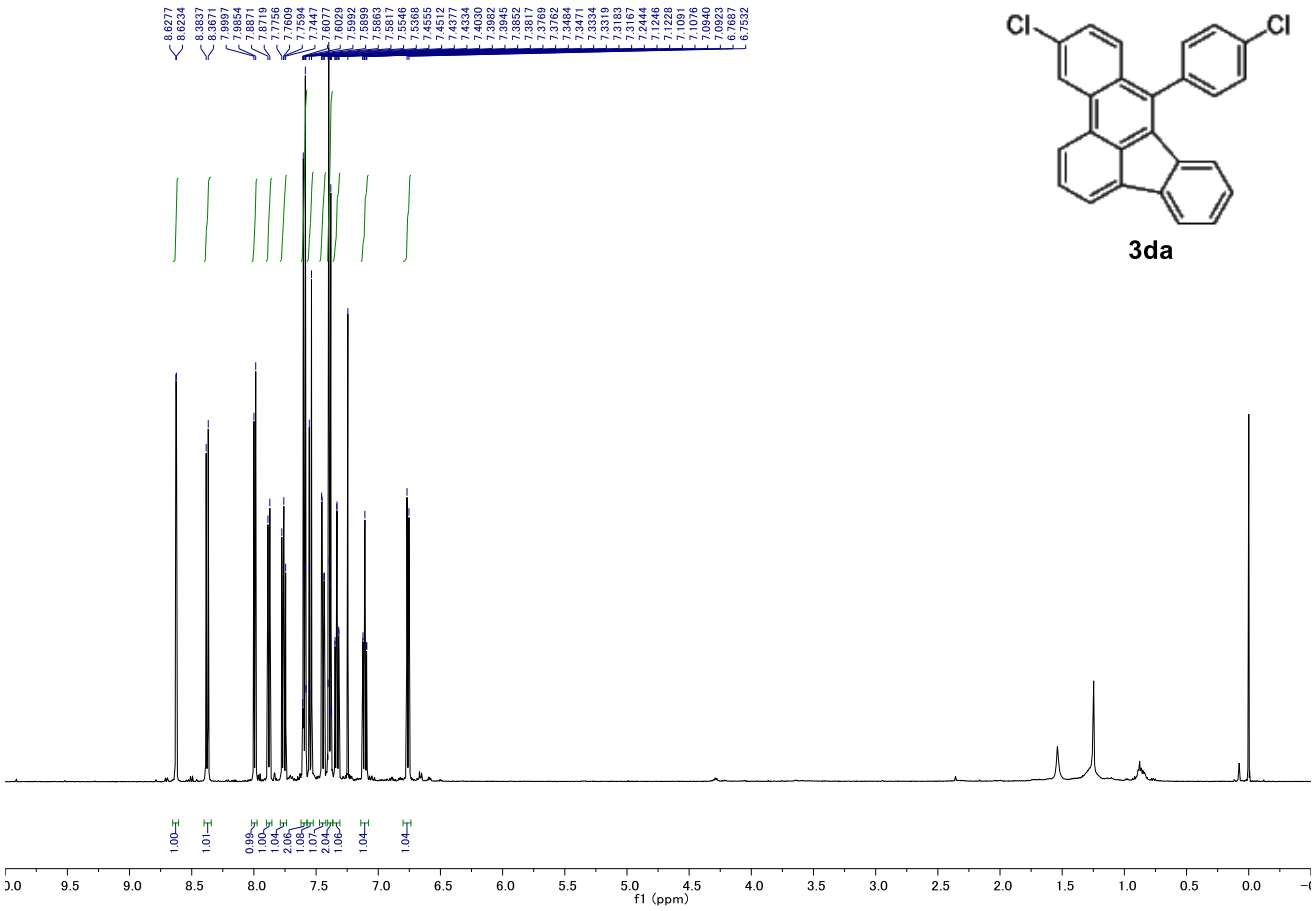
138.0578
137.1144
136.0916
134.6778
133.2227
133.0006
132.6980
132.2394
131.9414
129.9371
129.8928
128.3268
127.9749
127.4954
127.1198
126.4473
124.3691
122.7861
121.5279
121.2384
120.1726
21.6571
f1 (ppm)


Cl
OMe
3ca
