

Supporting Information:

Substituent Effects of Bridged Binaphthyl-Type Chiral Dopants on the Helical Twisting Power in Dopant-Induced Chiral Liquid Crystals

Yu Narazaki,^a Hiroya Nishikawa,^b Hiroki Higuchi,^b Yasushi Okumura^b and
Hirotsugu Kikuchi^{*,b}

^a *Interdisciplinary Graduate School of Engineering Sciences, Kyushu University, 6-1, Kasuga-koen, Kasuga, Fukuoka 816-8580, Japan*

^b *Institute for Materials Chemistry and Engineering, Kyushu University, 6-1, Kasuga-koen, Kasuga, Fukuoka 816-8580, Japan. E-mail: kikuchi@cm.kyushu-u.ac.jp*

Helical senses of synthesized chiral dopants

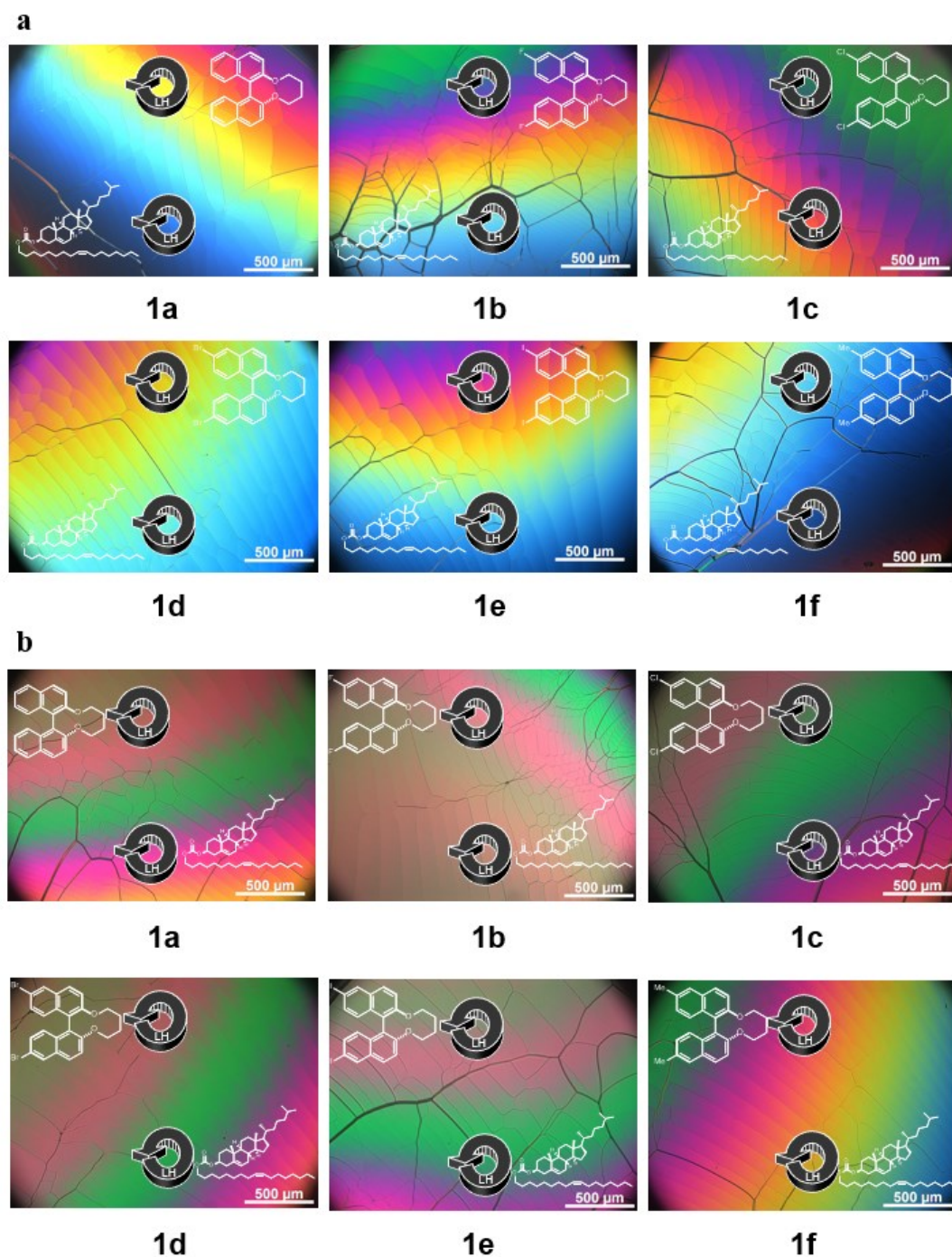


Figure S1 Contact methods: Optical textures of (a) 0.5wt% mixtures of **1a-1f** in JC-1041XX and (b) 0.5wt% mixtures of **1a-1f** in MBBA. The reference material denotes cholesteryl oleyl carbonate (COC) possessing a left-handed (LH) helical sense.

Experimental spectra

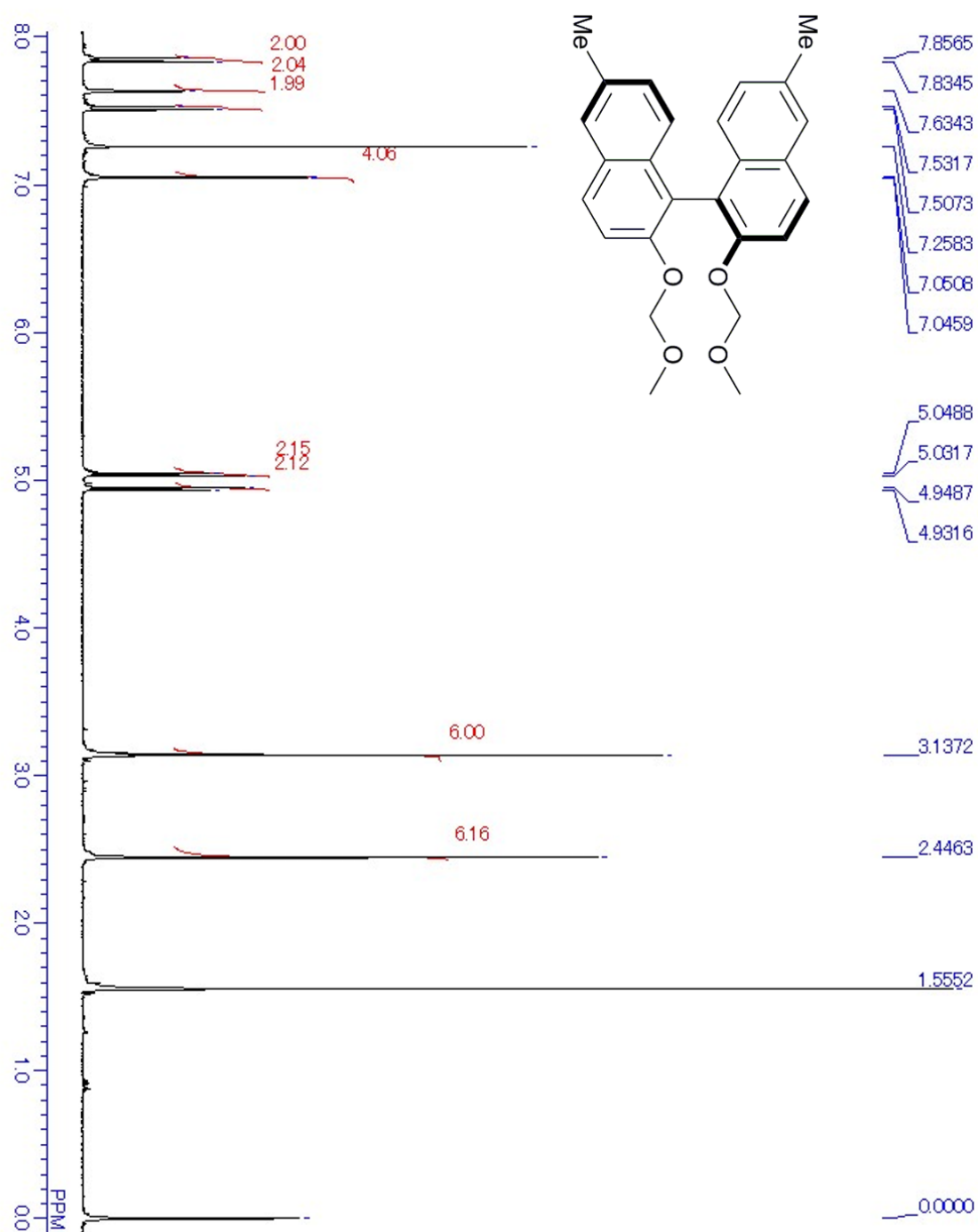


Figure S2 ^1H -NMR spectrum of **3**.

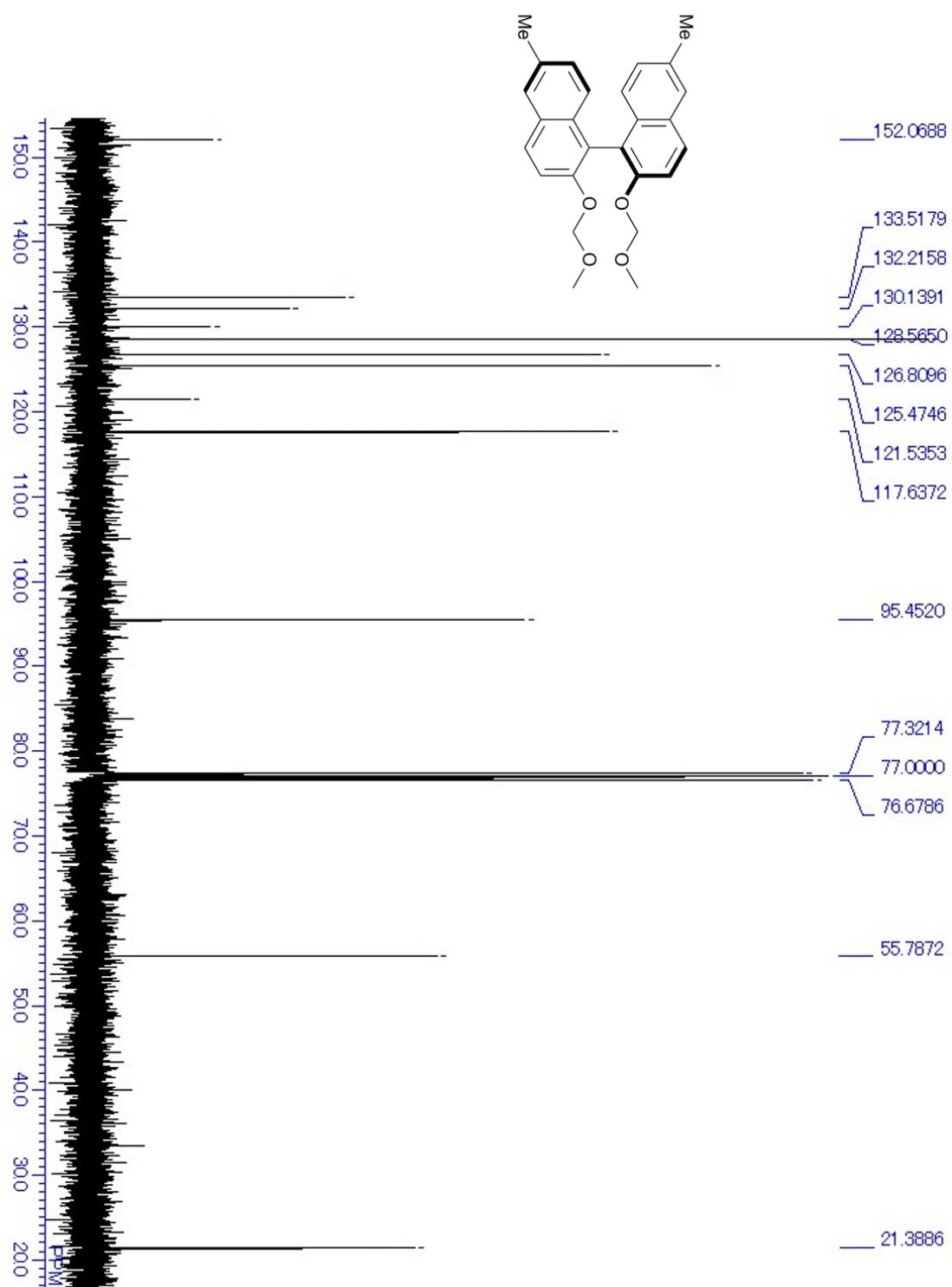
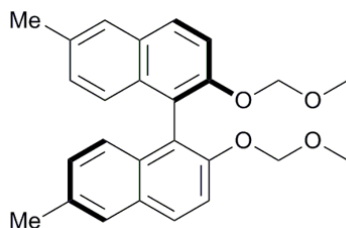


Figure S3 ^{13}C -NMR spectrum of **3**.