f1 (ppm)


f1 (ppm)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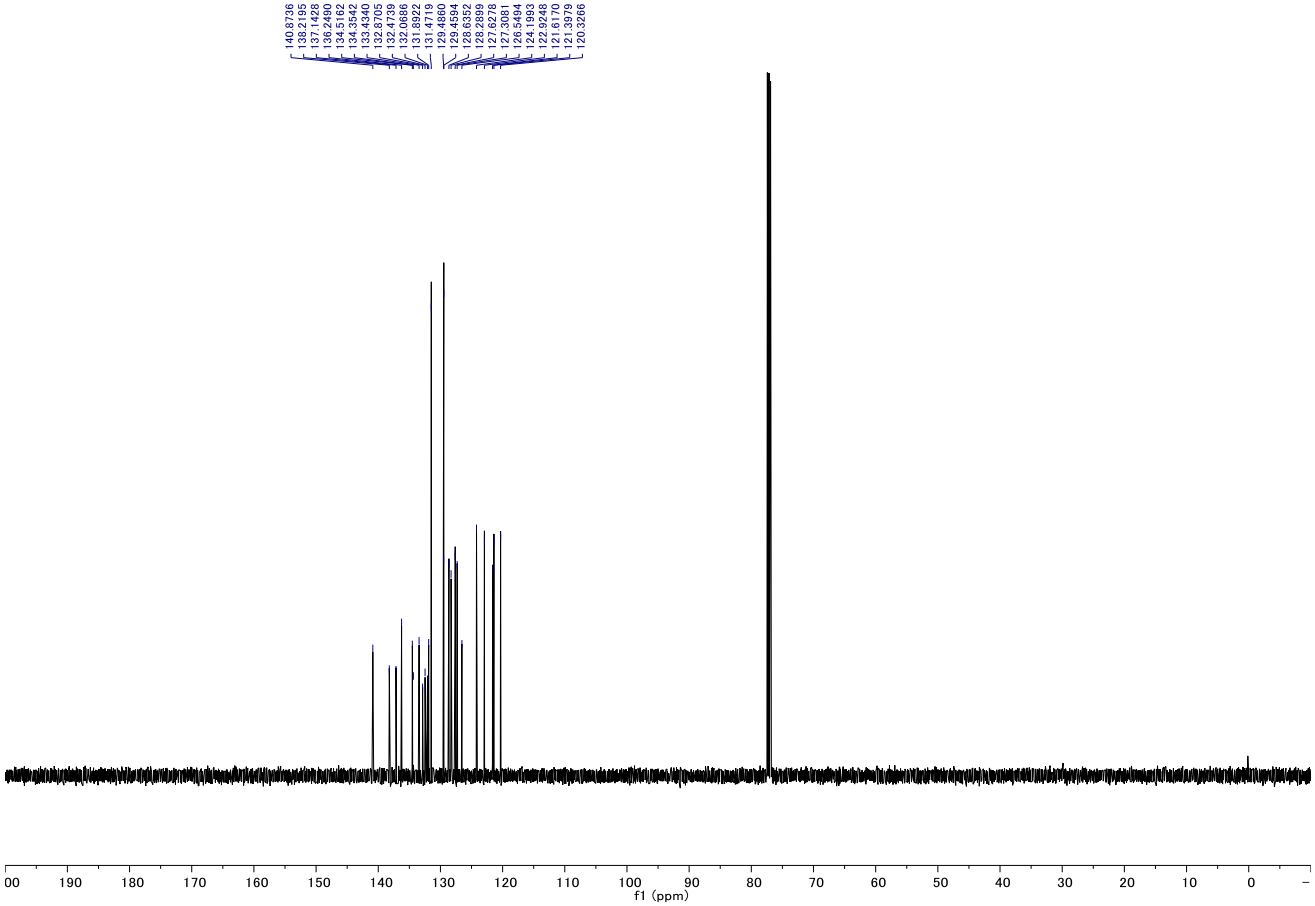
8.3837
8.3671
8.0997
7.9854
7.8871
7.8719
7.7756
7.7609
7.7594
7.7447
7.7077
7.6029
7.5892
7.5699
7.5863
7.5817
7.5546
7.5368
7.4555
7.4512
7.4377
7.4334
7.4030
7.3982
7.3945
7.3852
7.3817
7.3769
7.3762
7.3484
7.3471
7.3334
7.3319
7.3163
7.3157
7.2444
7.1246
7.1228
7.1091
7.1076
7.0940
7.0923
6.7687
6.7532
1.00
1.01
0.99
1.00
1.04
2.06
1.08
1.07
2.04
1.06
1.04
1.04
f1 (ppm)

Cl
Cl

3da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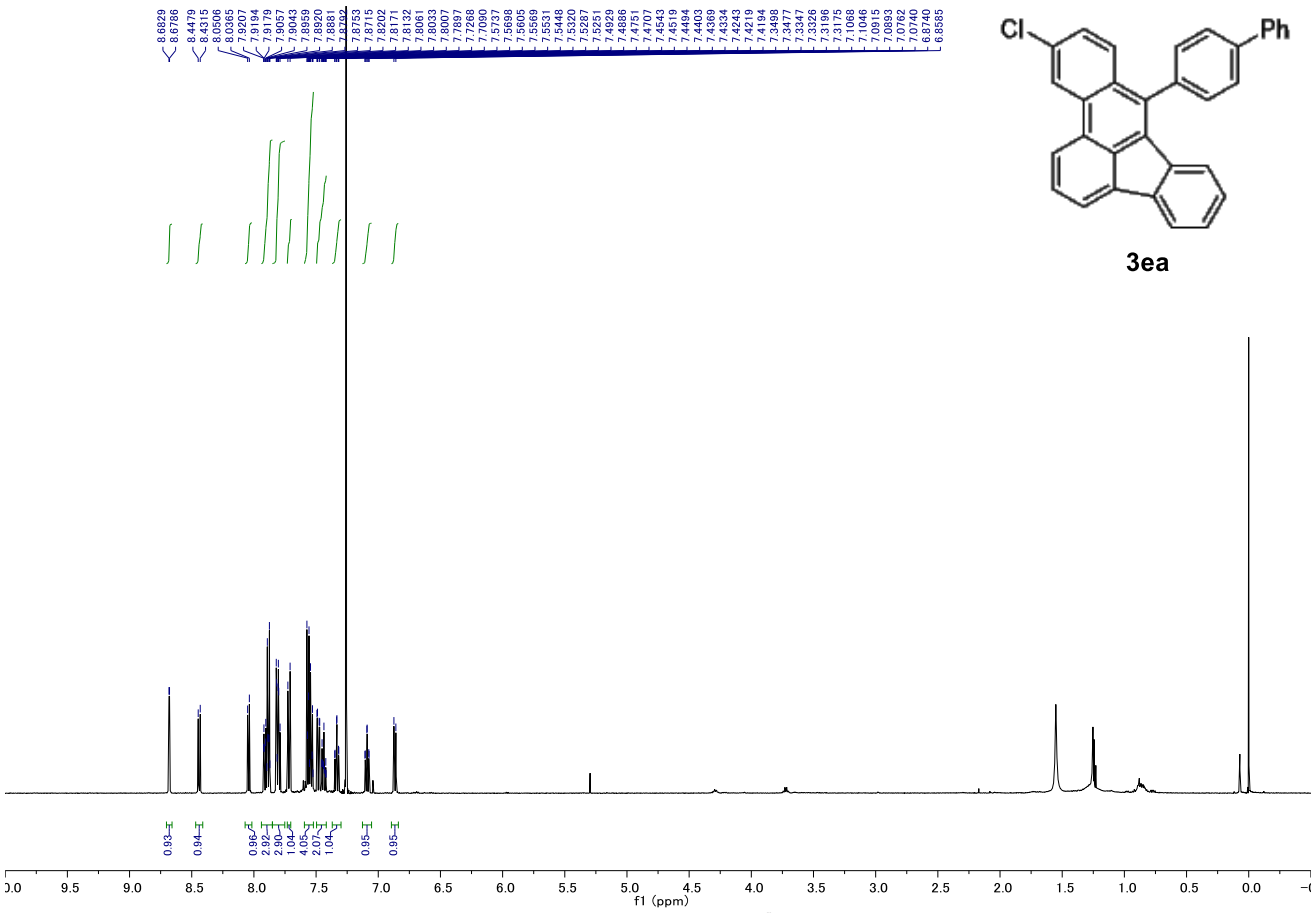
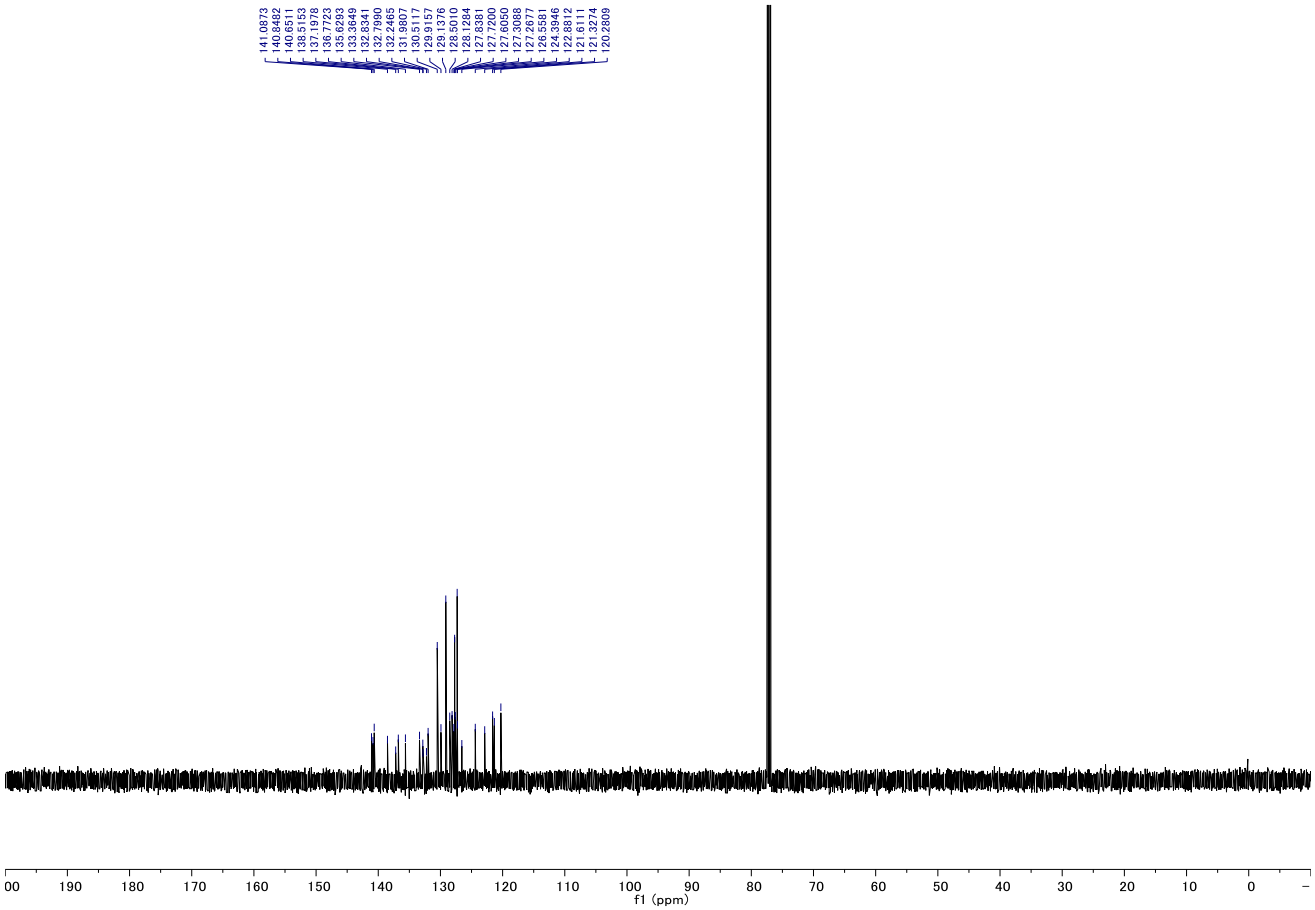
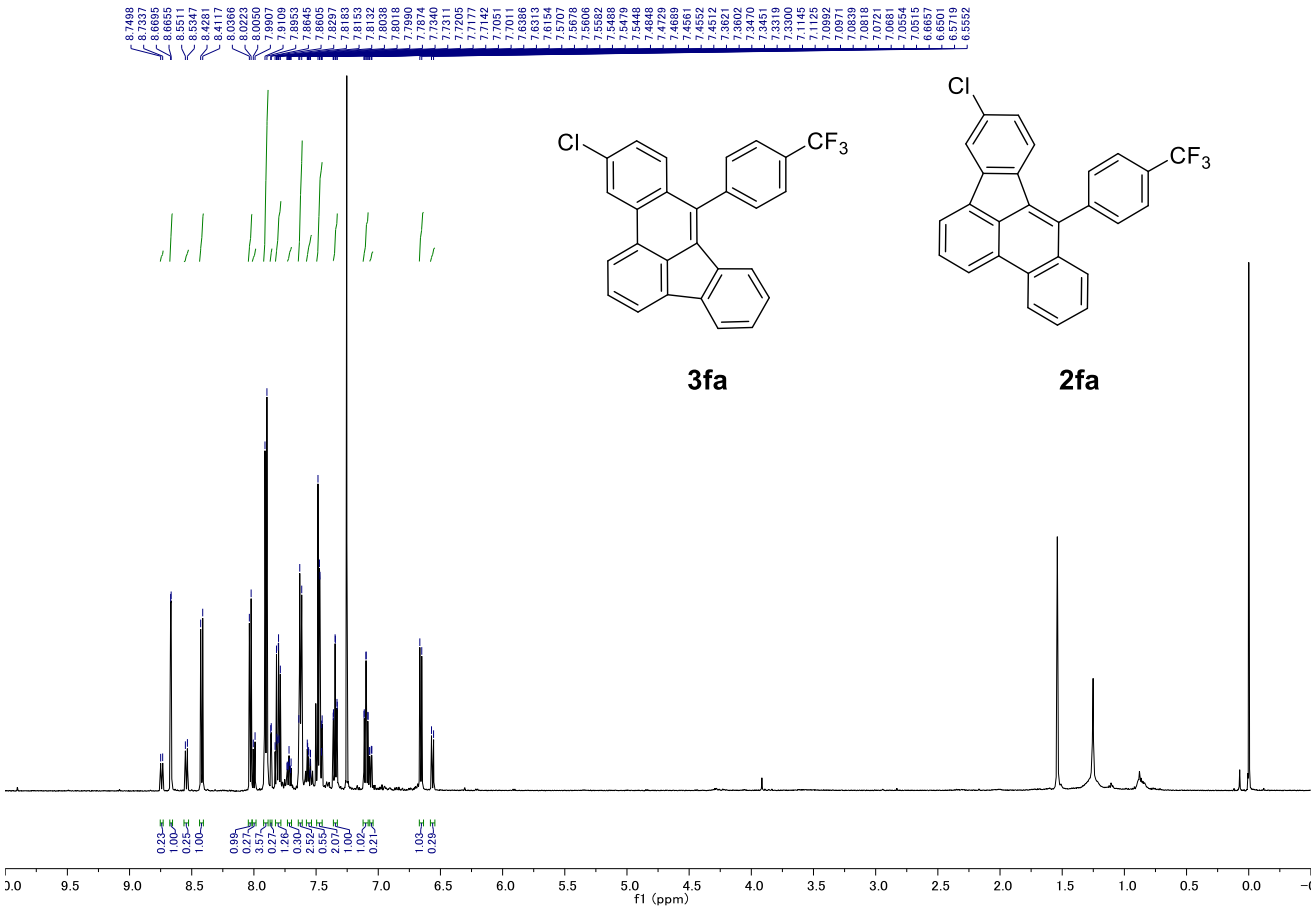
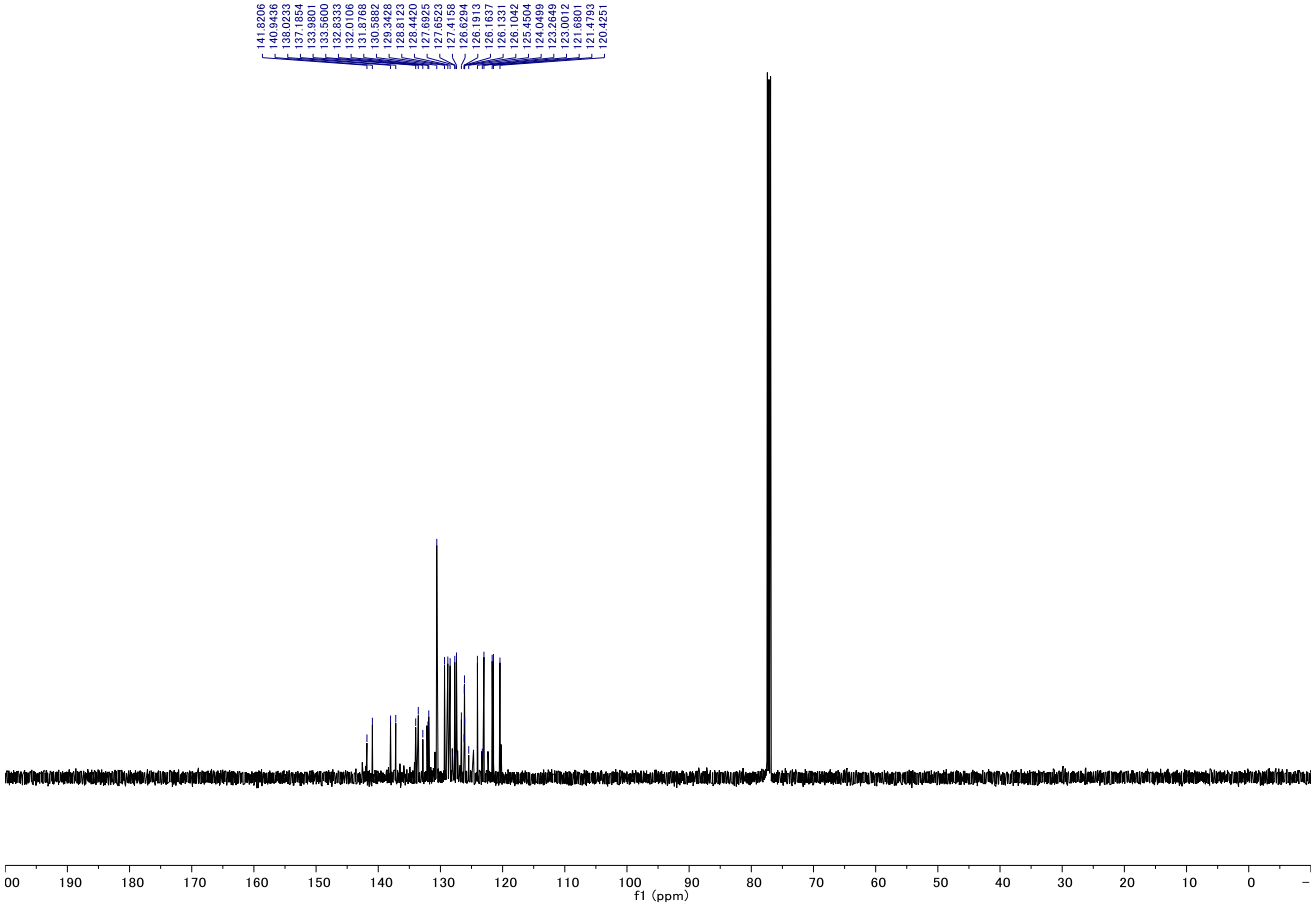
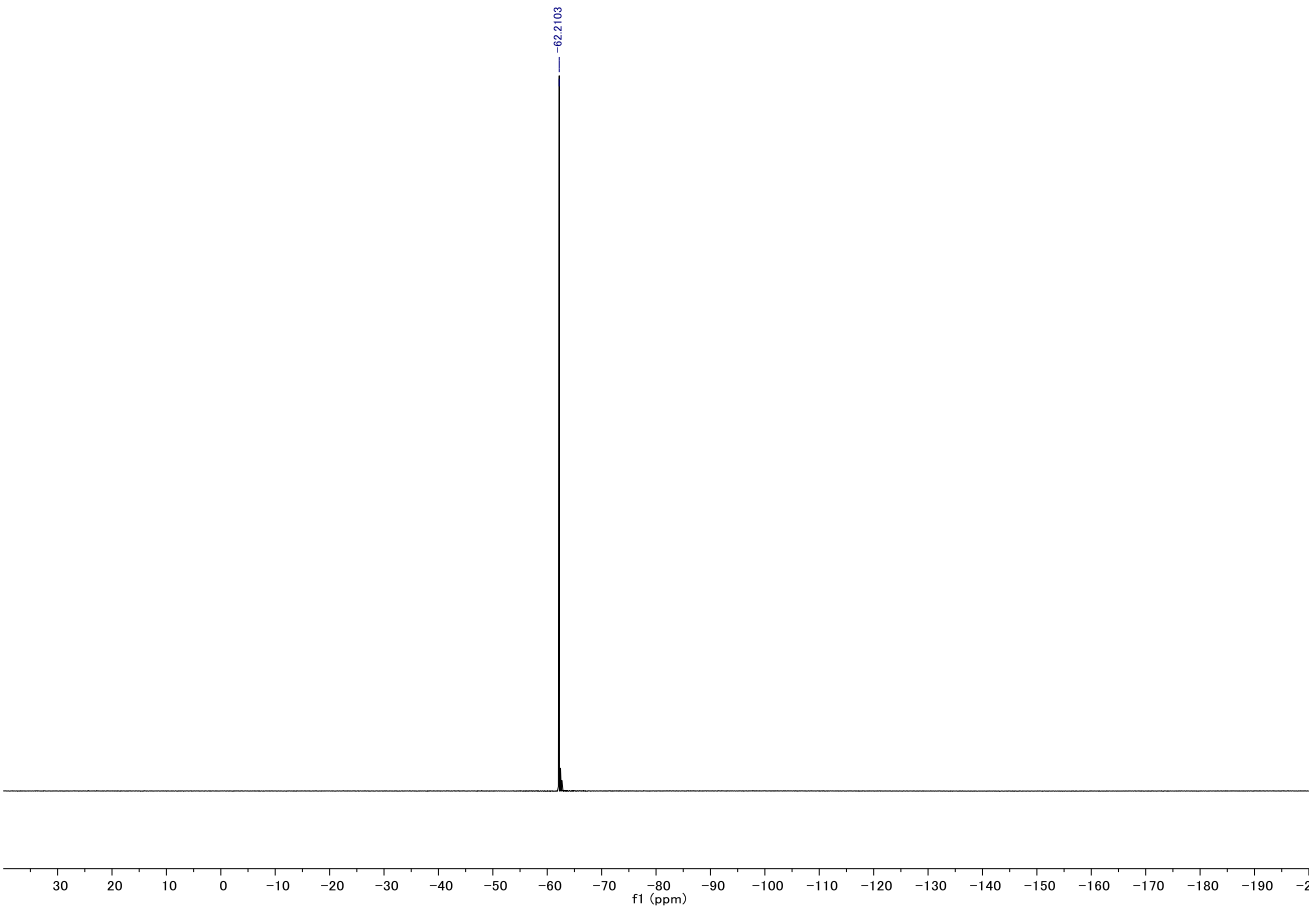
136.2490
134.5162
134.3542
133.4340