Chemical Formula: $C_{26}H_{26}O_4$

Exact Mass: 402.1831

Molecular Weight: 402.4900

m/z: 402.1831 (100.0%), 403.1865 (28.1%),
404.1898 (2.7%), 404.1898 (1.1%)

[Molecular Formula]

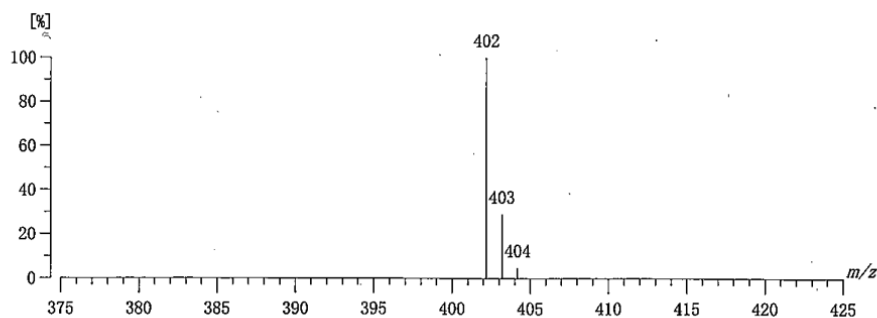
Data : Me-MOMBINOL-EIposi-HR Date : 15-Nov-2016 09:46

RT : 1.63 min Molecular Formula : $C_{26}H_{26}O_4$

Elements : C 26/0, H 26/0, O 4/0

Mass Tolerance : 10mmu

Unsaturation (U.S.) : -0.5 - 20.0



[Mass Spectrum]

Data : Me-MOMBINOL-EIposi-HR Date : 15-Nov-2016 09:46

Instrument : Station

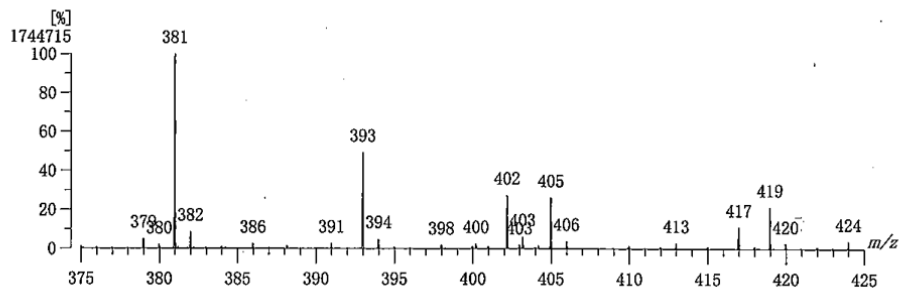
Note : MStation : IMCE Kyushu Univ.

Ion Mode : EI+

Scan# : 37

Cut Level : 1.00 %

Internal standard: PFK



	Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
1	402.1831	27.42	-0.0 / -0.0	14.0	$C_{26}H_{26}O_4$

Figure S4 High resolution mass spectrum of 3.

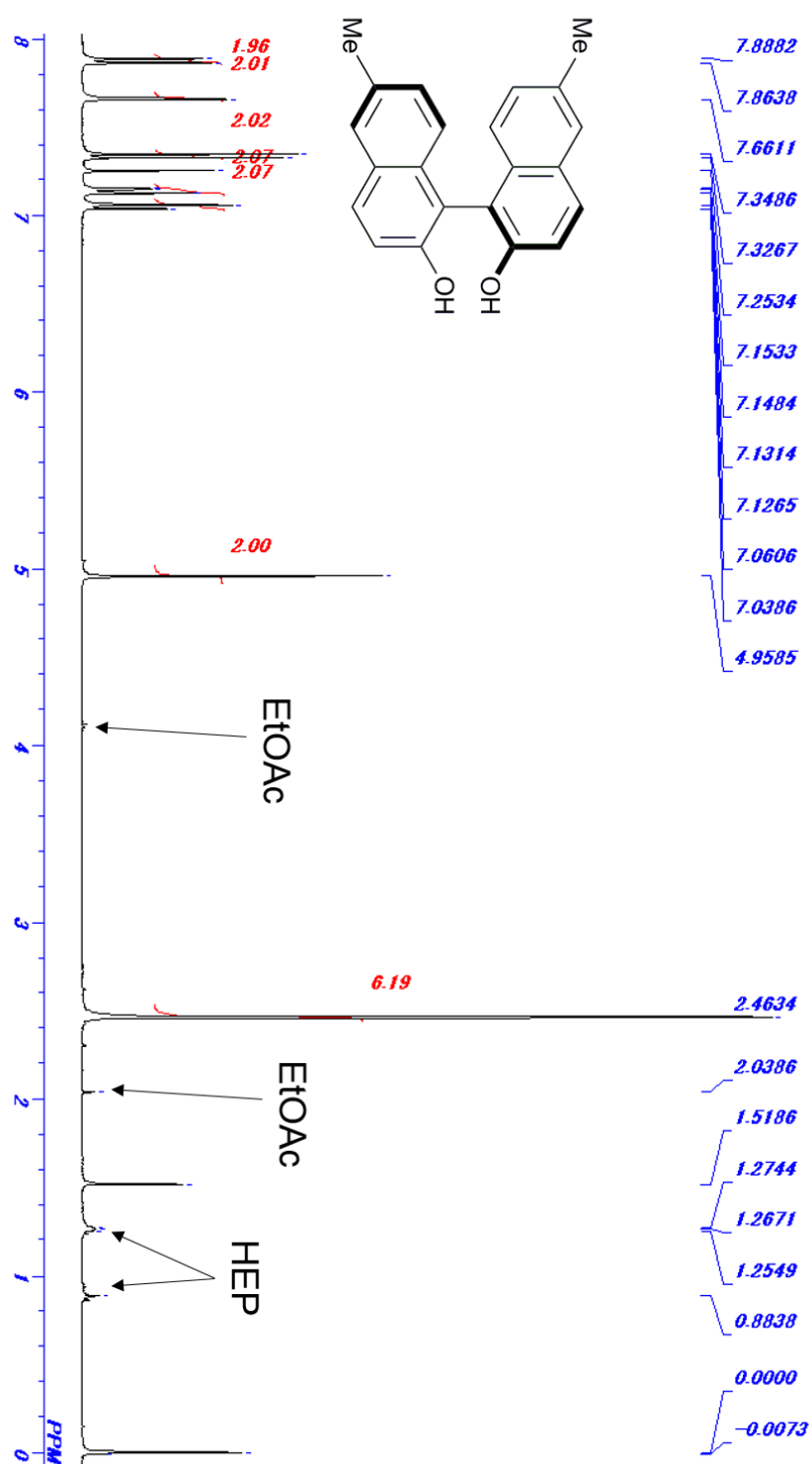


Figure S5 ¹H-NMR spectrum of 4f.

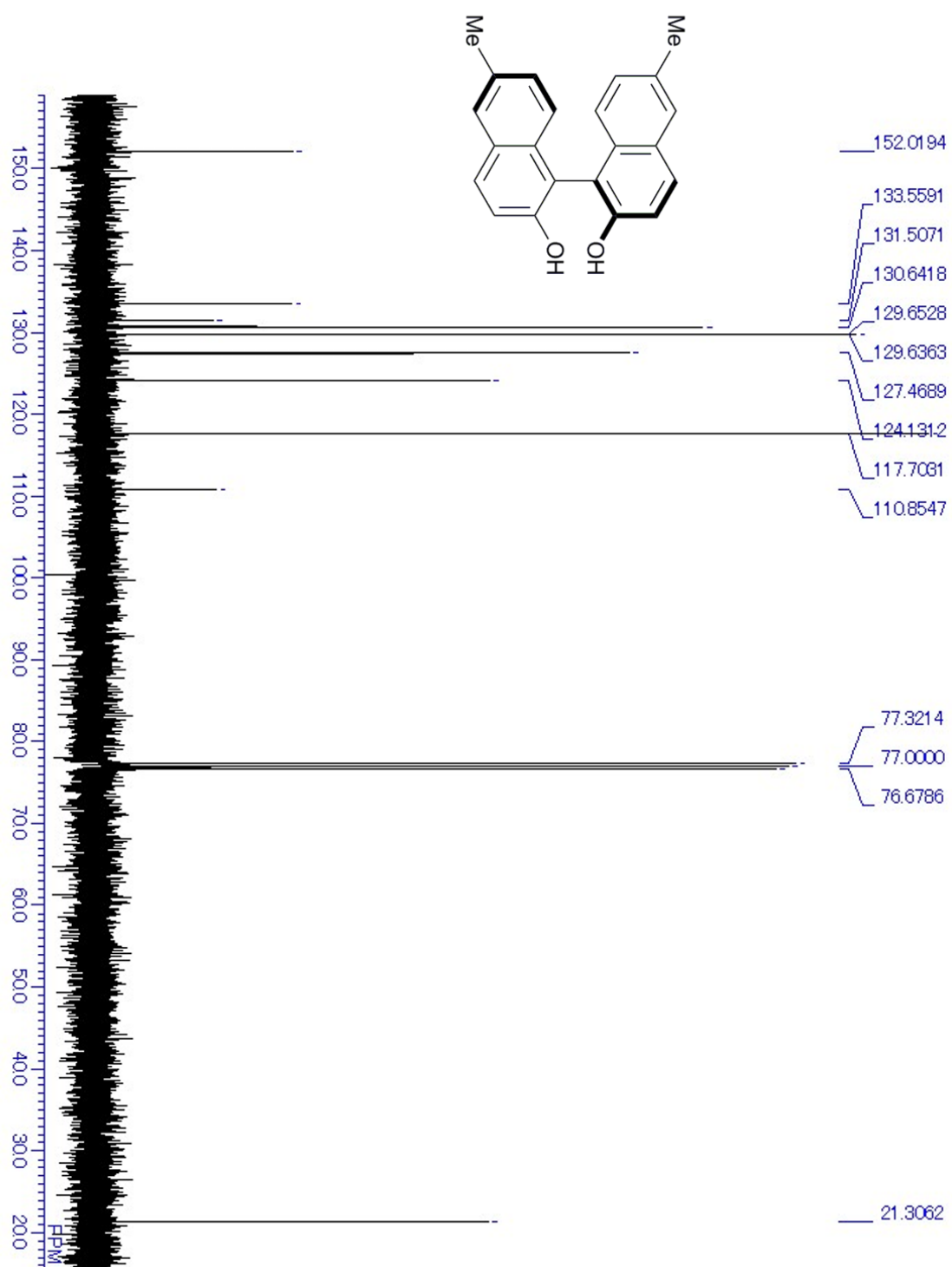
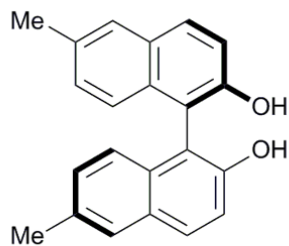


Figure S6 ^{13}C -NMR spectrum of **4f**.