132.8705
132.4739
132.0686
131.8922
131.4719
129.4860
129.4594
128.6352
128.2899
127.6278
127.2091
126.5494
124.1993
122.9248
121.6170
121.3979
120.3266
f1 (ppm)


Cl
Ph
3ea
f1 (ppm)


f1 (ppm)


Cl
CF3
3fa
Cl
CF3
2fa
f1 (ppm)


f1 (ppm)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20
10
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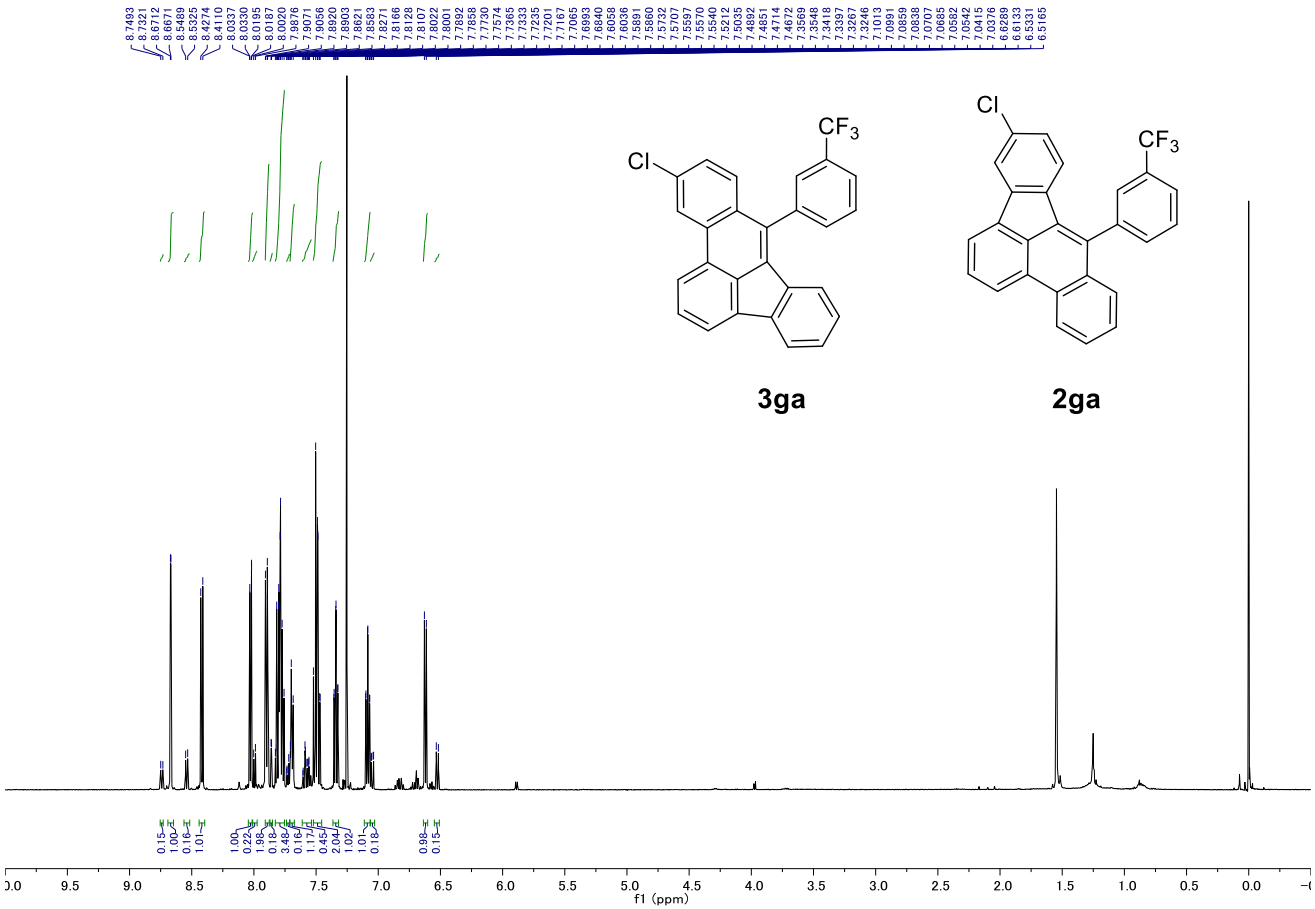
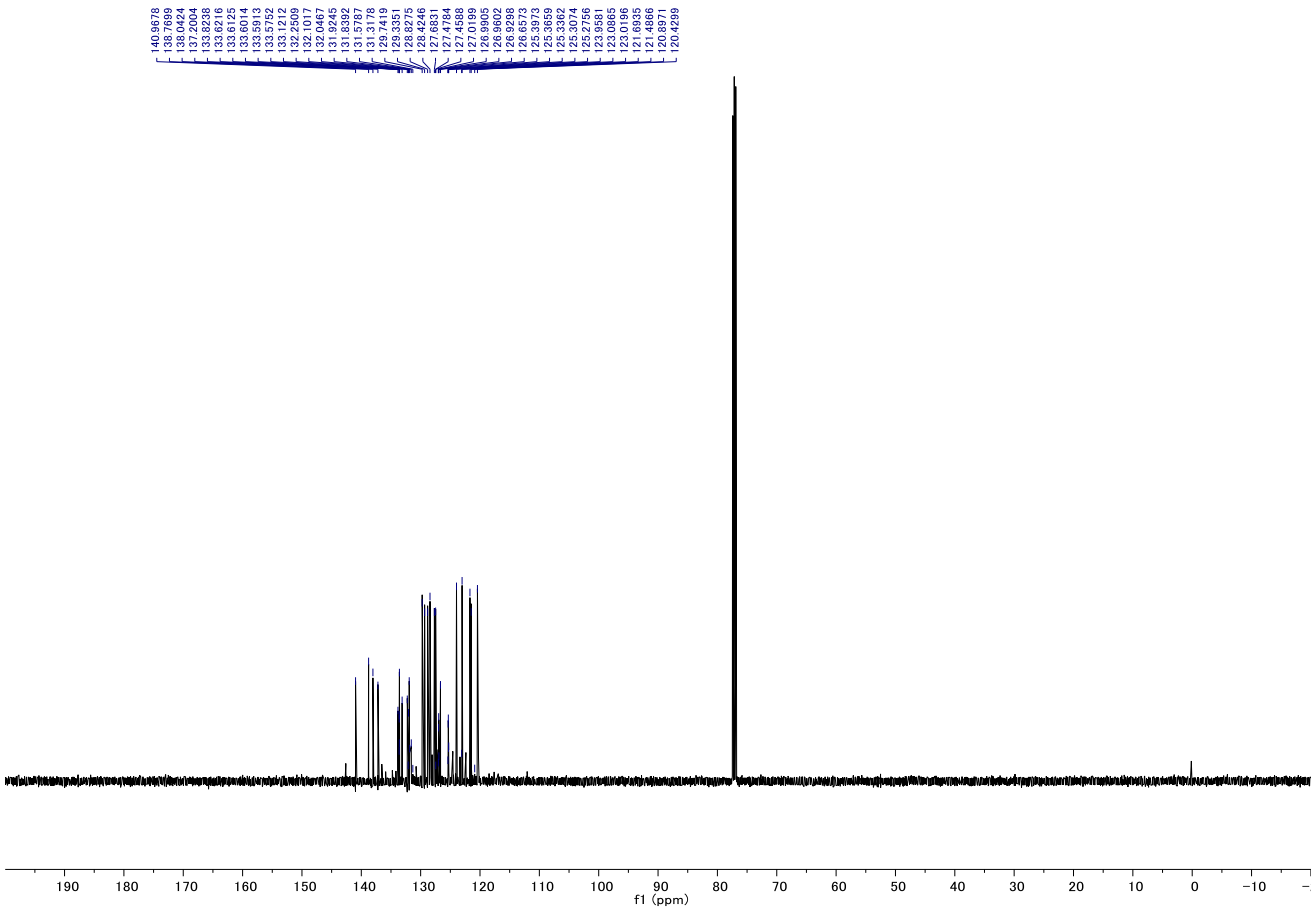
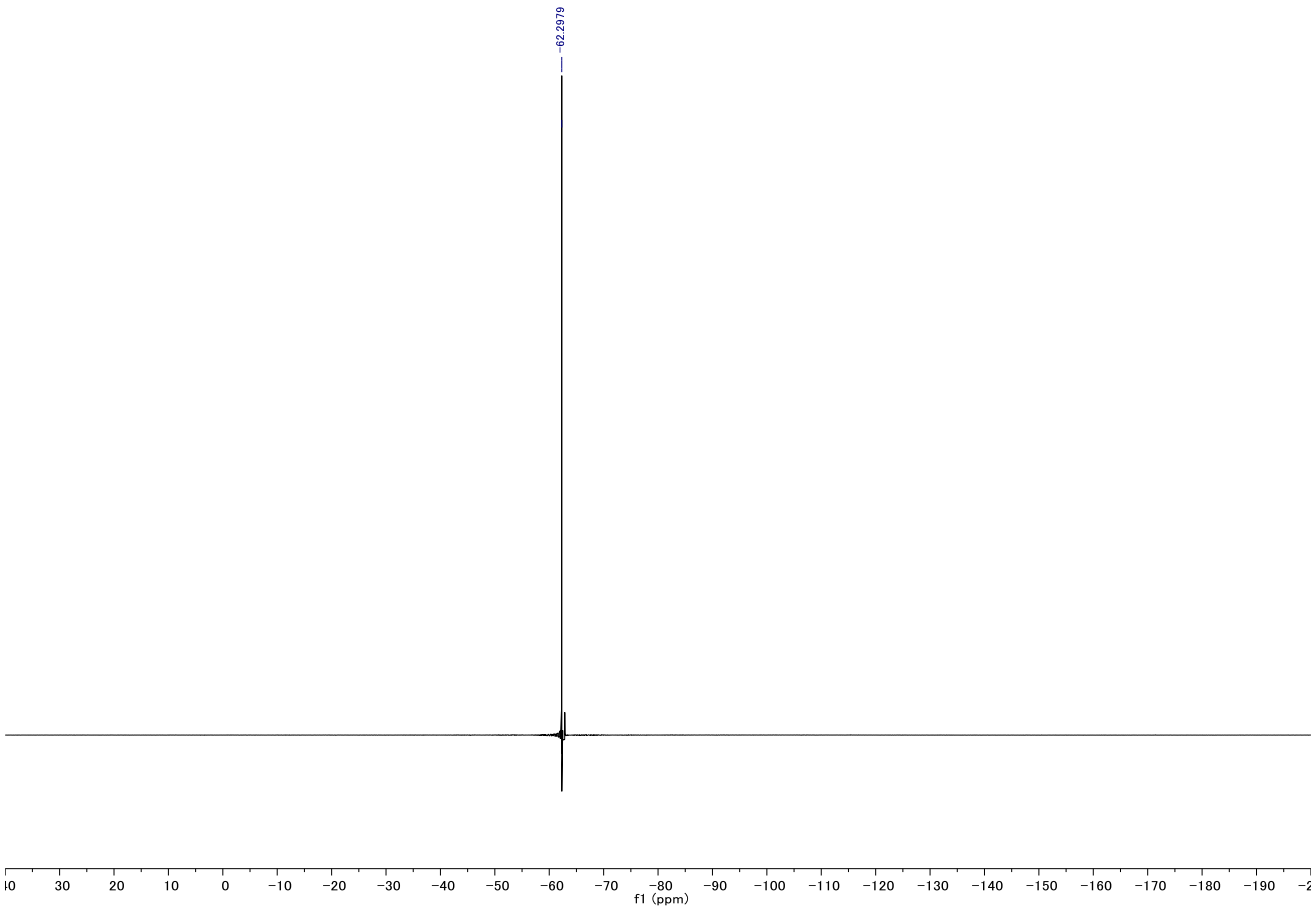
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
f1 (ppm)


Cl
CF3
3ga
Cl
CF3
2ga
f1 (ppm)


f1 (ppm)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20
10
0
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−60
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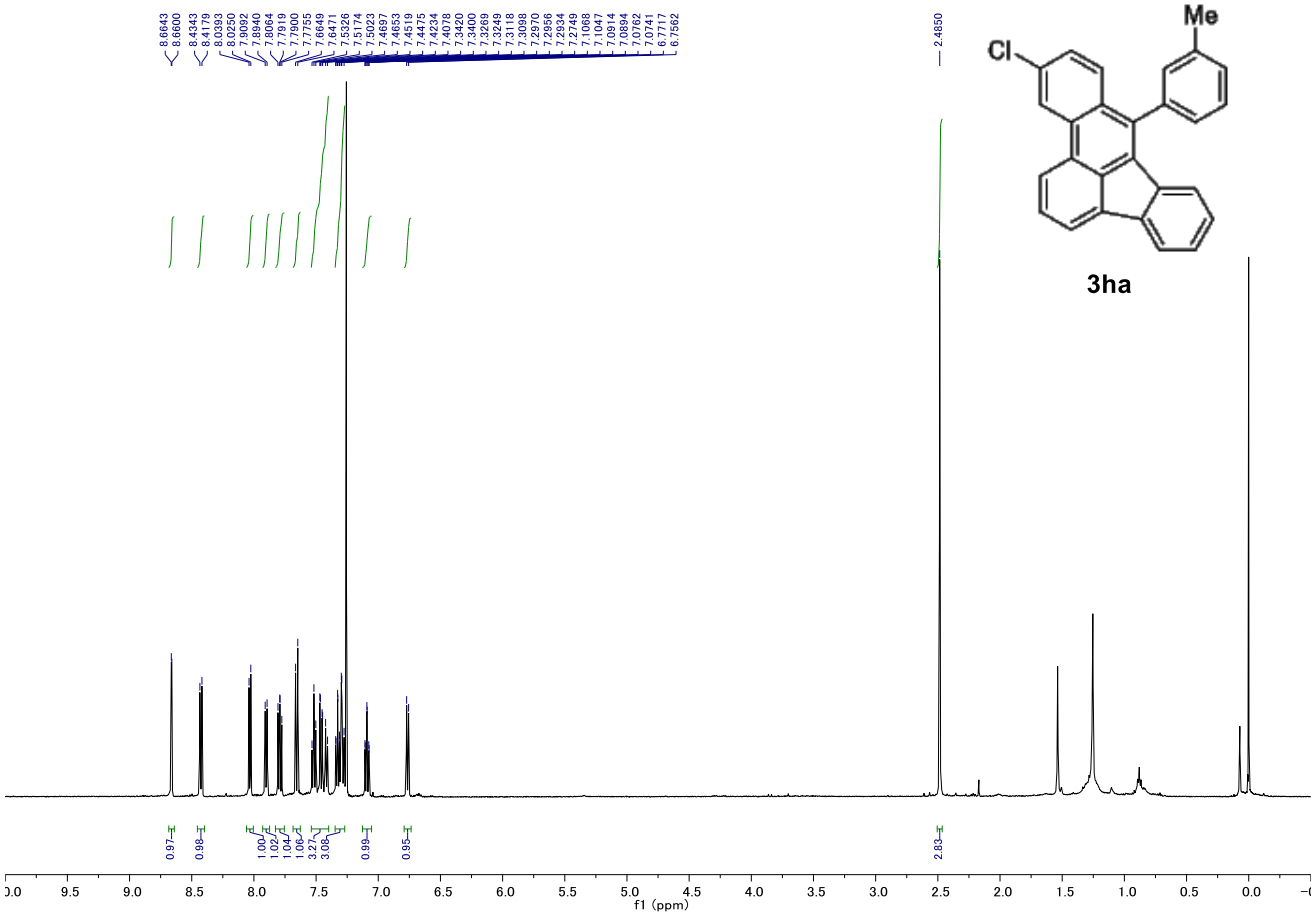