Chemical Formula: $C_{22}H_{18}O_2$

Exact Mass: 314.1307

Molecular Weight: 314.3840

m/z : 314.1307 (100.0%), 315.1340 (23.8%), 316.1374 (2.7%)

[Molecular Formula]

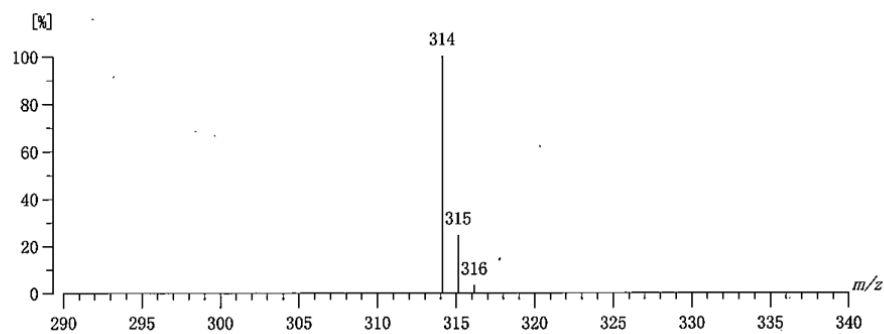
Data : Me-BINOL-EIposi-HR Date : 01-Dec-2016 13:32

RT : 0.21 min Molecular Formula : $C_{22}H_{18}O_2$

Elements : C 22/0, H 18/0, O 2/0

Mass Tolerance : 10mmu

Unsaturation (U.S.) : -0.5 - 20.0



[Mass Spectrum]

Data : Me-BINOL-EIposi-HR Date : 01-Dec-2016 13:32

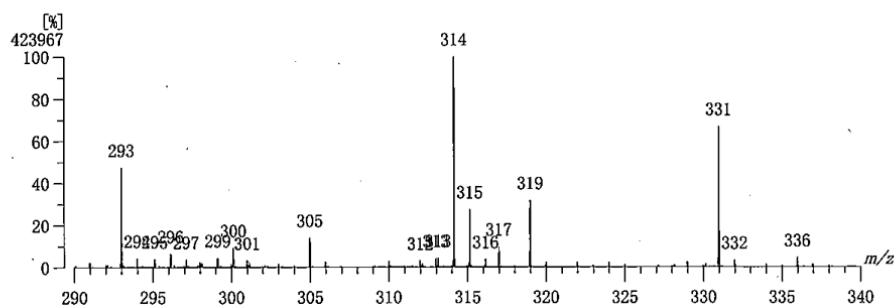
Instrument : Station

Note : MStation : IMCE Kyushu Univ.

Ion Mode : EI+

Scan# : 5

Cut Level : 1.00 %



Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
1 314.1308	100.00	+0.4 / +0.1	14.0 C22 H18 O2

Figure S7 High resolution mass spectrum of **4f**.

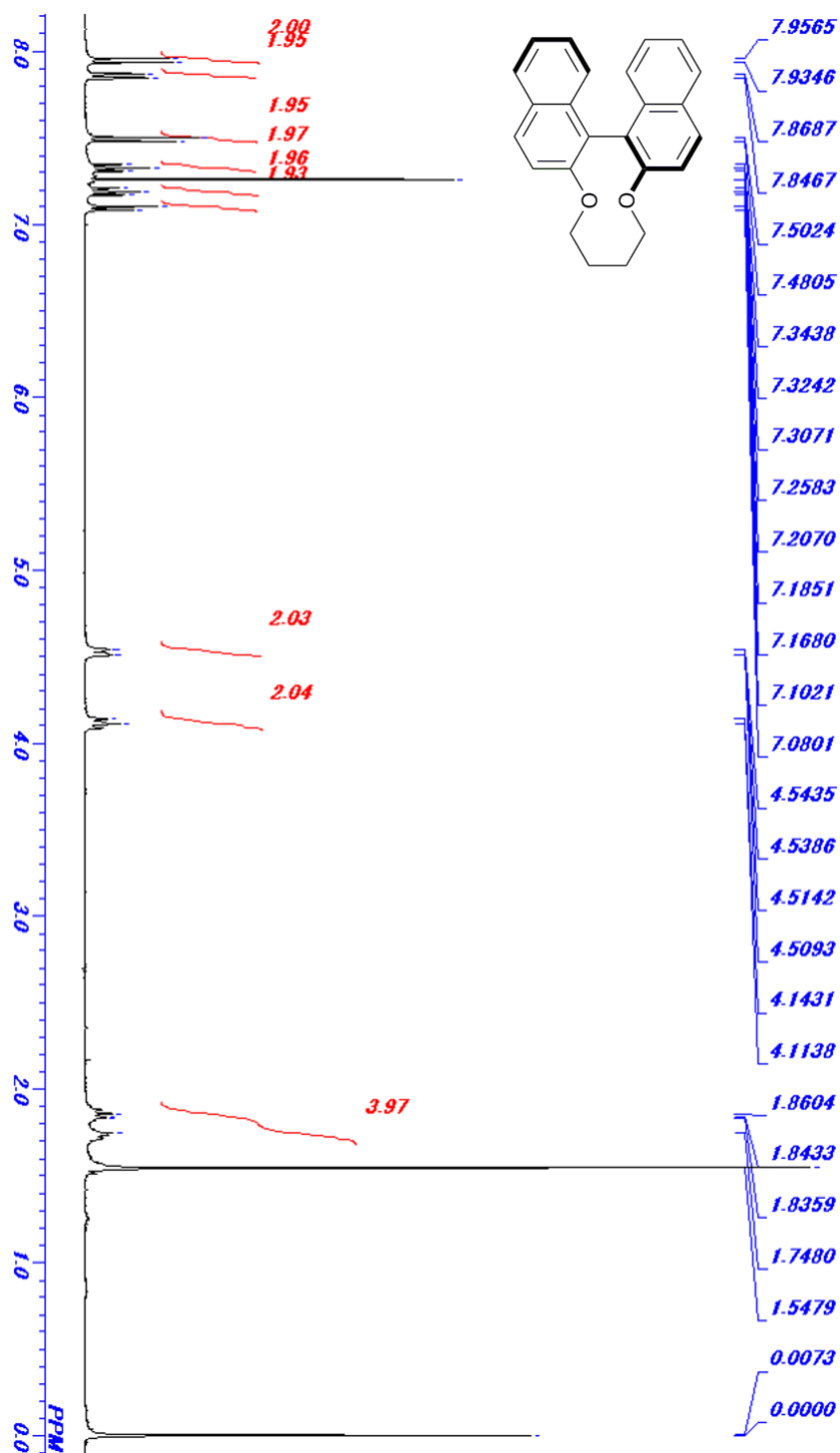


Figure S8 ¹H-NMR spectrum of 1a.

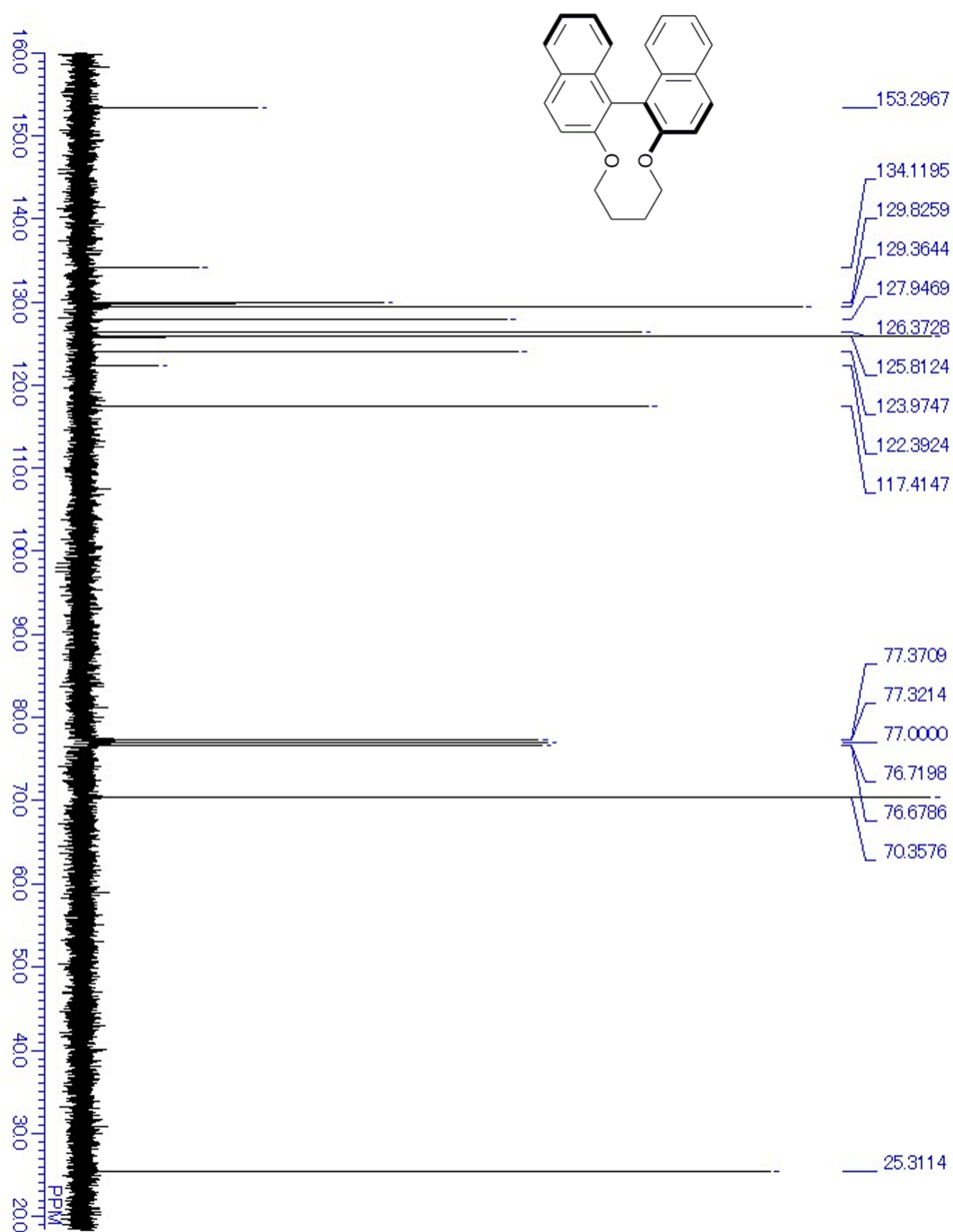
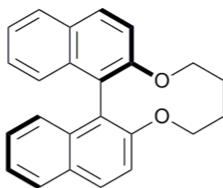


Figure S9 ¹³C-NMR spectrum of 1a.



Chemical Formula: $C_{24}H_{20}O_2$

Exact Mass: 340.1463

Molecular Weight: 340.4220

m/z: 340.1463 (100.0%), 341.1497 (26.0%), 342.1530 (3.2%)

[Molecular Formula]

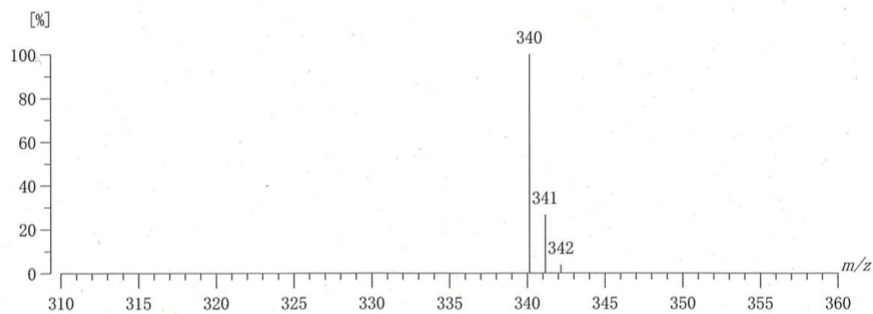
Data : Closed-H-EIposi-HR Date : 12-Oct-2017 13:51

RT : 0.92 min Molecular Formula : $C_{24}H_{20}O_2$

Elements : C 24/0, H 20/0, O 2/0

Mass Tolerance : 10mmu

Unsaturation (U.S.) : -0.5 - 20.0



[Mass Spectrum]

Data : Closed-H-EIposi-HR Date : 12-Oct-2017 13:51

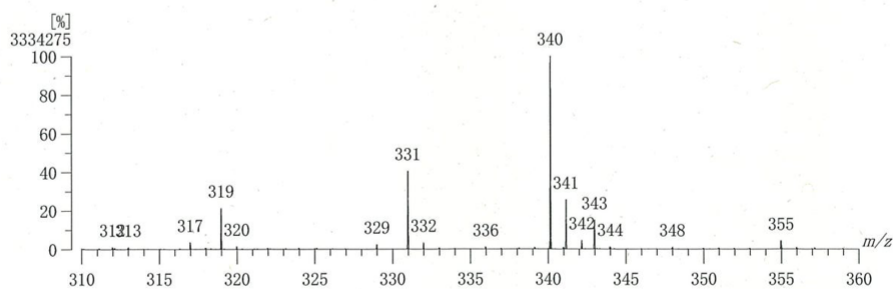
Instrument : Station

Note : MStation : IMCE Kyushu Univ.

Ion Mode : EI+

Scan# : 19

Cut Level : 1.00 %



Observed m/z	Int%	Err[ppm / mmu]	U.S. Composition
1 340.1464	100.00	+0.2 / +0.1	15.0 C24 H20 O2

Figure S10 High resolution mass spectrum of **1a**.

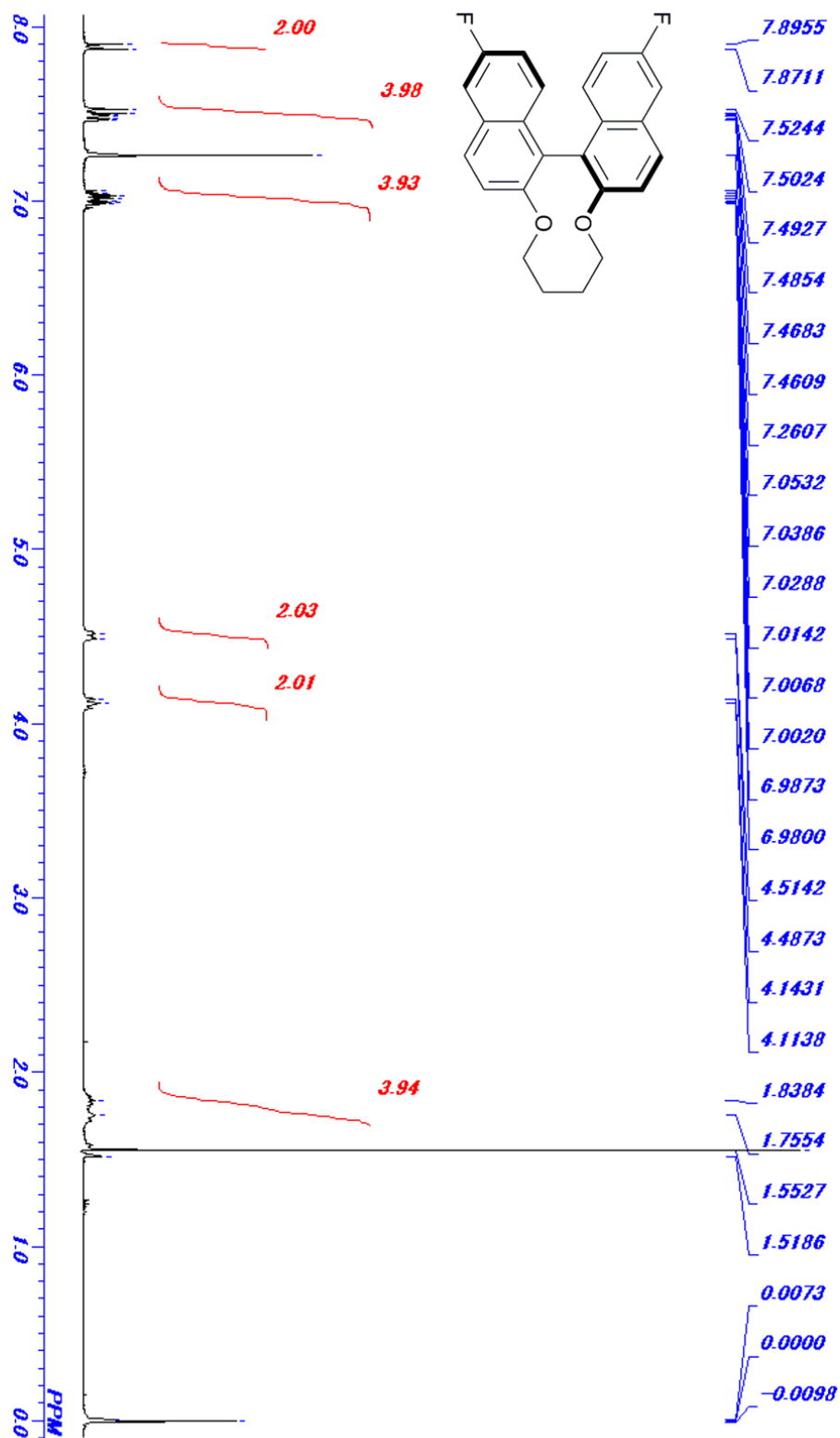


Figure S11 ¹H-NMR spectrum of 1b.

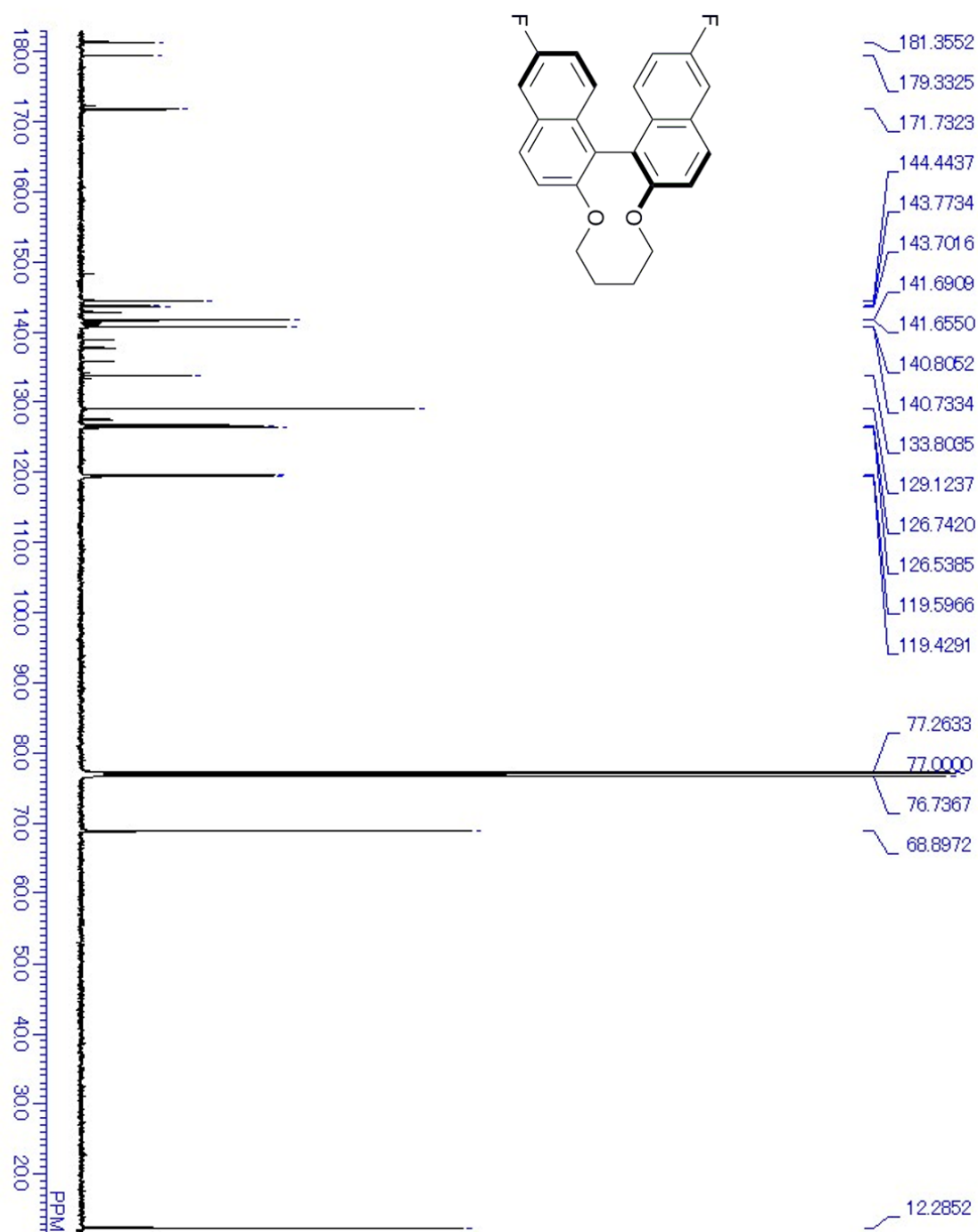


Figure S12 ¹³C-NMR spectrum of **1b**.

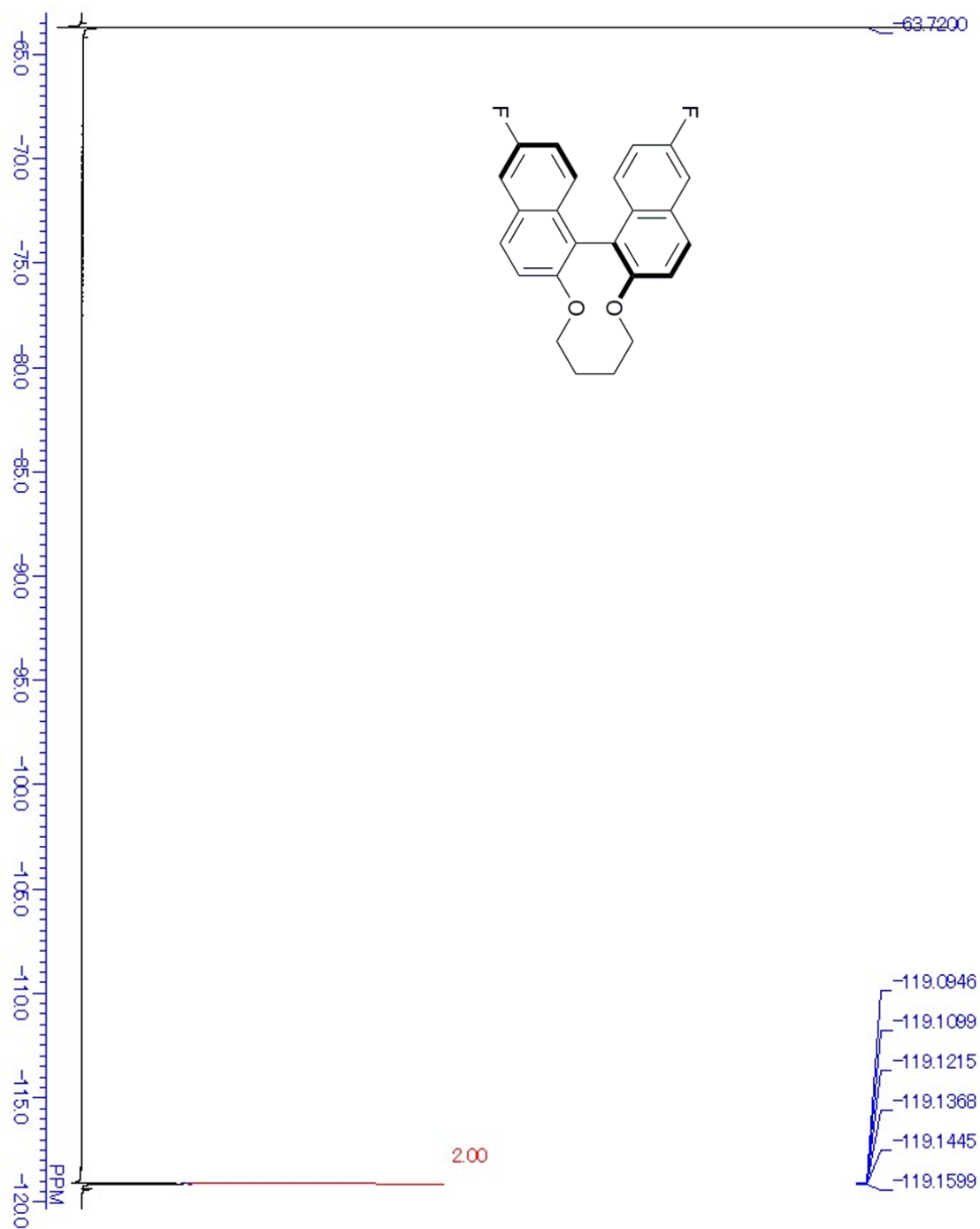
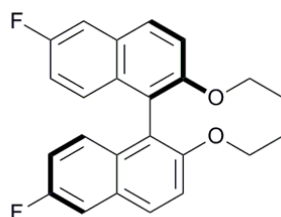


Figure S13 ^{19}F -NMR spectrum of **1b**.