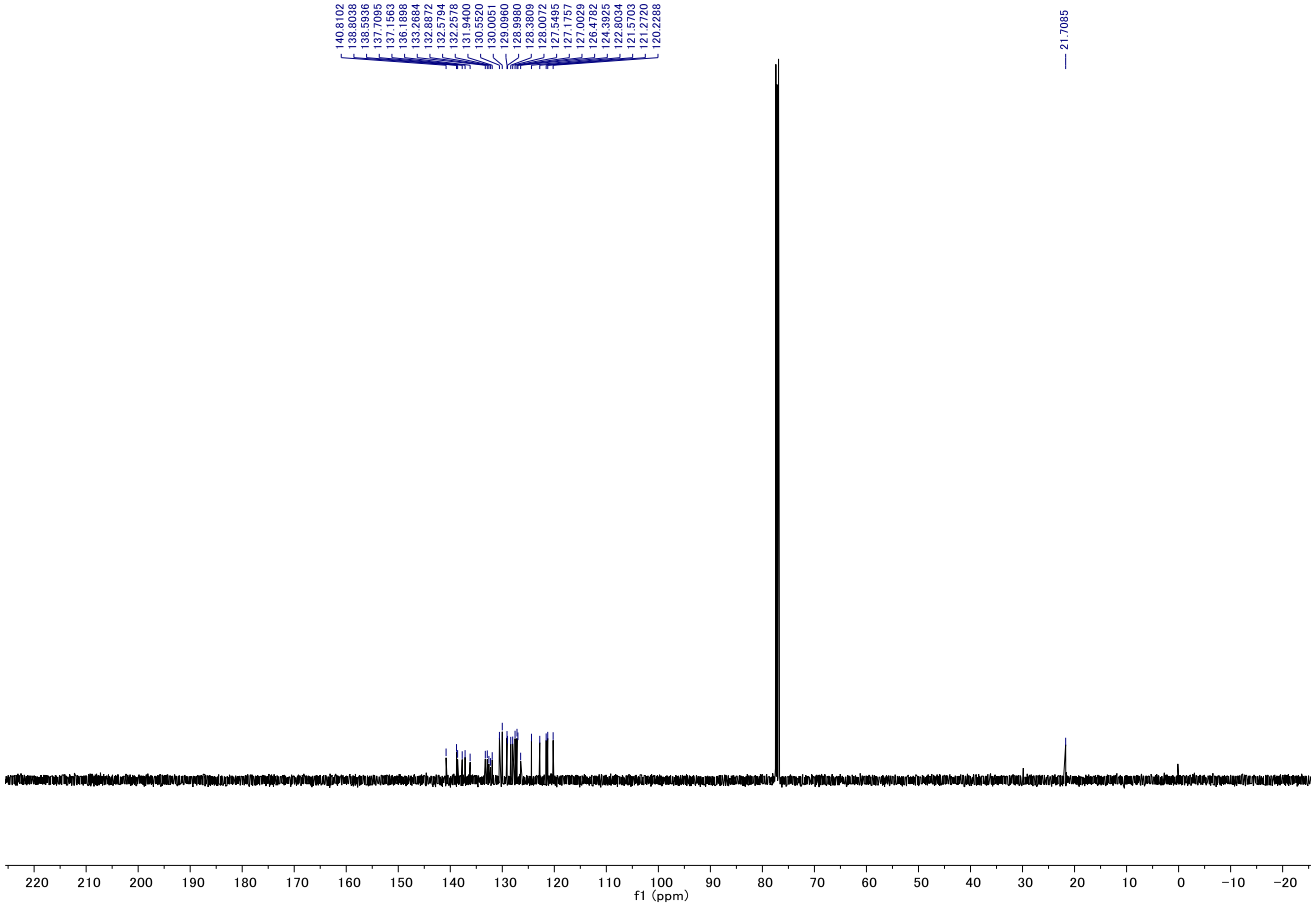
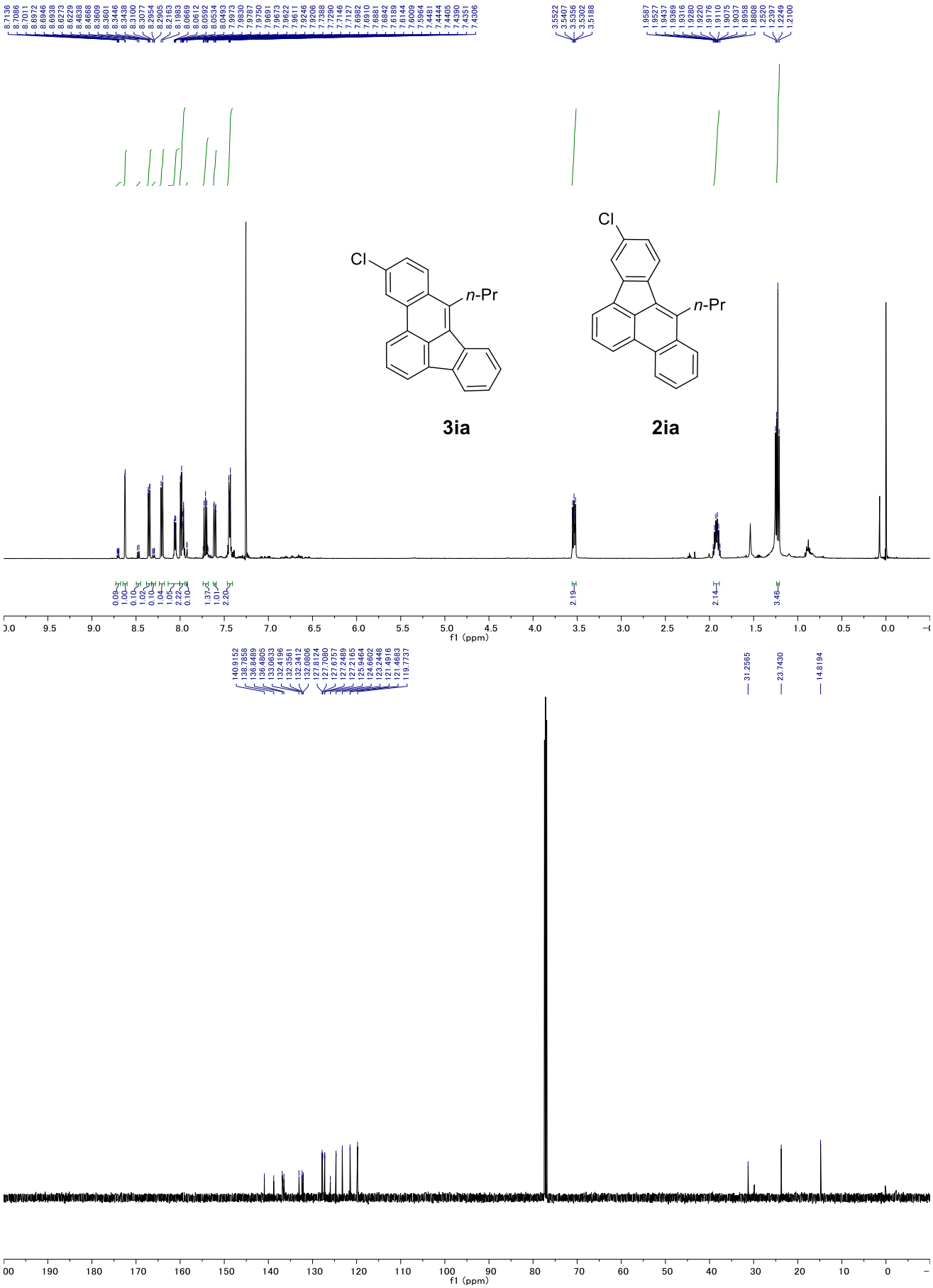
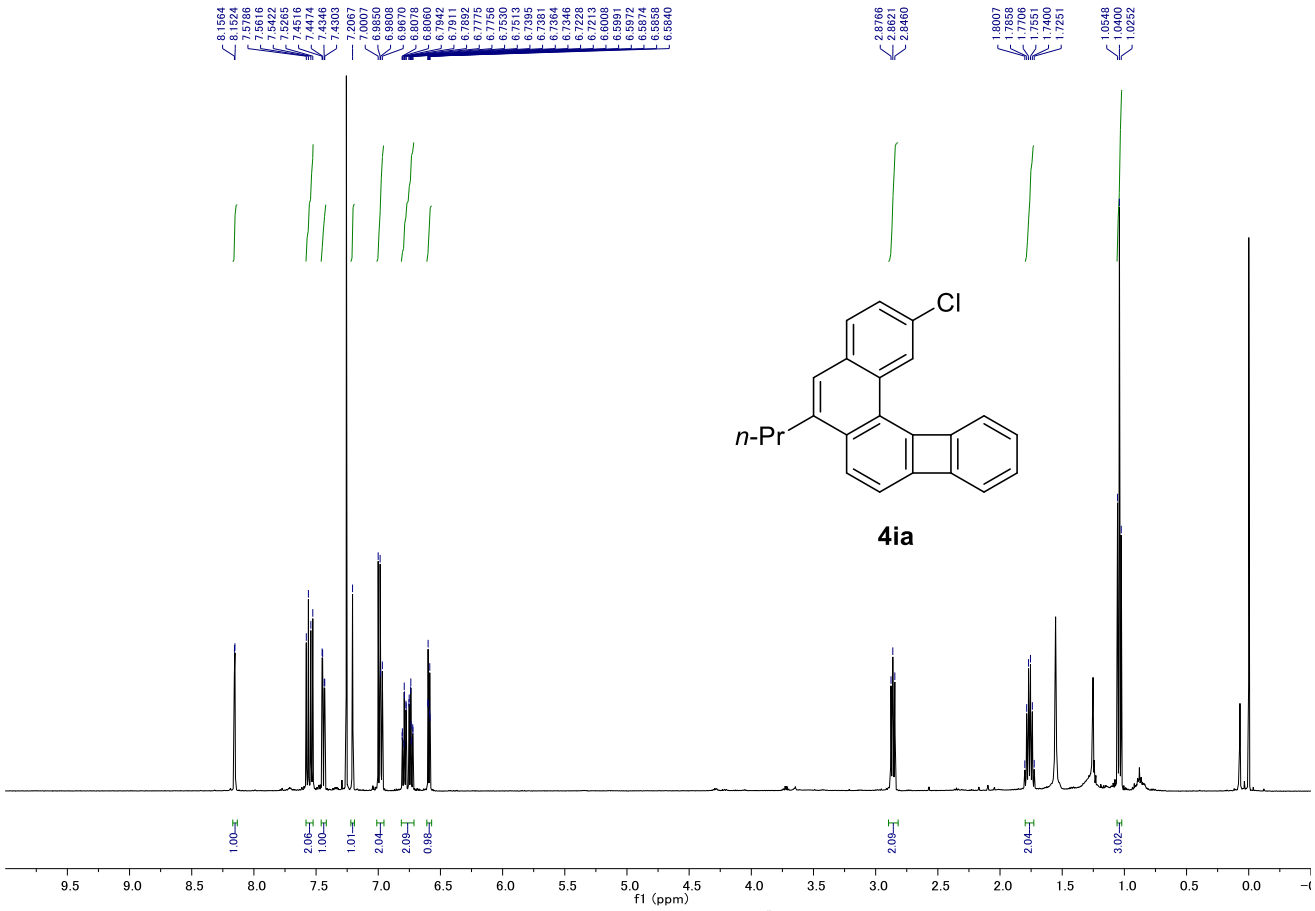
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
f1 (ppm)


Me
Cl
3ha
f1 (ppm)


f1 (ppm)


Cl
n-Pr
3ia
Cl
n-Pr
2ia
f1 (ppm)
f1 (ppm)



4ia