Chemical Formula: $C_{24}H_{18}F_2O_2$

Exact Mass: 376.1275

Molecular Weight: 376.4028

m/z : 376.1275 (100.0%), 377.1308 (26.0%), 378.1342 (3.2%)

[Molecular Formula]

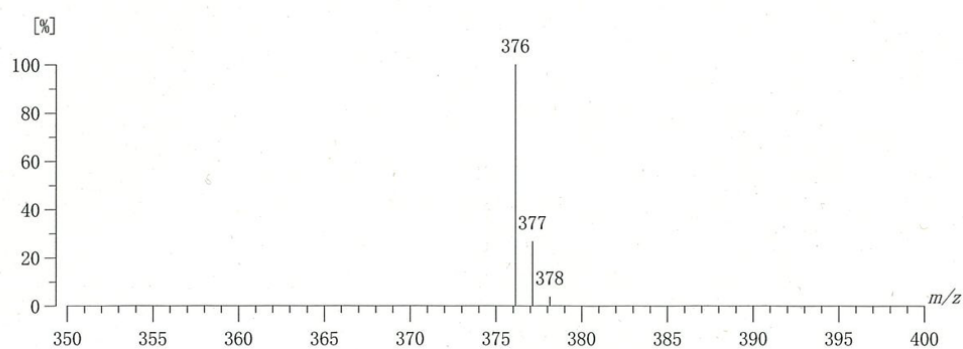
Data : Closed-F-EIposi-HR Date : 12-Oct-2017 15:21

RT : 1.15 min Molecular Formula : $C_{24}H_{18}F_2O_2$

Elements : C 24/0, H 18/0, F 2/0, O 2/0

Mass Tolerance : 10mmu

Unsaturation (U.S.) : -0.5 - 20.0



[Mass Spectrum]

Data : Closed-F-EIposi-HR Date : 12-Oct-2017 15:21

Instrument : Station

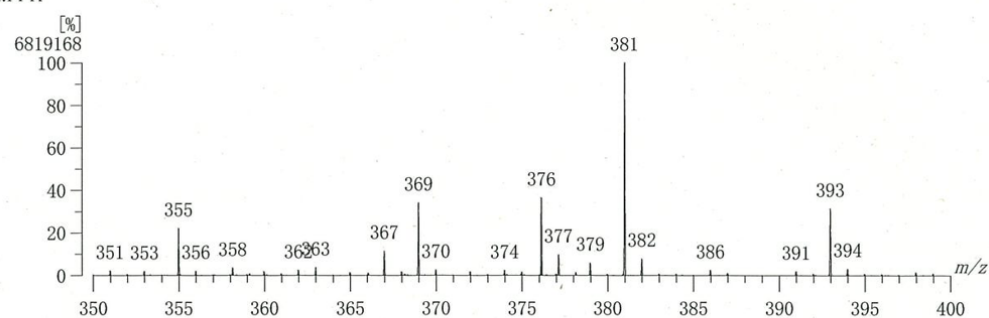
Note : MStation : IMCE Kyushu Univ.

Ion Mode : EI+

Scan# : (25,30)

Cut Level : 1.00 %

Internal standard:PFK



	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	376.1275	36.47	+0.0 / +0.0	15.0	C24 H18 F2 O2

Figure S14 High resolution mass spectrum of **1b**.

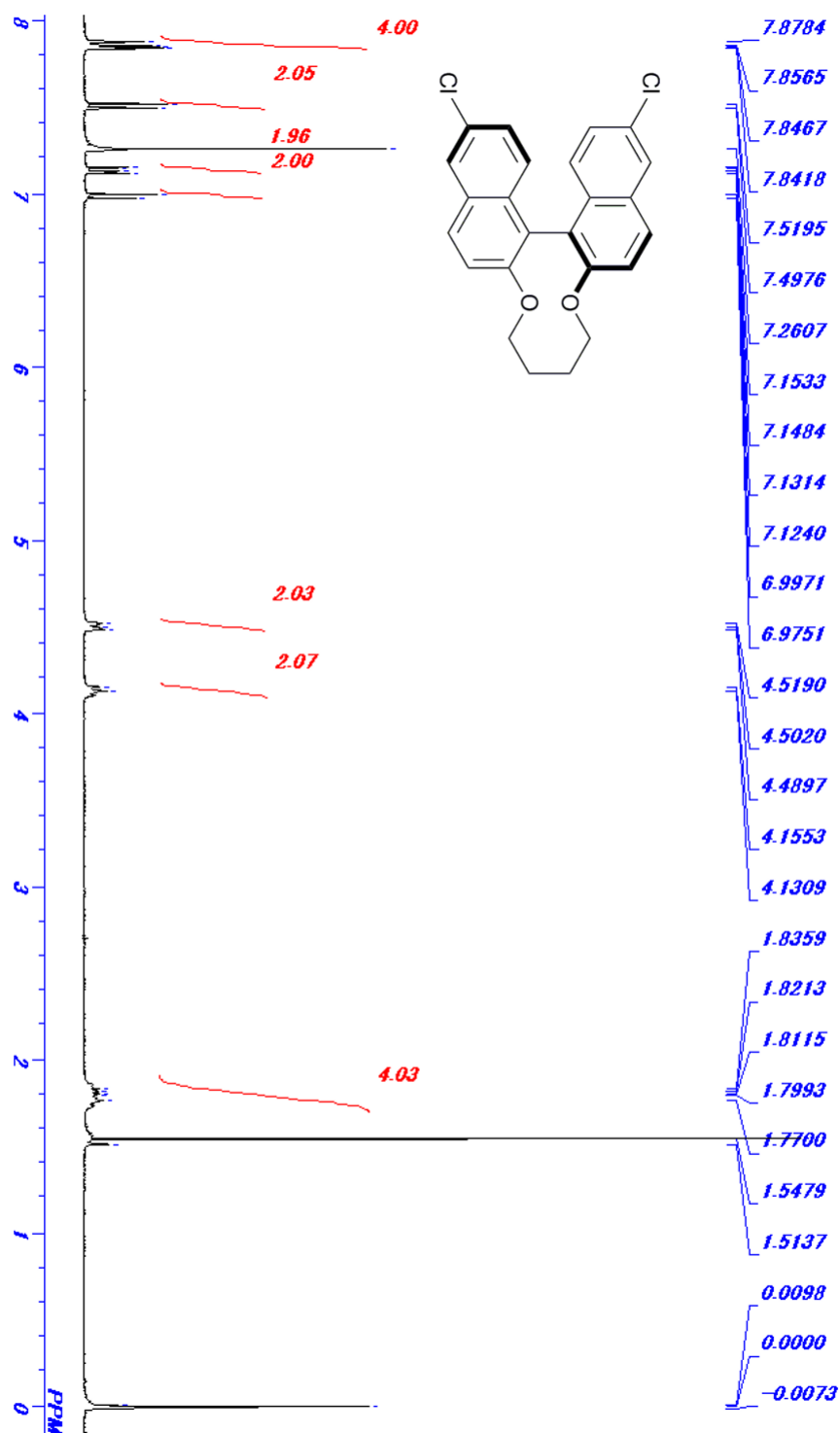


Figure S15 ^1H -NMR spectrum of **1c**.

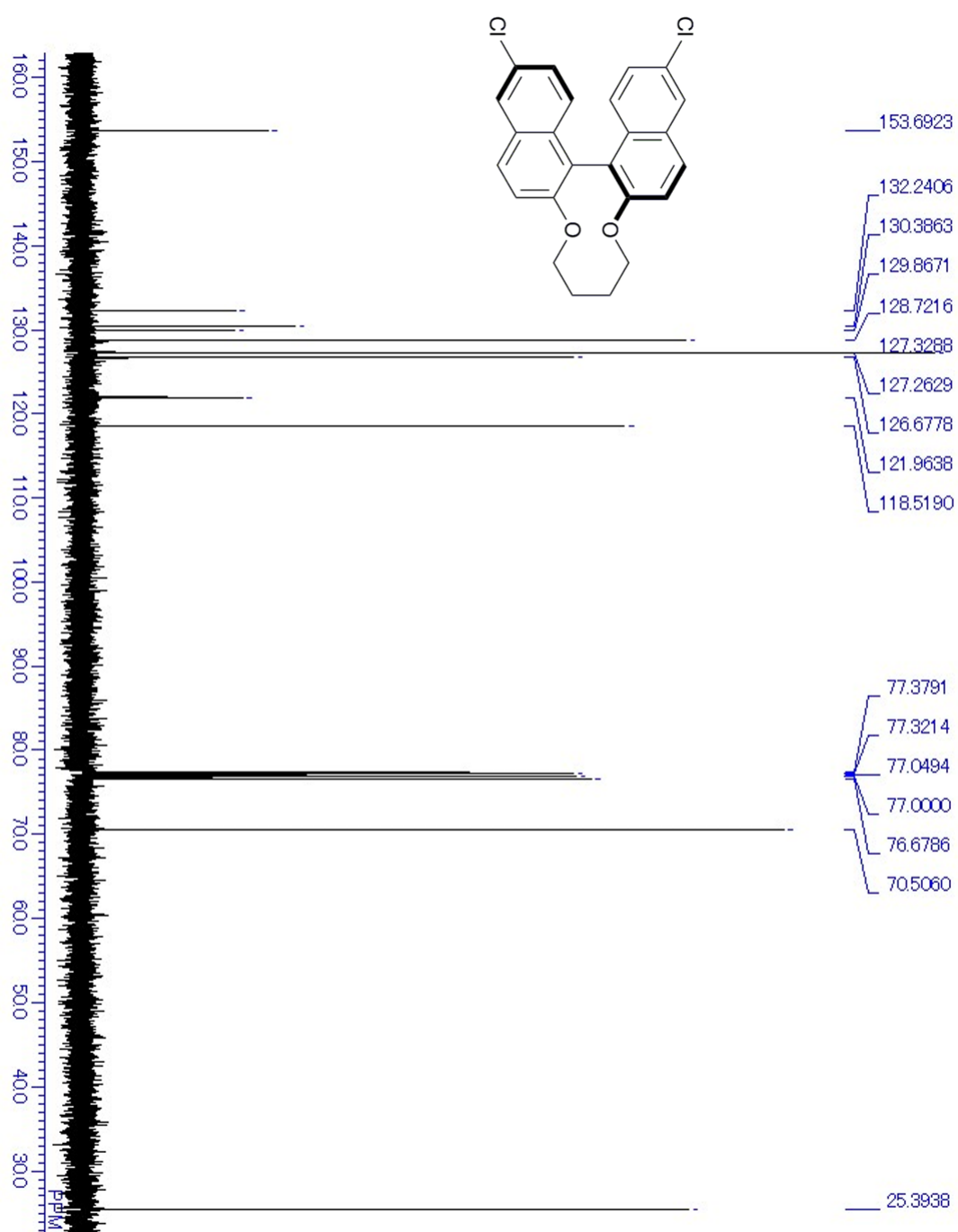
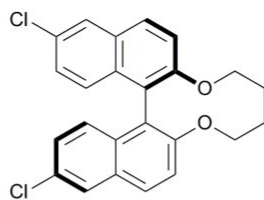


Figure S16 ^{13}C -NMR spectrum of **1c**.



Chemical Formula: $C_{24}H_{18}Cl_2O_2$

Exact Mass: 408.0684

Molecular Weight: 409.3060

m/z : 408.0684 (100.0%), 410.0654 (63.9%), 409.0717 (26.0%),
411.0688 (16.6%), 412.0625 (10.2%), 410.0751 (2.7%),
413.0658 (2.7%), 412.0721 (1.7%)

[Molecular Formula]

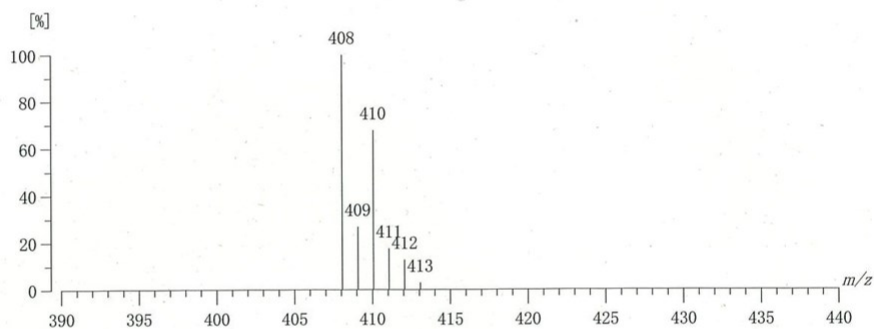
Data : Closed-Cl-EIposi-HR Date : 13-Oct-2017 09:33

RT : 1.09 min Molecular Formula : $C_{24}H_{18}Cl_2O_2$

Elements : C 24/24, H 18/18, 35Cl 2/0, 37Cl 2/0, O 2/0

Mass Tolerance : 10mmu

Unsaturation (U.S.) : -0.5 - 20.0



[Mass Spectrum]

Data : Closed-Cl-EIposi-HR Date : 13-Oct-2017 09:33

Instrument : Station

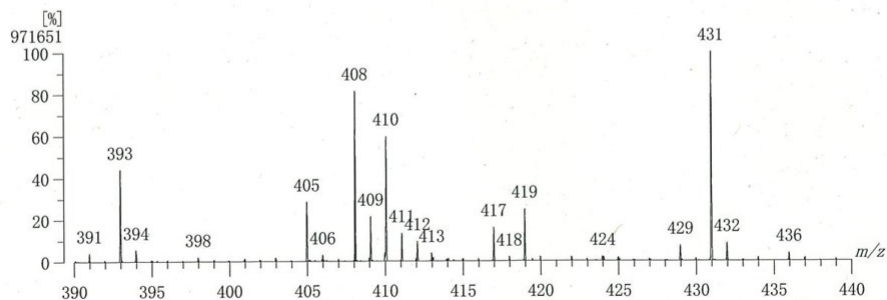
Note : MStation : IMCE Kyushu Univ.

Ion Mode : EI+

Scan# : 26

Cut Level : 1.00 %

Internal standard: PFK



Observed m/z	Int%	Err[ppm / mmu]	U.S. Composition
1 408.0684	81.46	+0.0 / +0.0	15.0 C ₂₄ H ₁₈ 35Cl ₂ O ₂

Figure S17 High resolution mass spectrum of **1c**.

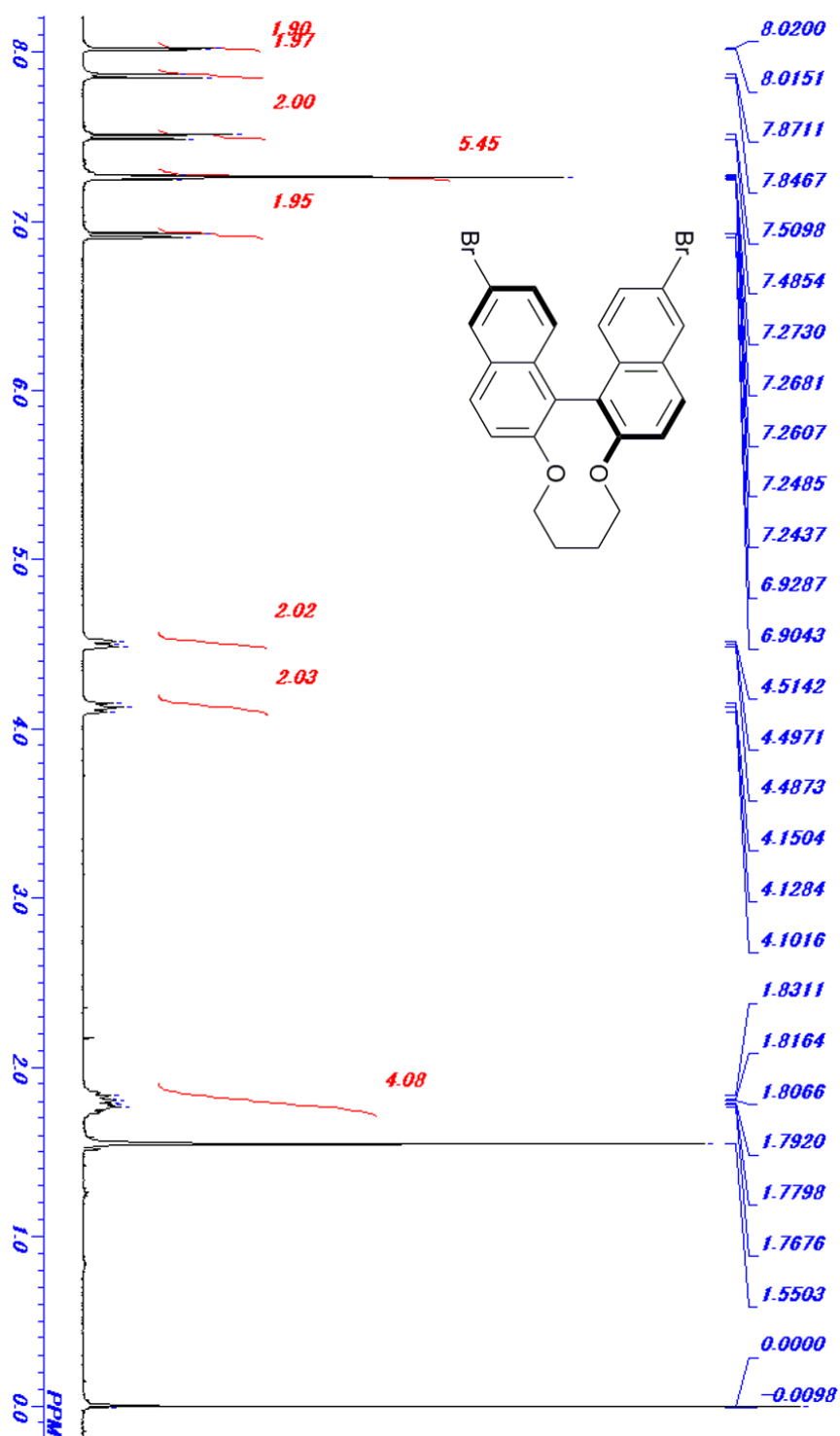


Figure S18 ^1H -NMR spectrum of **1d**.

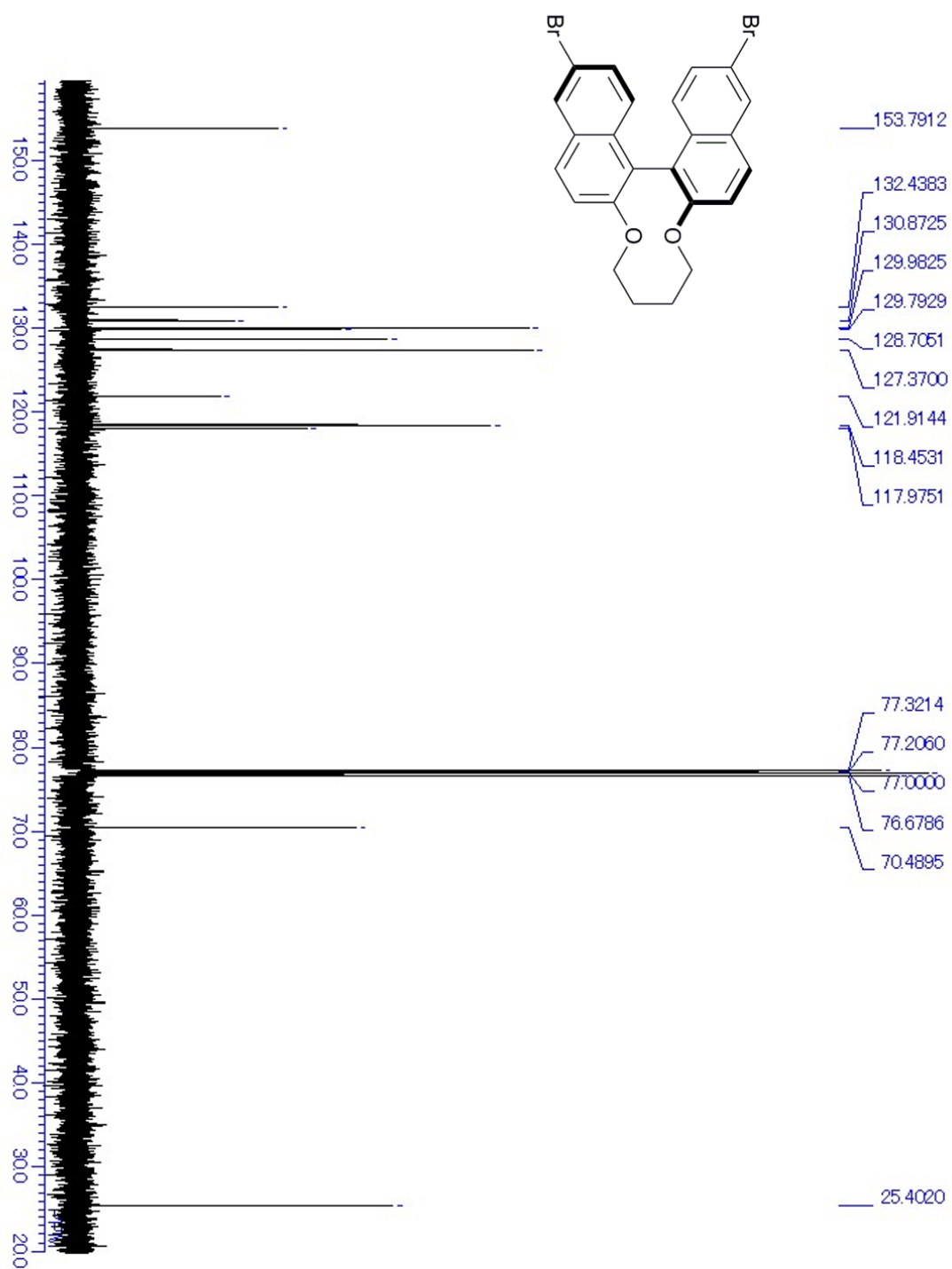
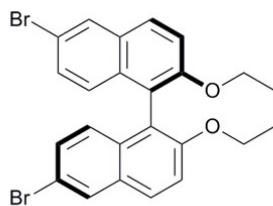


Figure S19 ¹³C-NMR spectrum of **1d**.



Chemical Formula: $C_{24}H_{18}Br_2O_2$

Exact Mass: 495.9674

Molecular Weight: 498.2140

m/z : 497.9653 (100.0%), 495.9674 (51.4%), 499.9633 (48.6%),
498.9687 (16.2%), 500.9666 (12.6%), 498.9687 (9.7%), 496.9707 (8.9%),
496.9707 (4.4%), 499.9720 (1.8%), 501.9700 (1.4%), 499.9720 (1.2%)

[Molecular Formula]

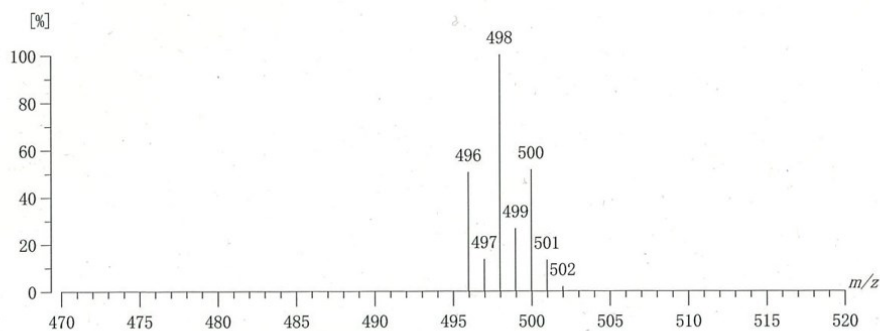
Data : Closed-Br-EIposi-HR Date : 13-Oct-2017 10:05

RT : 0.70 min Molecular Formula : $C_{24}H_{18}Br_2O_2$

Elements : C 24/24, H 18/18, 79Br 2/0, 81Br 2/0, O 2/0

Mass Tolerance : 10mmu

Unsaturation (U.S.) : -0.5 - 20.0



[Mass Spectrum]

Data : Closed-Br-EIposi-HR Date : 13-Oct-2017 10:05

Instrument : Station

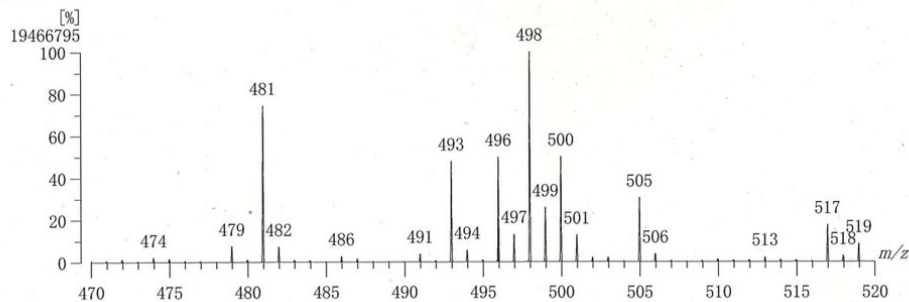
Note : MStation : IMCE Kyushu Univ.

Ion Mode : EI+

Scan# : (20,30)

Cut Level : 1.00 %

Internal standard:PFFK



Observed m/z	Int%	Err[ppm / mmu]	U.S. Composition
1 495.9673	49.85	-0.1 / -0.1	15.0 C24 H18 79Br2 O2

Figure S20 High resolution mass spectrum of **1d**.

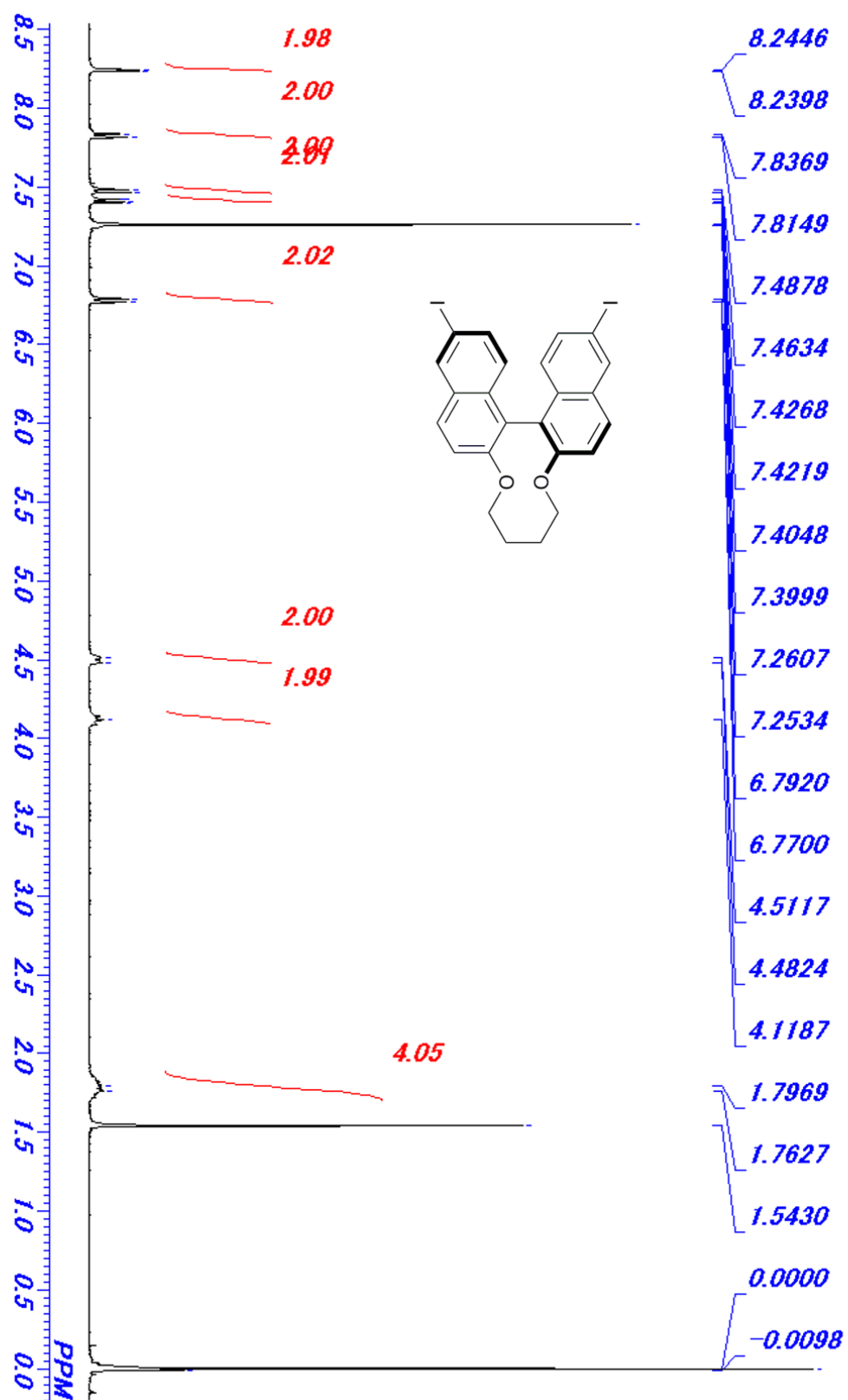


Figure S21 ¹H-NMR spectrum of **1e**.

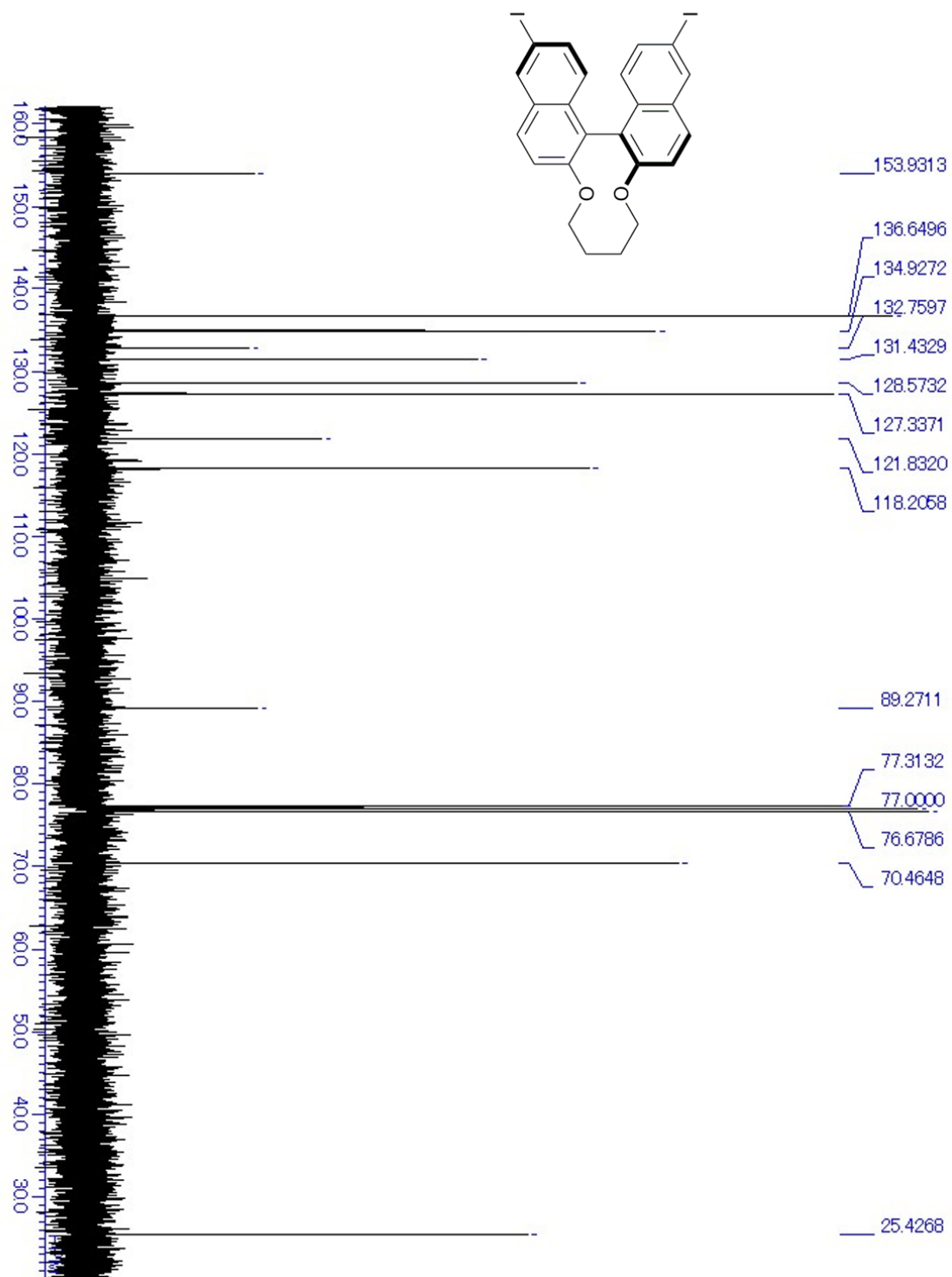
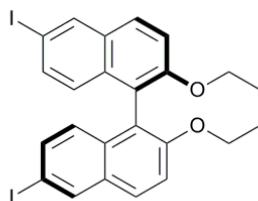


Figure S22 ^{13}C -NMR spectrum of **1e**.



Chemical Formula: $C_{24}H_{18}I_2O_2$

Exact Mass: 591.9396

Molecular Weight: 592.2149

m/z : 591.9396 (100.0%), 592.9430 (26.0%), 593.9463 (3.2%)

[Molecular Formula]

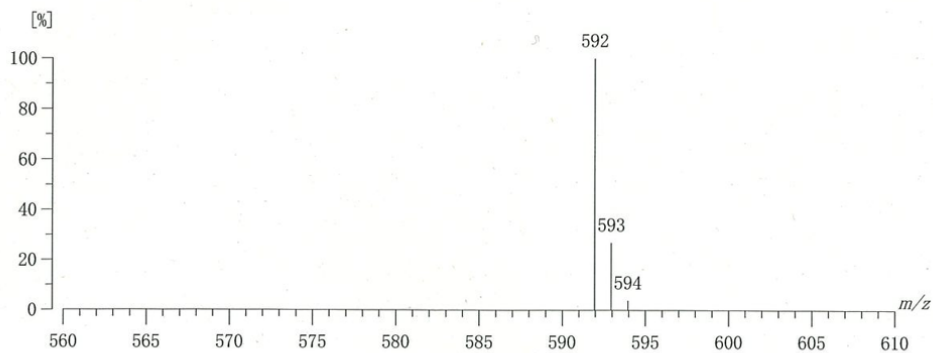
Data : Closed-I-EIposi-HR Date : 13-Oct-2017 10:40

RT : 1.07 min Molecular Formula : $C_{24}H_{18}O_2I_2$

Elements : C 24/24, H 18/18, O 2/0, I 2/0

Mass Tolerance : 1000ppm, 10mmu if $m/z < 10$, 50mmu if $m/z > 50$

Unsaturation (U.S.) : -0.5 - 20.0



[Mass Spectrum]

Data : Closed-I-EIposi-HR Date : 13-Oct-2017 10:40

Instrument : Station

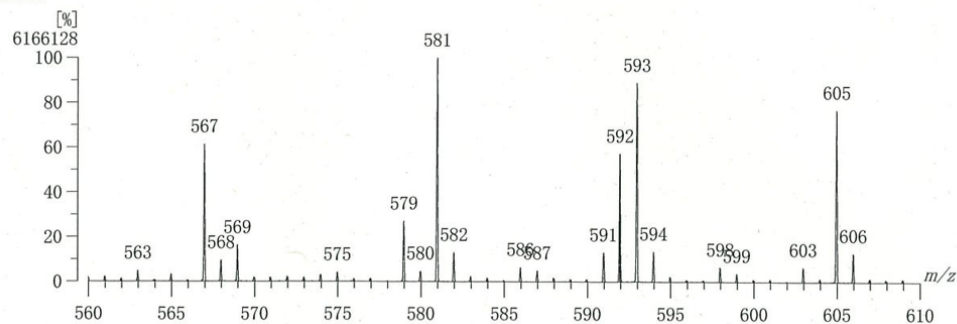
Note : MStation : IMCE Kyushu Univ.

Ion Mode : EI+

Scan# : (35,45)

Cut Level : 1.00 %

Internal standard: PFK



	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	591.9395	57.28	-0.2 / -0.1	15.0	$C_{24}H_{18}O_2I_2$

Figure S23 High resolution mass spectrum of **1e**.

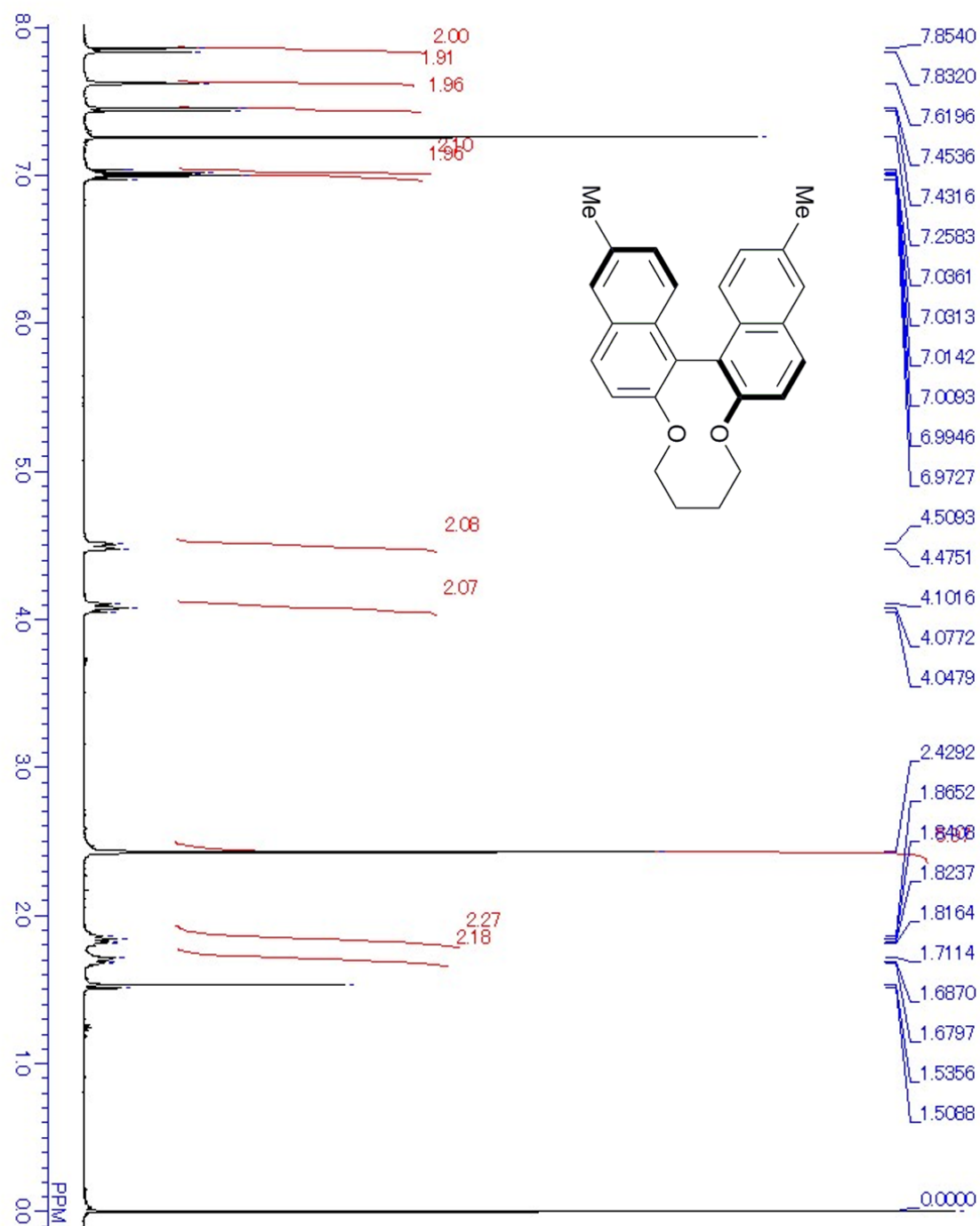


Figure S24 ¹H-NMR spectrum of **1f**.

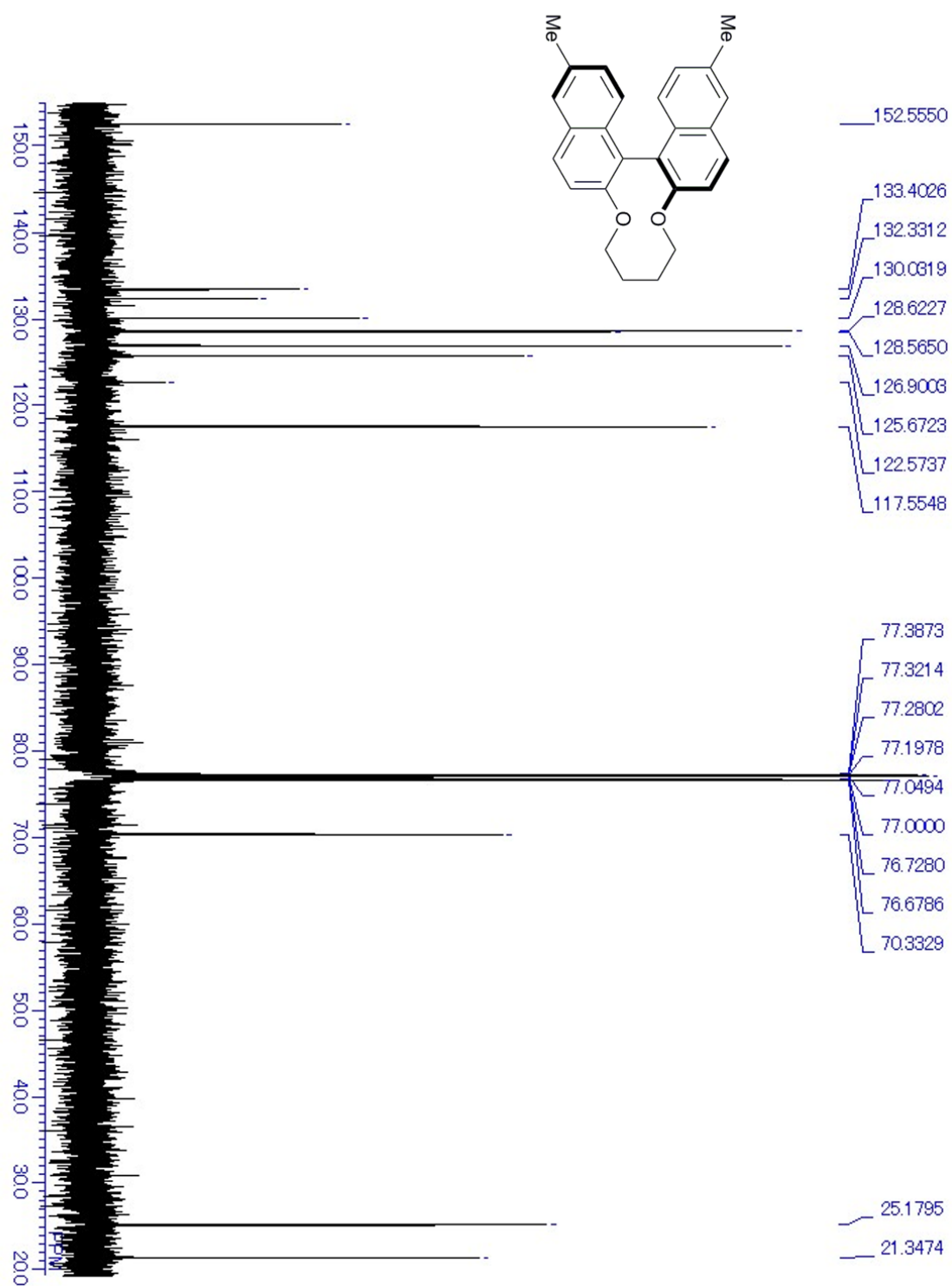
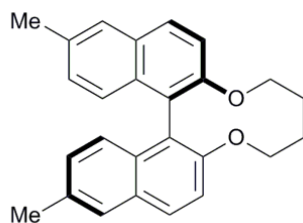


Figure S25 ¹³C-NMR spectrum of 1f.



Chemical Formula: $C_{26}H_{24}O_2$

Exact Mass: 368.1776

Molecular Weight: 368.4760

m/z : 368.1776 (100.0%), 369.1810 (28.1%), 370.1843 (3.8%)

[Molecular Formula]

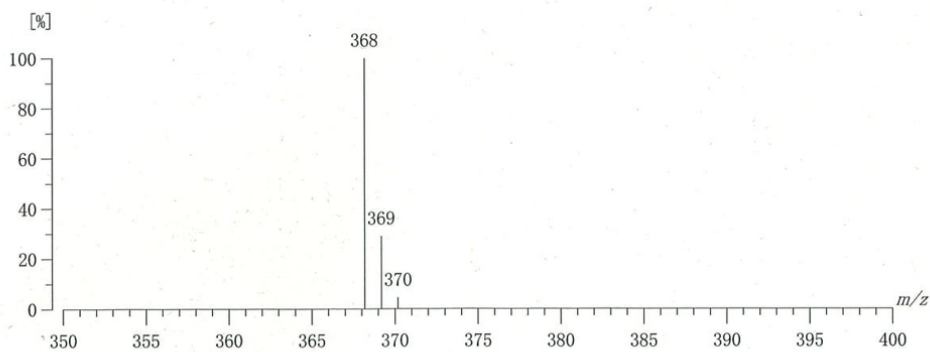
Data : Closed-Me-EIposi-HR Date : 12-Oct-2017 14:21

RT : 0.67 min Molecular Formula : $C_{26}H_{24}O_2$

Elements : C 26/0, H 24/0, O 2/0

Mass Tolerance : 10mmu

Unsaturation (U.S.) : -0.5 - 20.0



[Mass Spectrum]

Data : Closed-Me-EIposi-HR Date : 12-Oct-2017 14:21

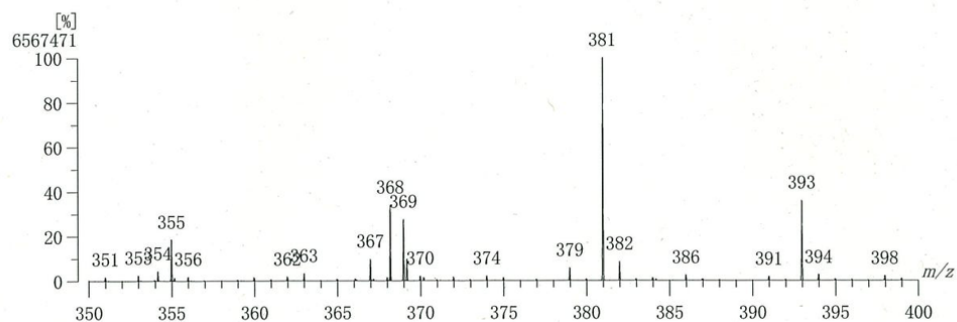
Instrument : Station

Note : MStation : IMCE Kyushu Univ.

Ion Mode : EI+

Scan# : (15,20)

Cut Level : 1.00 %



	Observed m/z	Int%	Err[ppm / mmu]	U.S. Composition
1	368.1778	33.99	+0.5 / +0.2	15.0 C ₂₆ H ₂₄ O ₂

Figure S26 High resolution mass spectrum of **1f**.